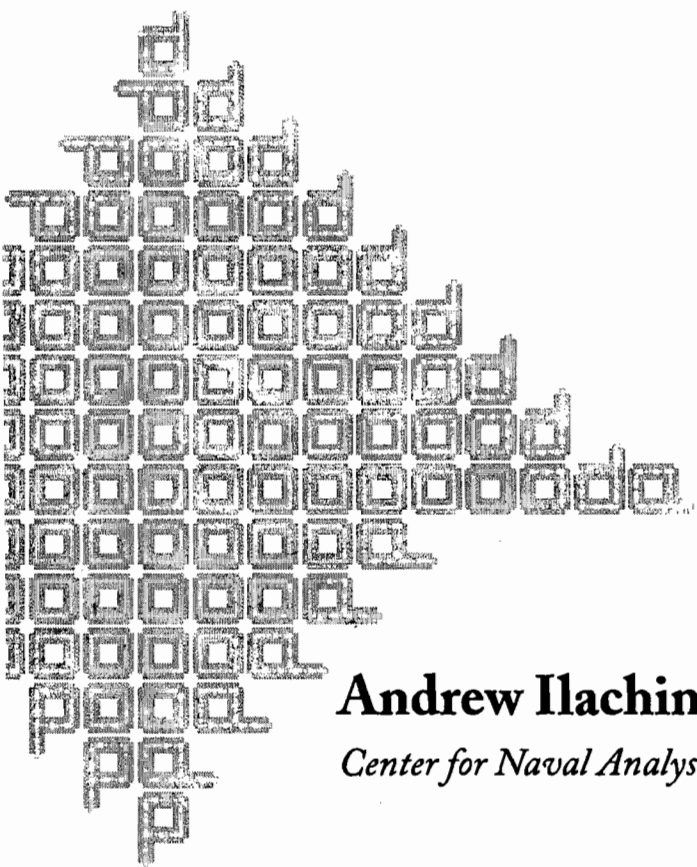


Cellular Automata

A Discrete Universe



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This book is dedicated to my two most precious companions in life,
without whose love, support and gentle encouragement it would
never have seen the light of day:

My beautiful wife and soul-mate *Irene*

&

My “little man”

(at least at the time when the book was finally finished ;-)

Noah!

Contents

Acknowledgments	xxi
Preface	xxiii
Foreword	xxvii
Chapter 1 Introduction: Preliminary Musings	1
1.1 Complex Systems	2
1.1.1 Short History	3
1.2 Cellular Automata	5
1.2.1 CA & Computation	6
1.2.2 Why Study CA?	7
1.2.2.1 CA as Powerful Computation Engines	7
1.2.2.2 CA as Discrete Dynamical System Simulators	8
1.2.2.3 CA as Conceptual Vehicles for Exploring Pattern Formation	8
1.2.2.4 CA as Original Models of Fundamental Physics	9
1.2.3 Example #1: One-dimensional CA	9
1.2.4 Example #2: Conway's Life	13
1.2.5 Example #3: Belousov-Zhabotinski Reaction	15
1.2.6 Example #4: Lattice Gases	15
1.2.7 Example #5: Collective Behavior in Higher Dimensions	16
1.2.8 Other Variants	17
1.3 Outline of Book	18
Chapter 2 Formalism	21
2.1 Mathematical Preliminaries	21
2.1.1 Set Theory	21
2.1.2 Information Theory	28
2.1.3 Graph Theory	30
2.1.4 Groups, Rings and Fields	35

2.1.5	Abstract Automata	38
2.2	Dynamical Rules: Notation and Definitions	40
2.2.1	One-dimensional CA	41
2.2.2	Two-dimensional CA	49
Chapter 3	Phenomenological Studies of Generic CA	53
3.1	One-dimensional Systems	53
3.1.1	Space-Time Patterns	54
3.1.2	Behavioral Classes	63
3.1.2.1	Difference Patterns	64
3.1.2.2	Blocking Transformations	66
3.1.3	General Properties of Elementary CA	71
3.1.3.1	Local Properties	71
3.1.3.2	Global Properties	75
3.1.4	A Small Sampling of Rules	82
3.1.4.1	The $k=2$, $r=1$ rule R22: Just How Complex Is It? . . .	83
3.1.4.2	The $k=2$, $r=1$ rule R30: Just How Random Is It? . . .	85
3.1.4.3	Critical-Like Behavior	86
3.1.4.4	Particle-Like Behavior	87
3.1.4.5	Reversible Rules	94
3.2	Parameterizing the Space of CA Rules	98
3.2.1	Langton's λ Parameter	98
3.2.2	Qualitative Overview of Behavior as a Function of λ	99
3.2.3	Quantitative Overview of Behavior as a Function of λ	100
3.2.3.1	Difference Pattern Spreading Rates	100
3.2.3.2	Entropy	102
3.2.4	Mutual Information	104
3.2.5	Discussion	106
3.2.5.1	Large $\mathcal{N}$ Limit	106
3.2.5.2	Large k Limit	106
3.2.5.3	Complexity Resides in the Transition Region?	107
3.3	Dependence on Lattice Topology	107
3.3.1	Natural Topology	107
3.3.2	Transitional Lattice Construction	110
3.3.3	$[2 : 2 : 2]$ Dynamical Profiles	112
3.3.4	$[3 : 3 : 3]$ Dynamical Profiles	114
3.3.5	Dynamical Profiles for Range Dependent Rules	115
3.3.6	Discussion	116
3.4	Two-dimensional Systems	116
3.4.1	Simple Seeds	119
3.4.2	Random Seeds	123
3.4.3	Voting Rules	124

3.4.3.1	Percolating Rules	125
3.4.3.2	Nucleating Rules	125
3.4.3.3	Variations on a Theme	128
3.4.4	Conway's <i>Life</i> Rule	130
3.4.4.1	Definition of <i>Life</i>	130
3.4.4.2	What's so Special About <i>Life</i> ?	131
3.4.4.3	<i>Life</i> 's Zoology	132
3.4.4.4	Ingredients for Universality	140
3.4.5	Sketch of a Proof that Conway's <i>Life</i> -rule is Universal	141
3.4.5.1	Bits $\iff$ Gliders	143
3.4.5.2	Thin Glider Gun	143
3.4.5.3	Logic Gates	145
3.4.5.4	Time Delays	145
3.4.5.5	A Glider-Stream Copier	145
3.4.5.6	Memory Storage	149
3.4.6	Three-dimensional <i>Life</i> ?	151
3.4.6.1	Analogues of Conway "Objects" in 3D	154
Chapter 4	Dynamical Systems Theory Approach	167
4.1	Dynamical System Theory	168
4.1.1	Discrete-time Poincaré Maps	168
4.1.2	Phase Space Volumes	169
4.1.3	A Generic Chaotic System — The Bernoulli Shift Map	172
4.1.4	Dissipative Systems	177
4.1.4.1	The Logistic Map	177
4.1.4.2	Hénon Map	184
4.1.5	Conservative Systems	187
4.1.5.1	Integrability	188
4.1.5.2	Phase Portraits and Stability	190
4.1.5.3	Prototypical Hamiltonian Mapping — Standard Map	192
4.2	Symbolic Dynamics	195
4.2.1	Basic Theory	196
4.2.2	CA-like Representation of Real-valued Maps	198
4.2.3	Real-valued Representation of CA Evolution	199
4.3	Lyapunov Characteristic Exponents	201
4.3.1	Continuous Flows	201
4.3.2	n-Dimensional Discrete Maps	203
4.3.3	Information-Theoretic Interpretation	205
4.3.4	CA Analogs	206
4.4	Invariant Measures	207
4.5	Entropies and Dimensions	209
4.5.1	Continuous Dynamical Systems	209

4.5.1.1	Fractal Dimension, D_F	210
4.5.1.2	Information Dimension, D_I	211
4.5.1.3	Correlation Dimension, D_C	211
4.5.1.4	Generalized Fractal Dimensions	212
4.5.2	CA Systems	215
4.5.2.1	Spatial Measures for Infinite Lattices	216
4.5.2.2	Temporal Measures for Infinite Lattices	220
4.5.2.3	Spatio-Temporal Measures for Infinite Lattices	222
Chapter 5	Analytic Approach	225
5.1	Deduction of Properties of General Rules	225
5.1.1	Cycle-State Structure from Global Eigenvalue Spectrum	225
5.1.2	Mathematical Characterization of Elementary CA	228
5.1.2.1	Implicit Deterministic Structures	228
5.1.2.2	Periodicity of Temporal Sequences	229
5.1.2.3	Rule Inverses	231
5.1.2.4	Homogeneous States	231
5.1.3	Enumeration of Limit Cycles	233
5.1.3.1	Invariance Matrix, A	233
5.1.3.2	Limit Cycle Enumeration	235
5.1.4	Shift Transformations	236
5.2	Algebraic Properties	237
5.2.1	An Example: Elementary Rule R90	238
5.2.1.1	Topology of the State Transition Graph	241
5.2.1.2	Cycle Length Distribution	242
5.2.2	CA over $\mathcal{F}_p$, p Prime	245
5.3	Local Structure Theory	247
5.3.1	Blocks, Measures and Bayesian Extensions	248
5.3.2	LST for One-dimensional Lattices	252
5.3.3	LST for d -Dimensional Lattices, $d > 1$	258
5.4	Dependence on Lattice Topology	260
5.4.1	Natural Topology	260
5.4.2	General Solution in $\mathcal{F}[q]$	261
5.4.3	Connection with Lattice Topology	264
5.4.4	Simplifications in $\mathcal{F}[2]$	269
5.4.5	Discussion	273
5.5	Lyapunov Functions and Threshold CA Rules	274
5.5.1	Generalized Threshold Automata	275
5.5.2	Lyapunov Functions	276
5.5.3	Characterization of Orbits	276
5.5.4	Bound on Possible Transient Lengths	277
5.5.4.1	A Is an Integer Valued Symmetric Matrix	279

5.5.4.2	A is a Binary Valued Symmetric Matrix	279
5.5.5	One-dimensional Majority Rules	280
5.5.5.1	Cyclic States	280
5.5.5.2	Transient Length	281
5.5.6	Two-dimensional Majority Rules	281
5.5.6.1	Cyclic States	282
5.5.6.2	Transient Length	283
5.5.7	Additional Remarks	283
5.5.7.1	A is Anti-Symmetric	284
5.5.7.2	Multithreshold Rules	284
5.5.7.3	Sequential Updating	285
5.5.7.4	Spin Glasses	286
5.6	Appendix 5-A	288
5.7	Appendix 5-B	289
Chapter 6	Cellular Automata and Language Theory	291
6.1	Formal Language Theory: A Primer	292
6.1.1	Regular Languages/ Finite Automata	294
6.1.2	Context-Free Languages/ Push-Down Automata	296
6.2	Relationship Between CA and Formal Languages	298
6.2.1	CA Rule $\longrightarrow$ Finite State Transition Graph	298
6.2.2	The Myhill-Nerode Theorem and the Minimization Algorithm	300
6.2.3	Regular Language Complexity	302
6.2.4	Entropy	303
6.2.5	What Happens as $t \rightarrow \infty$?	303
6.3	Power Spectra of Regular Languages	304
6.3.1	Numerical Estimates	305
6.3.2	Li's Algorithm for Generating Power Spectra	306
6.4	Reversible Computation	309
6.4.1	Universal Logic Gates	312
6.4.2	Universal Reversible Logic Gates	313
6.4.2.1	The Fredkin Gate	314
6.4.2.2	Conservative Logic Circuits	316
6.4.3	The Billiard Ball Model	317
6.4.3.1	Classical Mechanical Incarnation	317
6.4.3.2	The BBM CA	320
Chapter 7	Probabilistic CA	325
7.1	Critical Phenomena: A Heuristic Discussion	325
7.1.1	Boltzman Distribution	326
7.1.2	Free Energy	327
7.1.3	Stochastic Dynamics	328
7.1.3.1	Monte Carlo Dynamics	328

7.1.4	Critical Exponents	329
7.1.4.1	Universality	329
7.1.4.2	Scaling Hypothesis	330
7.1.5	Ising Model	332
7.1.5.1	General	333
7.1.5.2	One Dimensional Ising Model	334
7.1.6	Mean-Field Approximation	336
7.1.7	Spin Glasses	337
7.2	PCA $\longleftrightarrow$ Spin Model Equivalence	341
7.3	Critical Behavior of PCA	345
7.3.1	Peripheral PCA	345
7.3.1.1	Critical Exponents	346
7.3.1.2	Reduction to a One-Parameter Model	347
7.3.2	Totalistic PCA	348
7.4	Mean-Field Theory	349
7.4.1	General Rules	350
7.4.1.1	Binary Site Variables	351
7.4.2	Linear PCA	351
7.4.3	Totalistic PCA	352
7.4.4	Detailed Balance	353
7.4.5	Minimally Diluted Deterministic Rules	355
7.4.5.1	Numerical Results	357
7.5	CA Simulations of Spin Models	358
7.5.1	Why a “Naive” CA Approach Does Not Work	358
7.5.1.1	Metropolis Prescription	359
7.5.1.2	Microcanonical Prescription	359
7.5.2	Creutz’s Demons	361
7.5.2.1	Randomly Traveling Demons	361
7.5.2.2	Localized Demons	361
7.6	A Stochastic Version of Conway’s <i>Life</i> Rule	363
7.6.1	Zero-Temperature Limit	364
7.6.2	Finite Temperature	367
Chapter 8 Generalized Models		369
8.1	Reversible CA	369
8.1.1	Invertibility versus Time-Reversal Invariance	370
8.1.2	Historical Overview	371
8.1.3	A Sampling of Synthesis Techniques	372
8.1.3.1	Conserved Landscape Permutations	374
8.1.3.2	The Fredkin ‘Second-Order’ Construction	374
8.1.3.3	Partitioning CA	375
8.1.4	Elementary Reversible CA	376

8.1.5	Additive Invariants	378
8.1.5.1	Noether's Theorem	378
8.1.5.2	Invariants of <i>Fredkin-Reversible Rules</i>	379
8.1.5.3	Local Conservation Laws	383
8.1.6	Thermodynamic Behavior	385
8.1.6.1	Realizability of the Canonical Distribution	385
8.2	Coupled-Map Lattices	386
8.2.1	Stability of Homogeneous Solutions	387
8.2.2	Temporal Evolution of Inhomogeneous Initial States	389
8.2.3	Period-Doubling	390
8.2.4	Kink Diffusion	391
8.2.5	Quantitative Measures: An Overview	394
8.2.5.1	Power Spectra	394
8.2.5.2	Pattern Distribution	394
8.2.5.3	Entropy	395
8.2.5.4	Concluding Comments	397
8.2.6	Spatio-Temporal Intermittency	397
8.2.7	Soliton Turbulence	399
8.2.8	CA Approximation of Coupled-Map Lattices	401
8.2.8.1	First Order Approximation	404
8.2.8.2	Higher Order Approximations	405
8.3	Quantum Cellular Automata	406
8.3.1	QCA-I	407
8.3.1.1	General Properties	408
8.3.1.2	A Conservation Law	409
8.3.2	QCA-II	411
8.3.2.1	$k = 2$ Systems	413
8.3.2.2	$k = 3$ Systems	415
8.3.2.3	General Properties	416
8.4	Reaction-Diffusion Systems	419
8.4.1	The Belousov-Zhabotinskii Reaction	420
8.4.2	Greenberg-Hastings Model	420
8.4.3	Hodgspode Rule	422
8.5	Applications to Immunology	426
8.5.1	Normal Immune Response	426
8.5.2	Immune Disease: AIDS	428
8.6	Random Boolean Networks	429
8.6.1	Overview of the Dynamics of (N, κ) Nets	430
8.6.1.1	$\kappa = 1$	430
8.6.1.2	$\kappa = 2$	432
8.6.1.3	$\kappa > 5$	434
8.6.1.4	$\kappa = N$	434

8.6.2	Random Mappings	435
8.6.2.1	Average Cycle Length	435
8.6.2.2	Average Number of Length- a Cycles	436
8.6.2.3	Average Cycle Number	436
8.7	Self-Organized Criticality	437
8.7.1	Sandpile CA Model	437
8.7.2	One Dimensional Sandpiles	438
8.7.2.1	Resultant Dynamics	439
8.7.3	d -Dimensional Sandpiles	440
8.7.3.1	Spatial Power-Law Distribution	441
8.7.3.2	Temporal Power-Law Distribution	441
8.8	Structurally Dynamic Cellular Automata	443
8.8.1	The SDCA Model	444
8.8.2	An Example	447
8.8.3	Emerging Patterns and Behaviors	451
8.9	Mobile CA	457
8.9.1	Models of Combat	457
8.10	Appendix: Origins of Irreversibility — <i>The Kac Ring Model</i>	458
Chapter 9 CA Models of Fluid Dynamics		463
9.1	Continuum Fluid Dynamics	463
9.1.1	Continuity Equation	465
9.1.2	Euler's Equation	465
9.1.2.1	Momentum Flux Tensor	466
9.1.3	Navier-Stokes Equations	467
9.1.4	Reynold's Number	469
9.1.5	Fluid Flow as a Function of Reynolds Number	470
9.1.6	Routes to Turbulence	472
9.1.6.1	Landau-Hopf Route	472
9.1.6.2	Ruelle-Takens-Newhouse Route	473
9.1.6.3	Pomeau-Manneville Route	474
9.1.6.4	Feigenbaum Route	475
9.1.7	Kinetic Theory: Boltzman's Equation	475
9.1.8	Equilibrium Solutions of Boltzman's Equation	477
9.1.9	Conservation Laws $\rightarrow$ Equations of Hydrodynamics	481
9.1.9.1	Continuity Equation	482
9.1.9.2	Euler's Equation	482
9.1.9.3	Navier-Stokes Equations	483
9.1.9.4	Heat Conduction Equation	485
9.2	Lattice Gas Models	486
9.2.1	A Short History	488
9.2.2	HPP Model	489

9.2.2.1	Conservation Laws	491
9.2.2.2	Behavior	491
9.2.3	FHP Models	492
9.2.4	Equations for Macroscopic LG Behavior	494
9.2.4.1	Boltzman's Equation	494
9.2.4.2	Continuity Equation	496
9.2.4.3	Euler's Equation	497
9.2.4.4	Navier-Stokes Equations	500
9.2.5	LG Computers	503
9.2.5.1	Dynamic Range	503
9.2.5.2	Accuracy	503
9.2.5.3	Memory Efficiency	504
9.2.5.4	Programming Efficiency	505
9.2.5.5	Reynold's Number Scaling	505
Chapter 10	Neural Networks	507
10.1	Introduction	507
10.1.1	Connection Between Neural Nets and CA	508
10.1.2	A Short History	509
10.2	Biological Origins	510
10.3	McCulloch and Pitts	511
10.4	Hebbian Learning Rule	512
10.5	Perceptrons	512
10.5.1	Learning Rule	514
10.5.2	Linear Separability: the XOR Problem	515
10.6	The Hopfield Model	518
10.6.1	Associative Memory	518
10.6.2	The Model	520
10.6.3	Energy Function	521
10.6.4	Learning Rule	522
10.6.5	Spurious Attractors	524
10.6.6	Memory Storage Capacity	525
10.6.7	Variants of the Basic Model	528
10.7	Stochastic Nets	528
10.8	Boltzman Machines	532
10.8.1	Simulated Annealing	532
10.8.2	Learning Rule	534
10.9	Multi-Layered Perceptrons	536
10.9.1	The XOR Function Revisited	537
10.9.2	Backpropagation	540
10.9.2.1	Derivation	541
10.9.2.2	Variations of the Basic Rule	544

10.9.3	Model Development: A Short Primer	546
10.9.3.1	Kolmogorov's Theorem	549
10.9.3.2	Capacity	550
10.9.3.3	Ability to Generalize	551
10.9.4	Applications	552
10.9.4.1	NETtalk	552
10.10	Further Topics and Suggested Reading	554
Chapter 11	Artificial-Life	557
11.1	Introduction	557
11.2	Local vs. Global	558
11.3	Self-Organization	559
11.4	Emergence	560
11.4.1	Boids	561
11.4.2	Collective Sorting	561
11.5	Edge-of-Chaos	562
11.6	Agent-Based Models	564
11.6.1	Agent-Based Simulations vs. Traditional AI	566
11.6.2	Swarm	568
11.7	Self-Reproducing Automata	570
11.7.1	Just How Complex Must a Self-Reproducing Automaton Be?	572
11.7.2	Langton's Self-Reproducing Loop	573
11.8	Lindenmeyer Systems	576
11.8.1	Context Free L-Systems	576
11.8.2	Recursive Growth Models	577
11.8.3	Context Sensitive L-Systems	579
11.9	Vants	580
11.10	Genetic Algorithms	583
11.10.1	Genetic Operators	584
11.10.2	The Fitness Landscape	585
11.10.2.1	NK-Landscapes	587
11.10.3	The Basic Recipe	587
11.10.3.1	A Simple Example	588
11.10.4	How Do GAs Work?	589
11.10.4.1	The <i>Building-Block</i> Hypothesis	590
11.10.5	High-Level CA Rule Extraction	591
11.11	An Artificial-Life CA Model of Combat	592
11.11.1	Background	592
11.11.1.1	Land Combat as a Complex Adaptive System?	593
11.11.2	Combat Agents	594
11.11.3	Local "Personality" Rules	594
11.11.3.1	Meta-Rules	595

11.11.4	Combat	596
11.11.5	Sample Behavior	596
11.11.5.1	Sample # 1: Fluid-like Collisions	597
11.11.5.2	Sample # 2: Non-Monotonic Behavior	598
11.11.5.3	Sample # 3: GA-Bred Tactics	600
11.11.6	Payoffs to Using Agent-Based Models of Combat	601
Chapter 12	Is Nature, Underneath it All, a CA?	603
12.1	CA are Catalysts... But of What?	605
12.1.1	Further Reading	607
12.2	CA As Embodiments of a Paradigm Shift	608
12.3	Physics of Complexity	611
12.3.1	What is Complexity?	611
12.3.1.1	First Ask: "What is a Complex System?"	612
12.3.1.2	Then Ask: "What is "Complex Behavior?"	613
12.3.2	Towards a Definition of Complexity	614
12.3.2.1	Complexity as Information?	616
12.3.2.2	Complexity of a Graph	617
12.3.2.3	Complexity of a Simplicial "Complex"	619
12.3.2.4	Complexity of Hierarchical Systems	620
12.3.2.5	Computational Complexity	623
12.3.2.6	Algorithmic Complexity	624
12.3.2.7	Logical Depth	626
12.3.2.8	Thermodynamic Depth	627
12.3.3	Emergence	629
12.4	Physics of Information	632
12.4.1	Just What <u>is</u> Information?	633
12.4.2	A Few Hints to Get us Started	634
12.4.2.1	Thermodynamics and Information Theory	634
12.4.2.2	The Quantum Measurement Problem	636
12.4.2.3	Black Holes	636
12.4.2.4	Discrete Physics	638
12.4.3	Feynman's Challenge	638
12.4.4	Pregeometry?	639
12.4.4.1	Pregeometry as a "Bucket of Dust"	639
12.4.4.2	Pregeometry as the "Calculus of Propositions"	640
12.4.4.3	Pregeometry as "It from Bit"	640
12.4.4.4	The Combinatorial Hierarchy	641
12.4.4.5	Other Attempts at Pregeometry	642
12.4.5	Kantor's "Information Mechanics"	643
12.4.6	Stonier's "Information Physics"	643
12.4.7	Frieden's <i>Extreme Physical Information</i> Principle	646

12.5	Lattices and Field Theories	647
12.5.1	Field Theory Reformulated as a CA: I	648
12.5.2	Field Theory Reformulated as a CA: II	651
12.5.3	Field Theory Reformulated as a CA: III	654
12.5.3.1	Locality	655
12.5.3.2	Classical Mechanics	655
12.5.3.3	Nonrelativistic Quantum Mechanics	656
12.5.3.4	Scalar Fields on a Random Lattice	657
12.6	Is the Universe a CA?	660
12.6.1	A Teasingly Suggestive “Parable”	661
12.6.2	Speculations I: Minsky	662
12.6.2.1	Particle Interactions	663
12.6.3	Speculations II: Zuse	664
12.6.4	Speculations III: Fredkin	665
12.6.4.1	Digital Mechanics	666
12.6.4.2	DM Processes	667
12.6.4.3	Causality	667
12.6.4.4	Putting DM to the Test	668
12.7	Reversible Computers	672
12.7.1	Quantum Mechanical Computers	674
12.8	Computability and Physics	678
12.8.1	Turing’s <i>Halting Theorem</i>	679
12.8.2	Computational Irreducibility	680
12.8.3	Noncomputability	681
12.8.3.1	Church–Turing Thesis	682
12.8.3.2	Computation and Phase Transitions	683
12.8.4	A Simple Coincidence or is Something Really Interesting Going on Here?	685
12.9	Have We Gone Far Enough or is the World Crazier Still?	688
12.9.1	A Discrete Form of Geometrodynamics?	688
12.9.2	A Small Sampling of “Crazier Still...” Ideas	690
12.9.2.1	DiMarzio	690
12.9.2.2	Jourjine	691
12.9.2.3	Kaplunovsky and Weinstein	691
12.9.2.4	Chew and Stapp	691
12.9.2.5	Dadic and Pisk	692
12.9.2.6	Caianiello	692
12.9.2.7	Structurally Dynamic Cellular Automata (SDCA)	693
12.10	Final Musings & Speculations	694
12.10.1	What is Real?	700
12.10.2	A Glimpse of a New Physics?	705
	Postscript	711

Appendix A	CA Research Tools	713
A.1	Hardware	713
A.1.1	CAM-6	713
A.1.2	CAM-8	715
A.1.3	RAP1	716
A.1.4	Connection Machine	717
A.2	Software	717
A.2.1	CA Lab	717
A.2.2	CAM-PC	718
A.2.3	CAPOW	718
A.2.4	CellMaster	718
A.2.5	Cellsim	719
A.2.6	Discrete Dynamics Lab	719
A.2.7	Fractint	719
A.2.8	LCAU	720
A.2.9	Life32	720
A.2.10	Lifemn	720
A.2.11	MCell	720
A.2.12	StarLogo	721
A.2.13	WinCA	721
A.2.14	Symbolic Math Packages	721
Appendix B	Complex Systems Theory Resources	723
B.1	General Sources	723
B.2	Artificial Intelligence	724
B.3	Artificial Life	724
B.4	Artificial Life Simulation and Research Groups	724
B.5	Autonomous Agents	725
B.6	Cellular Automata	725
B.7	Chaos	725
B.8	Fractals	726
B.9	Fuzzy Logic	726
B.10	Genetic Algorithms	726
B.11	Genetic Programming	727
B.12	Intelligent Software Agents	727
B.13	Neural Nets	727
B.14	Nonlinear Dynamics	728
B.15	Software	728
B.16	Time Series Analysis	728
	Bibliography	729
	Index	801

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*Whose morning coffee chats about physics, engineering and cosmology kept my sanity in check.

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My sincere, humble apologies to all those that belong on this short list, but cannot find their name so listed. Know that your absence from these acknowledgments conveys no other conscious message other than the obvious evidence it provides of the author's fallible memory.

My deepest thanks, of course, goes to my family: to my mom and dad, *Sam & Katy Ilachinski*, who are two of the most loving and humblest creatures ever to grace this world; to my wife *Irene*, who has so infinitely enriched my life that I feel as though I've been blessed with a glimpse of heaven; and to my son *Noah*, who (at the tender age of two) has already taught me that love has no bounds and that mother nature is infinitely wiser than we know. Without my family's unconditional love, support and patience this book truly could not have been completed,

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Third, *Rich Bronowitz*, who has been the most important teacher, and mentor, in my professional career. I owe Rich an unpayable debt for unreservedly believing in, and allowing me to explore — virtually unencumbered by otherwise ubiquitous bureaucratic obstacles — my vision of introducing cellular automata into the arsenal of mathematical tools used by the operations research community and of applying agent-based modeling techniques to help understand the fundamental processes of conflict. A heartfelt thanks for all you've done, Rich. Know that you have played a far more important, and *active*, role in my development as an analyst, and as a person, than you allow yourself credit for.

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Preface

In memory of my teacher, friend and mentor, Max Dresden

The book that you-kind reader-are holding in your hand represents a labor of love, in the purest sense, for most of the five-and-a-half years that it took to write; and the additional five years that, because of various setbacks and self-imposed periods of inactivity, it took me to struggle through in order to have it finally see the light of day. In the time that the book has matured from a vague but interesting idea—first brought up by the author’s thesis advisor while waiting for dessert to arrive during a casual luncheon—to its final unintentionally massive form, I have myself evolved dramatically from an idealistic, 28-year-old, sadly underpaid graduate physics student to a husband, father and senior defense analyst working for a naval think-tank,[†] currently developing one of the first cellular-automata-based *artificial-life* simulations of combat. I would like to briefly share a few personal notes about how this book came to be.

I received my Ph.D. in theoretical physics from the *Institute of Theoretical Physics (ITP)* at the State University of Stony Brook in 1988. My thesis research, entitled “Computer Explorations of Discrete Complex Systems,” was conducted under Professor Max Dresden, who was at the time nearing the end of his professional career; a career that began when Max was studying for his own Ph.D. under Uhlenbeck (of spin fame). I was, in fact, Max’s last Ph.D. student, and it was Max who one day suggested to me during one of our frequent lunches that he and I ought to write a book on cellular automata together.

At the time, Max had just had his well-received biography of the Dutch physicist

[†]The *Center for Naval Analyses (CNA)* is a not-for-profit federally funded research & development center.

Kramers[†] published, and was, I suspect, anxious to start a new writing project. The year was 1987: four years after Wolfram's groundbreaking review article on cellular automata that appeared in *Reviews of Modern Physics* [wolf83a], and three years after the founding of the *Santa Fe Institute*, now arguably one of the world's leading centers for complex systems research.

My own interest in cellular automata manifested itself during my first year as a physics graduate student, while I was exploring the conceptual foundations of physics by looking into novel approaches to unifying quantum field theory and relativity. What was then, and remains today, an essentially open problem (string theory notwithstanding), is the unification of quantum mechanics—whose laws operate on the microscopic level—with general relativity—which describes phenomena on the very macroscopic level.

An idea that I had been tinkering with, in early 1983, involved re-writing some microscopic equations of motion on a discrete dynamic lattice representation of space-time. I wanted to see if one could construct a toy universe in which the fundamental distinction between *figure* (i.e. particles) and *ground* (i.e. space-time) is blurred (or disappears completely). Though I did not know it at the time (this was many months prior to Wolfram's review article, and whatever else I may have read on cellular automata certainly was not memorable enough in my own mind to start its own cognitive meme), the formalism I was struggling with to create and understand was precisely that of cellular automata!

The day that Wolfram's article appeared at ITP's library is forever etched in my mind as one of those proverbial milestone events in one's life. I knew instantly that cellular automata embodied a profound new approach to looking at physics and the world; and that cellular automata were a subject about which I had to do a lot of thinking. I will forever be indebted to Max for allowing me to pursue musings that seemed—certainly to those making up the intellectual inner-circle of ITP at the time—comical, at best and childishly unphysics-like, at worst. So...

It was with great pleasure that—three years later, and at the tail-end of completing my dissertation—I accepted Max's kind offer to jointly write a book on CA. "One or two years," I thought, "is all it will take." I was wrong.

Following my successful thesis defense in early 1988, I moved down to Washington, D.C. to start what has become a more than decade-long professional occupation as research analyst for the US Navy. My new job was, (and still is!) profoundly time consuming. My official duties soon took me to several (many-week-long) naval exercises at sea, included an intensive several-month-long reconstruction effort of *Operation Desert Storm* (which itself included virtually around-the-clock work days), and culminated in a multi-year stint as CNA's field representative at the naval air station located on Whidbey Island in Washington state (during which time many of my duties introduced me to the unhappy sport of prolonged sleep deprivation).

[†]Max Dresden, *Kramers: Between Tradition and Revolution*, Springer-Verlag, 1987.

Needless to say, the time (and energy) that remained for making any progress on this book after the long work days that characterized this period of my life, kept taking increasingly bigger hits.

Adding to these difficulties of writing a book, Max's own schedule had also undergone significant changes, and he was soon to back off from making a deeper commitment. Soon after I received my Ph.D., Max retired to Professor Emeritus status at Stanford University in California. He became engrossed in editing journals, working on several new physics projects with a fresh set of post Docs, and lecturing throughout the country on extended trips.[§] His schedule thus, unfortunately, left precious little time for writing. Though we had contract offers from two distinguished and reputable publishing houses (we accepted the one from Springer-Verlag), the co-authored project that began in earnest in 1989, was first converted to single authorship (namely, mine), and not long afterward, began languishing from a terminal case of *much, much too much to do in too short a time!*

The premature end of the project seemed to finally come when I learned in 1995 that Max had been diagnosed with an inoperable form of cancer. At the time, I had completed roughly 80% of the book, and the reality of actually completing the Herculean task no longer seemed so farfetched. However, without Max—without his encouragement and always happy outlook—I found that, for psychological reasons, it was difficult for me to continue. The book thus remained in its semi-complete form for several years following Max's sad announcement. Max died a few years later in 1997. As all of us who were graced by this gentle soul know well, Max was a profoundly gifted and inspiring teacher. He will be intensely missed.

What finally saw the book through to its conclusion? I confess to not having a solid answer. However, I am fairly certain that, had it not been for a serendipitous intervention of Jungian synchronicity, the book would never have been completed. In my professional capacity as a research analyst for the US Navy (working for a think tank that also does work for the Marine Corps), I had the distinct privilege and honor of getting to know a truly visionary military thinker: *Lt.Gen (Ret) Paul van Riper*.

General van Riper, during the time when he was Commanding General at the Marine Corps Concept Development Command at Quantico, VA. (1994-1996), approached CNA with an idea for a study that asked, *What do all of these new ideas I've been hearing about – nonlinearity, complexity, complex adaptive systems – have to do with combat?* Since many at CNA knew of my deep interest in the subject, I was soon asked to direct a project addressing this question; a project that has since spawned a follow-on multi-year effort sponsored by the *Office of Naval Research* to develop an artificial-life model of combat.[¶] To say that Lt.Gen van Riper's appear-

[§]Max was particularly fond of giving (always well received) talks at frequently held Chautauqua conferences for schoolteachers.

[¶]Those parts of this research that involve cellular automata are described in chapter 11 of this book. For additional details, including all approved-for-public-release documentation, see

ance on the scene was “welcome” would be a gross understatement. His vision has led me down many interesting new intellectual paths I would likely otherwise have never encountered.

Thus, slowly, at first, then more strongly, my CNA complexity project eventually re-ignited the passion I had inexplicably lost for my *other* complexity project: this book! Thus, to both Max and Gen van Riper, I owe an absolutely enormous, sincerely heartfelt, thanks. To Max for originally igniting and encouraging what was to become a life-long passion; to Paul van Riper for reminding me, more recently, and just as forcefully, of the passion that life’s circumstances had somehow, inadvertently and – as it turns out – only temporarily, dislodged. Thank you both!

I conclude this preface with an observation. Despite the very long gestation period for this book (nearly ten years, from original concept to publication), no other graduate-level book on cellular automata, comparable to the length and scope of this one, has appeared in the interim. Most likely, this is a direct reflection of the very broad scope, along with the relative immaturity, of the field. In any case, I am humble enough to know that my own effort will likely prove to be neither definitive nor complete. This book is intended solely to provide the interested reader with a self-contained reference summarizing some of the groundbreaking work that has been done by a great many researchers.

My greatest pleasure will come from learning that, for those of you who are not immediately put off by the daunting sight of a behemoth of a book sitting on your favorite bookseller’s shelf, this book has inspired a few of you to muse about cellular automata on your own. I am convinced that CA, in one form or another, will eventually be found lurking at the very heart of how our universe really works.

Andy Ilachinski
Springfield, Virginia
March, 2001

Foreword

Cellular automata (CA) are among the simplest mathematical representations of complex systems; where, for the moment, we may take “complex system” to mean any dynamical system that consists of more than a few—typically nonlinearly—interacting parts. As such, CA are extremely useful idealizations of the dynamical behavior of many real systems, including physical fluids, neural networks, molecular dynamical systems, natural ecologies, military command and control networks, and the economy, among many others. Because of their underlying simplicity, CA are also powerful conceptual engines with which to study general pattern formation. They have already provided critical insights into the self-organization of chemical reaction-diffusion systems, crystal growth, pattern formation on seashells, and phase-transition-like phenomena in vehicular traffic flow, to name but a few examples. On a more practical side, CA may provide the basis for extremely powerful encryption algorithms, a subject about which there has recently been much heated debate. There is even some serious speculation that CA may provide the backbone of a radically new discrete fundamental physics (an idea that we will focus our attention on in Chapter 12).

While the history of CA can be traced back to early *Systems’ Theory* and rigorous mathematical analyses conducted primarily by Russian researchers in the 1930s and 40s, their more recent incarnation as simple models of complexity in nature can arguably be traced to a single landmark review paper published by Wolfram in the *Reviews of Modern Physics* in 1983 [wolf83a].

Indeed, the sudden, almost explosive, emergence of CA as a major scientific and intellectual discipline is one of the most important developments in the decade from 1975-1985. It is always difficult and, in fact, a bit arbitrary to pinpoint particular dates as the definitive starting point of a new development, but it is striking how after a slow beginning, much influenced by the scientific demands of World War II, ideas leading to CA and computers entered the literature at an increasing rate. Around 1970, about 300 to 400 mathematically oriented papers dealing with automata were published; at the same time, the number of physics papers was at most a tenth of that. Some ten years later (~ 1980), evidence of a

shift in interest was already appearing: the numbers of mathematics and physics oriented papers was now roughly comparable, 50 to 100 each. In the succeeding five years the physics, or physically motivated, papers increased dramatically (400 to 500), while the number of mathematics papers slowly declined. The number of physics papers continues to increase even today. It is clear that CA can be anticipated to play an increasingly significant, if not major, role in future physics, and these developments should be analyzed and evaluated.

In spite of the large number of papers published on CA, their direct impact on the *mainstream* of physics was (and, depending on what researcher you ask today, still is), rather minor. Although many research studies make use of the computer experience and expertise which has been (and continues to be) developed in connection with CA, this influence remains primarily technical and computational rather than conceptual or philosophical. The contributions of CA have so far consisted of somewhat disjoint investigations which are largely isolated from modern physics—although they are arguably an integral component of an emerging new interdisciplinary research genre, that includes physics, called *complexity theory* (about which we will have more to say later). Complexity theory—as defined by, say, research being done at the *Santa Fe Institute* in New Mexico—is very much an immature, even infant science. This fact, along with it being a fundamentally interdisciplinary field, precludes us from branding it as mainstream physics. However, as this book hopes to show, CA are being increasingly recognized as important both for natural ability to simulate the dynamics of real physical systems and for providing powerful conceptual models with which to build (possibly radically new) physical theories.

Whenever a new field emerges, many different individuals contribute to its development. This is of course also true for CA, yet three persons stand out as originating and shaping the field: Alan Turing (1936), John von Neumann (1948) and Stephen Wolfram (1983). In addition, Stanislaw Ulam (1950) and John Conway (1969) each made specific, original contributions of long-lasting fundamental significance. It is interesting that four of these founders were mathematicians, while the sole physicist worked in particle physics and cosmology (rather than many-body theory or macroscopic physics, where current CA techniques find their primary use).

The scientific, mathematical orientation of these founding fathers had a major impact on the early development of CA. It is most remarkable that von Neumann, arguably the dominant figure, came to CA via the unlikely path of an interest in formal logic and the foundations of mathematics. In the 1920s, many of the usual procedures in classical mathematics were severely criticized by Brouwer and Weyl, who argued that the methodology and philosophy of set theory were fundamentally unsound. The intuitionist dogma was that all mathematical results should be constructive: proofs and derivations should be obtained via finite algorithms. Hilbert suggested a systematic program to counter this intuitionist criticism.

John von Neumann, under Hilbert's influence, actually produced a paper in which he showed that a subsystem of classical analysis could be obtained in a fini-

tistic manner. He further showed, by finitistic means, that this system is free of contradictions. He hoped, and even conjectured, that this proof and general conclusion could be extended to all analysis. Kurt Godel's well known proof of the incompleteness theorem, completed a few years later (1931), showed that von Neumann's conjecture was wrong and that Hilbert's program to show the contradiction-free character of mathematics by intuitionist methods was hopeless.

An important consequence of von Neumann's familiarity with finite mathematical schemes was its close, if not direct, connection with numerical analysis. von Neumann, unlike the Bourbaki school of mathematics, had a deep personal interest in numerical results, as well as in qualitative results outside of pure mathematics. He strongly believed that numerical results could provide novel insights into many phenomena; insights which were not obtainable by exclusively analytical or abstract means. (He even believed that mathematical innovation itself had to originate—at least in part—from extra-mathematical sources: economic, biological, neurological, etc.) It was the confluence of these disparate factors, a knowledge of finite mathematical algorithms, and a deep interest in—and respect for—numerical results, that led to von Neumann's epoch making investigations of computers and automata.

It is perhaps a fortuitous but interesting coincidence that while in Princeton, von Neumann became well acquainted with Turing, who wrote his thesis on the "The Decision Problem," another one of Hilbert's problems in formal logic. von Neumann was clearly impressed by Turing: he asked Turing to be his assistant for the academic year 1938-1939. Although Turing did not accept the position, von Neumann was familiar with Turing's work; his general approach played an important role in von Neumann's later efforts to construct computers which could reproduce themselves. Thus, the succeeding explosive development of electronic computers is the curious progeny of a profound analysis of the logical foundations of mathematics on the one hand, and a highly personal interest in numerical results on the other. As unlikely (and presumably as incompatible) a lineage as one could possibly imagine! Yet these two factors were fundamental in starting the computer revolution and the emergence of CA. von Neumann used to say, "The computer changed intuitionistic mathematics from ideology to reality."

Although precursors of CA were studied in a rigorously mathematical context by Russian mathematician in the late 1920s and 1930s, CA, as such, were first introduced in discussions between Ulam and von Neumann in the fall of 1951. von Neumann was interested in finding a reductionist model for biological evolution. His ambitious scheme was to abstract a set of primitive local interactions necessary for the evolution of complex forms of organization essential for life. It was Ulam's felicitous suggestion to emphasize discrete systems and dynamics, which—since that time—is automatically included as a characterizing feature of CA and which initiated the explosive growth of the field.

During the succeeding summer of 1952, Fermi, Pasta and Ulam showed that the use of a computer, even when applied to a presumably well understood physical

situation in classical mechanics, can lead to unanticipated phenomena; phenomena that are not always easy to explain, even though the basic rules are simple. Using the rapidly increasing power of computers, many models could now be analyzed and discussed. Perhaps the best known model is Conway's *Life* game, a CA which, while based on almost absurdly simple rules, can exhibit extraordinarily complex and even bizarre behavior. Since the *Life* game can be played using rather modest computing facilities, it became very popular for a time—acquiring an almost cult-like following among computer “hackers” in the early 1970s. There was even a journal devoted exclusively to the publication of computer results (and their interpretations) of the *Life* game.^{||} Although this game did a great deal to publicize CA, the effect on the physics, mathematics and general scientific community was rather mixed. Whether causally related or not, the number of purely mathematical papers on CA dropped sharply after the publication of Conway's *Life* game in 1970.

For physicists, applied mathematicians, biologists, etc., the general popularity of the *Life* games raises an important question: *What do these games, or more generally, the processes generated by CA (in spite of their suggestive names), actually have to do with phenomena—physical or otherwise?* For actual applications and for the ultimate importance of CA as an autonomous scientific method, this is clearly a very basic question. Although a general answer to this question cannot yet be given, there are many indications that it is reasonable to hope that a thorough, deep understanding of CA may well lead to an alternative, possibly more profound, and more useful, formulation of the basic laws of nature. As a very minor hint, it has been observed by many physicists that CA are intimately related to discrete statistical models. Since these models are constructed to elucidate basic ideas and general principles of statistical mechanics, it is reasonable to expect that the corresponding CA possess a similar physical interpretation, and have similar physical relevance.

It is, of course, far from obvious that all or even most of the fundamental physics can be phrased in terms of discrete CA. In fact, in current particle and high energy physics, symmetries, gauge symmetries, groups, Lie groups, and differential geometry—all of which stress *continuity* and not discrete features—play increasingly important roles. Yet, even in fundamental physics, attempts are made (in fact, with surprising regularity!) to discretize space and time and to express the basic laws as difference equations. Even though none of these efforts have been spectacularly successful, it is still too early to categorically dismiss such attempts as being misdirected and necessarily pointless.

It is worth pointing out, that in one of the more successful areas of particle physics, *Quantum Chromodynamics* (QCD), where basic physical principles are

^{||}*Lifeline*: A Quarterly Newsletter for Enthusiasts of John Conway's game of *Life*, edited by Robert Wainwright, #'s 1-11, 1971-1973; available on the internet at URL address <http://members.aol.com/lifeline/life/lifepage.htm>. See also *Time* magazine, January 21, 1974: “The game of *Life*,” which is a lively account of hackers versus serious computer time.

presumably all known, the resulting equations are of such complexity that they can be explored only by using extensive computer simulations. In fact, the actual analysis is almost always performed in terms of a lattice gauge theory. The system is put on a lattice and treated numerically. This is not exactly a reduction to a problem in CA dynamics, but it is beginning to approach it. Certainly, many interpretation questions in lattice gauge theory contain elements CA theory. It is a highly nontrivial problem, for example, to decide whether solutions to the *discrete* problems—obtained numerically—are indeed legitimate (albeit approximate) solutions of the original *continuous* problems. The precise relation between a continuous problem and an approximate treatment of a related discrete problem is quite delicate and subtle. This, in spite of the claim made some time ago that the only problem remaining in strong interaction physics is to “get enough money for a supercomputer.” The precise arguments needed to assess the meaning of the results obtained by a numerical analysis of the discretized version of the theory, lead to discussions which involve many formal aspects of CA.

These two examples are just illustrations of the ubiquitous role of CA in many different, unrelated areas of physics. Through the important work of Wolfram [wolf83a], which strongly ignited the recent explosive development as far as physics is concerned, it has become clear that many highly complex phenomena are the result of the collective, cooperative dynamics of a very large number of—typically very simple—individual parts. In these emerging complex patterns, recognizable macroscopic features may appear that have no simple, visible, or immediate relation to the original microscopic rules. The mathematical analysis of these patterns and their underlying dynamics involves algebra, number theory, graph theory, logic, topology, as well as techniques originating from dynamical systems theory. (It is interesting, and a little ironic, that many of the questions arising from the study of such systems are closely related to the kind of problems von Neumann and Turing considered in their own studies of computability and the foundations of mathematics). Much of the current serious work with CA centers around the question of how simple rules produce complex patterns. It is certainly eminently reasonable to expect that these investigations will lead to important results. They already have. This alone would justify a serious systematic discussion.

But there still could be doubts. *Are CA merely an amusing form of computer graphics, a sophisticated computer game for scientists, or do they indeed herald a new beginning for a conceptually new and distinct approach to science generally and physics in particular?*

This book is intended to mitigate these doubts. There is already enough of a structure to the theory of CA to show that they provide an effective and practical basis for the treatment of specific, as well as general, questions. In this monograph, the physical, formal and mathematical framework will be systematized to such an extent, that the framework becomes the natural setting for an effective description of the natural world. Just to what extent the fundamental laws of physics can, or

should, all be phrased in terms of CA is impossible to say at this juncture. The subject is interesting enough, promising enough, and important enough, however, that a scientific field (or an individual scientist) ignores it at his or her own risk.

Chapter 1

Introduction: Preliminary Musings

Cellular automata (CA) are, fundamentally, the simplest mathematical representations of a much broader class of complex systems (where, for the moment, “complex system” means any dynamical system that consists of more than a few – typically nonlinearly – interacting parts). As such, CA have proven to be extremely useful idealizations of the dynamical behavior of many real complex systems, including physical fluids, neural networks, molecular dynamical systems, natural ecologies, military command and control networks, and the economy, among many others. Because of their underlying simplicity, CA are also powerful conceptual engines with which to study general pattern formation. They have already provided critical insights into the self-organization of chemical reaction-diffusion systems, crystal growth, pattern formation on seashells, and phase-transition-like phenomena in vehicular traffic flow, to name but a few examples. On a more practical side, CA may provide the basis for extremely powerful encryption algorithms, a subject about which there has recently been much heated debate. There is even some serious speculation that CA may provide the backbone of a radically new discrete fundamental physics (an idea that we will focus our attention on in Chapter 12). While the history of CA can be traced back to early *Systems’ Theory* ([bert68], [jant75]) and the rigorous (but almost impenetrably dry) mathematical analyses conducted primarily by Russian researchers in the 1930s and 40s, their more recent incarnation as simple models of complexity in nature can arguably be traced to a single landmark review paper published by Wolfram in the *Reviews of Modern Physics* in 1983 [wolf83a]. Before embarking in earnest on our journey to explore some remarkable properties of CA in this book, we begin by giving in this introductory chapter a short historical overview and gentle first exposure to a few simple examples.

The fundamental challenge of physics has always been the understanding of the phenomenologically observed complexity in nature using a minimal set of simple principles. This reductionist program has historically—and for obvious reasons—concentrated mostly on studies of comparatively simple systems, deliberately avoiding *more complex descriptions and phenomena*.

Two powerful paradigms for studying natural systems have been provided by *statistical mechanics*, which deals with an infinite number of degrees of freedom and uses central limit theorems for computing desired observables, and *dynamical systems theory*, which deals with systems having only a relatively few degrees of freedom. During the last two decades there has been a veritable explosion of applications of nonlinear dynamics to physical systems. In particular, very simple dissipative deterministic classical systems have been shown to possess remarkable chaotic dynamical properties. Dynamical systems theory provides the tools for studying these systems, *provided* that their response to external probes is constrained to lie in some low-dimensional subspace of phase space. Neither traditional paradigm, however, is capable of dealing adequately with the collective behavior of *complex systems*, which—although consisting of large, often infinite, number of degrees of freedom—can behave in ways such that central limit theorems do not apply. In contrast to our understanding of irregular motions in continuous systems, a comprehensive analytical description of discrete complex systems, constructed out of large numbers of simple components undergoing nonlinear local interactions, is presently out of reach.

1.1 Complex Systems

What are complex systems? While difficult to define without first introducing a few technical concepts, we can see examples of complex systems just about everywhere we look in nature; from the turbulence in fluids to global weather patterns to beautifully intricate galactic structures to the complexity of living organisms. All such systems share at least this one property: they all consist of a large assemblage of interconnected, mutually (and typically nonlinearly) interacting parts. Moreover, their aggregate behavior is *emergent*. That is to say, the properties of the *whole* are not possessed by, nor are they directly derivable from, any of the *parts* – a water molecule is not a vortex, and a neuron is not conscious. A complex system must therefore be understood not just in terms of the set of components out of which it is constructed, but the topology of the interconnections and interactions among those components.

Gases, fluids, crystals, and lasers are all familiar kinds of complex systems from physics. Chemical reactions, in which a large number of molecules conspire to produce new molecules, are also good examples. In biology, there are DNA molecules built up from amino acids, cells built from molecules, and organisms built from cells. On a larger scale, the national and global economies and human culture as a whole are also complex systems, exhibiting their own brand of global cooperative behavior. One of the most far-reaching ideas of this sort is James Lovelock's controversial "Gaia" hypothesis, which asserts that the entire earth—molten core, biological ecosystems, atmospheric weather patterns and all—is essentially one huge, complex organism, delicately balanced on the edge-of-chaos [love79].

Perhaps the quintessential example of a complex system is the human brain, which, consisting of something on the order of 10^{10} neurons with 10^3 - 10^4 connec-

tions per neuron, is arguably the most complex complex system on this planet. Somehow, the cooperative dynamics of this vast web of “interconnected and mutually interacting parts” manages to produce a coherent and complex enough structure for the brain to be able to investigate its own behavior.

The emerging new sciences of complexity and complex adaptive systems explore the important question of whether (and/or to what extent) does the behavior of the many seemingly disparate complex systems found in nature—from the very small to the very large—stem from the same fundamental core set of universal principles.

References include monographs (Badii and Politi [badii97], Kauffman [kauff93], Holland [holl95], Mainzer [main93], Weisbuch [weis91]), popularizations (Lewin [lewin92], Waldrop [wald93], and Gell-Mann [gell94]), conference proceedings (Cowan [cowan94], Varela [varela92a], Yates [yates87a]) and a series of lecture notes from the Santa Fe Institute ([stein89], [jen90a], [nadel91], [nadel92], [nadel93], and [nadel95]). An eloquent exegesis of the complexity “worldview” is Kauffman’s *Investigations* [kauff00].

1.1.1 Short History

Whenever a new field emerges, many different individuals contribute to its development. This is of course also true of complex systems theory, yet three persons stand out as originating and shaping much of the field: *Alan Turing* [turing36], *John von Neumann* [vonN51], and *Stephen Wolfram* [wolf83a]. In addition, *Stanislaw Ulam* [ulam62] and *John Conway* [berk82] each made specific, original contributions of long-lasting fundamental significance. Table 1.1 shows a brief chronology of a few milestone events in the study of complex systems.

Turing, in 1936, published a landmark proof of what has come to be known as the **Halting Theorem**. Turing’s theorem fundamentally limits what one is able to know about the running of a program on a computer by asserting that there is in general no way to know in advance if an arbitrary program will ever stop running. In other words, there is, in general, no quick and dirty short-cut way of predicting an arbitrary program’s outcome; this is an example of what is called computational irreducibility. About five decades later, Wolfram suggested that computational irreducibility is actually a property not just of computers, but of many real physical systems as well [wolf85e].

Cellular automata were conceived in 1948 by John von Neumann, whose motivation was in finding a reductionist model for biological evolution [vonN51]. His ambitious scheme was to abstract the set of primitive logical interactions necessary for the evolution of the complex forms of organization essential for life. In a seminal work, completed by Burks, von Neumann followed a suggestion by Ulam to use discrete rather than continuous dynamics and constructed a two-dimensional automaton capable of self-reproduction. Although it obeyed a complicated dynamics and had a rather large state space, this was the first discrete parallel computational model formally shown to be a universal computer (which implies, in turn, that it is also computationally irreducible). Twenty years later, the mathematician John Conway introduced his well-known Life game, which remains among the simplest

Year	Researcher	Discovery
1936	Turing	Formalized concept of computability; universal turing machine
1948	von Neumann	Abstracted the logical structure of life; introduced self-reproducing automata as a means towards developing a reductionist biology
1950	Ulam	Proposed need for having more realistic models for the behavior of complex extended systems
1966	Burks	Completed and described von Neumann's work
1967	von Bertalanffy, <i>et al</i>	<i>System theory</i> applied to human systems
1969	Zuse	Introduced concept of "computing spaces," or digital models of mechanics
1970	Conway	Introduced two-dimensional cellular automaton Life rule
1977	Toffoli	Applied cellular automata directly to modeling physical laws
1983	Wolfram	Wrote a landmark review article on properties of cellular automata that effectively legitimized the field as research endeavor for physicists
1984	Cowan, <i>et al</i>	Santa Fe Institute founded, serving as a pre-eminent center for the interdisciplinary study of complex systems
1984	Toffoli, Wolfram	First cellular automata conference held at MIT, Boston
1987	Langton	First artificial life conference held at the Santa Fe Institute
1992	Varela, <i>et al</i>	First European conference on artificial life

Table 1.1 Some landmark historical developments in the study of cellular automata and complex systems.

known models proven to be computational universal [berk82].

Other important historical landmarks include the founding, in 1984, of the Santa Fe Institute,* which is one of the leading interdisciplinary centers for complex systems theory research; the first conference devoted solely to research in cellular automata (which is a prototypical mathematical model of complex systems), organized by Farmer, Toffoli and Wolfram at MIT in 1984 [farmer84]; and the first artificial life conference, organized by Chris Langton at Los Alamos National Laboratory, in 1987 [lang89].

*See the *Santa Fe Institute's* web site at <http://www.santafe.edu>.

1.2 Cellular Automata

Cellular automata (CA) are a class of spatially and temporally discrete, deterministic mathematical systems characterized by local interaction and an inherently parallel form of evolution. First introduced by von Neumann in the early 1950s to act as simple models of biological self-reproduction, CA are prototypical models for complex systems and processes consisting of a large number of identical, simple, locally interacting components. The study of these systems has generated great interest over the years because of their ability to generate a rich spectrum of very complex patterns of behavior out of sets of relatively simple underlying rules. Moreover, they appear to capture many essential features of complex self-organizing cooperative behavior observed in real systems.

Although much of the theoretical work with CA has been confined to mathematics and computer science, there have been numerous applications to physics, biology, chemistry, biochemistry, and geology, among other disciplines. Some specific examples of phenomena that have been modeled by CA include fluid and chemical turbulence ([d'Hum86], [gerh89]), plant growth [linde89] and the dendritic growth of crystals [kess90], ecological theory [prip92], DNA evolution, the propagation of infectious diseases [segel99], social dynamics [axtel96], forest fires [bak90], and patterns of electrical activity in neural networks [fran92]. CA have also been used as discrete versions of partial differential equations in one or more spatial variables. They have most recently been used to simulate some aspects of military combat (see [wood88] and [ilach97]).

The best sources of information on CA are conference proceedings and collections of papers, such as the one's edited by Boccara [bocc93a], Gutowitz [guto90a], Preston [prest84] and Wolfram ([wolf83b], [wolf94a]). An excellent review of how CA can be used to model physical systems is given by Toffoli and Margolus [marg87].

While there is an enormous variety of particular CA models—each carefully tailored to fit the requirements of a specific system—most CA models usually possesses these five generic characteristics:

- **Discrete lattice of cells:** the system substrate consists of a one-, two- or three-dimensional lattice of cells.
- **Homogeneity:** all cells are equivalent.
- **Discrete states:** each cell takes on one of a finite number of possible discrete states.
- **Local interactions:** each cell interacts only with cells that are in its local neighborhood.
- **Discrete dynamics:** at each discrete unit time, each cell updates its current state according to a transition rule taking into account the states of cells in its neighborhood.

There is a deceptive simplicity to these characteristics. In fact, as we shall see repeatedly in this book, such systems are capable of extremely complicated behavior. For example, although obeying local rules and having no intrinsic length scales other than the size of the neighborhoods about each site, CA can generate global patterns with very long-range order and correlation. CA are dynamically rich enough to be seriously considered as alternative mathematical models for a variety of physical systems.

While one is free to think of CA as being nothing more than formal idealizations of partial differential equations, their real power lies in the fact that they represent a large class of *exactly computable models*: since everything is fundamentally discrete, one need never worry about truncations or the slow accumulation of round-off error. Therefore, any dynamical properties observed to be true for such models take on the full strength of theorems [toff77a].

Exact computability in this sense, however, is achieved only at the cost of being able to obtain approximate solutions. Perturbation analysis, for example, is rendered virtually meaningless in this context. It is not surprising that traditional investigatory methodologies are not very well suited to studies of complex systems. Since the behavior of such models can generally be obtained *only* through explicit simulation, the computer becomes the one absolutely indispensable research tool.

1.2.1 CA & Computation

Since CA are totally discrete information processors, a useful analogy almost immediately presents itself between such models and conventional computers. Simply identify the initial state value specification in a CA with the initial *data* of a computer program, and identify the uniquely prescribed rule by which the sites evolve with the *program* itself. Running the program is equivalent to using the CA rule to evolve generations from the initial state, with successive configurations representing intermediate results of the computation. Unlike the serial computations making up the CPU cycles in conventional computers, however, CA process information in a fully parallel manner. Basic theoretical results have been obtained by exploiting this formal equivalence between CA and computers [wolf85e].

von Neumann's construction of a two-dimensional automaton capable of self-reproduction was the first discrete parallel computational model shown formally to be a *universal computer*. Twenty years later, John Conway introduced his (now, well studied) *Life* rule, which remains among the simplest known models proven rigorously to be a computationally universal system (see example # 2 below).

Computational universality is the ability to implement any finite algorithm and thus evaluate any computable function [wolf85e]. This property can be proven either by showing that the given system is formally equivalent to another system known to be a universal computer or by directly identifying the dynamics of intrinsically generated structures with the state transitions in a *Turing Machine* [garey79].

Apart from granting systems the same formal computational power as conventional digital computers, computational universality places a severe restriction on possible theoretical predictions of system behavior [toff77a]: because universal com-

puters all require the same order of magnitude times and data storage capacities to process particular algorithms, no computational method can exist with which a shortcut route is taken to a particular dynamical outcome. In the strongest possible terms, the long time behavior of computationally universal dynamical systems can be obtained only by direct simulation. No general predictive procedure is possible, even in principle. This implies, for example, that for systems such as von Neumann's self-reproducing automaton, there can neither be an analytical expression that exactly describes its asymptotic behavior nor an equation that defines the long-term behavior that itself can be solved in a time less than it would take the system to evolve (modulo a polynomial function of the number of iteration steps necessary for it to reach its final state). All such computationally irreducible systems share the property that their own evolution effectively defines the most efficient simulation of their behavior.

1.2.2 *Why Study CA?*

There are at least four partially overlapping motivations for studying CA, which we order according to increasing levels of theoretical significance:

- *As powerful computation engines*
- *As discrete dynamical system simulators*
- *As conceptual vehicles for studying pattern formation and complexity*
- *As original models of fundamental physics*

1.2.2.1 *CA as Powerful Computation Engines*

CA allow very efficient parallel computational implementations to be made of lattice models in physics and thus for a detailed analysis of many concurrent dynamical processes in nature. Indeed, dedicated hardware represents one of the most promising practical applications of CA modeling. With the help of such hardware, many heretofore intractable but technologically important problems such as fluid flow near and around airplane wings, are becoming computationally accessible for the first time. Weisbuch has aptly compared such dedicated CA processors to being the numerical equivalents of wind tunnels [weis91]. More ambitiously, Toffoli and Margolus foresee hardware implementations of CA systems as embodying the concept of *programmable matter* [toff91]; that is to say, a computationally amorphous "machine" that can be "programed" to act as a numerical wind tunnel one moment, or a sea of fermions the next. Their CAM-8 machine, a powerful new descendent of their earlier CAM-5 and CAM-6 CA simulators, comes close to realizing this exciting possibility.[†] The CAM-6, for example, which is still available commercially as a plug-in card for the PC, provides a 256-by-256 two dimensional array in which each site may contain up to four bits of data and the entire array is scanned, updated and displayed sixty times every second. Its speed is comparable in performance

[†]See MIT's *Information Mechanics Group* web page on the CAM-8 at <http://www.im.lcs.mit.edu/cam8/>.

to that of a CRAY-1 for this kind of application. A new generation of CA-based massively parallel computing machines is ushering in a new era in computational physics and applied mathematics.

1.2.2.2 CA as Discrete Dynamical System Simulators

CA allow systematic investigation of complex phenomena by embodying any number of desirable physical properties. Reversible CA,[†] for example, can be used as laboratories for studying the relationship between microscopic rules and macroscopic behavior—exact computability ensuring that the memory of the initial state is retained exactly for arbitrarily long periods of time. The behavior of computationally universal reversible rules, such as Fredkin’s *Billiard Ball* model [fredkin82], are of more than passing interest since they can conceivably avoid the fundamental lower bound on dissipation associated with the reversibility of logic elements in conventional computers [keyes70].

Suitably generalized discrete models have thus far been constructed and studied for dendritic crystal growth [kess90], spatial patterns generated by reaction-diffusion systems (such as the Belousov-Zhabotinsky reaction [madore83]; see example # 3 below), Ising models [creutz86], self-organization in neural networks [fran92], discrete multiple soliton-structure dynamics [aizawa90], and turbulence in hydrodynamical systems [chenh88]. Discrete models of turbulence are particularly impressive in that they clearly show that very simple finite dynamical implementations of local conservation laws (defined so that the discrete system is computationally universal) are capable of exactly reproducing continuum system behavior on the macroscale.

1.2.2.3 CA as Conceptual Vehicles for Exploring Pattern Formation

CA can be treated as abstract discrete dynamical systems embodying intrinsically interesting, and potentially novel, behavioral features. The central motivation is to abstract the general principles governing self-organizing structure formation. Haken ([haken77],[haken83]) has pioneered the interdisciplinary study of self-organization, coining the term *synergetics* to describe this emerging new discipline. Because of their underlying simplicity, CA offer a powerful theoretical and simulation research tool. Related interests include formal classification of the dynamical behavior of complex systems; a better understanding of the relationship between the dynamics of continuous and discrete systems; and the quantification of complexity—as a system property. All of these questions are particularly accessible through studying the generic behavior of CA systems.

[†]Reversible CA are characterized by the property that each site value has a unique predecessor neighborhood configuration.

1.2.2.4 CA as Original Models of Fundamental Physics

CA allow studies of radically new discrete dynamical approaches to microscopic physics, exploring the possibility that nature locally and digitally processes its own future states. The entire last chapter of this book is devoted to a prolonged discussion of such potentially ground breaking models of physics. Using the fact that computationally universal systems are capable of arbitrarily complicated behavior (in the sense that they can mimic any computation performed by a conventional computer), the idea is to construct fundamentally discrete field theories to compete with existing continuous models. The emphasis in this class of models is emphatically *not* to construct a lattice-gauge-like theory; rather, in the same way as lattice-gas CA successfully reproduce continuous fluid flow despite never having heard of the Navier-Stokes equations, so the hope is to abstract a set of microphysical laws that reproduce known behavior on the macro scale. A number of interesting ideas have recently been explored. Fredkin [fredkin93] has arguably gone to the furthest extreme by asserting that the universe is, at its core, a CA! We will offer a few of our own speculations on this subject in the last chapter.

1.2.3 Example #1: One-dimensional CA

For a one-dimensional CA, the value of the i^{th} cell at time t – denoted by $c_i(t)$ – evolves in time according to a rule F that is a function of $c_i(t)$ and other cells that are within a range r (on the left and right) of $c_i(t)$:

$$c_i(t) = F(c_{i-r}(t-1), c_{i-r+1}(t-1), \dots, c_{i+r-1}(t-1), c_{i+r}(t-1)). \quad (1.1)$$

Since each cell takes on one of k possible values—that is, $c_i(t) \in \{0, 1, 2, \dots, k\}$ —the rule F is completely defined by specifying the value assigned to each of the k^{2r+1} possible $(2r+1)$ -tuple configurations for a given range- r neighborhood:

$c_{i-r}(t-1)$	$\dots$	$c_i(t-1)$	$\dots$	$c_{i+r}(t-1)$	$c_i(t)$
0		0		0	$F(0,0,\dots,0)$
0		0		1	$F(0,0,\dots,1)$
$\vdots$		$\vdots$		$\vdots$	$\vdots$
k		k		k	$F(k,k,\dots,k)$

Since F itself assigns any of k values to each of the k^{2r+1} possible $(2r+1)$ -tuples, there are a total of $k^{k^{2r+1}}$ possible rules, which is an exponentially increasing function of both k and r . For the simplest case of nearest neighbors (range $r=1$) and $k=2$ ($c_i = 0$ or 1), for example, there are $2^8 = 256$ possible rules. Increasing the number of values each cell can take on to $k=3$ (but keeping the radius at $r=1$) increases the rule-space size to $3^{3^3} \approx 7 \cdot 10^{12}$.

Figure 1.1 shows the time evolution of a nearest-neighbor (radius $r=1$) rule where c is equal to either 0 or 1. The row of eight boxes at the top of the figure shows the explicit rule-set, where – for visual clarity – a box has been arbitrarily colored

black if the value $c=1$ and white if $c=0$. For each combination of three adjacent cells in generation 0, the rule F assigns a particular value to the next-generation center cell of the triplet. Beginning from an initial state (at time=0) consisting of the value zero everywhere except the center site, that is assigned the value 1, F is applied synchronously at each successive time step to each cell of the lattice. Each generation is represented by a row of cells and time is oriented downwards. The first image shows a blowup of the first five generations of the evolution. The second shows 300 generations. The figure illustrates the fact that simple rules can generate considerable complexity.

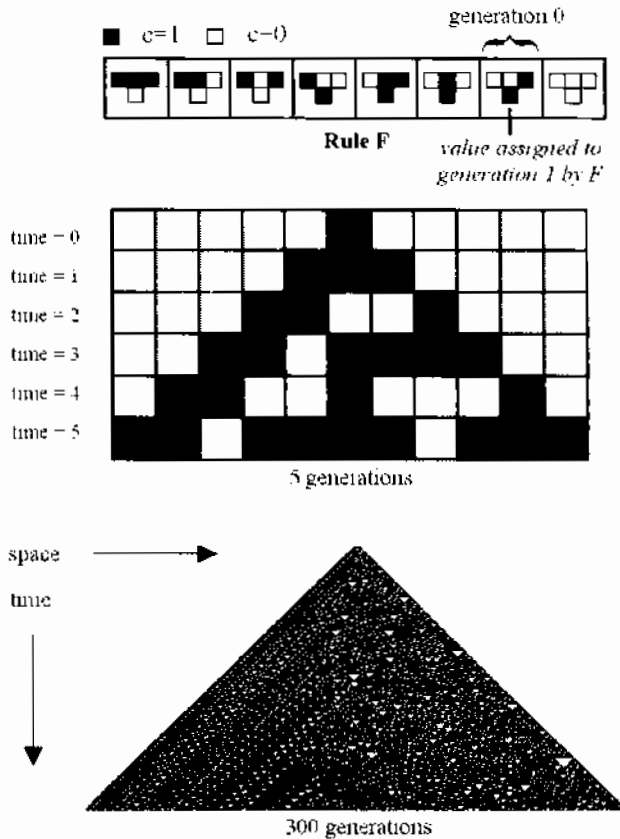


Fig. 1.1 Example of a one-dimensional CA starting from a single nonzero seed.

The space-time pattern generated from a single nonzero cell by this particular rule has a number of interesting properties. For example, it consists of a curious mixture of ordered behavior along the left-hand-side and what appears to be disordered behavior along the right-hand-side, separated by a corrugated boundary moving towards the left at a "speed" of about $1/4$ cells per "clock" tick. In fact, it can be shown that, despite starting from an obviously non-random initial state and evolving according to a fixed deterministic rule, the temporal sequence of ver-

tical values is completely random. Systems having the ability to deterministically generate randomness from non-random input are called autoplectic systems.

As another example, consider the rule shown at the top of figure 1.2. Its space-time evolution, starting from a random initial state, is shown at the bottom of the figure. Note that this space-time pattern can be described on two different levels: either on the cell-level, by explicitly reading off the values of the individual cells, or on a higher-level by describing it as a sea of particle-like structures superimposed on a periodic background. In fact, following a small initial transient period, temporal sections of this space-time pattern are always of the form "...BBBBPBB...BB...BBBP'BB...BBBP"BBB...", where "B" is a state of the periodic background consisting of repetitions of the sequence "10011011111000" (with spatial period 14 and temporal period 7), and the P's represent "particles." The particle pattern $P = "11111000"$, for example, repeats every four steps while being displaced two cells to the left; the particle $P = "11101011000"$ repeats every ten steps while being displaced two cells to the right.

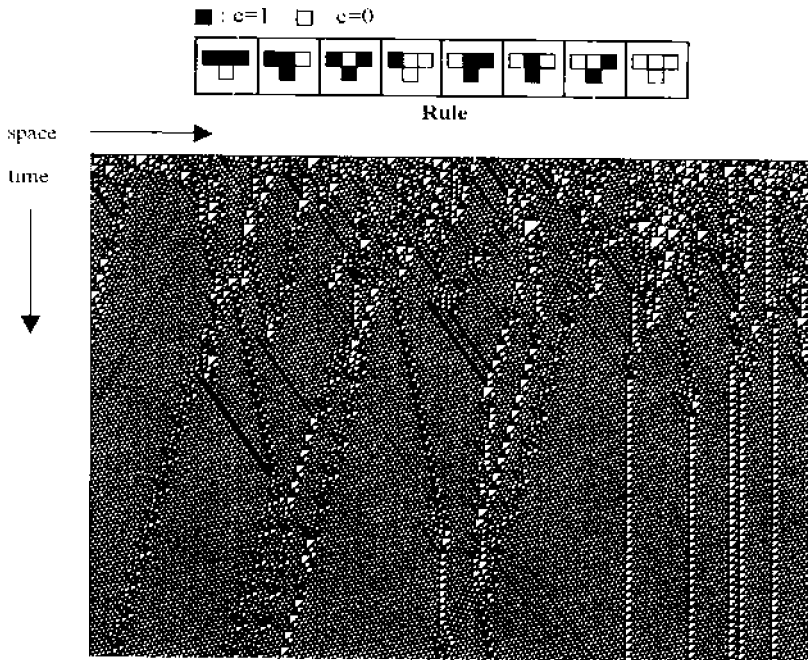


Fig. 1.2 Evolution of a one-dimensional CA starting from a random initial state.

Although the underlying dynamics describing this system is very simple, and entirely deterministic, there is an enormous variety, and complexity, of emergent particle-particle interactions. Such simple systems are powerful reminders that complex higher-level dynamics need not have a complex underlying origin. Indeed, suppose that we had been shown such a space-time pattern but were told nothing whatsoever about its origin. How would we make sense of its dynamics? Perhaps

the only reasonable course of action would be to follow the lead of any good experimental particle-physicist and begin cataloging the various possible particle states and interactions: there are N particles of size s moving to the left with speed v ; when a particle p of type P collides with q of type Q , the result is the set of particles $\{p_1, \dots, p_n\}$; and so on. It would take a tremendous leap of intuition to fathom the utter simplicity of the real dynamics.

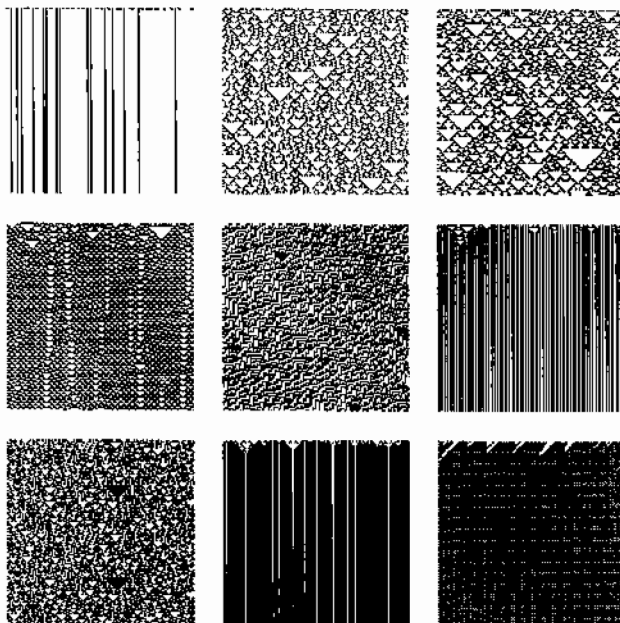


Fig. 1.3 Space-time evolution of nine different nearest neighbor one-dimensional CA starting from random initial states.

In general, the behavior of CA is strongly reminiscent of the kinds of behavior observed in continuum dynamical systems, with simple rules yielding steady-state behaviors consisting of fixed points or limit cycles, and complex rules giving rise to behaviors that are analogous to deterministic chaos. In fact, there is extensive empirical evidence suggesting that patterns generated by all (one-dimensional) CA evolving from disordered initial states fall into one of only four basic behavioral classes [wolf83a]:

- Class 1: *Evolution leads to a homogeneous state, in which all cells eventually attain the same value.*
- Class 2: *Evolution leads to either simple stable states or periodic and separated structures.*
- Class 3: *Evolution leads to chaotic nonperiodic patterns.*

- **Class 4:** *Evolution leads to complex, localized propagating structures.*

All CA within a given class yield qualitatively similar behavior. While the behaviors of rules belonging to the first three rule classes bear a strong resemblance to those observed in continuous systems – the homogeneous states of class 1 rules, for example, are analogous to fixed-point attracting states in continuous systems, the asymptotically periodic states of class 2 rules are analogous to continuous limit cycles and the chaotic states of class 3 rules are analogous to strange attractors – the more complicated localized structures emerging from class 4 rules do not appear to have any obvious continuous analogues (although such structures are well characterized as being soliton-like in their appearance).

Figure 1.3 shows a few examples of the kinds of space-time patterns generated by binary ($k = 2$) nearest-neighbor ($r = 1$) in one dimension and starting from random initial states.

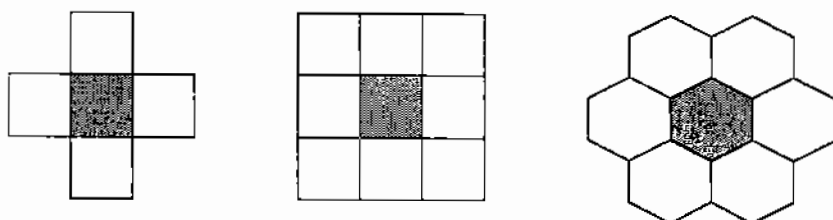


Fig. 1.4 Examples of CA neighborhoods in two dimensions.

Figure 1.4 shows examples of some commonly used neighborhood structures in two dimensions. These include the von Neumann neighborhood, which consists of the four cells that are horizontally and vertically adjacent to the center cell (left-most graphic appearing in figure 1.4), (2) the Moore neighborhood, that consists of all eight nearest-neighbor cells on a two-dimensional Euclidean lattice (center graphic in figure 1.4), and (3) the Hexagonal neighborhood, that consists of all nearest-neighbor cells on a hexagonal lattice (right-most graphic in figure 1.4).

1.2.4 Example #2: Conway's Life

"Its probable, given a large enough Life space, initially in a random state, that after a long time, intelligent self-reproducing animals will emerge and populate some parts of the space." – John H. Conway [berk82]

Perhaps the most widely known CA is the game of Life, invented by John H. Conway, and popularized extensively by Martin Gardner in his "Mathematical Games" department in *Scientific American* in the early 1970s (see, for example, [gardner70]).

Life is "played" using the 9-neighbor Moore neighborhood (see center graphic in figure 1.4), and consists of (1) seeding a lattice with some pattern of "live" and "dead" cells, and (2) simultaneously (and repeatedly) applying the following three

rules to each cell of the lattice at discrete time steps:

- **Birth:** replace a previously dead cell with a live one if exactly 3 of its neighbors are alive.
- **Death:** replace a previously live cell with a dead one if either (1) the living cell has no more than one live neighbor (i.e. it dies of isolation), or (2) the living cell has more than three neighbors (i.e. it dies of overcrowding).
- **Survival:** retain living cells if they have either 2 or 3 neighbors.

One of the most intriguing patterns in Life is an oscillatory propagating pattern known as the “glider.” Shown on the left-hand-side of figure 1.5, it consists of 5 “live” cells and reproduces itself in a diagonally displaced position once every four iterations.

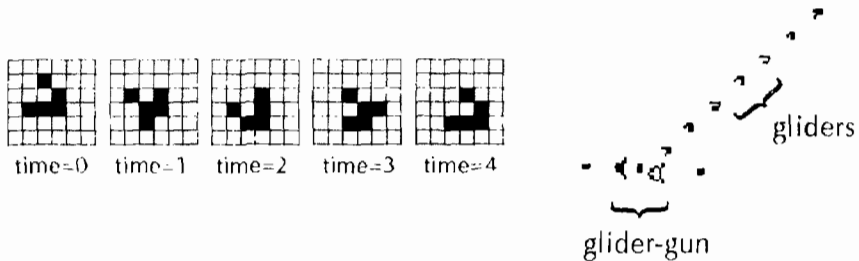


Fig. 1.5 Glider patterns in Conway's Life.

When the states of Life are projected onto a screen in quick succession by a fast computer, the glider gives the appearance of “walking” across the screen. The propagation of this pseudo-stable structure can also be seen as a self-organized emergent property of the system. The right-hand-side of figure 1.5 shows a still-frame in the evolution of a pattern known as a “glider-gun,” which shoots-out a glider once every 30 iteration steps.

What is remarkable about this very simple appearing rule is that one can show that it is capable of universal computation. This means that with a proper selection of initial conditions (i.e. the initial distribution of “live” and “dead” cells), Life can be turned into a general purpose computer. This fact fundamentally limits the overall predictability of Life's behavior.

The well known *Halting Theorem*, for example, asserts that there cannot exist a general algorithm for predicting when a computer will halt its execution of a given program [gary79]. Given that Life is a universal computer – so that the Halting Theorem applies – this means that one cannot, in general, predict whether a particular starting configuration of live and dead cells will eventually die out. No shortcut is possible, even in principle. The best one can do is to sit back and patiently await Life's own final outcome.

Put another way, this means that if you want to predict Life's long-term behavior with another “model” or by using, say, a partial differential equation, you

are doomed to fail from the outset because its long-term behavior is effectively unpredictable. Life – like all computationally universal systems – defines the most efficient simulation of its own behavior.

1.2.5 Example #3: Belousov–Zhabotinski Reaction

The Belousov-Zhabotinski (BZ) reaction is a chemical reaction consisting of simple organic molecules that is characterized by spectacular oscillating temporal and spatial patterns [zhabo64]. One variant of the BZ reaction involves the reaction of bromate ions with an organic substrate (typically malonic acid) in a sulfuric acid solution with cerium (or some other metal-ion catalyst). When this mixture is allowed to react exothermally at room temperature, interesting temporal and spatial oscillations (i.e. chemical waves) result. The system oscillates, changing from yellow to colorless and back to yellow about twice a minute, with the oscillations typically lasting for over an hour (until the organic substrate is exhausted).

These patterns are an example of what are sometimes called *dissipative structures*, which arise in many complex systems. Dissipative structures are dynamical patterns that retain their organized state by persistently dissipating matter and energy into an otherwise thermodynamically open environment.

Figure 1.6 shows a sample evolution of a CA model of this reaction, in which cells are identified with the reacting molecules, and are colored *black* if they are “active” and *white* if they are “inactive,” according to the reaction rules. The spatial and temporal patterns that emerge from the initially random mixture of states are also a good general example of how CA can be used to model self-organization. The rule shown here is due to Gerhardt and Schuster ([gerh89]; also see color plate 4 in the appendix to chapter three).

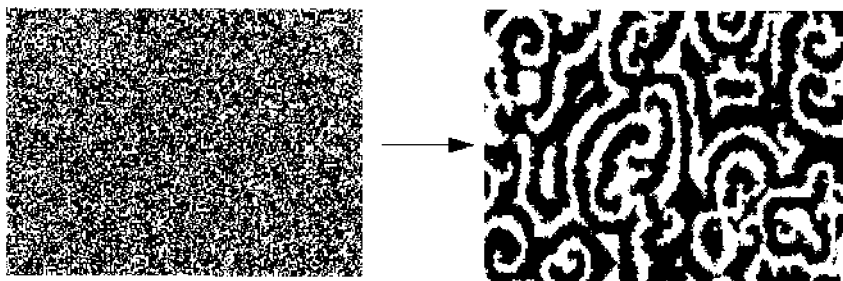


Fig. 1.6 Example of self-organization in a two-dimensional CA.

1.2.6 Example #4: Lattice Gases

Lattice gases are micro-level rule-based simulations of macro-level fluid behavior. Lattice-gas models provide a powerful new tool in modeling real fluid behavior ([doolen90], [doolen91]). The idea is to reproduce the desired macroscopic behavior of a fluid by modeling the underlying microscopic dynamics.

It can be shown that three basic ingredients are required to achieve an emergence of a suitable macrodynamics out of a discrete microscopic substrate [hass89]: (1) local thermodynamic equilibrium, (2) conservation laws, and (3) a “scale separation” between the levels at which the microscopic dynamics takes place (among kinetic variables living on a micro-lattice) and the collective motion itself appears (defined by hydrodynamical variable on a macro-lattice). Another critical feature is the symmetry of the underlying lattice.

While there are many variants of the basic model, one can show that there is a well-defined minimal set of rules that define a lattice-gas system whose macroscopic behavior reproduces that predicted by the Navier-Stokes equations exactly.[§] In other words, there is critical “threshold” of rule size and type that must be met before the continuum fluid behavior is matched, and once that threshold is reached the efficacy of the rule-set is no longer appreciably altered by additional rules respecting the required conservation laws and symmetries.

Figure 1.7 shows a few snapshots of the evolution of a two-dimensional lattice gas starting from an initial condition in which there is a tightly packed region of particles at the center of the lattice. Notice how this central region expands rapidly outward, and is very reminiscent of the effect a dropped stone has on an initially stagnant pool of water. The most striking feature is the circular sound wave, which is circular despite the fact that the microscopic dynamics takes place on a square lattice. The lattice gas rules thus force a symmetry that is not present in the microscopic dynamics to emerge on the macro-scale.

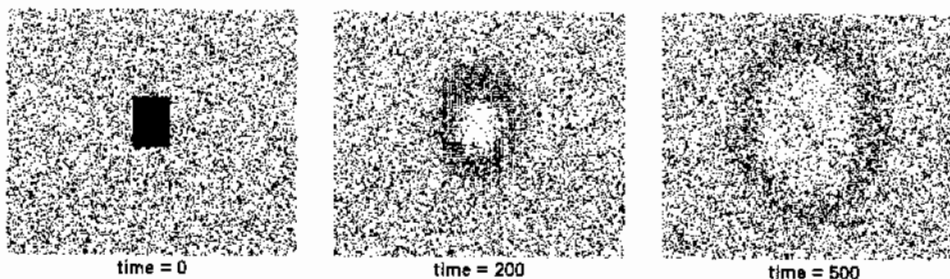


Fig. 1.7 Two-dimensional lattice-gas simulation of a fluid.

1.2.7 Example #5: Collective Behavior in Higher Dimensions

Chate and Manneville [chate92] have examined a wide variety of cellular automata that live in dimensions four, five and higher. They found many interesting rules that while being essentially featureless locally, nonetheless show a remarkably ordered global behavior.

Here again we see a pristine example of the three basic elements of emergence: (1) the global phenomenon (in this case the cell-value density) emerges out of an

[§]The Navier-Stokes equations are the fundamental equations describing incompressible fluid flow; see Chapter 9.

interaction of a large number of simple components (lattice cells of a cellular automaton), (2) there is no evidence of the global phenomenon on the local level, and (3) the global phenomenon obeys a separate dynamics (in this case, quasi-periodicity).

Figure 1.8, for example, plots the probability that a cell has value 1 at time $t+1$ – labeled P_{t+1} – versus the probability that a cell had value 1 at time t – labeled P_t – for a particular four dimensional cellular automaton rule. The rule itself is unimportant, as there are many rules that display essentially the same kind of behavior. The point is that while the behavior of this rule is locally featureless – its space-time diagram would look like noise on a television screen – the global density of cells with value 1 jumps around in quasi-periodic fashion. We emphasize that this quasi-periodicity is a *global* property of the system, and that no evidence for this kind of behavior is apparent in the local dynamics.

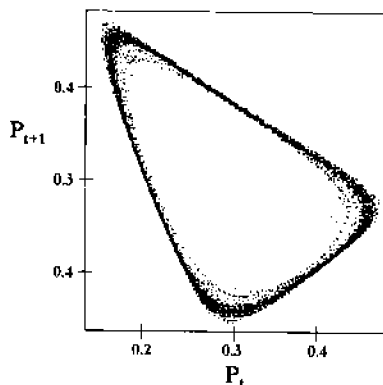


Fig. 1.8 Collective behavior of a four dimensional CA (after [chate92]).

1.2.8 Other Variants

There are at least as many variants of the basic CA algorithm as there are ways of generalizing the characteristics of a typical CA system. Here are a few general models:

Asynchronous CA. CA rules are typically defined so that all lattice sites update their values simultaneously throughout the lattice on each time step. A natural generalization is to lift this restriction by allowing *asynchronous* updates [inger84].

Coupled-map Lattices. Another obvious generalization is to lift the restriction that sites can take on only one of a few discrete values. Coupled-map lattices are CA models in which continuity is restored to the state space. That is to say, the cell values are no longer constrained to take on only the values 0 and 1 as in the examples discussed above, but can now take on arbitrary real values. First introduced by Kaneko [kaneko83]-[kaneko93], such systems are simpler than partial differential equations but more complex than generic CA. Coupled-map lattices are discussed in chapter 8.

Probabilistic CA. Probabilistic CA are cellular automata in which the deterministic state-transitions are replaced with specifications of the probabilities of the cell-value assignments. Since such systems have much in common with certain statistical mechanical models, analysis tools from physics are often borrowed for their study. Probabilistic CA are introduced in chapter 8.

Non-homogeneous CA. These are CA in which the state-transition rules are allowed to vary from cell to cell. The simplest such example is one where there are only two different rules randomly distributed throughout the lattice. Kauffman [kauff84] has studied the other extreme in which the lattice is randomly populated with all possible Boolean functions of k inputs.

Mobile CA. These are CA in which some (or all) lattice sites are free to move about the lattice. In effect, mobile CA are primitive models of mobile robots. Typically, their internal state space reflects some features of the local environment within which they are allowed to move and with which they are allowed to interact. An example of mobile CA used to model some aspects of military engagements is discussed in Chapter 12.

Structurally Dynamics CA. Most of the CA that we will encounter throughout this book (indeed, most that are currently being studied!) assume that the underlying lattice remains a passive and static object. The lattice is thus typically an arena for activity, not an active participant in the dynamics. What if the lattice were somehow made an integral part of the dynamics? That is to say, what if the topology – the sites and connections among sites – evolved alongside the value states? Structurally dynamic CA are discussed in Chapter 8.

1.3 Outline of Book

The remainder of the book is divided into eleven largely self-contained chapters. Chapter 2 introduces some basic mathematical formalism that will be used throughout the book, including set theory, information theory, graph theory, groups, rings and field theory, and abstract automata. It concludes with a preliminary mathematical discussion of one and two dimensional CA.

Chapter 3 provides a phenomenological introduction to generic CA. The narrative includes both a mathematical description of one, two and three dimensional CA along with guided-tour through a graphics-gallery of typical space-time patterns. Simple ways of parameterizing the space of CA rules are described, and a sketch of the proof of the computational universality of Conway's famous two-dimensional *Life*-rule is also provided.

Chapter 4 covers much of the same ground as chapter 3 but from a more formal dynamical systems theory approach. The discrete CA world is examined in the context of what is known about the behavior of continuous dynamical systems, and a number of important methodological tools developed by dynamical systems theory (i.e. Lyapunov exponents, invariant measures, and various measures of entropy and

dimension) are used to characterize the behavior of simple CA systems.

Chapter 5 provides some examples of purely analytical tools useful for describing CA. It discusses methods of inferring cycle-state structure from global eigenvalue spectra, the enumeration of limit cycles, the use of shift transformations, local structure theory, and Lyapunov functions. Some preliminary research on linking CA behavior with the topological characteristics of the underlying lattice is also described.

Chapter 6 is a short primer on CA and language theory, and provides a basic discussion of formal language theory, the relationship between CA and formal language theory, power spectra of regular languages and reversible computation.

Chapter 7 discusses a variety of topics all of which are related to the class of probabilistic CA (PCA); i.e. CA that involve some elements of probability in their state and/or time-evolution. The chapter begins with a physicist's overview of critical phenomena. Later sections include discussions of the equivalence between PCA and spin models, the critical behavior of PCA, mean-field theory, CA simulation of conventional spin models and a stochastic version of Conway's *Life* rule.

Chapter 8 describes a number of generalized CA models, including reversible CA, coupled-map lattices, quantum CA, reaction-diffusion models, immunologically motivated CA models, random Boolean networks, sandpile models (in the context of self-organized criticality), structurally dynamic CA (in which the temporal evolution of the *value* of individual sites of a lattice are dynamically linked to an evolving lattice *structure*), and simple CA models of combat.

Chapter 9 provides an introductory discussion of a research area that is rapidly growing in importance: *lattice gases*. Lattice gases, which are discretized models of continuous fluids, represent an early success of CA modeling techniques. The chapter begins with a short primer on continuum fluid dynamics and proceeds with a discussion of CA lattice gas models. One of the most important results is the observation that, under certain constraints, the macroscopic behavior of CA models *exactly* reproduces that predicted by the Navier-Stokes equations.

Chapter 10 covers another important field with a great overlap with CA: *neural networks*. Beginning with a short historical survey of what is really an independent field, chapter 10 discusses the Hopfield model, stochastic nets, Boltzman machines, and multi-layered perceptrons.

Chapter 11 contains a very brief introduction to what is rapidly becoming one of the central research areas in complex systems theory; namely, *artificial-life* (AL). Owing its origins to von Neumann's early explorations in self-reproducing automata, AL has blossomed in the last decade from consisting of a few toy worlds hardly more sophisticated than Conway's *Life*-rule universe to intricately rendered 3D artificial universes populated with interacting creatures undergoing an open-ended evolution. Topics include a brief survey of von Neumann's original work, Lindenmeyer systems, Langton's *vants* model, a short primer on genetic algorithms. The chapter concludes with a discussion of an artificial-life-like mobile CA model of land warfare.

The last chapter is a broad survey of a speculative proposition that CA just might one day prove to be even more profound in what they say about how our universe is organized than has heretofore been appreciated. The essence of the

proposition, borrowed from musings by Feynman [feyn82], Fredkin [fredkin90], Minsky [minsky82], Wheeler [wheel90] and others, is that the universe is fundamentally discrete and obeys, at its core, a simple CA-like dynamics. *Thus begin some final musings and a perhaps a glimpse of a new cosmogony!*

Appendix A provides a brief description of several existing hardware and software tools designed for CA research. Appendix B contains a useful list of CA and more general complexity-related information sources available on the World Wide Web (WWW), subject-sorted into a total of 91 WWW Universal Resource Locator (URL) links in 16 categories. The book is indexed and includes an extensive bibliography.

Chapter 2

Formalism

From a physicist's (or applied mathematician's) point of view, CA can be effectively thought of as being nothing more than very simple and elegant sets of rules that can be *played with* on a computer. However, a sincere understanding of their depth and elegance can come only from an appreciation of the great variety of different fields and mathematical formalisms to which they owe much of their history and substance. This introductory chapter briefly introduces some of the more important mathematical techniques that we will often use in our discussion. Specific formalisms will be subsequently developed in greater detail as needed in later chapters.

2.1 Mathematical Preliminaries

2.1.1 *Set Theory*

Sets

We shall often be dealing with *sets* of objects of some kind. A *set*, which we will label by capital letters $A, B, \dots$, is a collection of objects, denoted by lowercase letters $a, b, \dots$, which are *members* (or *elements*) of the set. Finite sets may be defined by explicitly listing all of their members: if the set A consists of the three elements a, b, c , for example, we would write $A \equiv \{a, b, c\}$. We also write $a \in A$ to mean that ' a ' belongs to the set A . Arbitrary sets may sometimes be more conveniently specified by some *property* $\mathcal{P}$, which is shared by all of their members. For example, the set

$$B \equiv \{x \mid x \text{ is an even integer} \}, \quad (2.1)$$

is the set consisting of all objects ' x ' such that ' x ' is an even integer. To indicate that a set C consists of all elements of some specific set $\mathcal{S}$ sharing the property $\mathcal{P}$, we can write $C = \{x \in \mathcal{S} \mid \mathcal{P}(x)\}$.

A set A is a *subset* of B , written as $A \subset B$, if every element of A is also an element of B . One special kind of set is the *null* (or *empty*) set, which is “the set having no elements”. The null set is the subset of every set A and is denoted by the symbol ϕ . The *power set* of A , $\mathcal{P}(A) = 2^A$, is defined as the set of all subsets of A : $\mathcal{P}(A) = \{B \mid B \subset A\}$. We observe that sets are *completely defined by their elements*: two sets A and B are *equal* if they have the exactly the same elements; i.e. $A = B$ if and only if $A \subset B$ and $B \subset A$.

Operations on Sets

From any two sets, one can form a third set by using a variety of set operations. The *union* of two sets A and B , for example, is the set C consisting of all elements in A or B or in both A and B ,

$$C = A \cup B \equiv \{x \mid x \in A \text{ or } x \in B\}, \quad (2.2)$$

and obeys the following properties:

$$\begin{aligned} \mathbf{U1}: & A \cup B = B \cup A \\ \mathbf{U2}: & A \cup A = A \text{ and } A \cup \phi = A \\ \mathbf{U3}: & A \cup (B \cap C) = (A \cup B) \cap C \\ \mathbf{U4}: & A \cup B = B \text{ if and only if } A \subset B \end{aligned} \quad (2.3)$$

A union of an arbitrarily large number of sets is handled in a straightforward manner: let $A_1, A_2, \dots, A_n$ be sets. Then

$$\bigcup_{i=1}^n A_i \equiv A_1 \cup A_2 \cup \dots \cup A_n = \{x \mid x \in A_i \text{ for at least one } i\}. \quad (2.4)$$

We can similarly form the *intersection* of A and B , which is the set C consisting of elements common to both:

$$C = A \cap B \equiv \{x \mid x \in A \text{ and } x \in B\} \quad (2.5)$$

The properties obeyed by intersection are analogous to those of the union:

$$\begin{aligned} \mathbf{I1}: & A \cap B = B \cap A \\ \mathbf{I2}: & A \cap A = A \text{ and } A \cap \phi = \phi \\ \mathbf{I3}: & A \cap (B \cup C) = (A \cap B) \cup C \\ \mathbf{I4}: & A \cap B = B \text{ if and only if } A \subset B, \end{aligned} \quad (2.6)$$

as is the definition of an arbitrary number of intersections:

$$\bigcap_{i=1}^n A_i \equiv A_1 \cap A_2 \cap \dots \cap A_n = \{x \mid x \in A_i \text{ for each } i = 1, 2, \dots, n\}. \quad (2.7)$$

The union and intersection are related by two distributive laws:

$$\begin{cases} A \cup (B \cap C) = (A \cup B) \cap (A \cup C) & \leftrightarrow \cup - \text{distributive} \\ A \cap (B \cup C) = (A \cap B) \cup (A \cap C) & \leftrightarrow \cap - \text{distributive} \end{cases} \quad (2.8)$$

A third operation on two sets A and B is the *difference*, $A - B$, consisting of elements of A which are not elements of B :

$$C = A - B \equiv \{x \mid x \in A \text{ and } x \notin B\}. \quad (2.9)$$

The difference operator has the following properties:

$$\begin{aligned} \mathbf{D1}: & A - \phi = A \text{ and } A - A = \phi \\ \mathbf{D2}: & A - B = \phi \text{ if and only if } A \subset B \\ \mathbf{D3}: & A - B = A \text{ if and only if } A \cap B = \phi \\ \mathbf{D4}: & A - B = A - C \text{ if and only if } A \cap B = A \cap C \\ \mathbf{D5}: & A - (B \cap C) = (A - B) \cup (A - C) \\ \mathbf{D6}: & A - (B \cup C) = (A - B) \cap (A - C) \end{aligned} \quad (2.10)$$

Properties **D5** and **D6** are sometimes referred to as the *DeMorgan Laws*.

Finally, we mention an important operation called the *cartesian* (or *direct*) product of two sets, $A \times B$, which is the set of ordered pairs of the form (a, b) , where $a \in A$ and $b \in B$:

$$C = A \times B \equiv \{(a, b) \mid a \in A \text{ and } b \in B\}. \quad (2.11)$$

Note that the cartesian product $A \times B$ is *not the same* as the product $B \times A$. A simple example is the two-dimensional coordinate plane $\mathcal{R} \times \mathcal{R}$, where $\mathcal{R}$ is the set of real numbers. Each point of the plane is specified by the ordered pair (x, y) of real numbers; $(x, y) = (y, x)$ if and only if $x = y$. Let $A_1, A_2, \dots, A_n$ be sets. Then

$$\mathbf{X}_{i=1}^n A_i \equiv A_1 \times A_2 \times \dots \times A_n = \{\vec{x} = (x_1, x_2, \dots, x_n) \mid x_i \in A_i\}, \quad (2.12)$$

where x_i is called the i^{th} *coordinate* of $\vec{x}$.

An important concept is that of the *size* of a set. Let $\mathcal{N}$ denote the set of *natural numbers*, and $\mathcal{N}_n$ denote the set $\{1, 2, \dots, n\}$. Then a set A is *finite* if $A = \phi$ or it is in one-to-one correspondence with $\mathcal{N}_n$, for some ' n '; in the latter case, the size (*i.e.* the number of elements) of A is equal to ' n ': $|A| = n$. The following three properties are elementary:

$$\begin{aligned} \mathbf{S1}: & |\mathcal{P}(A)| = 2^{|A|} \\ \mathbf{S2}: & |A \cup B| + |A \cap B| = |A| + |B| \\ \mathbf{S3}: & |A \times B| = |A| |B| \end{aligned} \quad (2.13)$$

A set which is not finite is called *infinite*. Although it is meaningless to speak of the 'number of elements' of such sets, we say that two infinite sets have the same *cardinality* if their respective elements can be put into a one-to-one correspondence.

In particular, sets for which there exists a one-to-one mapping to the set $\mathcal{N}$ are called *countable* (or *countably infinite*).

EXAMPLES: countable sets include the *integers* $\mathcal{Z}$ (simply use the 1 : 1 correspondence $f : \mathcal{N} \rightarrow \mathcal{Z}$, $f(n) = \lfloor n/2 \rfloor (-1)^n$, where $\lfloor x \rfloor$ is the greatest integer not exceeding x); *prime integers* (use $2 \leftrightarrow 1$, $3 \leftrightarrow 2$, $5 \leftrightarrow 3$, etc.) and the set of *rational*s $\mathcal{Q}$ of the form p/q , $p, q \in \mathcal{Z}$ (the easiest way to see this is to imagine an infinite square lattice array, each point of which represents a rational number, and to ‘count’ the points by following a zig-zag motion from the origin outwards).

Not every infinite set is countable, of course. For example, there can be no one-to-one correspondence between $\mathcal{N}$ and its power set $\mathcal{P}(\mathcal{N})$. That the set of reals, $\mathcal{R}$, is an also uncountable set can be demonstrated by using Cantor’s *diagonal* argument: consider just the $\mathcal{R} \in [0, 1]$, and assume that each real in this interval can be put into one-to-one correspondence with an integer ‘ n ’. We then have the matching $n \longleftrightarrow R(n)$. Representing each of the reals, $R(1)$, $R(2)$, $R(3)$, ..., by an infinitely long decimal expansion, we form another real, R^* , by the following prescription: its i^{th} digit is *any digit other than the one found in the i^{th} position of the decimal expansion of $R(i)$* . It should be clear that R^* cannot be an element of our presumably exhaustive set of reals, and therefore cannot be mapped to an integer: *i.e.* $\mathcal{R}$ is uncountable.

Topology

A *topology* $\mathcal{T}$ on a set X is defined to be a collection $\mathcal{T}$ of subsets of X with

$$\begin{cases} \phi, X \in \mathcal{T} \\ \bigcup t_i \subset T, \quad \forall t_i \in \mathcal{T} \\ \bigcap t_i \subset T, \quad \forall t_i \in \mathcal{T}, \end{cases} \quad (2.14)$$

where $\phi \equiv$ *empty set*. A subset $U \subset X$ is an *open set* U of X if $U \in \mathcal{T}$. There are three distinct kinds of topologies of interest to us, and which will be used later to provide a topological characterization of CA: *discrete*, *product* and *metric* topologies.

A *discrete* topology is a collection of all subsets of X . To define the *product* topology we first introduce the notion of a basis for a topology: a basis β for a topology $\mathcal{T}$ on X is a collection of subsets of X such that

$$\begin{cases} \forall x \in X, \exists \text{ at least one } b \in \beta \text{ containing } x \\ \text{if } x \in (b_1 \cap b_2) \text{ then } \exists b_3 \text{ containing } x \mid b_3 \subset (b_1 \cap b_2) \end{cases} \quad (2.15)$$

Now, β can be used to generate a topology $\mathcal{T}(\beta)$: a subset U is *open* in X (*i.e.* $U \in \mathcal{T}(\beta)$) if $\forall x \in U \exists b \in \beta \mid x \in b \text{ and } b \subset U$. Then, the *product topology* on $X \times Y$ is the topology having as basis the collection β of all sets of the form $U \times V$, where U and V are open sets of X and Y , respectively.

In order to define the *metric* topology, we must first introduce the notion of *metric*: a function $\partial : X \times X \rightarrow \mathcal{R}$ is a metric on a set X if and only if it satisfies

the following three properties:

$$\begin{cases} \partial(x, y) \geq 0, \quad \forall x, y \in X; \quad \partial(x, y) = 0 \leftrightarrow x = y \\ \partial(x, y) = \partial(y, x) \\ \partial(x, y) + \partial(y, z) \geq \partial(x, z). \end{cases} \quad (2.16)$$

Using the ϵ -ball $b(x, \epsilon) \equiv \{y | \partial(x, y) < \epsilon\}$, we define the metric topology $\mathcal{T}_\partial$, induced by the metric ∂ , as the topology having as basis the collection $\{b(x, \epsilon) | \forall x \in X, \epsilon > 0\}$. That is, a set U is open in $\mathcal{T}_\partial$ if and only if $\forall u \in U \exists \delta > 0$ such that $b(u, \delta) \subset U$. Generally, topological spaces that arise from metric space are said to be *metrizable*.

A fundamental theorem states that a function $f : \mathcal{T}_1 \rightarrow \mathcal{T}_2$ between two metric topologies is *continuous* if and only if for all open sets $U \in \mathcal{T}_2$, the set $f^{-1}(U)$ is open in $\mathcal{T}_1$. In particular, if two different metrics, ∂_1 and ∂_2 , give rise to the same family of open sets then any function which is continuous under ∂_1 will also be continuous under ∂_2 .

EXAMPLES: (1) Consider the metric function

$$\partial(x, y) = \begin{cases} 1 & \text{if } x \neq y \\ 0 & \text{else.} \end{cases} \quad (2.17)$$

Then the basis elements are given by $b(x, 1) = x$ which defines the *discrete* topology.

(2) $\partial(x, y) = \{\sum_{i=1}^n (x_i - y_i)^2\}^{1/2} \doteq \|\vec{x} - \vec{y}\|$ is the usual *Euclidean* metric on $\mathcal{R}^n$.

(3) If $\partial(x, y)$ is a metric and ' α ' is any positive real number, then $\partial_r(x, y) \equiv \alpha\partial(x, y)$ is also a metric.

(4) A very useful distance measure between ordered sets of discrete valued elements is the *Hamming distance*, ∂_H . Given two sets, $\vec{x} = (x_1, \dots, x_n)$ and $\vec{y} = (y_1, \dots, y_n)$,

$$\partial_H(\vec{x}, \vec{y}) \equiv \sum_{i=1}^n \chi_i, \quad (2.18)$$

where $\chi_i = 1$ if $x_i \neq y_i$ and $\chi_i = 0$ otherwise. Thus ∂_H indicates in how many positions two vectors are different.

Fractal Sets and Dimensions

Consider a subset $A \subset X$ and an arbitrary metric ∂ . Let $N(A, \epsilon)$ be the smallest number of ϵ -balls needed to cover the set A ; i.e.,

$$N(A, \epsilon) = \text{smallest integer 'n' such that } A \subset \bigcup_{i=1}^n b(x_i, \epsilon), \quad (2.19)$$

for some distinct set of points $\{x_i, i = 1, 2, \dots, n\}$. If $N(A, \epsilon)$ increases as $N(A, \epsilon) \sim \epsilon^{-D}$ for $\epsilon \rightarrow 0$ then D is called the *fractal dimension* (sometimes also called the *capacity*) of the set A ; 'solving' for D , we find that

$$D_{\text{fractal}} = \lim_{\epsilon \rightarrow 0} \frac{\ln N(A, \epsilon)}{\ln (1/\epsilon)}. \quad (2.20)$$

That D_{fractal} gives the expected result for simple sets in Euclidean space is easy to see. If A consists of a single point, for example, we have $N(A, \epsilon) = 1, \forall \epsilon$, and thus that $D_{\text{fractal}} = 0$. Similarly, if A is a line segment of length L , then $N(A, \epsilon) = L/\epsilon$ so that $D_{\text{fractal}} = 1$. In fact, for the usual ' n ' dimensional Euclidean sets, the fractal dimension equals the topological dimension. There are more complicated sets, however, for which the two measures differ.

Consider the *triadic Cantor set* construction on the real line: let $x_0 = [0, 1]$ and x_1 be the set obtained from x_0 by deleting the open interval $(\frac{1}{3}, \frac{2}{3})$. Let x_2 be the set obtained from x_1 by deleting the 'middle thirds' $(\frac{1}{9}, \frac{2}{9})$ and $(\frac{7}{9}, \frac{8}{9})$. Continue in this fashion, letting $x_n = x_{n-1} - \bigcup_{i=0}^{\infty} (\frac{1+3i}{3^n}, \frac{2+3i}{3^n})$ (see figure 2.1). Then the Cantor set is the intersection $C = \bigcap_{n=0}^{\infty} x_n$; it is totally disconnected, compact, and uncountable.

Although the *length* of the Cantor set is zero -

$$L = 1 - \frac{1}{3} - \frac{2}{9} - \frac{4}{27} - \dots = 1 - \frac{1}{3} \sum_{i=0}^{\infty} \left(\frac{2}{3}\right)^i = 0, \quad (2.21)$$

- its fractal dimension is *greater* than zero: since at the n^{th} step of the construction $N(\epsilon) = 2^n$ balls of size $\epsilon = (1/3)^n$ are needed to cover the set, we see immediately that

$$D_{\text{fractal}}(\text{Cantor}) = \lim_{n \rightarrow \infty} \frac{\ln 2^n}{\ln 3^n} \sim 0.6309. \quad (2.22)$$

Although it is not the only such measure, the fractal dimension does quantify the intuitive belief that the Cantor set is somewhere 'in-between' a point and a line. We will consider generalizations of D_{fractal} as needed in later chapters.



Fig. 2.1 First six steps of the construction of the triadic *Cantor Set*. The infinite-time limit point set has *fractal dimension* $D_{\text{fractal}} = \ln 2 / \ln 3$.

Consider a general sequence of transformations $\mathcal{T}$ applied to a set A ,

$$A_0 \rightarrow A_1 = \mathcal{T}A_0 \rightarrow A_2 = \mathcal{T}A_1 \rightarrow \cdots \rightarrow A_n = \mathcal{T}^n A_0, \quad (2.23)$$

where the scale of resolution at the n^{th} step is ϵ_n . If an arbitrary measurable quantity of interest $\mathcal{Q}$ (mass, area, volume, *etc.*), scales in self-similar fashion we can write

$$\mathcal{Q}(A_{n+1}(\epsilon_{n+1})) = \left\{ \frac{\epsilon_n}{\epsilon_{n+1}} \right\}^D \mathcal{Q}(A_n(\epsilon_n)), \quad (2.24)$$

where $\mathcal{Q}(A_n(\epsilon_n))$ is quantity $\mathcal{Q}$ measured in units of ϵ_n . Since, in the general case, this relation may only be satisfied in the limit as $n \rightarrow \infty$ we obtain

$$D_{\text{fractal}} = \lim_{n \rightarrow \infty} \frac{\ln [\mathcal{Q}(A_{n+1}(\epsilon_{n+1}))/\mathcal{Q}(A_n(\epsilon_n))]}{\ln (\epsilon_n/\epsilon_{n+1})}. \quad (2.25)$$

Thus, whenever the set A has a manifest *self-similarity*, so that, like the Cantor set, it can be defined by a recursive geometric construction, D_{fractal} can be easily calculated from this relation. The *Koch Curve*, for example, the first three steps in the construction of which are shown in figure 2.2, has a length L which scales as

$$L_{n+1}(\epsilon_{n+1} = \epsilon_n/3) = 4 L_n(\epsilon_n), \quad (2.26)$$

so that $D_{\text{fractal}}(\text{Koch}) = \ln 4 / \ln 3 \sim 1.262$.

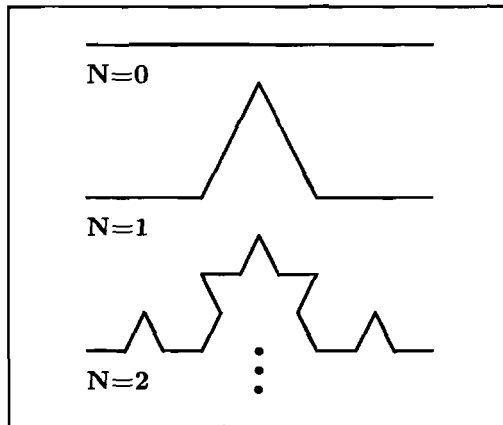


Fig. 2.2 First three steps in the construction of the *Triadic Koch Curve*. The fractal curve is obtained in the limit $N \rightarrow \infty$ and has a fractal dimension $D_{\text{fractal}} = \ln 4 / \ln 3 \sim 1.26$.

2.1.2 Information Theory

Like the physically ‘primitive’ notions of *spin* and *energy* of a particle, the *information content*, $\mathcal{I}$, of an arbitrary measurement or message composed of particular symbol sequences, is itself a primitive concept. While the roots of information theory extend back to the definition of the classical entropy of a physical system introduced by Clausius in 1864 and Boltzman’s probabilistic re-interpretation of classical entropy in 1896, the mathematical formalism for measuring $\mathcal{I}$ is due largely to a seminal 1948 paper by Claude E. Shannon (see [shann49]). Within the context of sending and receiving messages in a communication system, Shannon was interested in finding a measure of the information content of a received message. His approach was to obtain a measure of the *reduction of uncertainty* given some *a-priori* knowledge of the symbols being sent.

Information Capacity

Suppose we are given a situation in which there are N different and *a-priori* equally likely possible outcomes. In the case of a roll of a single die, for example, $N = 6$ and the probability, $p_i = 1/6$ for $i = 1, \dots, 6$. The outcome of throwing the die may be interpreted as receiving a ‘message’; heuristically, the larger the number N , the greater the uncertainty is in predicting the outcome and the greater the information gain upon receiving the message. A measure of this information gain, $\mathcal{I}$, is obtained by requiring that $\mathcal{I}$ is *additive for independent events*. That is to say, if there are two independent sets of outcomes, N_1 and N_2 , so that the total number of outcomes is $N = N_1 \cdot N_2$, it is required that

$$\mathcal{I}(N_1 \cdot N_2) = \mathcal{I}(N_1) + \mathcal{I}(N_2). \quad (2.27)$$

This requirement is *uniquely* satisfied by the function

$$\mathcal{I} = c \log N, \quad (2.28)$$

where ‘ c ’ is an arbitrary constant. The value of this constant is conventionally fixed by considering a binary sequence of length n ; by a binary sequence we mean one in which each symbol takes on one of only two values (*heads or tails, up or down, etc.*). By defining the information content of such a binary sequence to be equal to its *length*, n , we find $\mathcal{I} \equiv n = c \log N = c n \log 2 \implies c = \log_2 10$, where $N = 2^n$ is the total number of possible binary sequences of length n . With this value of ‘ c ’, equation 2.28 becomes

$$\mathcal{I} = \log_2 N \quad (\text{bits}), \quad (2.29)$$

where $\log_2$ is the logarithm base-2.

Average Information Gain

Equation 2.29, giving the maximum information content of a system with N equally likely possible outcomes, may be generalized to the case of N possible outcomes with

unequal probabilities. Consider a binary sequence of length N containing N_1 0's and N_2 1's, with $N = N_1 + N_2$. The total number of possible sequences that may be constructed, for *fixed* N_1 and N_2 , is given by $\mathcal{N} = N!/(N_1!N_2!)$. Using Stirling's approximation for factorials, $\log n! \approx n \log n - n$, we find that the *average information per symbol*, is

$$\begin{aligned} I &= \frac{\mathcal{I}}{N} = \frac{\log_2 \mathcal{N}}{N} \approx N(\log_2 N - 1) - N_1(\log_2 N_1 - 1) - N_2(\log_2 N_2 - 1), \\ &\approx \frac{N_1}{N} \log_2 \frac{N}{N_1} + \frac{N_2}{N} \log_2 \frac{N}{N_2}, \\ &\approx -(p_1 \log_2 p_1 + p_2 \log_2 p_2), \end{aligned} \quad (2.30)$$

where $p_i = N_i/N$, $i = 1, 2$, is the probability of finding each of the two possible symbols. The generalization of this result to a system with more than two symbols is Shannon's measure of average information gain: Given, *a-priori*, that a total of n possible events (or states) may occur with individual probabilities p_i , the *average information gained** by repeatedly measuring the outcome state of the system is given by

$$I^{(n)}(p_1, p_2, \dots, p_n) = -\sum_{i=1}^n p_i \log_2 p_i \quad (\text{bits/symbols}). \quad (2.31)$$

By extending $x \log_2 x$ to the origin by continuity, we define $p_i \log_2 p_i = 0$ if $p_i = 0$.

An increase in the accuracy of a measurement increases the information gain. Suppose we are measuring the position of a point along some line segment. This may be done by partitioning the segment into n equal intervals and noting which one contains the chosen point. Since the probability that it is in any of the segments is $p_i = 1/n$, the information gain of the measurement is $I^{(n)} = \sum_i \frac{1}{n} \log_2 n = \log_2 n$. Thus, as the resolution (*i.e.*, n) increases, the information increases.

$I^{(n)}$ may be considered as being an average over the *self-information*, $I_i = -\log_2 p_i$ (*bits*), contained in the i^{th} outcome. Note that this definition is an 'intuitive' one: if we observe outcome ' i ', whose *a-priori* probability is known to be $p_i \sim 1$, we do not gain much information since we already expected to see it; if $p_i \sim 0$, on the other hand, the i^{th} outcome is a rare event an observation of which therefore yields a significant amount of information. If all N events are equally likely, $p_i = 1/N$ for all ' i ', and $I_i = I = \log_2 N$, consistent with the information content defined in equation 2.29 above.

Properties of $I^{(n)}$: We list a few basic properties of $I^{(n)}$ without proof; most are either obvious or straightforward to verify (for details see ([aczel75] and [guiasu77]).

P1. Since $\log_2 p_i \leq 0$ for $0 < p_i \leq 1$, $I^{(n)} \geq 0$. $I^{(n)} = 0$ if and only if all of the p_i except one are equal to zero.

*Also called the *uncertainty* or – because of its formal similarity to the entropy function used in statistical mechanics – *Shannon entropy*.

P2. $I^{(n+1)}(p_1, p_2, \dots, p_n, 0) = I^{(n)}(p_1, p_2, \dots, p_n)$.

P3. For a given n , $I^{(n)}(p_1, p_2, \dots, p_n) \leq I^{(n)}(\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n}) = \log_2 n$. (This property is a simple consequence of the *convexity* property of the logarithm, $\log_2 x \leq x - 1$).[†]

P4. $I^{(n)}(\mathbf{p})$ is a *concave* function of $\mathbf{p}$.

P5. The average information is additive for *independent events*: $I^{(n)}(p_1, p_2, \dots, p_n) = \sum_{i=1}^n I^{(1)}(p_i)$. In general, $I^{(n)}(p_1, p_2, \dots, p_n) \leq \sum_{i=1}^n I^{(1)}(p_i)$.

2.1.3 Graph Theory

We shall extensively employ the notation of graph theory; it provides a powerful and elegant formalism for the description of both the 'structure' of the discrete lattices on which the CA live, and the complete 'dynamics' (*i.e.* the *global state transitions*) induced by those structures. Graph theory also allows the correspondence between CA configurations and the words of a regular language to be made in a very natural fashion.

Basic Terminology

A graph $G(N, M)$ (also called a *linear*, or *ordinary graph*), is a finite, nonempty set $V(G) = \{v_1, \dots, v_N\}$ of *vertices* together with (a possibly empty) set $E(G) = \{e_1, \dots, e_M\}$ of *edges*. Each edge $e = e(i, j) \in E(G)$, *connects* vertex ' i ' to vertex ' j '. If the edges represent *ordered* pairs of vertices, then G is a *directed graph*: each $e(i, j)$ defines an edge *directed from* ' i ' *to* ' j ', and is denoted by $e(i, j) = i\bar{j}$. If, on the other hand, $e_n(i_n, j_n) = e_n(j_n, i_n)$ for all ' n ', then G is an *undirected graph*, and all edges are denoted simply by $e(i, j) = ij = ji$. Two vertices, ' i ' and ' j ', are said to be *adjacent* if $e(i, j) \in E(G)$.

Intuitively, a graph can be realized geometrically in a three-dimensional Euclidean space: vertices are represented by *points* and edges are represented either by *lines* (in the case of undirected graphs) or *arrows* (in the case of directed graphs). In this book, we will be concerned with both kinds of graphs; *multiple edges* (*i.e.* when vertices are connected by more than one line or arrow), however, are not allowed.

The *order* of a graph G is the number of vertices of G : $|G| = |V(G)| = N$. The *size* of G is the total number of edges in G : $||G|| = |E(G)| = M$. In principle, the order and size of G may both be infinite, but we will mostly consider the case in which they are both finite. Clearly, for every M , $0 \leq M \leq \binom{N}{2}$, there is a graph $G(N, M)$. The graph of order N and size $\binom{N}{2}$ is called a *complete N -graph*; it is

[†]A function f is called *convex* if a straight line between any two points of the graph of f never falls below the graph of f : *i.e.*, if

$$f(\alpha x_1 + (1 - \alpha)x_2) \leq \alpha f(x_1) + (1 - \alpha)f(x_2),$$

for all x_1, x_2 and all $0 < \alpha < 1$. A function f is *concave* if $-f$ is convex.

denoted by K_N .

A graph $G(N, M)$ is *labeled* if all of its N vertices are associated with N distinct labels in a one-to-one manner. An *edge-labeled* graph is defined in an analogous fashion.

It is very important to understand what is meant by two graphs being the ‘same’ or ‘different’. For this purpose we introduce the notion of graph isomorphism. Two graphs, G_1 and G_2 , are *isomorphic*, which we write as $G_1 \cong G_2$, if there exists a bijection $\psi : V_1 \rightarrow V_2$ which preserves adjacency (*i.e.* such that $e(i, j) \in E_1$ if and only if $e(\psi(i), \psi(j)) \in E_2$). Isomorphic graphs necessarily must have the same order and size. It is easy to see that *isomorphism* is an *equivalence* relation on graphs: it divides the collection of all graphs into equivalence classes, for which any two member graphs must have the same structure.

Since all graphs in the same class are in this sense *topologically equivalent*, a representative member of each class, devoid of explicit vertex (or edge) labels, defines a unique *unlabeled graph*. Figure 2.3, for example, shows all of the undirected and unlabeled graphs of order 4.

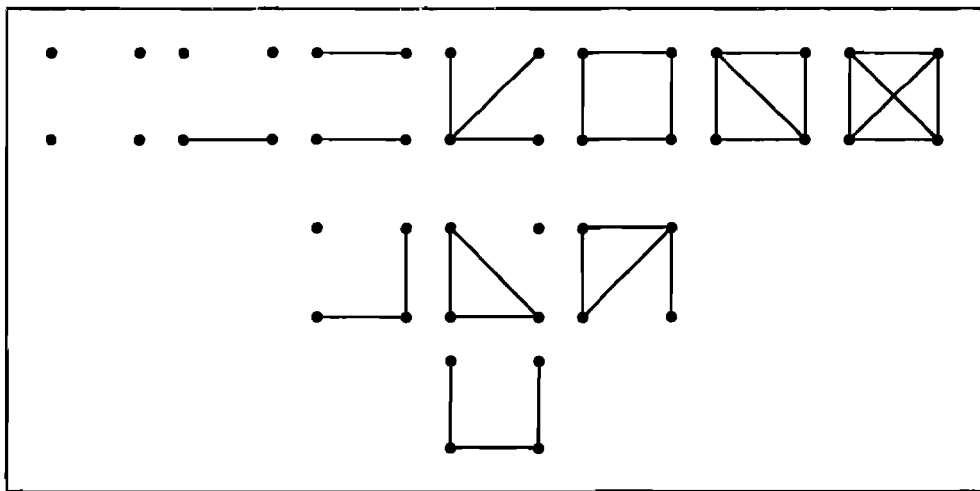


Fig. 2.3 All undirected, unlabeled graphs G of order $|G| = 4$.

Suppose π is a permutation of the N labels, $1, 2, \dots, N$ and G is a labeled graph of order N . Let $\pi(G)$ represent the graph obtained from G by relabeling each vertex ‘ i ’ by ‘ $\pi(i)$ ’. Then the set $\mathcal{A}(G)$, consisting of all permutations ‘ π ’ such that G and $\pi(G)$ are identical graphs is called the *automorphism* group of G . Since any graph G can be labeled in any of $n!$ distinct ways, the order of the automorphism group, $|\mathcal{A}(G)|$, tells us how many of these labelings will be topologically equivalent: *i.e.*

the number of ways of labeling an unlabeled graph is given by

$$\alpha(G_{\text{unlabeled}}) = \frac{n!}{|\mathcal{A}(G_{\text{unlabeled}})|}.$$

It is easy to show that the number of graphs of order N , $\mathcal{G}_N = 2^{\binom{N}{2}}$, and the number of graphs of order N and size q , $\mathcal{G}_{N,q} = \binom{\binom{N}{2}}{q}$.

$\tilde{G} = (\tilde{V}, \tilde{E})$ is a *subgraph* of $G = (V, E)$, written $\tilde{G} \subset G$, if $\tilde{V} \subset V$ and $\tilde{E} \subset E$. If $\tilde{G}$ contains *all edges* of G that join two vertices in $\tilde{V}$, then $\tilde{G}$ is the subgraph induced (or *spanned*) by $\tilde{V}$, and is denoted by $G[\tilde{V}]$. A subgraph $\tilde{G}$ of G is an *induced subgraph* if $\tilde{G} = G[\tilde{V}(\tilde{G})]$. $\tilde{G}$ is a *spanning subgraph* of G if $\tilde{V} = V$.

The set of vertices adjacent to a vertex $i \in V(G)$ is denoted by $\Gamma(i)$. The *degree* of ' i ', $d(i)$, is defined to be the number of vertices adjacent to ' i ': $d(i) = |\Gamma(i)|$. Note that, for undirected graphs, the sum of the degrees is exactly *twice* the number of edges: $\sum_{i=1}^N d(v_i) = 2M$. We will denote the *minimum* degree of G by $\delta(G)$, and the *maximum* degree by $\Delta(G)$.

Examples of Graphs

A *walk* from the vertex v_1 to vertex v_{i+1} is a finite sequence of edges of the form $(v_1, v_2), (v_2, v_3), \dots, (v_i, v_{i+1})$ (also written as $(v_1, v_2) \rightarrow (v_2, v_3) \rightarrow \dots \rightarrow (v_i, v_{i+1})$). In general, a given vertex or edge can be visited any number of times. A walk in which each vertex is distinct is called a *path*. A *path of length n* is therefore a graph $\mathcal{P}_n$ consisting of the distinct sequence of vertices $\{v_1, \dots, v_n\}$ and edges $\{(v_1, v_2), (v_2, v_3), \dots, (v_{n-1}, v_n)\}$. If the edge (v_n, v_1) is added, the path becomes a *circuit of length n* , $\mathcal{C}_n$. If we substitute the *arrows* (or *arcs*) $(v_i \rightarrow v_{i+1})$ for the lines (v_i, v_{i+1}) , the circuit becomes a *cycle of length n* , $\mathcal{C}_n$. If a graph G contains at least one cycle which itself contains all of the vertices of G , then G is said to be *Hamiltonian*.

A graph G is *connected* if for every pair of distinct vertices in G there exists at least one path along existing edges. The connected (undirected) graph of order N which has the smallest size is called a *tree*. In fact, a tree T is equally well characterized by any of the following properties:

- $$\left\{ \begin{array}{l} \bullet \text{ } T \text{ contains no circuits and has } N - 1 \text{ edges} \\ \bullet \text{ } T \text{ is connected and has } N - 1 \text{ edges} \\ \bullet \text{ any two vertices of } T \text{ are connected by} \\ \quad \text{exactly one path} \\ \bullet \text{ } T \text{ contains no circuits; the addition of any} \\ \quad \text{new edge creates exactly one circuit.} \end{array} \right.$$

A *spanning tree* in G is an edge-subgraph of G which has $N - 1$ edges and contains no circuits.

If $\delta(G) = \Delta(G) = r$ (i.e. each vertex of G has the same degree $d = r$) then G is an *r -regular graph*. A *circuit*, for example, can be alternatively defined as a 2-regular connected graph.

Graph Matrices

Although most graphical properties are most easily distinguished by means of a diagram, there are many instances when a *matrix representation* of a graph is extremely helpful, particularly when a more formal analytic understanding is desired.

There are a variety of different matrices that can be defined; we mention two of the most important.

Adjacency Matrix: The adjacency matrix $A(G)$ of an order N graph G with $V(G) = \{v_1, v_2, \dots, v_N\}$ is an $N \times N$ matrix $[a_{ij}]$ with entries $a_{ij} = 1$ if $(v_i, v_j) \in E(G)$ and $a_{ij} = 0$ otherwise. $A(G)$ is therefore a symmetric ($a_{ij} = a_{ji}$) $(0, 1)$ -matrix with trace $\text{Tr}(A) = 0$ (i.e. A has all zeros on the diagonal).

Note that this is an exact correspondence: i.e. the set of all $N \times N$ matrices satisfying these properties represents the class of all (labeled) graphs G of order N .

The entries of the n^{th} power of $A(G)$ have a very simple interpretation: $[a_{ij}^{[n]}]$, $n \geq 1$ is the number of different walks from v_i to v_j of length ' n ' in G . In particular, $a_{ij}^{[2]}$, $i \neq j$ is the number of $v_i - v_j$ paths of length two and $a_{ii}^{[2]} = \deg v_i$.

While the rows and columns of A obviously depend on a particular choice of vertex labels, the generic structural properties of G must remain invariant under a permutation of rows and columns. Much of this structural information can in fact be extracted from the *spectrum* of G : the spectrum of a graph G ,

$$\mathbf{Sp}(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \cdots & \lambda_s \\ m(\lambda_1) & m(\lambda_2) & \cdots & m(\lambda_s) \end{pmatrix},$$

is the set of eigenvalues, λ_i of $A(G)$, together with their multiplicities, $m(\lambda_i)$. Since $A(G)$ is *real* and symmetric, we know that the eigenvalues λ_i must also be *real*. For example, the spectrum of the complete graph of order ' n ', $\mathbf{Sp}(K_n) = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}$. Two non-isomorphic graphs, G_1 and G_2 , are *cospectral* if $\mathbf{Sp}(G_1) = \mathbf{Sp}(G_2)$.

The relationship between the topological properties of graphs and the set of eigenvalues of the adjacency matrix is an intensely studied field. For some questions, the spectrum yields a wealth of knowledge; for other questions, it may tell very little. Although it used to be believed that an arbitrary graph G is uniquely specified by $\mathbf{Sp}(G)$, this conjecture was later shown to be very wrong. In 1973, for example, it was proven that the probability that an order N tree T belongs to a cospectral pair tends to *one* as $N \rightarrow \infty$; i.e. the probability that T is characterized by $\mathbf{Sp}(T)$ approaches *zero* as $N \rightarrow \infty$.[†]

Some structural information about G can be obtained directly from the *characteristic polynomial* of $A(G)$:

$$\chi_G(\lambda) \equiv \det(A - \lambda I) = \sum_{i=0}^N a_i \lambda^{N-i}.$$

[†]A.J.Schwenk, in *New Directions in the Theory of Graphs*, ed. by F.Harary, Academic Press (1973), pp 275-307.

Since the coefficients a_i can be interpreted as sums of principal minors of $A(G)$, it is easy to check that (i) $a_1 = 0$, (ii) $a_2 = \text{the number of edges in } G$, and (iii) $a_3 = \text{twice the number of triangles in } G$. A more powerful version of this result will be presented and used in chapter 5.

Incidence Matrix: The incidence matrix $B(G)$ of an order N graph G with $V(G) = \{v_1, \dots, v_N\}$ and $E(G) = \{e_1, \dots, e_M\}$ is an $N \times M$ matrix $[b_{ij}]$ for which

$$b_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is the initial vertex of edge } e_j, \\ -1 & \text{if } v_i \text{ is the terminal vertex of edge } e_j, \\ 0 & \text{otherwise.} \end{cases}$$

$B(G)$ is often used to define the *complexity* of a graph G , $\kappa(G)$, equal to the number of spanning trees of G .[†] It turns out that

$$\kappa(G) = \det(J + BB^t) = \det(J + D - A),$$

where J is an $N \times N$ matrix all of whose entries are equal to one, D is an $N \times N$ diagonal matrix in which $[d_{ii}] = d(v_i)$, 'det' is the determinant and B^t is the transpose of B . Note that this result shows the simple relationship which holds between the adjacency and incidence matrices; namely, that $BB^t = D - A$.

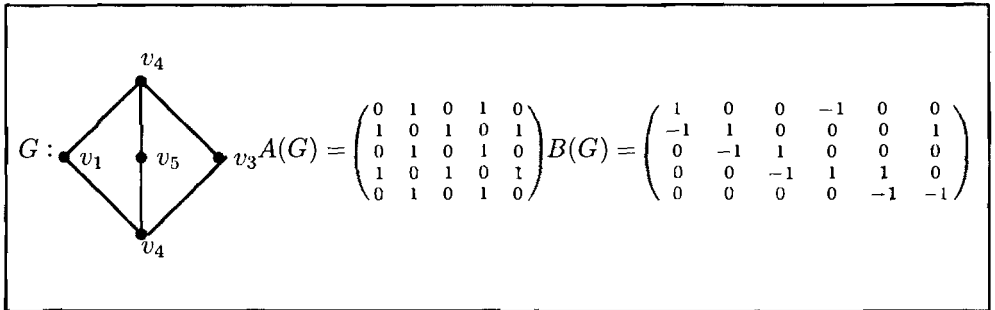


Fig. 2.4 The adjacency ($A(G)$) and incidence ($B(G)$) matrices of an order-5 directed graph G .

Random Graphs

The theory of random graphs—developed principally by Erdős and Rényi [erdos60]—offers an appropriate framework for posing questions about the general topological structures of computational systems and the expected mathematical behavior of certain random dynamical systems. The basic idea is to think of a graph as a living organism which develops by acquiring more and more edges and explore how its

[†]See H. Temperley, *Proc. Phys. Soc.* **83** (1964), 3.

various topological features emerge, often in a dramatically abrupt and unexpected fashion.

In order to show the emergence of some specific property $\mathcal{P}$ of a graph G , a probability space of graphs should first be formed, in which the probability that G has this property is positive. We define two frequently used models.

Model A: the sample space, Ω_A , consists of all order- N labeled graphs $G(N, M)$ of size M . The probability of G is given by

$$P(G) = \left(\binom{N}{2} \right)^{-1} \binom{M}{M},$$

so that each such graph is equally likely to occur.

Model B: the sample space, Ω_B , consists of all order- N graphs $G(N)$. If G has size M , then the probability of G is given by

$$P(G) = p^M (1 - p)^{\binom{N}{2} - M},$$

where ‘ p ’ is an independent probability, $0 \leq p \leq 1$, and is typically taken to be a function of N .

Note that **Model A** can be compared to the *microcanonical* ensemble in physics, in that it depends on the direct enumeration of possible configurations of a given graph; **Model B**, on the other hand, by assigning an independent probability to each edge, resembles the *canonical* ensemble. As for physical systems, these two models give the same results in the limit as $N \rightarrow \infty$. Depending on the problem at hand, the sample space can be generalized to include loops, multiple edges or even ensembles of graphs embedded in other topologies.

As alluded to earlier, as more and more edges are added to G (using **model A**), or the probability, ‘ p ’, of adding an edge is systematically increased (using **model B**), G successively passes through several well defined *structural* stages. If $M = cN$ in **model A** (or $p(N) = 2c/N$ in **model B**), for example, then an abrupt ‘phase transition’ occurs at $c = 1/2$: for $0 < c < 1/2$, G consists entirely of isolated points or small trees of order at most $\sim N \log N$; at $c = 1/2$, these small trees are suddenly replaced by a single tree spanning $\sim N^{2/3}$ vertices. An equally as dramatic a change occurs when $q = \frac{1}{2}cN \log N$ (or $p(N) = (c \log N)/N$): while G is almost always disconnected for $0 < c < 1$, for $c > 1$, G not only is almost always connected but is *hamiltonian* as well.

2.1.4 Groups, Rings and Fields

Groups

Let S be a set. A mapping $\phi : S \times S \rightarrow S$ is called a *binary* operation on S . A group $\mathcal{G} \equiv (G, \circ)$ is a set G together with a binary operation ‘ $\circ$ ’ on G such that the

following four properties hold:

$$\left\{ \begin{array}{ll} \text{Closure:} & \forall g_1, g_2 \in G, \quad g_1 \circ g_2 \in G \\ \text{Associativity:} & \forall g_1, g_2, g_3 \in G, \quad g_1 \circ (g_2 \circ g_3) = (g_1 \circ g_2) \circ g_3 \\ \text{Identity} & \exists e \in G, \text{ such that } \forall g \in G, \quad e \circ g = g \circ e = g \\ \text{Inverse:} & \forall g \in G \quad \exists g^{-1} \in G \text{ such that } g \circ g^{-1} = g^{-1} \circ g = e. \end{array} \right.$$

G is an *Abelian* group if, in addition to the above properties, for all $g_1, g_2 \in G$, $g_1 \circ g_2 = g_2 \circ g_1$.

Rings

The set R , together with the binary operations *addition* and *multiplication*, is a ring $\mathcal{R} \equiv (R, \circ, +)$ if it satisfies the following postulates:

$$\left\{ \begin{array}{ll} \text{Abelian:} & R \text{ is an abelian group with respect to '+'} \\ \text{Closure:} & \forall r_1, r_2 \in R, \quad r_1 \circ r_2 \in R \\ \text{Associativity:} & \forall r_1, r_2, r_3 \in R, \quad r_1 \circ (r_2 \circ r_3) = (r_1 \circ r_2) \circ r_3 \\ \text{Distributivity:} & \forall r_1, r_2, r_3 \in R, \quad r_1 \circ (r_2 + r_3) = r_1 \circ r_2 + r_1 \circ r_3 \\ & \forall r_1, r_2, r_3 \in R, \quad r_1 \circ (r_2 + r_3) = r_1 \circ r_2 + r_1 \circ r_3. \end{array} \right.$$

As for groups, R is a *commutative* ring if for all r_1, r_2 in R , $r_1 \circ r_2 = r_2 \circ r_1$. If there exists an integer n such that $nr = 0$ for all $r \in R$, then the least such integer n is called the *characteristic* of R . If no $n > 0$ exists then R is said to have characteristic 0. It is a simple exercise to show that if a ring $R \neq \{0\}$ which has an identity and no zero divisors (*i.e.* $ab = 0$ implies that either $a = 0$ or $b = 0$) has a positive characteristic, then it must have a prime characteristic.

Fields

Most of the analytical structure of the dynamics of linear CA systems emerges from their field-theoretic properties; specifically, those of finite fields and polynomials over fields. A brief summary of definitions and a few pertinent theorems will be presented (without proofs) to serve as reference for the presentation in subsequent sections.

A commutative ring $\mathcal{F}$ is called a *field* if, in addition to the properties given above, the following two postulates also hold true:

$$\left\{ \begin{array}{ll} \text{Identity:} & \exists \text{ an element } 1, \text{ such that } \forall f \in \mathcal{F}, \quad 1 \circ f = f \circ 1 \\ \text{Inverse:} & \forall \text{ nonzero } f \in \mathcal{F}, \quad \exists f^{-1} \text{ such that } f \circ f^{-1} = f^{-1} \circ f = 1. \end{array} \right.$$

Two simple examples of fields are the rational numbers, $\mathbb{Q}$ and the set of integers $\mathbb{Z}_p = \{0, 1, \dots, p-1\}$, where p is prime and addition and multiplication are defined *modulo* p . The latter is an example of a *finite* field – that is, of a field containing only a finite number of elements. Since CA are almost always defined so that individual sites take on one of a finite number of values, if those values happen to be elements of a finite field then the dynamics can be well understood by using some of the general properties of that field. An elementary property of finite fields

with q elements, written $\mathcal{F}_q$, is that $\mathcal{F}_q$ must have prime characteristic. Moreover, if the characteristic of $\mathcal{F}_q$ is p , then the number of elements of $\mathcal{F}_q$ must be a power of p : $q = p^n$, for some positive integer n .

We will have occasion to use both polynomials and matrices defined over some finite field $\mathcal{F}_q$. In the case of a polynomial $f(x)$, what is meant is simply that

$$f(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \cdots + \alpha_n x^n,$$

where $\alpha_i \in \mathcal{F}_q$. The set of all polynomials over $\mathcal{F}_q$ forms a ring, denoted by $\mathcal{F}[x]$. Similarly, a matrix over $\mathcal{F}_q$ is a matrix all of whose entries are elements of the field $\mathcal{F}_q$.

The *degree* of $f(x)$, denoted by $\partial[f]$, is the highest power of x with a nonzero coefficient; this coefficient is called the *leading coefficient* of $f(x)$. If the leading coefficient is '1', then $f(x)$ is called a *monic polynomial*. For any two polynomials, $f_1(x)$ and $f_2(x)$, one can uniquely write $f_1(x) = q(x)f_2(x) + r(x)$, where $0 \leq \partial[r] < \partial[f_2]$ or $r(x) = 0$. If $r(x) = 0$ then $q(x)$ is a *divisor* of $f_1(x)$. A polynomial $f(x)$ is *irreducible* if its only divisors are α and $\alpha f(x)$, where $\alpha \in \mathcal{F}$.

The *prime factorization theorem* states that any polynomial $f(x)$ can be written in the following form:

$$f(x) = [p_1(x)]^{\nu_1} [p_2(x)]^{\nu_2} \cdots [p_n(x)]^{\nu_n},$$

where ' $p_i(x)$ ' are distinct irreducible polynomials and $[p_i(x)]^{\nu_i}$ are the *prime factors* of $f(x)$. The factorization is unique up to a constant multiplier and the order in which the prime factors appear.

It is easy to show that every polynomial $f(x)$ (not divisible by x) over a finite field $\mathcal{F}_q$ is a factor of $1-x^n$, for some power ' n '. The *order* (sometimes also called the *period* or *exponent*) of $f(x)$, denoted by $\text{ord}(f)$, is the least such ' n '. If $f(x) = p(x)$ is an irreducible polynomial (other than x) with $\partial[f] = n$ then $\text{ord}(f)$ must divide $p^n - 1$. There are two important theorems concerning the orders of prime factors and products of relatively prime polynomials over $\mathcal{F}_q$:

Theorem 1: let $p(x) \in \mathcal{F}_q$, $p(0) \neq 0$, be irreducible, $\text{ord}(p)=n$, and $f(x) = [p(x)]^m$, with m a positive integer. Then $\text{ord}(f)=np^t$, where t is the smallest integer with $p^t \geq m$.

Theorem 2: Let $f_1, f_2, \dots, f_k$ be pairwise relatively prime nonzero polynomials over $\mathcal{F}_q$, and $f = \prod_i f_i$. Then $\text{ord}(f) = \text{lcm}(\text{ord}(f_1), \dots, \text{ord}(f_k))$.

The set of all polynomials over $\mathcal{F}_q$ which satisfies the property that any two polynomials, $f_1(x)$ and $f_2(x)$, are equal if and only if $f_1(x) - f_2(x) = \alpha a(x)$, where $\alpha \in \mathcal{F}_q$, constitutes a ring called the *ring of polynomials over $\mathcal{F}_q$ modulo $a(x)$* . The ring of polynomials over $\mathcal{F}_q$ modulo $p(x)$, where $p(x)$ is an irreducible polynomial, is also a field. If $\partial[p] = k$, then this field is represented by the set of all p^k polynomials of degrees $k-1$ or less over $\mathcal{F}_q$ and is called the *Galois field of order p^k* . Every finite field $\mathcal{F}_q$ is isomorphic (i.e. can be put into a one-to-one correspondence) with some

Galois field of order p^k .

2.1.5 Abstract Automata

Alphabets and Strings

Just as *points* and *lines* are formally undefined geometrical objects, a *symbol* represents an abstract undefined object. Typical representations include *letters* and *digits*. An *alphabet* is then simply a finite nonempty set A of symbols. An n -tuple of symbols of A is defined to be a *string* on A (also called a *word* on A). If $A = \{a_1, a_2, \dots, a_n\}$, for example, then we would write the string $s(A) = a_1 a_2 \cdots a_n$; the *length* of the string is the number of symbols of which it is composed, and is written $|s(A)| = n$. The *null* string, s_0 , is a unique string consisting of zero symbols (so that $|s_0| = 0$). Letting S^* denote the set of all strings, we introduce a binary *concatenation* operator: if $s_1, s_2 \in S^*$, then the concatenation $\overline{s_1 s_2}$ is obtained by placing the string ' s_2 ' after the string ' s_1 '. For example, if $s_1 = a_1 a_2 a_3$ and $s_2 = b_1 b_2$ then

$$\overline{s_1 s_2} = a_1 a_2 a_3 b_1 b_2 \neq \overline{s_2 s_1} = b_1 b_2 a_1 a_2 a_3. \quad (2.32)$$

It is clear that $\overline{s\phi} = \overline{\phi s} = s$. If ' s ' is a string and $n \in \mathcal{N}$, $n > 0$ then we write $s^{[n]} = \underbrace{ss \cdots s}_n$. By convention, $s^{[0]} = \phi$.

Define the set $\mathcal{S}(A)$ to be the set of all subsets on A . Then a *language on A* (or a *language with alphabet A*) is any subset of $\mathcal{S}(A)$. The set of all strings over a fixed finite alphabet A , for example, is a language; it is denoted by $\mathcal{L}(A)$. If $A = \{0, 1\}$, then $\mathcal{L}(A) = \{\phi, 0, 1, 00, 01, 10, 000, \dots\}$.

Formal Languages

Formal languages are subsets of $\mathcal{S}(A)$ formed according to definite grammatical rules. It is easy to see that sets of CA configurations can be considered to be formal languages; in chapter 6, we will in fact exploit the correspondence between the *words* and *configurations* by using the *finite* set of grammatical rules to analyze the *infinite* set of CA configurations.

A computer can be used to implement the grammatical rules to generate (or recognize) the strings in the formal language; different *types* of languages being distinguished by the required size of memory in the computer. The simplest example of an idealized computer is the abstract automaton:

DEFINITION: A finite automaton $\mathcal{M}$ is specified by three sets A , Σ and Σ^* and a state-transition function $\phi : \Sigma \times A \rightarrow \Sigma$, where

$$\begin{cases} A & = \{a_1, \dots, a_n\} \text{ is a finite input alphabet,} \\ \Sigma & = \{\sigma_1, \dots, \sigma_m\} \text{ is a finite set of states,} \\ \Sigma^* \subset \Sigma & \text{is the set of output (or accepting) states.} \end{cases}$$

Given an automaton $\mathcal{M}$ that starts in state σ_1 , and any finite string $s \in A^*$, $\phi^*(\sigma, s)$ will represent the final output state that $\mathcal{M}$ will enter after having processed s , one symbol at a time, from left to right. $\mathcal{M}$ is said to *accept* the word s if $\phi^*(\sigma_1, s) \in \Sigma^*$; the word s is *rejected* if and only if it is not accepted. Finally, we may define the *language* $\mathcal{L}(\mathcal{M})$ accepted by $\mathcal{M}$ as the set of all words $s \in A^*$ that are accepted by $\mathcal{M}$. A language $\mathcal{L}$ is called *regular* if there is a finite automaton $\mathcal{M}$ that accepts it.

The *grammars* for regular languages can be conveniently specified by *finite state transition graphs* for the finite automata that recognize them. The vertices of the graph represent the the system states $\sigma_i \in \Sigma$ and the arcs represent the possible input states $a_i \in A$. The arrows point to the next state that will result from the initial state when the input on the arc is applied.

EXAMPLE: Consider an automaton $\mathcal{M}$ with alphabet $A = \{0, 1\}$, state space $\Sigma = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4\}$ and transition rule ϕ given by

$$\left\{ \begin{array}{llll} \phi(\sigma_1, 0) = \sigma_2, & \phi(\sigma_1, 1) = \sigma_4, & \phi(\sigma_2, 0) = \sigma_2, & \phi(\sigma_2, 1) = \sigma_3, \\ \phi(\sigma_3, 0) = \sigma_4, & \phi(\sigma_3, 1) = \sigma_3, & \phi(\sigma_4, 0) = \sigma_4, & \phi(\sigma_4, 1) = \sigma_4. \end{array} \right\}$$

Assume that the initial state is σ_1 and that the accepting set is $\Sigma^* = \{\sigma_3\}$. It is easy to see that $\mathcal{M}$ will reject the strings $s_1 = 00110$ and $s_2 = 10011$ (since $\phi^*(\sigma_1, s_1) = \phi^*(\sigma_1, s_2) = \sigma_4$), and accept $s_3 = 00111$ (since $\phi^*(\sigma_3, s_3) = \sigma_3 \in \Sigma^*$). In fact, $\mathcal{M}$ accepts the regular language

$$\mathcal{L} = \{0^{[n]}1^{[m]}; \ n, m \geq 0\}.$$

The state transition graph for this example is given in figure 2.5.

Finite automata such as these are the simplest kind of computational model, and are not very powerful. For example, no finite automaton can accept the set of all *palindromes* over some specified alphabet. They certainly do not wield, in abstract terms, the full computational power of a conventional computer. For that we need a suitable generalization of the these primitive computational models. Despite the literally hundreds of computing models that have been proposed at one time or another since the beginning of computer science, it has been found that each has been essentially equivalent to just one of four fundamental models: *finite automata*, *pushdown automata*, *linear bounded automata* and *Turing machines*.

Each one of these four models can be thought of as defining the response of a black-box to a tape of symbols that is fed to it, cyclically, one cell at a time. During each cycle, the black-box reads the symbol at the appropriate cell, responds to that symbol according to a set of model-specific rules, and then moves the tape forward by one cell. What type of computational model the black-box represents depends on its general response. Although a more detailed discussion of each of these types will be given in chapter 6, we mention here that the four models make up what is conventionally called the *Chomsky hierarchy*[†]. Each type of computational

[†]Named after the linguist and philosopher of language, Noam Chomsky.

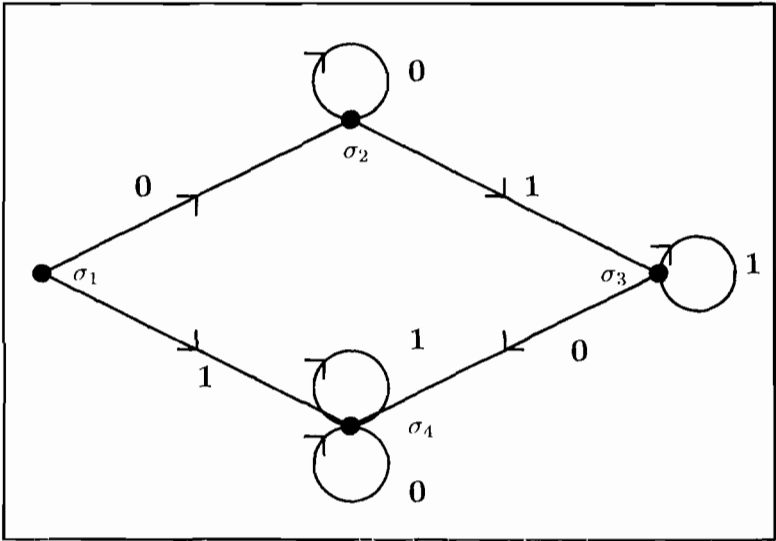


Fig. 2.5 State Transition graph for the regular language $\mathcal{L} = \{0^{[n]} 1^{[m]}\}$.

Level	Language Class	Class of Accepting Automata	Memory
0	Unrestricted	Universal computer	arbitrarily large
1	Context-Sensitive	linear-bounded	$\sim s_{\text{input}} $
2	Context-Free	pushdown	fixed length
3	regular	finite	none

Table 2.1 Chomsky Language Hierarchy.

model determines a particular language class, and, since each is more general than its predecessor, each language class must include the one that comes before it. Each level of the hierarchy is characterized by the amount of memory needed in an automaton that accepts it (see table 2.1).

2.2 Dynamical Rules: Notation and Definitions

Although there is an incredibly rich variety of specific CA systems, each of which is carefully defined or selected to fit the requirements of a particular model, the definition of any of these specific systems requires the specification of each of the following four generic characteristics:

Discrete Cellular State Space $\mathcal{L}$: the discrete lattice of cells or sites upon which CA ‘live’, and their dynamics unfolds. $\mathcal{L}$ can be one-dimensional, two-dimensional

(either rectangular or hexagonal), three-dimensional, or even random.

Local Value Space Σ : each cell of $\mathcal{L}$, indexed by the elements of the $\mathcal{L}$'s symmetry group, can assume only one of a finite number of different values:

$$\sigma_{\vec{i} \in \mathcal{L}}(t) \in \Sigma \equiv \{0, 1, 2, \dots, k-1\}, \quad (2.33)$$

where $\sigma_{\vec{i}}$ is the value of the $\vec{i}^{th}$ cell at time 't', and Σ is any finite commutative ring (usually taken to be the integers *modulo* 'k', $\mathbb{Z}_k$). If the CA evolves on a finite lattice of N cells, then the total number of *global* states is also finite, and is given by k^N .

Boundary Conditions: although CA are assumed to live on infinitely large lattices, computer simulations must necessarily be run on finite sets. For a one dimensional lattice with N cells, it is common to use *periodic boundary conditions*, in which σ_{N+1} is identified with σ_1 . Alternatively, all cells to the left and right of a finite block of N cells may be arbitrarily defined to possess value '0' for all time, so that their dynamics remains uncoupled with that taking place within the block. Similarly, in two dimensions, it is usual to have the dynamics take place on a *torus*, in which $\sigma_{i,M+1} = \sigma_{i,1}$ and $\sigma_{N+1,j} = \sigma_{1,j}$. As we will see later it turns out that boundary conditions often play an important role in shaping the form of the resulting dynamics.

Dynamical Rule ϕ : $\overbrace{\Sigma \times \Sigma \times \dots \times \Sigma}^n \longrightarrow \Sigma$, where 'n' specifies the number of cells needed to define the *neighborhood* of a given cell. Defining $\mathcal{N}\{\vec{i}\}$ to be the neighborhood about cell $\vec{i}$, the transition rule is most generally written as

$$\sigma_{\vec{i}}(t+1) = \phi(\sigma_{\vec{j}} \in \mathcal{N}\{\vec{i}\}). \quad (2.34)$$

State transitions are therefore *local* in both space and time: individual cells evolve iteratively according to a fixed, and usually deterministic, function of the current state of that cell and its neighboring cells. One *iteration step* of the dynamical evolution is achieved after the simultaneous application of the rule ϕ to each cell in the lattice $\mathcal{L}$.

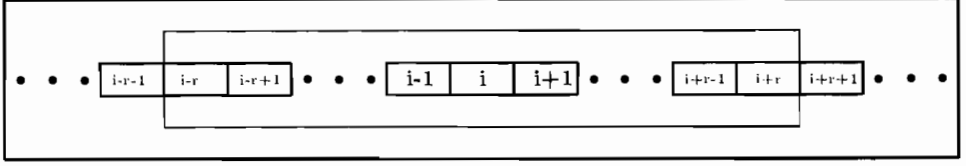
2.2.1 One-dimensional CA

An arbitrary *range-r* one-dimensional rule can be written as follows:

$$\sigma_i(t+1) = \phi(\sigma_{i-r}(t), \dots, \sigma_i(t), \dots, \sigma_{i+r}(t)), \quad \phi : S^{2r+1} \longrightarrow S, \quad (2.35)$$

where the range 'r' specifies the size of the neighborhood for each site.

Since each site can take one any of 'k' values, ϕ is completely defined by specifying the value assigned to each of the k^{2r+1} possible $(2r+1)$ -tuple configurations for a given neighborhood:

Fig. 2.6 One-dimensional *range-r* neighborhood of center site '*i*'.

$\sigma_{i-r}(t)$	$\dots$	$\sigma_i(t)$	$\dots$	$\sigma_{i+r}(t)$	$\longrightarrow$	$\sigma_i(t+1)$
0		0		0		$\phi(0, 0, \dots, 0)$
0		0		1		$\phi(0, 0, \dots, 1)$
0		0		2		$\phi(0, 0, \dots, 2)$
$\vdots$		$\vdots$		$\vdots$		$\vdots$
k		k		k		$\phi(k, k, \dots, k)$

For example, let $k = 2$ (so that $\sigma_i \in \{0, 1\}$) and range $r = 1$, and consider the rule $\phi : \{0, 1\}^3 \rightarrow \{0, 1\}$ defined by

$$\phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)) = \sigma_{i-1}(t) \oplus_2 \sigma_{i+1}(t), \quad (2.36)$$

where ' $\oplus_2$ ' is addition *modulo 2*. The explicit form of the dynamics is given by listing, for each of the eight possible local states that three adjacent cells can be in at time ' t ', the corresponding state at time ' $t+1$ ' that is assigned by ϕ to the central cell of this 3-tuple:

111	110	101	100	011	010	001	000
↓	↓	↓	↓	↓	↓	↓	↓
0	1	0	1	1	0	1	0

After choosing some specific initial global state

$$\vec{\sigma}(t=0) = (\sigma_1(0), \sigma_2(0), \dots, \sigma_N(0)), \quad (2.37)$$

the temporal evolution of this CA is then given by the simultaneous application of ϕ to each of the N lattice cells. After four iterations are applied to a size $N = 17$ lattice with periodic boundary conditions, and initial state $\vec{\sigma}(t=0) = '010111010110101'$, for example, we find that $\vec{\sigma}(t=0)$ evolves into $\vec{\sigma}(t=4) = '1000001101111000'$:

time (t)	$\vec{\sigma}(t)$															
0	0	1	0	1	1	1	0	1	0	1	1	0	1	0	1	0
1	0	0	0	1	0	1	0	0	0	1	1	0	0	0	0	0
2	0	0	1	0	0	0	1	0	1	1	1	1	0	0	0	0
3	0	1	0	1	0	1	0	0	1	0	0	1	1	0	0	0
4	1	0	0	0	0	0	1	1	0	1	1	1	1	1	0	0

Rule Composition

Rules may be combined by *composition*: i.e., two rules, ϕ_1 and ϕ_2 , may be combined to form the rule $\tilde{\phi} \equiv \phi_1\phi_2$. The set of rules obtained in this way is closed under composition, although the number of sites in the neighborhood will typically have to be increased. If a rule is composed with itself, then $\tilde{\phi} = (\phi\phi)$ generates patterns consisting of alternate time steps of the patterns of ϕ . In general, composition is noncommutative: $\phi_1\phi_2 \neq \phi_2\phi_1$.

Higher Order Time Dependence

Equation 2.35 defines an arbitrary range- r rule that is 1st-order in time. n^{th} -Order rules, for which a particular site value at time ' t ' depends on the r -neighborhood site values for the previous ' n ' iteration steps, may, of course, also be constructed:

$$\sigma_i(t) = \phi^{(n)}(\begin{matrix} \sigma_{i-r}(t-n+1), & \dots, & \sigma_i(t-n+1), & \dots, & \sigma_{i+r}(t-n+1), \\ \vdots, & & \vdots & & \vdots \\ \sigma_{i-r}(t), & \dots, & \sigma_i(t), & \dots, & \sigma_{i+r}(t) \end{matrix}) \quad (2.38)$$

By defining 'effective' site values $\tilde{\sigma} \equiv \sum_{j=0}^{n-1} k^j \sigma(t-j)$, and allowing for a larger neighborhood radius, an equivalent 1st-order rule, $\tilde{\phi}^{(1)}$, may always be constructed from a given n^{th} -order rule.

Figure 2.7, for example, shows how a 2nd-order radius $r = 1$ rule ϕ may be converted into a 1st-order radius $r = 2$ rule $\tilde{\phi}$. Effective values $\tilde{\sigma} \in \{0, 1, \dots, k^2\}$ define the states of the single remaining cell of a two-state collapse in time, and extra sites are added on to either side of the original neighborhood.

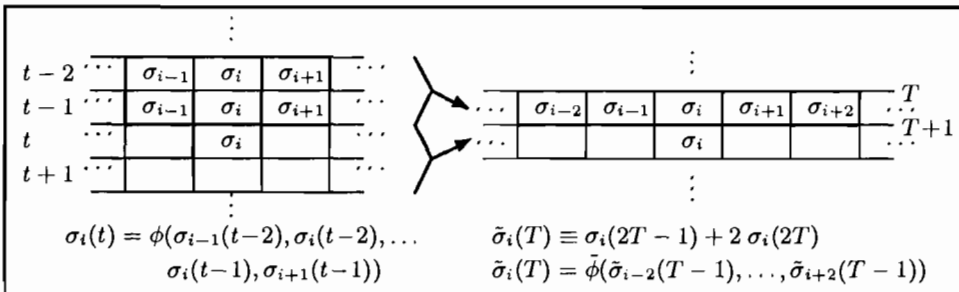


Fig. 2.7 Construction of equivalent radius $r = 2$ rule, $\tilde{\phi}$, that is 1st-order in time from a radius $r = 1$, 2nd-order rule, ϕ .

In general if a radius- r rule ϕ is n^{th} order in time, an equivalent 1st order rule will be defined on a neighborhood with radius $r' = nr$; if $\sigma \in \{0, 1, \dots, k\}$, then $\tilde{\sigma} \in \{0, 1, \dots, k^n\}$.

Rule Codes

Rather than being defined by lengthy explicit listings of their local action, rules are instead conventionally identified by a compact *code*. If the bottom eight binary digits of the $r = 1 \bmod 2$ rule in the example cited above are interpreted as the binary representation of a decimal number, then the code, $R[\oplus_2]$, is given by that base-10 equivalent:

$$\begin{aligned} R[\oplus_2] &= 0 \cdot 2^0 + 1 \cdot 2^1 + 0 \cdot 2^2 + 1 \cdot 2^3 + 1 \cdot 2^4 + 0 \cdot 2^5 + 1 \cdot 2^6 + 0 \cdot 2^7 \\ &= 90 \end{aligned} \quad (2.39)$$

This rule can then be alternatively referred to in the text as **R90**.

More generally, for an arbitrary rule ϕ of the form given in equation (2.3), we define the code

$$R[\phi] \equiv \sum_{\{\sigma_{i-r}, \dots, \sigma_{i+r}\}} \phi[\sigma_{i-r}, \dots, \sigma_{i+r}] k^{\sum_{j=-r}^r k^{r-j} \sigma_{i+j}}. \quad (2.40)$$

Since each explicit listing of the local action on each of the k^{2r+1} possible range- r neighborhoods defines a unique rule, and since there are $k^{k^{2r+1}}$ such distinct explicit listings, we find that there are, in general, $k^{k^{2r+1}}$ possible range- r rules (see table 2.1).

‘Legal’ and Other ‘Simplifying’ Forms of Rules

Because of the rather large total number of possible rules, it is frequently convenient to deal with more restricted classes. As we will later see, however, it is rather fortuitous that most, if not *all*, of the characteristic behavior of generic CA rules is nonetheless retained.

Legal Rules: Legal rules are those for which the following two properties hold:

$$\begin{cases} \text{Null state quiescence: } \phi(0, 0, \dots, 0) = 0 \\ \text{Reflection Symmetry: } \phi(\sigma_{i-r}, \dots, \sigma_{i+r}) = \phi(\sigma_{i+r}, \dots, \sigma_{i-r}). \end{cases} \quad (2.41)$$

Imposition of these ‘legality’ conditions for $r = 1$ reduces the set of 256 general rules to a set of 32 legal rules of the form

$$\begin{aligned} 111 &\rightarrow a, & 110 &\rightarrow b, & 101 &\rightarrow c, & 100 &\rightarrow d, \\ 011 &\rightarrow b, & 010 &\rightarrow e, & 001 &\rightarrow d, & 000 &\rightarrow 0, \end{aligned} \quad (2.42)$$

where $a, b, c, d, e \in \{0, 1\}$.

Totalistic Rules: Totalistic (**T**) rules, ϕ_{tot} , are functions of the *sums* of values of all sites in a particular neighborhood: $\phi_{\text{tot}} = \phi_{\text{tot}}(\sum_{j=-r}^r \sigma_{i+j})$. Here we define the totalistic code

$$\mathbf{T}[\phi_{\text{tot}}] \equiv \sum_{i=0}^{(2r+1)(k-1)} k^i \phi_{\text{tot}}(i). \quad (2.43)$$

k	r	TOTAL	LEGAL	TOTALISTIC	OUTER TOTALISTIC	ADDITIVE
2	1	256	32	8	8	8
2	2	$4 \cdot 10^9$	524288	32	32	32
2	3	$3 \cdot 10^{38}$	$2 \cdot 10^{21}$	128	128	128
3	1	$8 \cdot 10^{12}$	129140163	64	48	27
3	2	10^{116}	10^{64}	1024	768	243
.	.	.	.	.	.	.
k	r	$k^{k^{(2r+1)}}$	$k^{k^{r+1}(k^r+1)/2-1}$	$2^{(k-1)(2r+1)}$	$k2^{2r(k-1)}$	k^{2r+1}

Table 2.2 Number of possible rules of a specific type for a given 'k' and range 'r'.

If $r = 1$, $k = 2$ and $\sigma_i(t+1) = 1 \iff \sigma_{i-1}(t) + \sigma_i(t) + \sigma_{i+1}(t) \in \{1, 3\}$, for example, then $T = 2^1 + 2^3 = 10$ and we would cite the rule ϕ_{tot} as **T10**.

Outer-Totalistic Rules: Outer-totalistic (**OT**) rules, $\phi_{\text{out-tot}}$, are functions of both the value of a given site and the sum of values of all *remaining* sites in the neighborhood of that site. Thus, $\phi_{\text{out-tot}} = \phi_{\text{out-tot}}(\sigma_i, \sum_{j=-r}^r \sigma_{i+j} - \sigma_i)$, with general code given by

$$\mathbf{OT}[\phi_{\text{out-tot}}] \equiv \sum_{i=0}^{2r(k-1)} \sum_{j=0}^{k-1} k^{ki+j} \phi_{\text{out-tot}}(j, i). \quad (2.44)$$

Additive Rules: Rules belonging to the special class of *additive* rules, ' ϕ_{add} ', are linear functions of neighborhood sites:

$$\phi_{\text{add}} = \sum_{j=-r}^r \alpha_j \sigma_{i+j} \pmod{k}, \quad \alpha_j \in S. \quad (2.45)$$

The eight additive $r = 1$, $k = 2$ rules, for example, are of the general form

$$\begin{aligned} 111 &\rightarrow a, & 110 &\rightarrow b, & 101 &\rightarrow 0, & 100 &\rightarrow c, \\ 011 &\rightarrow b, & 010 &\rightarrow a, & 001 &\rightarrow c, & 000 &\rightarrow 0, \end{aligned} \quad (2.46)$$

where $a, b, c \in \{0, 1\}$ and $c = (a + b) \text{ modulo } 2$.

By exploiting the fact that such rules obey an additive superposition principle – namely, that if Φ_{add} is the *global* transition function, then $\Phi(\vec{\sigma}_A + \vec{\sigma}_B) = \Phi(\vec{\sigma}_A) + \Phi(\vec{\sigma}_B)$ – virtually all of the fundamental dynamical behavior of CA obeying this type of a rule can be obtained. We will discuss various methodologies for performing exact algebraic analyses of such systems, including the interesting question of the dynamical relationship between such rules and the underlying lattice topology, in chapter 5.

Feedback Shift Registers: Feedback shift registers are essentially one-dimensional finite state machines consisting of a linear array of sites $i = 1, 2, \dots, n$, with each site i carrying value σ_i . At each time step, the system evolves according to the following

two rules (see figure 2.8): (1) all of the sites are shifted one site to the right, $\sigma'_i = \sigma_{i-1}$, and (2) $\sigma'_0 = f(\sigma_{n-m+1}, \sigma_{n-m}, \dots, \sigma_n)$, where sites $i = n-m+1, n-m, \dots, n$ label the positions of the “taps” on the shift-register. A feedback shift register is called *linear* if f is a linear function:

$$f(\sigma_{n-m+1}, \sigma_{n-m}, \dots, \sigma_n) = \alpha_0 \sigma_{n-m+1} \oplus \alpha_1 \sigma_{n-m} \oplus \dots \oplus \alpha_m \sigma_n, \quad (2.47)$$

where $\alpha_i \in \{0, 1\}$ and *oplus*₂ is addition modulo-two.

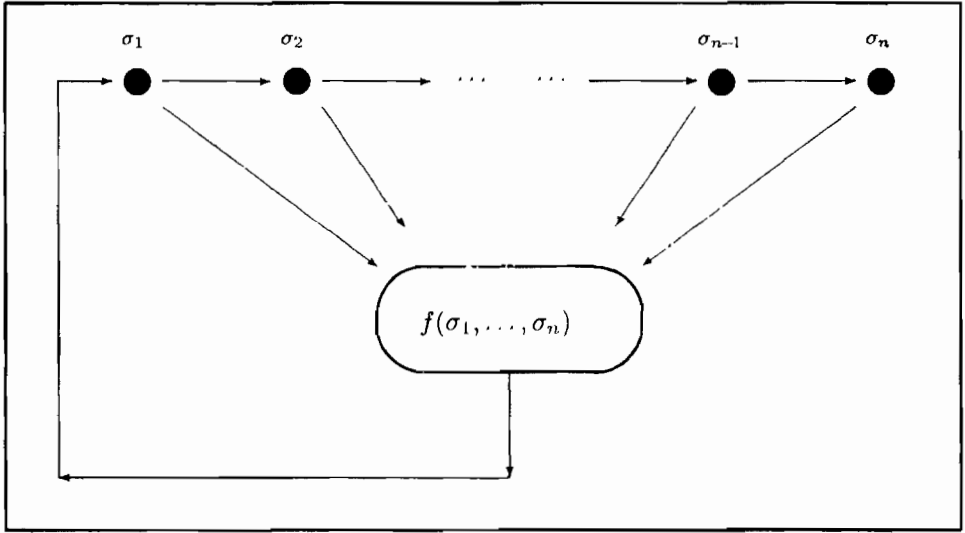


Fig. 2.8 Schematic diagram of a length- n feedback shift register.

It is easy to see that an elementary size- n one-dimensional CA rule ϕ is equivalent to a size- n feedback shift register with $\sigma \in \{0, 1\}$, taps at positions $n-2, n-1$ and n , and $f = \phi$. The only difference is that it takes n “shift-register” time-steps to reproduce a single “CA” time step.

Topological Characterization of Cellular Automata

Labeling each cell of the one-dimensional ‘lattice’ by $i \in \mathcal{Z}$, where $\mathcal{Z}$ is the set of integers, the collection of all *configurations* $\vec{\sigma}$ defines the CA *phase space*, and is denoted by $\Gamma \equiv \Sigma^{\mathcal{Z}}$.

If we give Σ the discrete topology and Γ the product topology, then Γ becomes a compact metric space homeomorphic to the Cantor set under the metric

$$\partial(\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}) = \sum_{i=-\infty}^{\infty} k^{-|i|} |\vec{\sigma}_i^{(1)} - \vec{\sigma}_i^{(2)}|, \quad \vec{\sigma}^{(1)}, \vec{\sigma}^{(2)} \in \Gamma. \quad (2.48)$$

Two configurations are *close*, under ‘ ∂ ’, if their components $\vec{\sigma}_i^{(1)}$ and $\vec{\sigma}_i^{(2)}$ are the same for $|i| < N$ for large N .

Open sets ‘ $\mathcal{O}$ ’ are defined as unions of n -cylinders: $\mathcal{O} \equiv \bigcup_i c_i^{(n)}$, where $c_i^{(n)} \equiv \{\vec{\sigma} \mid \vec{\sigma}_i = c_i, \dots, \vec{\sigma}_{i+n-1} = c_{i+n-1}\}$. Each n -cylinder may be put into a one-to-one correspondence with an n -block $B_n^{(i)} \equiv \{b_1 = c_i, b_2 = c_{i+1}, \dots, b_n = c_{i+n-1}\}$, each of which is simply an explicit list of a specified sequence of states.

We define two maps:

1. the *shift* operator $\gamma : \Gamma \longrightarrow \Gamma$, such that for any $\vec{\sigma} \in \Gamma$, $(\gamma\vec{\sigma})_i = \vec{\sigma}_{i+1}$. ‘ γ ’ is clearly a homeomorphism of Γ , and
2. the *dynamical* map $\Phi : \Gamma \longrightarrow \Gamma$, defined by

$$[\Phi(\vec{\sigma})]_i = \phi(\sigma_{i-r}, \sigma_{i-r+1}, \dots, \sigma_{i+r-1}, \sigma_{i+r}), \quad (2.49)$$

where $\phi : \Sigma^{2r+1} \longrightarrow \Sigma$ is a *range- r* local function.[†]

We see that (i) if $\vec{\sigma}^{(1)}$ is close to $\vec{\sigma}^{(2)}$, then $\Phi[\vec{\sigma}^{(1)}]$ will be close to $\Phi[\vec{\sigma}^{(2)}]$, so that ‘ Φ ’ is *continuous*, and (ii) the commutator $[\Phi, \gamma] = 0$. That the converse is also true—i.e. that if $\phi : \Gamma \longrightarrow \Gamma$ is a continuous map which commutes with ‘ γ ’, then it must be of the above form—was shown by Hedlund in 1969 [hedl69]. Specifically, he showed that the set of shift-commuting functions on $\Sigma^{\mathbb{Z}}$ which are continuous with respect to the metric ‘ ∂ ’, is identical to the set of cellular automata. Cellular automata can, therefore, be viewed as discrete dynamical systems whose temporal evolution is given by some continuous mapping of a Cantor set to itself; the dynamics of such maps can then be compared to the continuous dynamics of iterated maps $f : \mathcal{R}^n \longrightarrow \mathcal{R}^n$.

Observing that $\Phi\Gamma \subseteq \Gamma$, the fundamental problem is to describe the limit set $\Lambda_\Gamma \equiv \lim_{n \rightarrow \infty} (\Phi^n \Gamma)$. Such mappings have been studied previously as *shift-dynamical systems*, but largely without reference to any underlying physical motivation. It was only following the pioneering study of Wolfram in 1983 [wolf83a], that such dynamical systems were first brought to the full attention of the physics community.

Finite Lattice Dynamics

Although CA are most often assumed to *live* on infinitely large lattices, we can equally well consider lattices that are finite in extent (which is done in practice regardless, since all CA simulations are ultimately restricted by a finite computer memory). If a lattice $\mathcal{L}$ has N sites, there are clearly a finite number, k^N , of possible global configurations. The global dynamical evolution can then be represented by a finite *state transition graph* $G_{\mathcal{L}}$, much like the one considered in the description of an abstract automaton in section 2.1.4.

[†] ϕ is more formally defined by first choosing an arbitrary operator mapping $B_{2r+1} \longrightarrow B_1$, and then extending it, via the shift-operator γ , to a map $B_{2r+i} \longrightarrow B_i$, for any ‘ i ’. ϕ is then made to act on configurations ‘ $\vec{\sigma}$ ’ by infinite extension by ‘ γ ’.

The nodes of $G_{\mathcal{L}}$ represent specific global states, $\vec{\sigma}_i$, in $\mathcal{L}$, and there is a directed link from $\vec{\sigma}_i$ to $\vec{\sigma}_j$ if and only if $\Phi[\vec{\sigma}_i] = \vec{\sigma}_j$. Since there are a finite number of possible states, all finite systems must enter *cycles* – wherein a fixed subset of configurations is repeatedly visited – in a time $t \leq k^N$. We represent these subsets – or *attracting* states of the finite system – by a formal *cycle sum decomposition*

$$\mathcal{C}[\mathcal{L}] \equiv \sum_i^{N_{\max}} [n_i, \ell_i] = [n_1, \ell_1] + [n_2, \ell_2] + \cdots + [n_m, \ell_m] + \cdots + [n_{N_{\max}}, \ell_{N_{\max}}], \quad (2.50)$$

where n_i = number of cycles of length ℓ_i . Vertices corresponding to cyclic states may be roots of *trees*, which represent all *transient* configurations of the system. Whenever directed trees are present, we have a manifest irreversibility: although there is exactly one outwardly oriented link at each tree-vertex, a given vertex can have an arbitrary number of predecessor vertices. Peripheral vertices, or those having no incoming links, represent so-called *garden-of-eden* configurations which can occur only as initial states, and thus can never be generated in the course of the evolution.

Figure 2.9 shows a typical $G_{\mathcal{L}}$ topology, computed for a one-dimensional lattice consisting of four vertices and evolving according to totalistic rule **T2**.

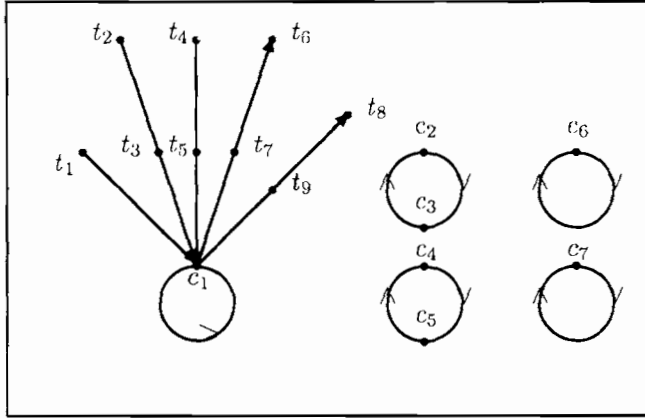


Fig. 2.9 The state transition graph $G_{\mathcal{L}}$, computed for a 1-dim lattice consisting of $N = 4$ points (with periodic boundary conditions), and totalistic rule ‘**T2**’. The vertices labeled ‘ t_i ’ represent transient configurations; those labeled ‘ c_i ’ represent cyclic states, and give rise to the formal cycle sum decomposition $\mathcal{C}[\mathcal{L}] = [3, 1] + [2, 2]$.

The explicit form of the $G_{\mathcal{L}}$ topology is analytically accessible for only a very few specific systems, most notably those defined by *additive* rules and relatively simple lattices. The method of calculation of these topologies will be presented in some detail in chapter 5.

2.2.2 Two-dimensional CA

There are a variety of different lattices and neighborhood structures that can be used by two-dimensional CA (see figure 2.10). The *von-Neumann* neighborhood, consisting only of the four cells which are horizontally and vertically adjacent to the center cell of interest, and the *Moore* neighborhood, consisting of all eight cells which are immediately adjacent to the center site, are both defined on a regular Euclidean lattice and have been studied most extensively. Their explicit forms are given as follows:

$$\left\{ \begin{array}{ll} \text{von-Neumann:} & \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i,j}^{(t)}, \sigma_{i-1,j}^{(t)}, \sigma_{i+1,j}^{(t)}, \sigma_{i,j-1}^{(t)}, \sigma_{i,j+1}^{(t)}) \\ \text{Moore:} & \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i-1,j-1}^{(t)}, \sigma_{i,j-1}^{(t)}, \sigma_{i+1,j-1}^{(t)}, \sigma_{i-1,j}^{(t)}, \sigma_{i,j}^{(t)}, \\ & \sigma_{i+1,j}^{(t)}, \sigma_{i-1,j+1}^{(t)}, \sigma_{i,j+1}^{(t)}, \sigma_{i+1,j+1}^{(t)}). \end{array} \right. \quad (2.51)$$

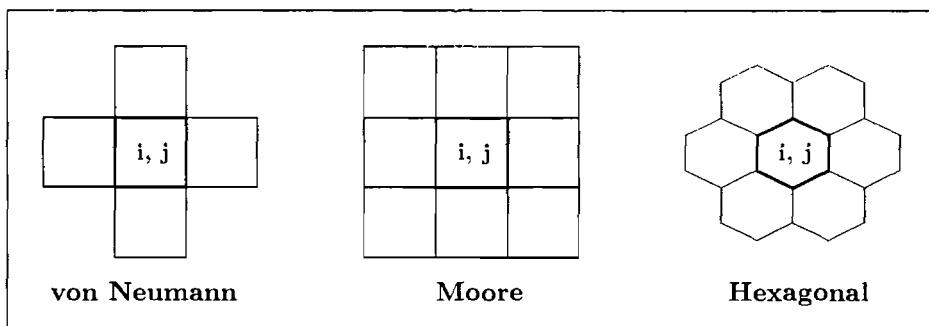


Fig. 2.10 Examples of possible two-dimensional neighborhoods of site ' i, j '.

Triangular and hexagonal lattices (which, along with the *von-Neumann* neighborhood, may be considered as special cases of the nine-neighbor *Moore* neighborhood), can also be used. *Totalistic*, *outer-totalistic*, and *additive* rules are defined exactly as in the one-dimensional case, while *legal* rules may now be generalized to include rotation, reflection, and completely symmetric rules. The various numbers of such two-dimensional rules, for $k = 2$, are given in table 2.2.

The extension of generic CA systems to two dimensions is significant for two reasons: first, the extension brings with it the appearance of many new phenomena involving behaviors of the boundaries of, and interfaces between, two-dimensional patterns that have no simple analogs in one-dimension. Secondly, two-dimensional dynamics permits easier (sometimes direct) comparison to real physical systems. As we shall see in later sections, models for dendritic crystal growth, chemical reaction-diffusion systems and a direct simulation of turbulent fluid flow patterns are in fact specific instances of 2D CA rules and lattices.

Rule Type	<i>von-Neumann</i>	<i>Moore</i>	<i>Hexagonal</i>
General	$4 \cdot 10^9$	10^{154}	$3 \cdot 10^{38}$
Reflection symmetric	$2 \cdot 10^7$	$5 \cdot 10^{86}$	10^{22}
Rotation symmetric	4096	10^{42}	$2 \cdot 10^{19}$
Completely symmetric	4096	$5 \cdot 10^{30}$	$3 \cdot 10^8$
Outer-Totalistic	1024	$3 \cdot 10^5$	16384
Totalistic	32	512	128

Table 2.3 Numbers of possible rules of various types for $k = 2$ two-dimensional CA with specified neighborhood structures.

Generalizations

The explicit forms of rules introduced thus far in this chapter have been essentially generic, in that they arguably represent the simplest possible form of a discrete dynamics. Although, as we will see very shortly, such generic systems already possess an impressive variety of complex behaviors, extensions and generalizations of these primitive systems must be made if one hopes to capture the essence of the actual patterns and structures underlying specific physical (or even social and behavioral) systems. We provide a general list here of what are some of the more important generalizations of the basic CA systems that have appeared in the literature, and indicate the corresponding chapters of this book in which more detailed accounts can be found.

Reversible Rules: almost any random rule that one writes down will give rise to *non-invertible* dynamics, in the sense that it will be impossible to determine what local configuration of site values at the *previous time step* gave rise to a particular value at the current step. Since real physical dynamical laws are *microscopically reversible* any honest attempts at simulating real physical systems can be made only if the underlying CA is itself reversible. Following a suggestion first made by Fredkin [fredkin82], it turns out to be fairly straightforward to write down a general form for such rules:

$$\sigma_{\vec{i}}^{(t+1)} = \phi(\sigma_{\vec{i}}^{(t)} \in \mathcal{N}\{\vec{i}\}) \ominus_k \sigma_{\vec{i}}^{(t-1)}, \quad (2.52)$$

where ‘ $\ominus_k$ ’ is the *modulo- k* difference, and ϕ is completely arbitrary. It should be clear that for such rules, any preceding or succeeding value of $\sigma_{\vec{i}}$ can be determined if the values at site $\vec{i}$ are known for two consecutive time steps; *i.e.*, the total information contained in the initial state is preserved for all time. Moreover, it turns out that reversible rules can be universal, which in turn leads to the intriguing new concept of *reversible computation*. These, and other issues, of reversible rules are discussed in chapters 4.3 and 6.3. *Ballistic Computation* – a CA implementation of Fredkin’s billiard-ball model of computation (BBMC) – is introduced in chapter 3.2.4.

Probabilistic CA (PCA): deterministic state-transitions may be replaced with

specifications of the *probabilities* of cell-value assignments. That is to say, rules ϕ are replaced by probabilities

$$\text{prob} \left\{ \sigma_i^{(t+1)} = \alpha, \text{ given the values } (\sigma_{i-1}^{(t)}, \sigma_i^{(t)}, \sigma_{i+1}^{(t)}) \text{ in } \mathcal{N} \right\}, \quad (2.53)$$

where $\alpha \in \Sigma$. Instead of studying particular evolutions of arbitrary initial states, such rules require that *ensembles* of CA trajectories be considered. An important application of PCA is to the well-studied *Ising model*; Domany and Kinzel [domany84], for example, have constructed an explicit mapping of a d -dim PCA onto an Ising model in $(d+1)$ -dimensions. Chapter 7.2.2 discusses the general relationship existing between PCA and statistical mechanical models.

Non-Homogeneous CA: a characteristic feature of all CA rules defined so far has been that of *homogeneity* – each cell of the system evolves according to the *same* rule ϕ . Hartman and Vichniac [hart86] were the first to systematically study a class of inhomogeneous CA (INCA), in which the state-transition rules are allowed to vary from cell to cell. The simplest such example is one where there are only two different ϕ 's, which are randomly distributed throughout the lattice. Kauffman has studied the other extreme in which the lattice is randomly populated with all 2^{2^k} possible boolean functions of k inputs. The results of such studies, as well as the relationship with the dynamics of *random mappings*, are covered in detail in chapter 8.3.

Coupled-Map Lattices: these are models in which continuity is restored to the state space:

$$x_i^{(t+1)} = \varepsilon f(x_i^{(t)}) + (1 - \varepsilon) (x_{i-1}^{(t)} + x_{i+1}^{(t)}); \quad x \in \mathcal{R}_{[0,1]}, \quad (2.54)$$

where $f(x) : \mathcal{R}_{[0,1]} \rightarrow \mathcal{R}_{[0,1]}$ is an arbitrary continuous function and ε is a coupling term. First introduced by Kaneko [kaneko83], they are simpler than partial differential equations, but more complex than generic CA. Their behavior is analyzed in chapter 8.

Structurally Dynamic CA: the only generalizations mentioned so far were generalizations of either the rules or state space. Another intriguing possibility is to allow for the lattice $\mathcal{L}$ itself to become a full participant in the dynamical evolution of the system, much as the classically ‘static’ physical space-time arena becomes a bona-fide dynamic element in general relativity. The idea is to study the behavior of systems evolving according to both value and local structure rules:

$$\begin{cases} \sigma^{(t+1)} &= \phi \left[\sigma^{(t)} \in \mathcal{N}, a_{i,j}^{(t)} \in A^{(t)}(\mathcal{L}) \right] \\ a_{i,j}^{(t+1)} &= \psi \left[\sigma^{(t)} \in \mathcal{N}, a_{i,j}^{(t)} \in A^{(t)}(\mathcal{L}) \right], \end{cases} \quad (2.55)$$

where $A^{(t)}(\mathcal{L}) = [a_{i,j}^{(t)}]$ is the adjacency matrix of the lattice at iteration step ‘ t ’. The kinds of lattice structures that emerge in such fully dynamic systems is examined in detail in chapter 8.1.

Quantum Cellular Automata (QCA): in order to address the possibly very fundamental role CA-like dynamics may play in the microphysical domain, some form of quantum dynamical generalization to the basic rule structure must be considered. One way to do this is to replace the usual time evolution of what may now be called classical site values σ_i , by unitary transitions between k -component complex probability- amplitude states, $|\sigma\rangle_i$ – defined in such a way as to permit superposition of states. As is standard in quantum mechanics, the absolute *square* of these amplitudes is then interpreted to give the probability of observing the corresponding classical value. Two independently defined models – both of which exhibit much of the typically quantum behavior observed in real systems – are discussed in chapter 8.2.

Chapter 3

Phenomenological Studies of Generic CA

The renaissance of CA research following Wolfram's pioneering review [wolf83a] would arguably not have occurred were it not for the existence of, and easy access to, affordable personal computers and graphics workstations. Most of the important but excessively technical mathematics of what were called tessellation-automata had already been published years before ([yamad69], [ostr71], and [amoro72]); it was not until the dynamics could be observed directly, however, that anything approaching an *intuition* for the behavior of these systems could finally be obtained. As has already been alluded to repeatedly, except for special-case rules, the behavioral properties of even the simplest CA systems can be exceedingly difficult to establish by direct mathematical analysis. Not surprisingly, the most prudent course of action has proven to be a direct phenomenological study of the systems in question: a particular CA rule and initial state are selected and the dynamical evolution—with an emphasis given to any observable generic properties—is traced directly by computer simulation. Such an approach, also used widely in the general study of continuous chaotic systems, is gaining a considerable respectability and really constitutes a fundamentally new experimental branch of mathematics. This chapter introduces the generic behavior of the simplest one and two dimensional CA systems by way of a guided-tour through a graphics gallery of their dynamical evolutions.

3.1 One-dimensional Systems

We recall from chapter 2 (section 2.1.1) that the general form of a range ‘ r ’ one-dimensional rule ϕ is given by

$$\sigma_i(t+1) = \phi(\sigma_{i-r}(t), \sigma_{i-r+1}(t), \dots, \sigma_{i+r-1}(t), \sigma_{i+r}(t)), \quad (3.1)$$

where $\sigma_j \in \{0, 1, \dots, k-1\}$, and ϕ is explicitly defined by assigning values to each of the k^{2r+1} possible $(2r+1)$ -tuple configurations for a given neighborhood. In the following, specific rules will be referred to more compactly by using the simple code given in equation 2.7.

3.1.1 Space-Time Patterns

Simple Seeds

We begin with the simplest CA of all; namely those whose site variables take on only one of two values and evolve according to rules which depend only on the previous values of a given site and those of its immediate left and right neighbors:

$$\sigma_i(t+1) = \phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)), \quad \sigma \in \{0, 1\}. \quad (3.2)$$

We recall, from equations 2.8 and 2.9, that only 32 so-called *legal* rules (out of the 256 total possible rules that can be defined), leave the zero-state $\vec{\sigma} = 0$ unchanged and are such that reflection-symmetric local states – ‘100’ and ‘001’, for example – yield the same values. We now examine the patterns generated by these types of rules.

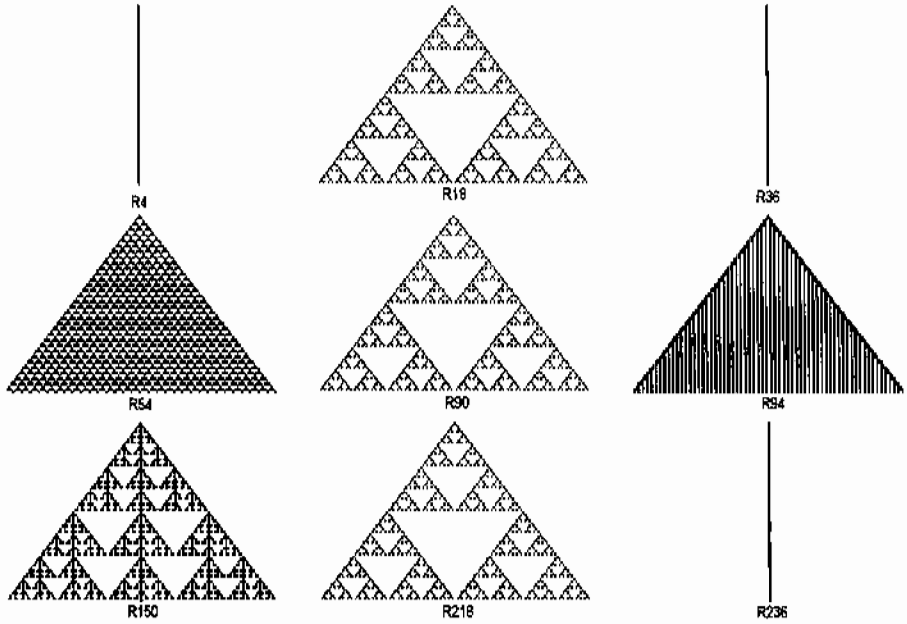


Fig. 3.1 Space-time patterns of a few elementary *legal* rules ($k = 2$, $r = 1$).

Figure 3.1 shows the evolution of a few legal rules, starting from an initial state consisting of a single nonzero value at the center site. In each case, and all such one-dimensional *space-time* patterns appearing in this book, the time axis runs from top to bottom and sites with value $\sigma_i = 1$ are colored *black*.

Several distinct classes of patterns, or behaviors, are evident:

- (i) the initial state remains unchanged for all time (**R4**, **R36**),

- (ii) the region of nonzero sites expands symmetrically to the right and left of the center value to produce essentially uniform structures (**R54**, **R94**), and
- (iii) the symmetrically expanding nonzero region forms a nontrivial complicated pattern of zero's and one's (**R18**, **R90**, **R150**, **R218**).

By virtue of being *local*, CA rules can define neither an intrinsic 'length' scale other than the size of the local neighborhood nor any intrinsic 'time' scale other than the discrete interval between successive configurational states. Since an initial state consisting of a single nonzero site itself defines no intrinsic length scale, the CA configurations appearing in figure 3.1 should also not exhibit an intrinsic scale, at least in the infinite time limit. While some rules yield obviously scale-invariant *uniform* final patterns, the scale invariance of the more complex patterns is more subtle.

Patterns of this third class in fact demonstrate a complex form of scale-invariance by their *self-similarity*; in the infinite time limit, different magnifications observed at the same resolution are indistinguishable. The pattern generated by rule **R90**, for example, matches that of the successive lines in Pascal's triangle: $\sigma_i(t)$ is given by the coefficient of x^i in the expansion of $(1+x)^t$ *modulo-two* (see figure 3.2).

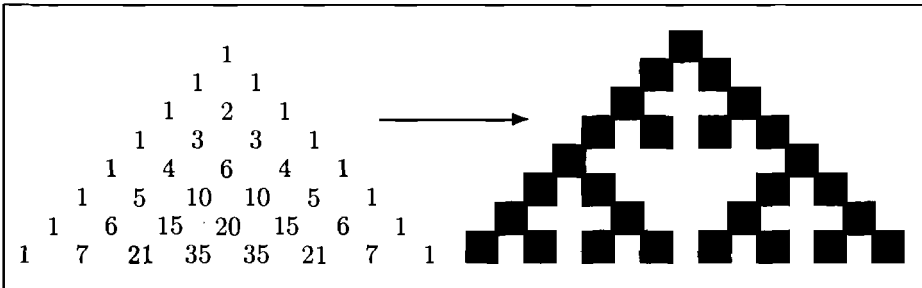


Fig. 3.2 Algebraic construction for the single-seed evolution under **R90**. The left side gives the values of the coefficients of x^n in the expansion of $(1+x)^n$; the right, which matches that of **R90**, are those same values *modulo-two*.

The resulting large-time limit pattern can be obtained by a simple recursive geometrical construction (see figure 3.3), and its manifest self-similarity can be quantitatively characterized by the *Hausdorff-Besicovitch* (or *fractal*) dimension defined in the previous chapter. We see that at each successive stage in the construction the number of triangles increases by a factor of three while their base-length decreases by a factor of two. Thus, defining $T(n)$ to be the number of triangles with base-length ' n ' ($n = 2^k$),

$$T(n/2) \sim 3 T(n) \implies D_{\text{fractal}}(\mathbf{R90}) = \frac{\ln 3}{\ln 2} \sim 1.5849. \quad (3.3)$$

While the patterns generated by rules **R18** and **R218** are essentially the same as

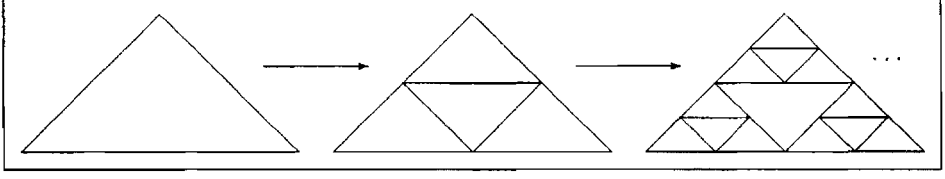


Fig. 3.3 First three steps in the recursive geometric construction of the large-time pattern induced by **R90** when starting from a simple nonzero initial state. The actual final pattern would be given as the infinite time limit of the sequence shown here, and is characterized by a fractal dimension $D_{\text{fractal}} = \ln 3 / \ln 2$.

the one resulting from **R90**, the single-seed pattern induced by **R150** can be shown to be equal to the sequence of coefficients of x^i in the expansion of $(1 + x + x^2)^t$ modulo-two, and can be geometrically constructed according to the scheme shown in figure 3.4. In this case, $T(n)$ satisfies a two-term recurrence relation

$$\begin{aligned} T(n = 2^k) &= 2T(2^{k-1}) + 4T(2^{k-2}), \quad T(2) = 4, \quad T(4) = 12, \\ &= \frac{(5+3\sqrt{5})(1+\sqrt{5})^k}{10} + \frac{(5+3\sqrt{5})(1-\sqrt{5})^k}{10}, \end{aligned} \quad (3.4)$$

so that, as $k \rightarrow \infty$, $T(n) \sim n^{-\log_2(1+\sqrt{5})} \implies D_{\text{fractal}}(\mathbf{R150}) \sim 1.6942$.

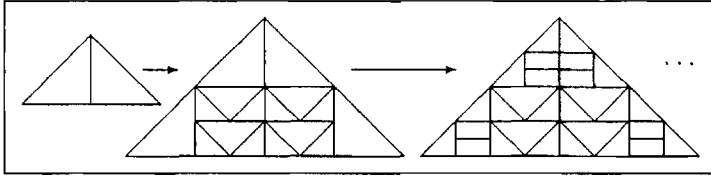


Fig. 3.4 First three steps in the recursive geometric construction of the large-time pattern induced by **R150** when starting from a simple nonzero initial state. The infinite time limit pattern is characterized by a fractal dimension $D_{\text{fractal}} \sim 1.69$.

In general, when starting from a single seed and independent of the value of the nonzero site, sum modulo- k rules for k equal to a *prime*,

$$\sigma_i(t+1) = \sum_{j=i-r}^{i+r} \sigma_j(t) \pmod{k}, \quad (3.5)$$

generate self-similar fractal patterns with fractal dimension given by

$$D_{\text{fractal}}(\oplus_k; \text{single-seed}) = \log_k \sum_{i=1}^k i = 1 + \log_k \left(\frac{k+1}{2} \right). \quad (3.6)$$

Figure 3.5 shows the time evolution of a few asymmetric (*i.e.*, *illegal*) $k=2$, $r=1$ rules. Doing away with the quiescence condition produces patterns in which $\bar{\sigma}$

alternates between $\vec{1}$ or $\vec{0}$ in successive time-steps; removing reflection symmetry, on the other hand, tends to 'shift' local patterns. Although self-similarity is still evident it is also sheared by shifting. With the one possible exception of rule **R30**, therefore – whose pattern is really a complicated mixture of periodicity and randomness and about which we will have more to say in a later section of this chapter, illegal rules generally do not appear to introduce any dramatically new qualitative dynamical features.

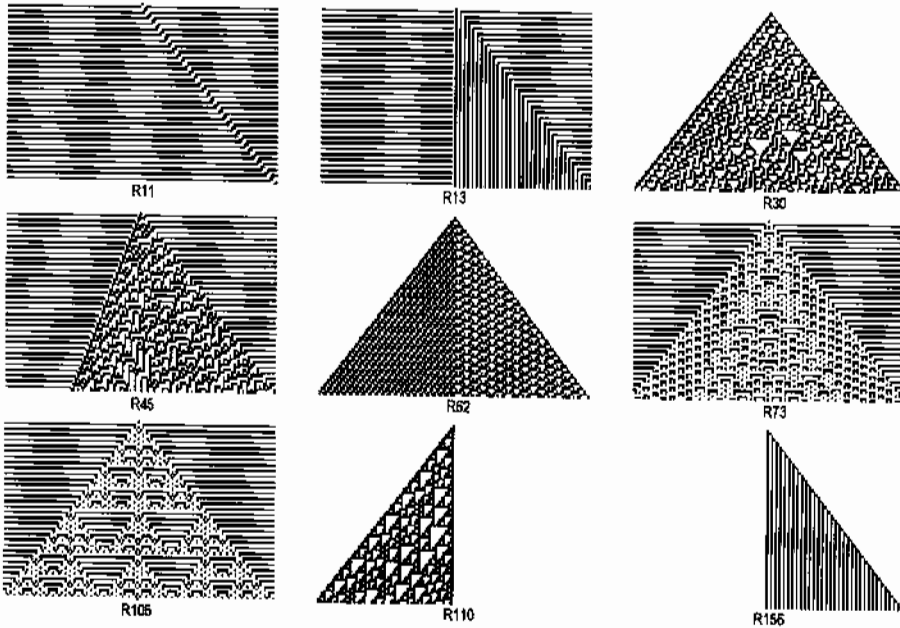


Fig. 3.5 Space-time patterns of a few asymmetric (i.e. *illegal*) $k = 2$, $r = 1$ rules.

Figure 3.6 shows the same legal rules appearing in figure 3.1 but starting from an initial state with nonzero sites occupying only a small central region.

For some rules (such as **R4** and **R94**) the patterns obtained from single seeds are stable under the addition of further nonzero sites. For other rules (such as **R218**) the pattern is unstable. Although the patterns for **R18** and **R150** retain much of their fractal structure, some of the details appear to be washed away. A similar contrast between the evolutionary behaviors of single and small nonzero region seeded rules can be observed for the $r = 2$ totalistic rules shown in figures 3.7 and 3.8.

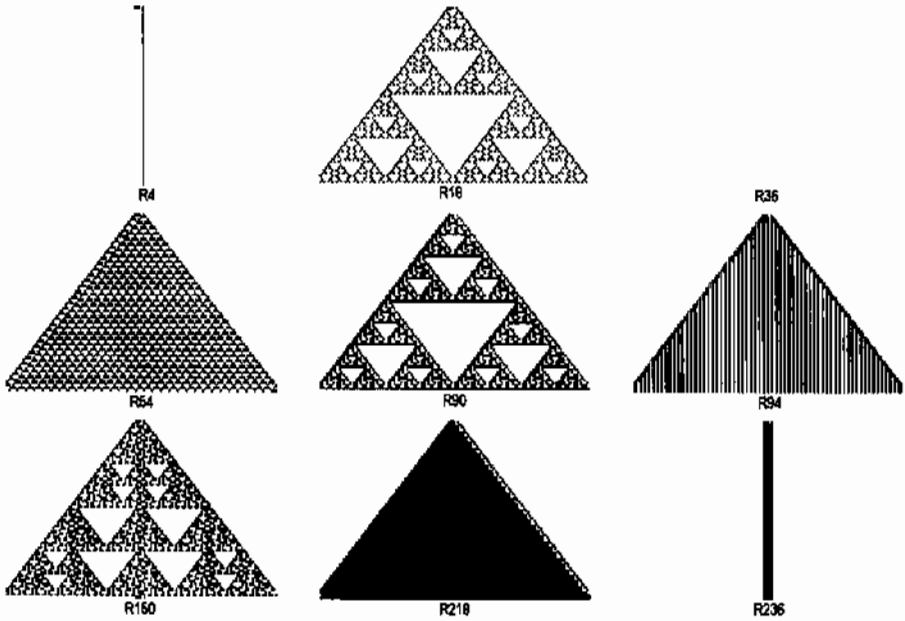


Fig. 3.6 Space-time plots of the same legal rules appearing in figure 3.5 but starting from an initial state with nonzero sites occupying only a small central region.

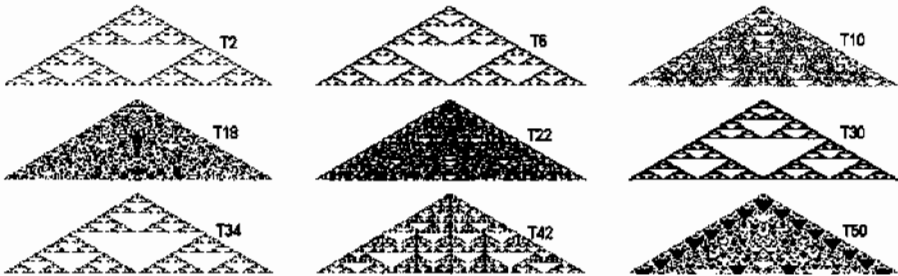


Fig. 3.7 Space-time plots $r = 2$ totalistic rules. The lattice consists of 256 sites and each rule is iterated 64 times. The initial condition, in each case, is a single non-zero site at the center.

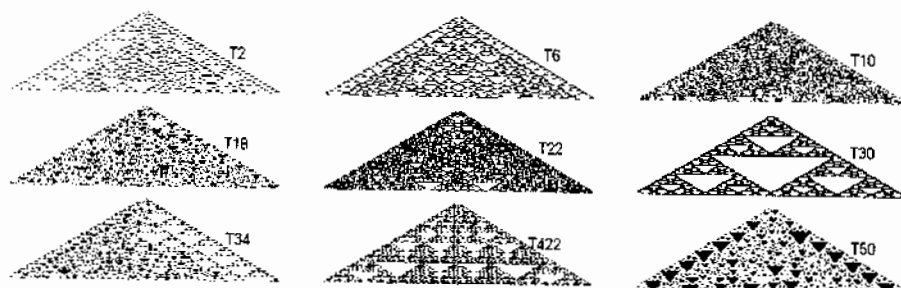


Fig. 3.8 Space-time plots $r = 2$ totalistic rules. The lattice consists of 256 sites and each rule is iterated 64 times. The initial condition, in each case, consists of five nonzero sites near the center.

It is important to point out that except for the obvious *necessary* two conditions that either

$$\begin{cases} \phi(\sigma_{i-r}, \sigma_{i-r+1}, \dots, \sigma_{i-1}, 0, \dots, 0) \neq 0, & \text{or} \\ \phi(0, \dots, 0, \sigma_{i+1}, \sigma_{i+2}, \dots, \sigma_{i+r}) \neq 0, \end{cases} \quad (3.7)$$

must be satisfied for some set of σ_i in order for there to be unbounded growth, there is no known simple general criterion by which the type of pattern to emerge can be predicted directly from ϕ . Similarly, a *necessary*, but not *sufficient*, condition for self-similar pattern formation is to have some sort of *growth inhibition*: the presence of nonzero site configurations must sometimes cause ϕ to yield zero.

Irregular Growth: Although, as we have seen, the nonzero region of most space-time patterns evolving from simple seeds propagates outward at a fixed speed of $c \leq r$ sites per time step, there exist rules for which the growth is much more irregular. Figure 3.9, for example, shows the evolution of the initial state $\vec{\sigma}(0) = \dots 0042400 \dots$ according the $k = 5$, $r = 1$ totalistic rule **T985707700**. The nonzero region, or *light-cone*, undergoes a series of alternating growths and decays, with an average expansion rate of about ~ 0.2 sites per time step.

Random Seeds

Figures 3.10-3.14 show the time evolution of a variety of $r = 1$, $r = 2$ and $r = 3$ rules for both $k = 2$ and $k = 3$ and all starting from a disordered or random configuration. The configurations are defined by randomly and independently assigning each site the value $\sigma = 0$ or $\sigma = 1$ with equal probability: $\text{prob}(\sigma = 0) = \text{prob}(\sigma = 1) = \dots = \text{prob}(\sigma = k - 1) = 1/k$.

We again see a variety of behaviors, including both uniform and complicated patterns. Generally speaking, rules for which fractal patterns emerge from single or simple seeds produce chaotic patterns when grown from larger seeds. The most interesting feature, however, is the fact that many rules destroy the independence of

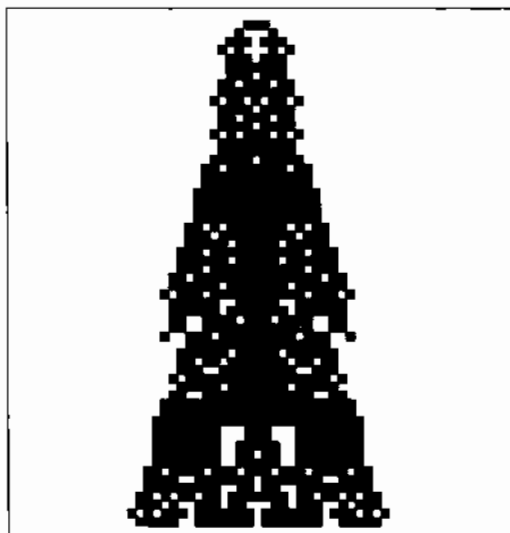


Fig. 3.9 Example of a slow *diffusive*-like growth from a simple seed. The initial state $\vec{\sigma} = \dots 0042400 \dots$ evolves according to the $k = 5$, $r = 1$ totalistic rule **T985707700**. All sites with $\sigma > 0$ are colored black.

the initial configuration and dynamically generate correlations between (often very far) separated sites.

Local regularities within random appearing patterns are associated with *invariants* of a given rule. For example, because the null configuration is invariant under all *legal* rules, any finite string of contiguous zeros can only be reduced in size by nonzero values propagating inward from the sides. Finite strings of zeros thus lead to the triangular clearings seen in the figures.

We have already seen that most CA rules are irreversible: a particular global configuration may have a number of different predecessors, so that the global mapping Φ is not one-to-one. Moreover, there also exist configurations (the so called *garden-of-eden* states) for which there are no predecessors, so that Φ is not onto. The contractive nature of most rules, therefore, implies that only some subset of the space of all possible configurations may occur at large times. What we are thus seeing these figures is rather dramatic (albeit crude) evidence of the phenomenon of *self-organization*, in which an initially random state evolves to a state exhibiting long-range correlations and whose overall space-time patterns contain manifestly *nonlocal* structure. The manifest irreversibility of a given rule results in a long time behavior which is effectively determined by the properties of some limit set consisting of a special subset of all possible states. It is the *universality* of the properties of these special subsets that we turn to next.

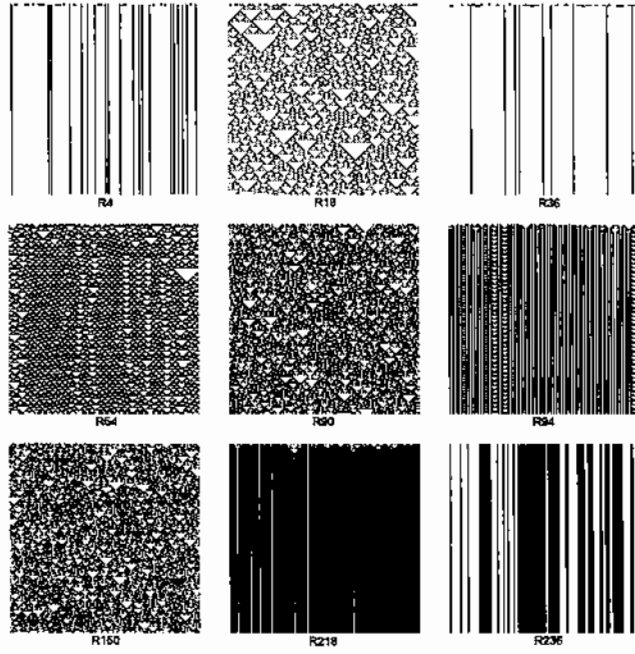


Fig. 3.10 One-dimensional $k = 2$, $r = 1$ rules starting with random initial conditions.

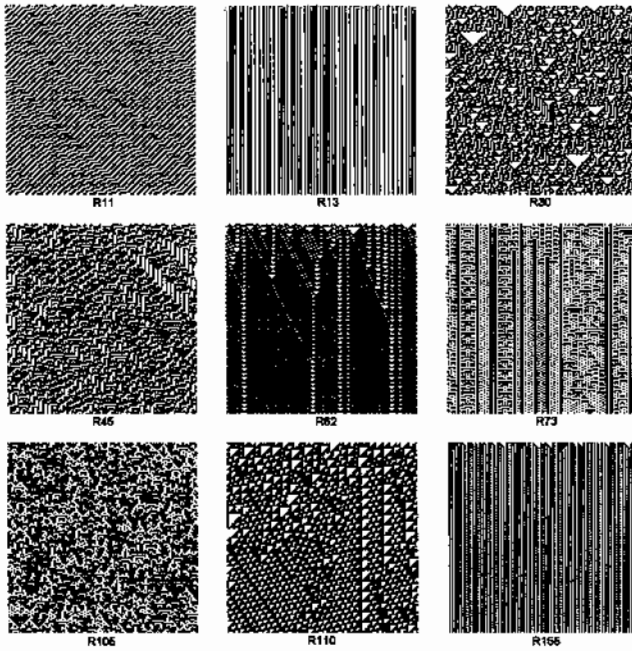


Fig. 3.11 One-dimensional $k = 2$, $r = 1$ rules starting with random initial conditions.

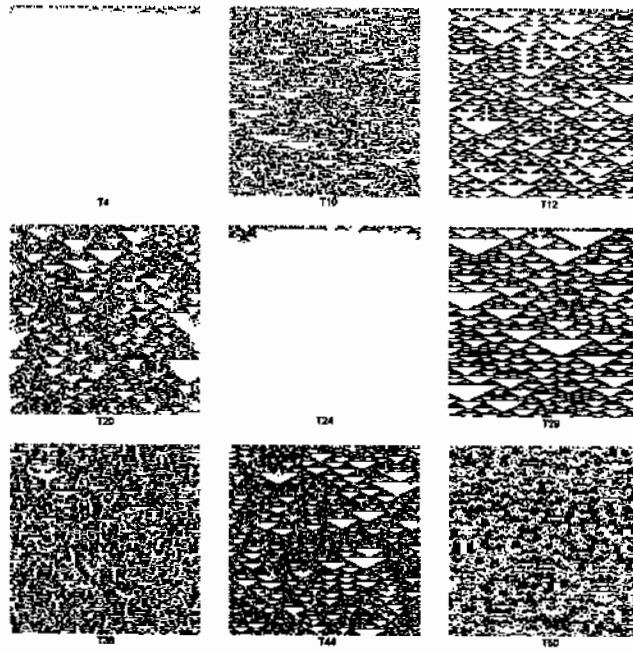


Fig. 3.12 *Totalistic* $d = 1$, $k = 2$, $r = 2$ rules; starting from random initial conditions.

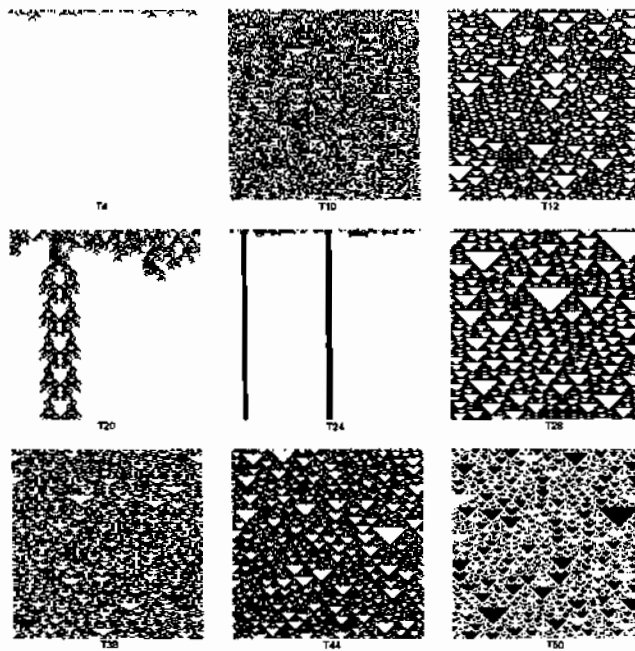


Fig. 3.13 *Totalistic* $d = 1$, $k = 2$, $r = 3$ rules; starting from random initial conditions.

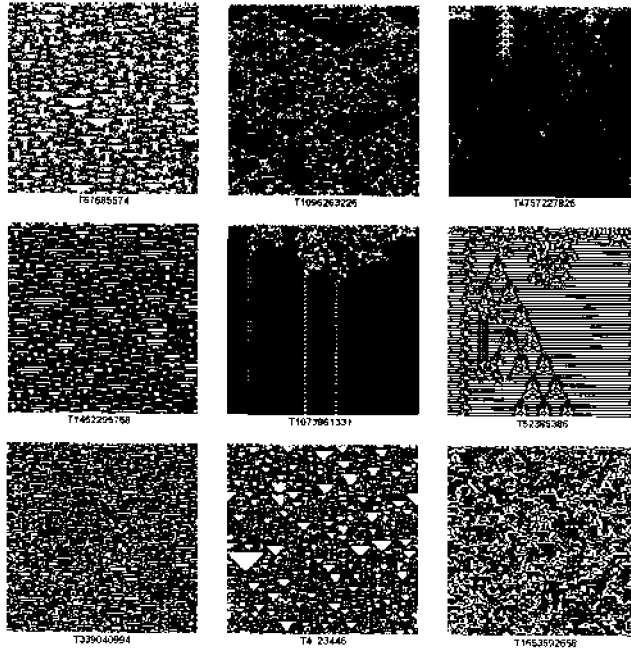


Fig. 3.14 Totalistic $d = 1$, $k = 3$, $r = 2$ rules; starting with random initial conditions.

3.1.2 Behavioral Classes

Although different initial configurations typically give rise to patterns which differ in the *details* of their appearance (see figures 3.10-3.11, for example), the gross overall characteristics of a given pattern appear unchanged: each particular rule yields its own unique and easily recognizable space-time pattern*. Indeed, there is extensive empirical evidence to support the conjecture that the patterns generated by *all* (one-dimensional) CA rules evolving from disordered initial states fall into one of only four basic qualitative behavioral classes ([wolf85b], [wolf85f]) :

Class c1: *All sites eventually attain the same value.*

Class c2: *Simple stable states or periodic and separated structures emerge.*

Class c3: *Chaotic nonperiodic patterns are generated.*

Class c4: *Complex, localized, propagating structures are formed.*

All CA within a given class, regardless of the precise specification of the evolution rule, yield qualitatively similar behavior. Except for rules in the **c4** class, the

*Exceptional initial states yielding distinctly different patterns from the same rule may exist but with low or zero probability.

behaviors bear a strong resemblance to those observed in continuous systems. The homogeneous final states occurring for all **c1** rules, for example, are essentially the same as a *fixed point* attracting final state. Similarly, the asymptotically periodic final states of all **c2** rules are analogous to continuous *limit cycles*, while the chaotic states generated by **c3** rules are analogous to the *strange attractors* appearing in continuous dynamical systems (see chapter 4.2 for details). The more complicated localized structures emerging from **c4** class rules, on the other hand, do not appear to have any obvious continuous analogs, although many are best described as being *soliton-like* in their appearance.

Alternative classification schemes are of course possible. Culik and Dube [culik89a], for example, provide an empirical refinement to class **c3** for $k = 2$, $r = 2$ totalistic rules, based on observations of evolutions starting from random finite initial configurations[†]; they observed that such rules actually form an almost continuous spectrum when classified on the basis of fractal-generation ability. A more formal approach based on observations of behavior starting from finite configurations is taken by Culik and Yu [culik88]. Among the several important, and unexpected, results reported there, are (i) it is undecidable whether all the finite configurations of a given CA eventually become quiescent, and (ii) it is undecidable to which class a given CA belongs, *even when choosing between the simplest two classes*.

3.1.2.1 Difference Patterns

Although the question of the quantitative characterization of these classes is taken up in earnest in chapter 4, we can here mention that an important tool will be a discrete *Green function*. Green functions measure *changes* in patterns generated by a given rule resulting from a small changes in the initial state, and give the average probability that sites a given distance away from the small area of differing initial values will be changed after a certain number of iteration steps. We can get a glimpse of the form of these Green functions for a selected rule by plotting various *difference patterns*.

Difference patterns are space-time patterns of the difference between two evolutions of the same rule starting from two different initial states. For example, the i^{th} site at the n^{th} step of a difference pattern for ($k = 2$ global) rule Φ in which the two different initial global states $\vec{\sigma}_1(0)$ and $\vec{\sigma}_2(0)$ differ only at a single site (see figure 3.15), is defined to be

$$\Delta_i^{[1]}(n) = \Phi^n [\vec{\sigma}_1(0)]_i \oplus \Phi^n [\vec{\sigma}_2(0)]_i. \quad (3.8)$$

The rate of growth of such patterns – which gives an idea of the speed with which various features in a CA pattern may propagate through the lattice – provides one quantitative measure that can be used to distinguish between the behaviors of different classes.

[†]By a *finite* initial configuration we mean one in which all but a finite number of sites in an infinite lattice are in the same quiescent state.

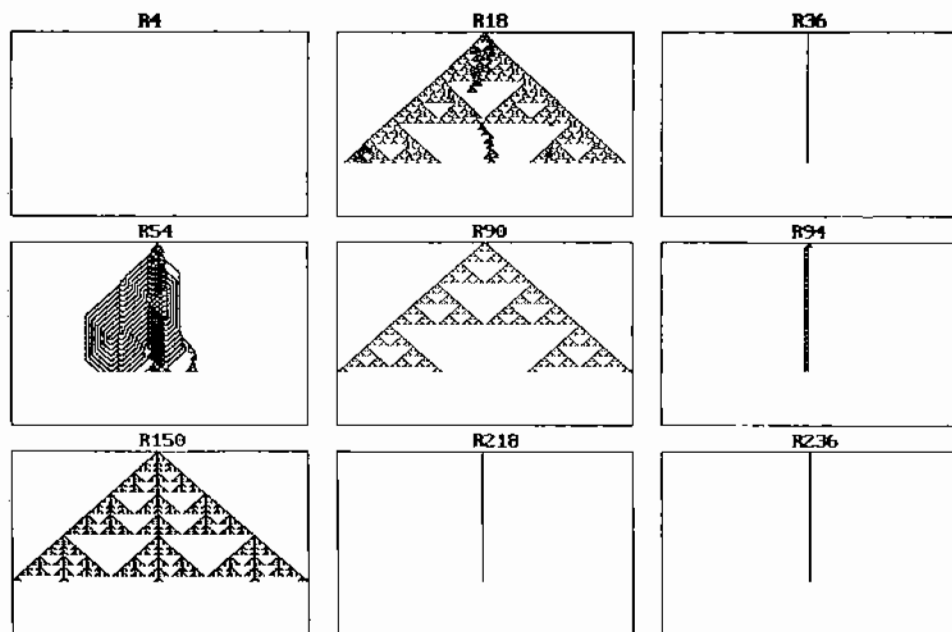


Fig. 3.15 *Difference patterns* for a few elementary $k = 2$, $r = 1$ rules; see text.

Class **c1** rules, for example, have unique final states which are unaffected by any change to the initial state. Similarly, **c2** rules are such that small changes in the initial state only affect a fixed finite region around the area in which the values were changed. A change in the value of even a single site for **c3** rules, on the other hand, affects a linearly increasing region of sites; given enough time, therefore, infinitely large lattices would have arbitrarily large regions affected by a minimal perturbation to the initial state.

The same structural irregularity of the space-time patterns of **c4** rules appears also in their difference patterns. While some perturbations on some initial configurations appear to propagate arbitrarily far, others die out rather quickly. Unlike the first three classes of rules, for which statistical averages of propagation speeds are easily obtained, the behavior of **c4** rules is so irregular that meaningful averages cannot be obtained. In particular, this means that Green functions cannot be properly defined for **c4** rules.

Table 3.1 (taken from reference [wolf86b]) gives the approximate fractions of a variety of legal totalistic rules belonging to each of the four behavioral classes. We see that rules generally become more likely to exhibit **c3** or **c4** behavior for larger ' k ' and ' r ', and that **c4** behavior does not appear at all in any of the *elementary* $r = 1$, $k = 2$ rules.

Since the speed of information propagation is, as we shall see in chapter 4, related to the Lyapunov exponent for the CA evolution, and is a direct measure of the sensitivity to initial conditions, it should not be surprising to learn that various rules can also be distinguished by the *degree of predictability* for the outcome of

CLASS	k=2, r=1	k=2, r=2	k=2, r=3	k=3, r=1
c1	0.50	0.25	0.09	0.12
c2	0.25	0.16	0.11	0.19
c3	0.25	0.53	0.73	0.60
c4	0.00	0.06	0.06	0.07

Table 3.1 Approximate fraction of legal totalistic rules belonging to each of the four behavioral classes.

CLASS	FINITE SEED	RANDOM SEED	DIFFERENCE PATTERN	PREDICTABILITY
c1	pattern disappears	all sites attain same value	no change	completely predictable
c2	evolves to fixed finite size	simple stable or periodic structures	changes only over finite region	locally predictable from local initial state
c3	grows indefinitely	chaotic aperiodic behavior	changes over ever expanding region	behavior depends on ever increasing initial region
c4	alternating growth and decay	complex localized structures	irregular changes	effectively unpredictable

Table 3.2 Characteristics of the four behavioral classes.

their evolution. Table 3.2 summarizes the qualitative differences among the four behavioral classes.

What has not yet been discussed is the reason for this behavioral universality. A possible mechanism may be provided by the apparently ubiquitous phenomenon of attractive rule simulation in *blocking transformation* networks, a description of which we turn to next.

3.1.2.2 Blocking Transformations

' T ' iterations of rule ' ϕ_1 ' are often *simulated* by ' nT ' ($n > 1$) iterations of another rule ' ϕ_2 ', provided that individual site values of the first system are replaced with particular blocks of sites in the second:

$$\begin{cases} 0 \longrightarrow B_0, \\ 1 \longrightarrow B_1. \end{cases} \quad (3.9)$$

As a simple example of this, consider the elementary rules **R18** and **R90**:

RULE	111	110	101	100	011	010	001	000
	↓	↓	↓	↓	↓	↓	↓	↓
R18	0	0	0	1	0	0	1	0
R90	0	1	0	1	1	0	1	0

Notice that any initial configuration that does not contain any '110' or '011' blocks will evolve in the same way under the two rules.

Provided that *two time steps* under **R18** are carried out for every *one time step* of rule **R90**, it is in fact easy to show that under the block transform

$$\begin{cases} 0 \rightarrow '00' \\ 1 \rightarrow '10', \end{cases} \quad (3.10)$$

the evolution of arbitrary starting configurations under **R90** is reproduced, or *simulated*, by **R18**.

Consider the global state $\vec{\sigma}_1 = '0011000'$, for example, which evolves into $\vec{\sigma}_2 = '0111100'$ under **R90**. $\vec{\sigma}_2$ could equally well be obtained by applying two iterations of **R18** to the block-transformed starting state $B(\vec{\sigma}_1) = '00001010000000'$:

$$\begin{aligned} \Phi_{\mathbf{R18}} [\Phi_{\mathbf{R18}} (B(\vec{\sigma}_1))] &= '00101010100000' \\ &= B(\vec{\sigma}_2) \\ &= B(\Phi_{\mathbf{R90}}[\vec{\sigma}_1]). \end{aligned} \quad (3.11)$$

Simulation of ϕ_1 by ϕ_2 implies the existence of a set $\lambda \subseteq \Lambda$ for which the evolution under the two rules ϕ_1 and ϕ_2 is the same. Since most CA rules are irreversible it may happen that *only the one subset of blocks corresponding to some particular simulated rule* will continue being generated at large times. If this happens, then it may be said that the behavior of the first rule is *attracted* to that of the second. Rule **R18**, for example, is attracted to rule **R90** in precisely this manner (see below).

Many, possibly all, rules appear to generate asymptotic states which are block-related to configurations evolving according to one of only a small subset of the set of all rules, members of which are left invariant under all block transformations. That is, the infinite time behavior appears to be determined by evolution towards *fixed point rule* behavior, and the statistical properties of all CA rules can then, in principle, be determined directly from the appropriate block transformations necessary to reach a particular fixed point rule.

Block-Defined 'Phases' of Behavior: The simulation of **R90** by **R18** also illustrates the appearance of distinct *phases* of behavior, separated by domain walls. Each *phase* corresponds to a particular set of configurations, such as those for which the given rule simulates some other rule.

We first observe that any random initial configuration '*S*' can be decomposed into two distinct sets:

$$S = \left(\bigcup_i S_i^{\text{even}} \right) \cup \left(\bigcup_j S_j^{\text{odd}} \right), \quad (3.12)$$

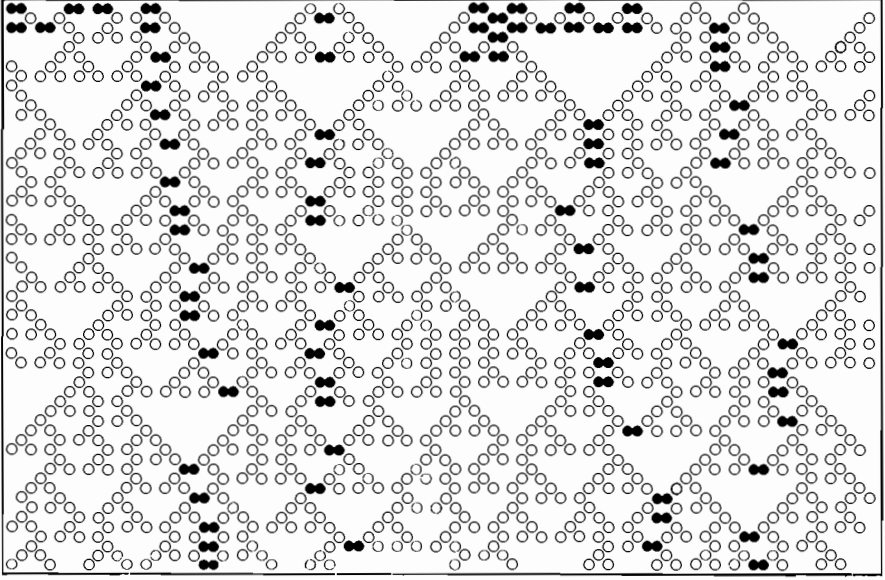


Fig. 3.16 Space-time pattern of $k = 2$, $r = 1$ rule **R18**; *kink-sites* (i.e. neighboring $\sigma = 1$ sites) are indicated in solid black. Notice the stochastic-like kink trajectories, despite the strictly deterministic rule.

where S^{even} and S^{odd} are configurations in which all *even* and all *odd* sites are zero, respectively. It is easy to see that

1. Both of the sets, S^{even} and S^{odd} , are *invariant* under **R18**, and
2. Each set, or *phase*, has the correct blocking form to simulate evolution under rule **R90**.

The domain walls (or *kinks*, consisting of pairs of sites with value $\sigma = 1$) that define the boundary between the two sets, however, *do not* evolve as they would under **R90** but instead undergo pairwise annihilating random walks (see figure 3.16). Indeed, numerical analysis [grass84a] has shown that, as $t \rightarrow \infty$, their density decreases like

$$\rho_{\text{kink}} \sim (4\pi t)^{-1/2}. \quad (3.13)$$

A similar kind of ‘kink-annihilation’ exists for rules **R122**, **R126**, **R146**, and **182**.[†]

[†]One may speculate on the fundamental importance of the following obvious, but no less intriguing, point: despite a fundamentally deterministic evolution taking place on the lower *site* level, a nondeterministic stochastic dynamics unexpectedly appears on the higher *kink* level. We are at least reminded once again that neither complex nor random behavior need have a complex

As time increases, S^{even} and S^{odd} take up arbitrarily large regions of the lattice. The behavior of rule **R18** thus approaches that of **R90** arbitrarily closely; *i.e.*, rule **R18** is *attracted*, to rule **R90**, via the block transformation defined by equation 3.10.

Rule $\mathcal{R}_1$	(Simulates) $\rightarrow \mathcal{R}_2$	$0 \rightarrow 'B_0'$	$1 \rightarrow 'B_1'$	Simulation Steps
22	0	11011000	11111000	4
	90	0000	1000	4
	146	00	01	2
58	0	101	100	3
	128	00	10	2
	170	11010	10110	5
	240	1100	1110	8
60	60	00	10	2
90	90	00	10	2
110	0	110100	101100	9
	170	10011000	11111000	16
	240	111000	100110	9
122	0	1010	1000	2
	90	00	11	2
	128	00	10	2
	204	11100	11110	2

Table 3.3 Block-Transformation Simulations for a few selected elementary rules.

Table 3.3 lists blocking transformations and equivalent simulation time steps for a few other rules.[†] Notice that some rules, like **R60** and **R90**, remain invariant under certain blocking transformations and can thus be considered *fixed points* of the transform. Essentially all rules whose blocking transformation properties have been studied thus far have been found to follow an attractive simulation path to one of the few fixed point rules. It has been suggested that the large time behavior of *all rules* tends towards that of the fixed point rules ([wolf83a], [wolf85a], [wolf85d]). If true then the set of fixed point rules accounts for the phenomenologically observed behavioral universality of CA: all class **c1** rules tend towards the null rule; all class **c2** rules are attracted towards the identity rule, and all class **c3** rules are attracted to the class **c3** fixed point rules.

We have just seen that rule **R18** has essentially one phase that takes two different forms. A general rule typically supports many different phases, each corresponding to simulations of different rules. Not all of these phases will be *stable* however. For example, of the two **R122** phases defined by block transforms $\mathcal{T}_1 = \begin{pmatrix} 0 \rightarrow 00 \\ 1 \rightarrow 11 \end{pmatrix}$ (for

dynamical origin.

[†]More complete tables of blocking transformations appear in [wolf83a] and in the appendix of reference [wolf85c].

which **R122** simulates the class **c3** rule **R90**) and $\mathcal{T}_2 = \begin{pmatrix} 0 \rightarrow 11100 \\ 1 \rightarrow 11110 \end{pmatrix}$ (for which **R122** simulates the class **c2** rule **R204**), only the former is stable.

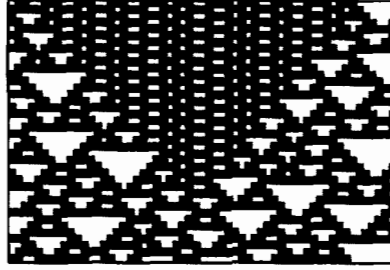


Fig. 3.17 Stable (class **c3**) and unstable (class **c2**) phases of rule **R122**.

Figure 3.17 shows the evolution of an initial state consisting only of blocks '11100' and '11110', except for two 'defects', '00' and '10', placed at the end (periodic boundary conditions are used). Starting from these defects, the stable class **c3** behavior expands approximately linearly in time to eventually dominate the overall pattern.

Blocked Space-Time Patterns: The intrinsic phase structure of a rule can sometimes be directly observed by graphing its *blocked pattern*. We can describe the space-time sets of the two ordered states of rule **R18** by

$$\begin{cases} \sigma_n^I(t) & \longleftrightarrow & n+t = \text{even} \\ \sigma_n^{II}(t) & \longleftrightarrow & n+t = \text{odd} \end{cases} \quad (3.14)$$

The two sets may thus be effectively disjoined from one another by plotting only *every-other* site, both spatially and temporally. Higher order blocked patterns may also prove useful. Various phases for systems with $k > 2$, on the other hand, are often evident even without resorting to blocked patterns.

Block-Transform Generation of Fractal Patterns: Blocking transformations provide an elegant 'explanation' of the self-similar, or scale-invariant, fractal patterns generated by rules such as **R90** and **R218** (see figure 3.1). If the (inverse) blocking transform $\mathcal{T} \equiv \begin{pmatrix} 00 \rightarrow 0 \\ 01 \rightarrow 1 \end{pmatrix}$ were applied to either of these two rules, for example, the resulting blocked-pattern would be reproduced by the same rule; *i.e.*, rules **R90** and **R218** are fixed points of $\mathcal{T}$. Since the rule and initial configuration are both invariant under $\mathcal{T}$, the resulting space-time pattern must also be; hence, the scale-invariance of the final figure. Similarly, any rule that simulates one of these rules using another block transform $\mathcal{T}'$ will also produce scale-invariant patterns when their initial states consist solely of the blocks in $\mathcal{T}'$.

3.1.3 General Properties of Elementary CA

Figures 3.10-3.15 present some qualitative evidence for the *self-organization* of space-time patterns emerging out of initial configurations of uncorrelated sites. In this section we introduce some of the quantitative characterizations of self-organization in elementary $r = 1$, $k = 2$ rules by examining these systems from two different points of view:

1. the local statistical properties of individual configurations, and
2. the global statistical properties of the ensemble of all possible configurations.

More general methodology applicable to a wider variety of complex rules is introduced in chapters 4 and 5.

3.1.3.1 Local Properties

As alluded to earlier, a given configuration may be considered *disordered* (or essentially random) if the values of different sites are statistically uncorrelated. Deviations of statistical measures from those obtained for disordered configurations signify the appearance of *order* and therefore mark the appearance of correlations between values of separated sites. While a completely disordered configuration is completely specified by a single parameter ' p ', representing the probability that a given site has value '1', the specification of ordered configurations requires additional parameters.

Density: The simplest statistical measure that can be used to characterize a configuration is the *density* $\rho_1(t)$, defined to be the *average fraction of sites with value $\sigma = 1$ at time t* . For a disordered configuration, for example, $\rho_1 = p$.

Consider, first, the density $\rho_1(t = 1)$, obtained from an initially disordered configuration by evolution for one time step. For a disordered configuration, $p = \rho_1 = 1/2$, so that all eight possible 3-tuple local neighborhoods occur with equal probability. The fraction of sites with value ' $\sigma = 1$ ' after one iteration of rule ' ϕ ' is given by the fraction of the eight possible neighborhoods that yield the value '1' according to the ' ϕ ':

$$\rho_1(1) = \frac{\#_1(\phi)}{\#_1(\phi) + \#_0(\phi)} = \frac{\#_1(\phi)}{8}, \quad (3.15)$$

where $\#_1(\phi)$ is the number of occurrences of the digit '1' in the binary representation of the rule ' ϕ '. The binary representation of **R122**, for example, is given by '01111010' so that $\#_1(\mathbf{R122}) = 5$ and, consequently, the density $\rho_1(1) = 5/8$ for an infinitely large configuration.

The generalization of this simple formula to the case when $p \neq 1/2$ is straightforward. In this case, each of the eight possible 3-tuple neighborhoods $\vec{\sigma} = \sigma_1\sigma_2\sigma_3$

must first be weighted by a factor

$$p(\vec{\sigma}) = p^{\#_1(\vec{\sigma})} (1-p)^{\#_0(\vec{\sigma})}, \quad (3.16)$$

where $\#_1(\vec{\sigma})$ is the number of occurrences of the digit '1' in the 3-tuple $\vec{\sigma}$. The density after one time step is then given by adding the probabilities for all $\vec{\sigma}$ which yield value '1' under ' ϕ ':

$$\rho_1(1) = \sum_{\{\vec{\sigma} \mid \phi(\vec{\sigma})=1\}} p(\vec{\sigma}). \quad (3.17)$$

Obtaining $\rho_1(t)$ for $t > 1$ is more difficult because of the correlations that are inevitably generated in the course of a typical evolution. In particular, since the independence assumption underlying the above derivation of $\rho_1(1)$ is generally invalid, derivations must usually be tailored to particular rules. An exception is the class of *additive rules*, which we recall obey the property of the *additive superposition*: configurations obtained by evolution from arbitrary initial states are given by adding (*modulo 2*) the evolutions of initial configurations having a single nonzero cell. Consider, for example, the additive rule **R90**.

An examination of figures 3.1 and 3.2 reveals that the number of sites with value '1' at time ' t ' obtained by an evolution of an initial state containing a single nonzero site according to rule **R90** is given by

$$N_1(t) = 2^{\#_1(t)}, \quad (3.18)$$

where $\#_1(t)$ is the number of occurrences of '1' in the binary representation of ' t '. The value of a site at time ' t ' is the sum *modulo 2* of the initial values of $N_1(t)$ sites, each of which has a probability $\rho_1(0)$ of having the value $\sigma = 1$. Since a site can have value $\sigma = 1$ only if the predecessor 3-tuple neighborhood had an *odd* number of sites with value '1', we merely have to calculate the probability, p_{odd} , that the sum of values of the sites is *odd*. If each of a set of ' k ' sites has value '1' with probability ' p ', then p_{odd} is given by

$$p_{\text{odd}} = \sum_{\{i \text{ odd}\}} \binom{k}{i} p^i (1-p)^{k-i} = \frac{1}{2} [1 - (1-2p)^k], \quad (3.19)$$

so that $\rho_1(t)$, obtained from an initially disordered state with density $\rho_1(0)$ according to **R90** is

$$\rho_1(t) = \frac{1}{2} [1 - (1-2\rho_1(0))^{2^{\#_1(t)}}]. \quad (3.20)$$

Note that for large ' t ', $\#_1(t) = \mathcal{O}(\log_2 t)$ except at a set of measure zero, so that $\rho_1(t) \rightarrow 1/2$ at $t \rightarrow \infty$ for almost all ' t '.

Asymptotic results obtained for additive rules can often be almost immediately extended to certain non-additive rules, by exploiting 'blocking-transformation' relationships. We recall from the discussion in the last section, for example, that the complex rule **R18** *simulates* **R90** under a transformation which associates with

each site an additional zero valued cell. This transformation thus effectively ‘dilutes’ the patterns evolving according to **R90**; specifically, if no kinks were present, $\rho_{1,\mathbf{R18}}(t)$ would equal $\frac{1}{2} \cdot \rho_{1,\mathbf{R90}}(t)$. Assuming that the system has evolved long enough according to **R18** to allow most of the *kinks* to annihilate, we may conclude that the asymptotic density $\rho_{1,\mathbf{R18}}(t \rightarrow \infty) = 1/4$.

For general rules, a first-order statistical approximation for limiting densities $\rho_1(t \rightarrow \infty)$ can be obtained by a method akin to the *mean-field* theory in statistical mechanics (more sophisticated approaches will be introduced in chapter 4).

Mean Field Approximation: as a first order approximation, we will ignore all correlations between values at different sites and parameterize configurations purely in terms of the average density at time ‘ t ’, ρ . The time evolution of ρ under an arbitrary rule ‘ ϕ ’ is then given by the master equation

$$\frac{\delta \rho}{\delta t} = f_{0 \rightarrow 1} - f_{1 \rightarrow 0}, \quad (3.21)$$

where $f_{i \rightarrow j}$ is the average fraction of sites whose value changed from $\sigma = i$ to $\sigma = j$. An explicit form for these fractions is obtained by observing that the probability ‘ P ’ of having the 3-tuple $\vec{\sigma} = \langle \sigma_1 \sigma_2 \sigma_3 \rangle$ appear in a neighborhood is

$$P(\sigma_1, \sigma_2, \sigma_3) = p^{\#_1(\vec{\sigma})} (1 - p)^{3 - \#_1(\vec{\sigma})}, \quad (3.22)$$

where, as before, $\#_1(\vec{\sigma})$ is the number of times ‘1’ appears in the string $\vec{\sigma}$. Thus,

$$\begin{cases} f_{0 \rightarrow 1} &= \sum_{\{\vec{\sigma} \mid \sigma_2=0\}} \phi(\sigma_1, \sigma_2, \sigma_3) P(\sigma_1, \sigma_2, \sigma_3), \\ f_{1 \rightarrow 0} &= \sum_{\{\vec{\sigma} \mid \sigma_2=1\}} [1 - \phi(\sigma_1, \sigma_2, \sigma_3)] P(\sigma_1, \sigma_2, \sigma_3). \end{cases} \quad (3.23)$$

The equilibrium, or *steady-state*, density $\rho_1(t \rightarrow \infty)$ is achieved when

$$\frac{\delta \rho}{\delta t} = 0. \quad (3.24)$$

For rule **R90**, for example, we find that

$$\begin{cases} f_{0 \rightarrow 1} &= P(0, 0, 1) + P(1, 0, 0) = 2(1 - p)^2 p, \\ f_{1 \rightarrow 0} &= P(0, 1, 0) + P(1, 1, 1) = (1 - p)^2 p + p^3. \end{cases} \quad (3.25)$$

Thus, $\delta \rho / \delta t = 0 \implies p(1 - 2p) = 0$, which has solutions $p = 0$ (or the *null* state) and $p = 1/2$. Similarly, for **R18**, we find that $p(1 - 4p + 2p^2) = 0$, with solutions $p = 0$ and $p \approx 0.293$. Both nonzero results appear to be consistent with our earlier observations.

Although differences between mean-field estimates and exact limiting densities are to be expected because of the presence of correlations in actual evolutions, the mean-field approach nonetheless typically comes to within about 10 – 20% of the exact values for all elementary complex rules.

Two point correlations: We have already mentioned several times that evolutions generally induce correlations between cell values at different sites; indeed, the presence of correlations is a telltale signature of self-organization. The average density discussed above, however, is too crude a measure to capture these finer details.

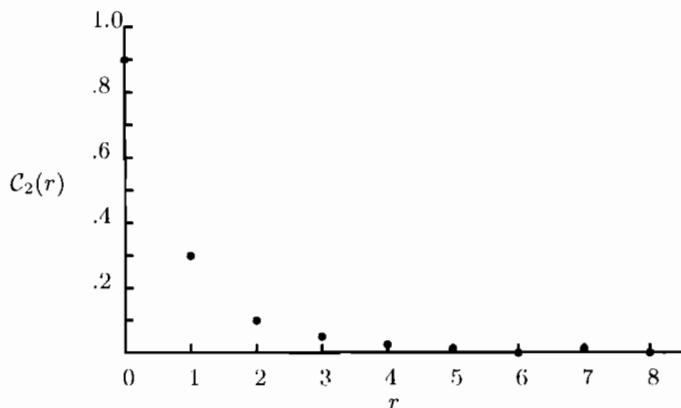


Fig. 3.18 Two point correlation function for large time ‘ t ’ for elementary $k = 2$, $r = 1$ rule **R22**.

In its place we can use the simplest correlation measure, the two point *correlation function*,

$$C_2(r) = \langle \zeta_i \zeta_{i+r} \rangle - \langle \zeta_i \rangle \langle \zeta_{i+1} \rangle, \quad (3.26)$$

where the average is taken over all possible sites ‘ i ’ at a fixed time ‘ t ’, and

$$\zeta_i = \begin{cases} +1 & \longleftrightarrow \sigma_i = 1, \\ -1 & \longleftrightarrow \sigma_i = 0. \end{cases} \quad (3.27)$$

A completely disordered configuration gives $C_2(r) = 0$ for $r \geq 1$, with $C(0) = \langle \zeta_i^2 \rangle - \langle \zeta_i \rangle^2 = \langle (2\sigma_i - 1)^2 \rangle - \langle 2\sigma_i - 1 \rangle^2 = 4p(1 - p)$. The periodicities frequently evident in complex patterns evolving from initial states with a single nonzero site, give rise to peaks in $C_2(r)$. For the class of additive rules, $C_2(r)$ at time ‘ t ’ is obtained by convolution of this result with the correlation function for an arbitrary disordered initial state, and thus remains equal to zero for all time. For nonadditive rules, however, there exists the possibility that short-range correlations may be built up from completely disordered initial configurations. The existence of a nonzero correlation length is our first quantitative evidence of the appearance of self-organization. Figure 3.18 shows the form of $C_2(r)$ for rule 22. We see that the correlation appears to fall off exponentially with a correlation length $\ell_c \approx 2$.

Although $\rho(t)$ and $C_2(r)$ do give some insight into the behavior of complex rules, even a casual glance at the earlier space-time patterns reveals a rich diversity of structure that these measures are incapable of capturing.

The most obvious feature is the frequent presence of triangular clearings of various sizes. These occur when a long string of cells all attain the value $\sigma = 1$ so that, if the rule is legal, all sites away from either end of the string revert to $\sigma = 0$ on the next time step. Thereafter, in successive time steps, the newly formed ‘clearing’ is progressively reduced in length as sites with $\sigma = 1$ steadily migrate in from the sides. What is not readily perceivable, however, is again a kind of universality in the numbers of such clearings.

Defining $\mathcal{T}(n)$ to be the *density of triangular clearings with base length ‘n’*, it has been found that, for large ‘n’ and for patterns generated from disordered initial states, $\mathcal{T}(n)$ behaves as

$$\mathcal{T}(n) \sim \begin{cases} 2^{-n} & \longleftrightarrow \text{additive rules,} \\ (\frac{4}{3})^{-n} & \longleftrightarrow \text{nonadditive rules.} \end{cases} \quad (3.28)$$

The spectrum of triangular clearings is therefore independent both of the particular initial configuration and evolutionary rule.

There are a number of additional local structures and properties that appear even in elementary CA systems. Grassberger [grass84b], for example, has observed that rule **R22** actually harbors very complex long-range effects, similar to a critical phenomenon (see section 3.1.4). Since the majority of these findings require the use of more general and sophisticated correlation measures than we have defined thus far, we will pick up our discussion of them in chapter 4.

3.1.3.2 Global Properties

The preceding section dealt with the statistical properties of the set of cell values in individual configurations. An alternative, and in some sense complementary, approach is to examine the statistical properties of the set of all possible configurations. Such a global view sets the stage for drawing comparisons between the evolution of CA and that of general dynamical systems.

Finite Lattices: Consider a finite CA having $N < \infty$ sites. The total number of possible configurations for this system is 2^N , with each configuration being uniquely specified by a binary string of length N whose digits give the values of each of the sites. For simplicity, we can assume periodic boundary conditions.

Since finite lattices harbor a finite number of possible states, we know that any sequence of configurations starting from an arbitrary initial state *must* become periodic after at most 2^N iterations.

Figure 3.19, for example, shows a few of the cycles that emerge on a size $N = 10$ lattice for a system evolving according to the class **c3** rule **R122**. In practice, and as suggested by this figure, many fewer iterations than the maximum $t_{\max} = 2^N$ are needed before a cyclic state is reached.

If, as is usually the case, the rule is *locally irreversible* – i.e., the rule is such that

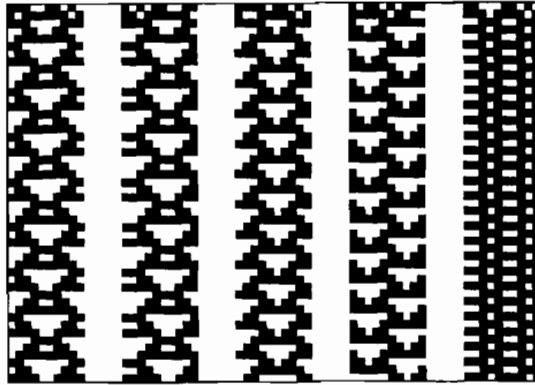


Fig. 3.19 Evolution of typical initial configurations on a size $N=10$ lattice with periodic boundary conditions according to rule 122.

a given local configuration may have more than one local predecessor state – there clearly must exist configurations which can only occur as initial states. On the other hand, local irreversibility does not preclude the overall system from being *globally reversible*. A system is said to be globally reversible if each global configuration has exactly one predecessor and exactly one successor state. Although not immediately obvious, a little thought will demonstrate that this is indeed possible even if the local rule is itself irreversible.

We have just identified three basic kinds of configurations that can conceivably occur in an evolution:

Garden-of-Eden States: which can never be dynamically generated in the course of the evolution and can therefore occur only as initial states. For the trivial *null* rule, for example, in which all local states get mapped to zero, all nonzero states are dynamically unreachable. Under the identity rule, **R204**, on the other hand, all configurations are reachable, making **R204** a trivially *reversible* rule. While a complete characterization of unreachable states for additive rules will be given in chapter 5, we mention here that the fraction of unreachable configurations for irreversible rules *tends to zero* at a rate λ^N , where $\lambda \approx 0.88$ for nonadditive rules.

Cyclic States: which are configurations that appear in cycles and are repeatedly visited over the course of the evolution; they are the *attractor* states of the system in the sense that they comprise the set toward which all evolutions ultimately lead. If *all* states are cyclic then the system is globally reversible.

Transient States: which can arise only in the first $t_T < 2^N$ time steps of an evolution. Since transient states do not lie on cycles, once a transient state is reached from a given initial state, it cannot be revisited later.

Figures 3.20, 3.21 and 3.22 show how the number of cyclic states (N_C), the average cycle length (C_{rmave}) and total fraction of states on cycles (f_C) changes as

a function of lattice size ‘ N ’ for a few representative elementary rules (**R32** is in the class **c1**; **R108** is in **c2**; **R122** and **R150** are both in **c3**).

Kaneko [kaneko86a] has, in fact, pointed out that, despite being strictly defined only for infinitely large systems, the four generic behavioral classes appear to be well characterized by the number and length of their attractors on finite lattices:[†]

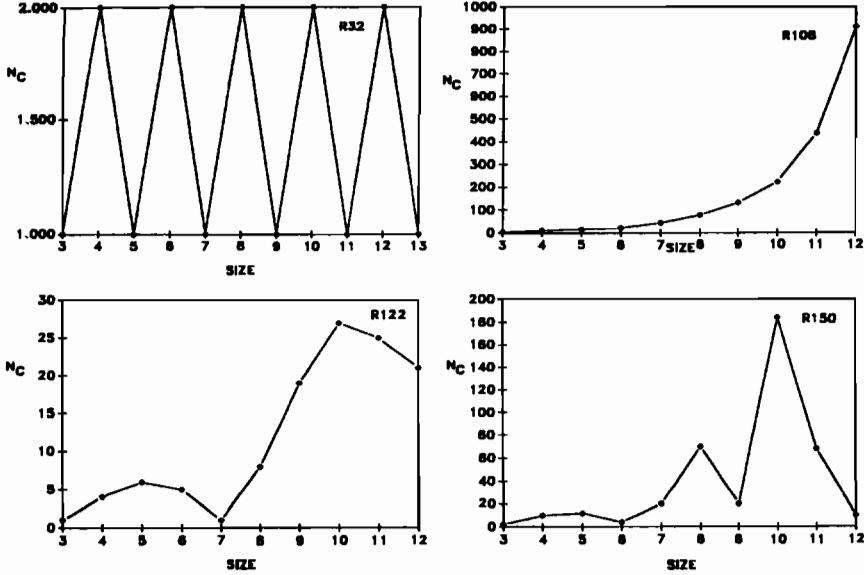


Fig. 3.20 Number of cyclic states as a function of lattice size for a few representative one-dimensional elementary rules; see text.

Class c1: *Small number of attractors with short periods.* The number of attractors typically remains very small ($\approx 1 - 3$), even for large N .

Class c2: *Large number of attractors with short periods.* The number of attractors $N_c \propto \exp(\alpha N)$, $\alpha \approx 0.2 - 0.4$.

Class c3: *Small number of attractors with long periods.* The number of attractors changes irregularly as N increases, and, at least for some rules, appears to depend on some number-theoretic properties of the size and rule. A singular behavior, for example, frequently occurs near $N = 2^k - i$, where $i = 0, 1$ or -1 , depending on the rule.

Class c4: *Large number of attractors with possibly long periods.* Kaneko has found that this class is characterized by an exponentially increasing number of attractors, although the increase is irregular.

[†]A *large number* here means some quantity which is exponential in lattice size ($\mathcal{O}(e^N)$), while a *small number* is anything less than the power of lattice size ($\mathcal{O}(N^a)$); the *period* is large if it is $\mathcal{O}(N)$ and is small if it is bounded by $\mathcal{O}(1)$.

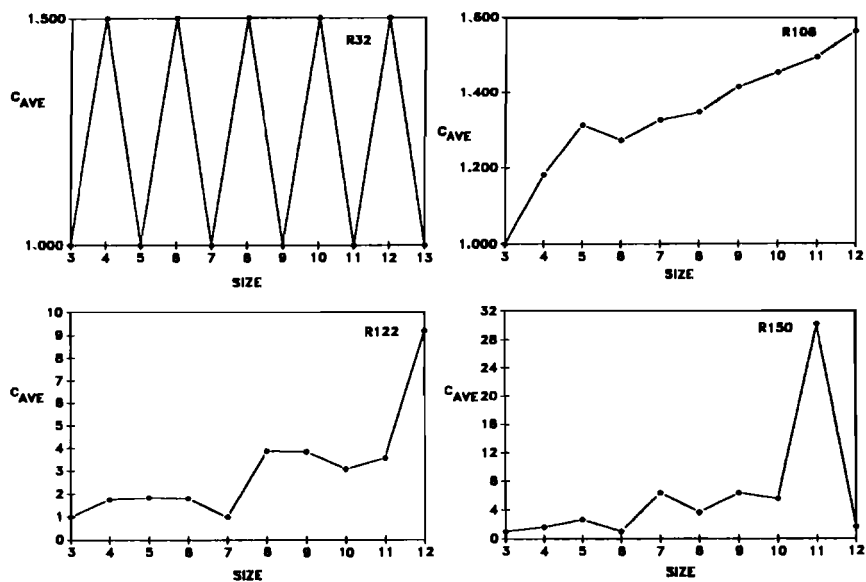


Fig. 3.21 Cycle length as a function of lattice size for a few representative one-dimensional elementary rules; see text.

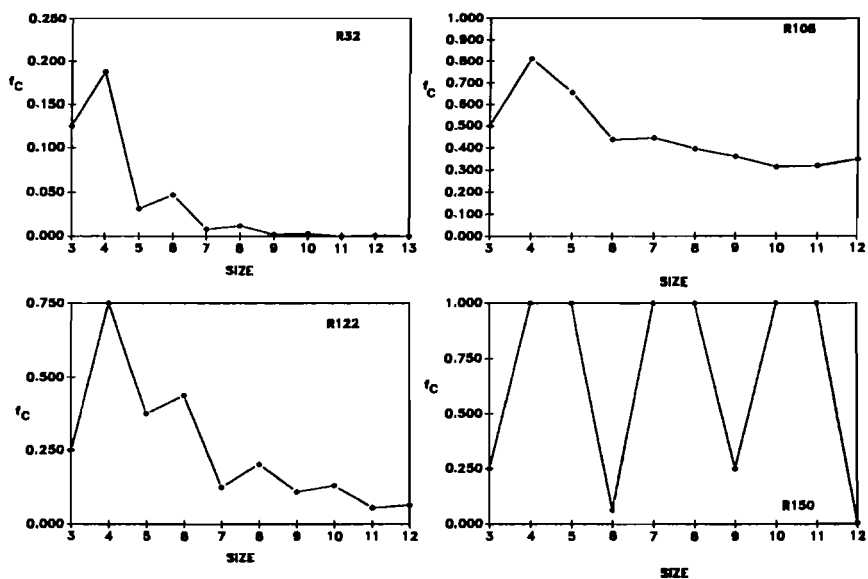


Fig. 3.22 Fraction of states on cycles as a function of lattice size for a few representative one-dimensional elementary rules; see text.

Stability: As was mentioned earlier, an important qualitative characterization of the four behavioral classes is provided by their sensitivity to small changes made to the initial states. A convenient measure for quantifying the difference between evolutions starting from two different binary valued initial states, $\vec{\sigma}^{(1)}$, and $\vec{\sigma}^{(2)}$, is provided by the *Hamming distance*, $H_{\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}}(t)$:

$$H_{\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}}(t) = \sum_{i=1}^N \sigma_i^{(1)}(t) \oplus_2 \sigma_i^{(2)}(t), \quad (3.29)$$

where ' $\oplus_2$ ' is addition *modulo two*.

$H(t)$ thus measures the number of sites at which the two evolutions differ at time ' t '. Since information propagates at a finite speed of r sites per step for a radius- r rule, $H(t)$ is bounded by $H(t) \leq (2rt + 1)$.

Consider two random initial configurations that differ at only one site, so that $H(t = 0) = 1$. The *difference plots* shown in figure 3.16 suggest that for class **c1** and **c2** rules, $H(t)$ rapidly approaches some small fixed value. Class **c3** rules, on the other hand, are *unstable* with respect to such small 'perturbations'; $H(t)$ generally grows with time. The rate of growth of $H(t)$ depends on whether the rules are *additive* or *nonadditive*.

For additive rules, which we recall from chapter two are those obeying an additive superposition principle, the difference at time t is equal to the t^{th} step in the evolution of the initial difference. $H(t)$ thus counts the number of 1's appearing in the t^{th} row of the characteristic fractal patterns generated from single seeds (see figure 3.1). For Rule **R90**, for example, it is easy to show that $H(t)$ is given explicitly by $H(t) = 2^{\#_1(t)}$, where $\#_1(t)$ is the number of times the digit '1' appears in the binary representation of the integer ' t '. The average Hamming distance, smoothed out over many iterations, is given approximately by $H(t) = t^{\log_2 3 - 1} \approx t^{0.59}$ [wolf83a] (see figure 3.23).

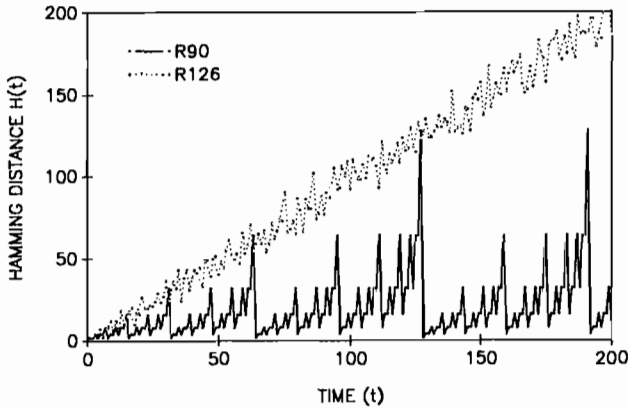


Fig. 3.23 *Hamming distance* as a function of time for elementary rule **R90**; see text.

For nonadditive rules, $H(t)$ can no longer be obtained by merely looking at the evolution of the initial difference state. A fairly typical nonadditive behavior is that of rule **R126**. We see that, apart from small fluctuations, $H(t)$ tends to steadily increase in a roughly linear fashion. This means that as time increases, the values of particular sites will depend on an ever increasing set of initial sites; *i.e.*, space-time patterns are *sensitively dependent on the initial conditions*. We will pick up this theme in our discussion of *chaos* in continuous systems in chapter 4.

Statistical Ensembles: A statistical ensemble of states can be constructed by assigning the probability for each of the 2^N possible configurations. By an *equiprobable ensemble*, we will mean a (maximally disordered) collection of states such that each configuration appears with equal probability. A self-organizing evolution under a particular rule ϕ modifies the *a-priori* equal probabilities for states of the ensemble to occur.

Figures 3.24 and 3.25, for example, show the probabilities for the 2^{10} possible configurations on an $N = 10$ lattice obtained at time $t = 10$ for evolutions by rules **R126** and **R30** (both in class **c3**), respectively. The figures show that the evolution modifies the probabilities of states from initially being equally likely to distributions in which individual configurations can have widely differing final probabilities. The properties of the more probable states will then tend to dominate the statistical averages over the ensemble.

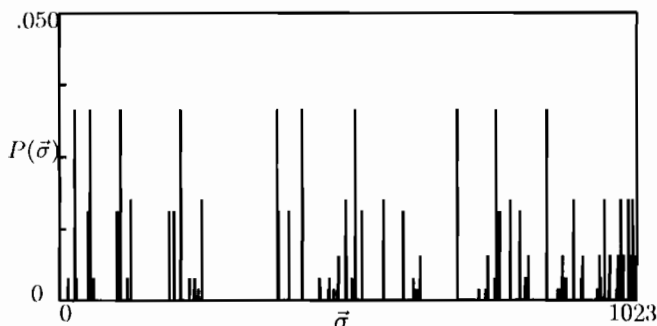


Fig. 3.24 Global configuration probabilities at $t=10$ computed for rule **R126**. The probability for the zero state, $P(\vec{\sigma} = \vec{0}) = .121$, is not shown.

Entropy: Much of the more technical discussion of the dynamical systems approach to CA in chapter 4 will depend on the notions of *information* and *entropy*. We here provide the groundwork for our later analysis by introducing the following two elementary measures:

$$\left\{ \begin{array}{ll} \text{Global Set Entropy:} & S_{\text{set}}(t) = \frac{1}{N} \log_2 \left(\sum_{j=1}^{2^N} \zeta(p_j^t) \right), \\ \text{Global Measure Entropy:} & S_{\text{meas}}(t) = -\frac{1}{N} \sum_{i=1}^{2^N} p_i^t \log_2 p_i^t, \end{array} \right. \quad (3.30)$$

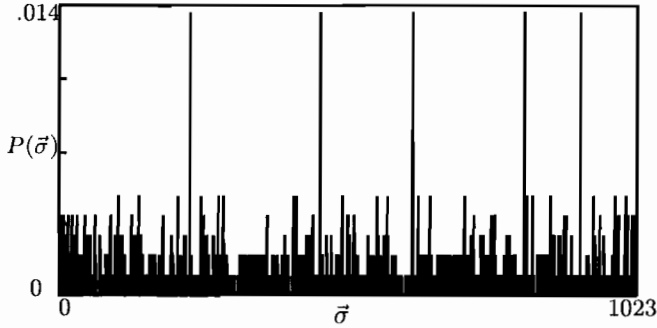


Fig. 3.25 Global configuration probabilities at $t=10$ computed for rule **R30**.

where p_i^t is the probability of the i^{th} state at iteration step ' t ' and $\zeta(p_j) = 1$ for $p_j > 0$ and $\zeta(0) = 0$.

Both measures obviously are related to certain global properties of the state transition graph. $S_{\text{set}}(t)$, for example, is determined by the fraction of possible configurations that can be reached at time ' t ' during the evolution. At large times, $S_{\text{set}}(t \rightarrow \infty)$ is therefore given by the fraction of states that are cyclic. $S_{\text{meas}}(t)$, on the other hand, is a *finer* entropic measure in that it makes use of the individual probabilities of states. Indeed, $S_{\text{meas}}(t)$ can be interpreted as being the *average number of binary bits that are necessary to completely specify a state in a statistical ensemble of all possible states*.

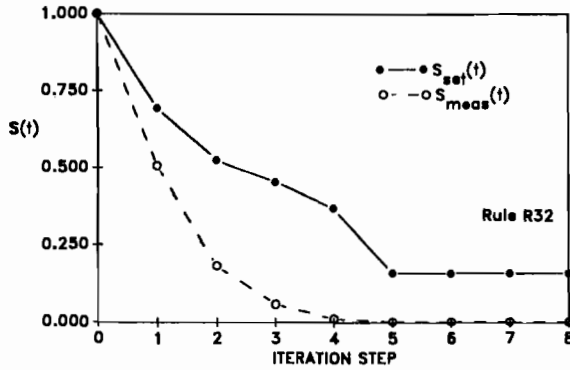


Fig. 3.26 Time evolution of the average entropy for elementary rule **R32**; see text.

The two measures satisfy the relation

$$0 \leq S_{\text{meas}}(t) \leq S_{\text{set}}(t) \leq 1. \quad (3.31)$$

Since entropy is maximum when the system is maximally disordered, $S_{\text{meas}}(t)$ takes its maximal value of *one binary bit per site* for an equiprobable ensemble: $S_{\text{set}}(t \rightarrow \infty) = 1$ only if all states are cyclic. If the system settles onto a unique cyclic

state (which must be the *null* state if the rule is legal), then $S_{\text{meas}}(t \rightarrow \infty) = 0$. $S_{\text{meas}}(t) = S_{\text{set}}(t)$ if and only if all nonzero state probabilities p_j^t are equal.

For reversible systems, evolution almost always leads to an increase in entropy. The evolution of irreversible systems, on the other hand, typically results in a decrease in entropy. Figures 3.26 and 3.27 show the time evolution of the average entropy for elementary rules **R32** (class **c1**) and **R122** (class **c3**) for an ensemble of size $N = 10$ CA starting with an equiprobable ensemble. We see that the entropy decreases with time in both cases, reaching a steady-state value after a transient period. This decrease is a direct reflection of the irreversibility of the given rules.

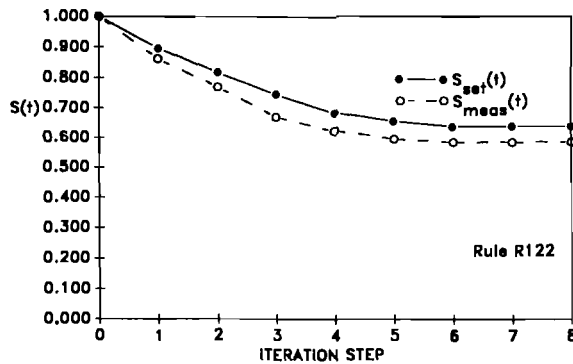


Fig. 3.27 Time evolution of the average entropy for elementary rule **R122**; see text.

Infinite Lattices: Although cyclic behavior is certain to occur under even class **c3** rules for finite systems, it is a rare occurrence for truly infinite systems: *cycles occur only with exceptional initial conditions*. For a finite sized initial seed, for example, the pattern either quickly dies or grows progressively larger with time. Most infinite seeds lead only to complex acyclic patterns. Under the special condition that the initial state is periodic with period ' m ', however, the evolution of the infinite system will be the same as that of the finite CA of size $N = m$; in this case, cycles of length $<< 2^N$ can occur.

Similarly, if the initial state consists of nothing but infinite repetitions of some invariant block of values, the space-time pattern will again be periodic. Figure 3.28, for example, shows sections of two infinite periodic patterns for elementary class rule **R30**, starting from the states ' $\dots 0101\dots$ ' and ' $\dots 00100110010011\dots$ '.

3.1.4 A Small Sampling of Rules

Perhaps the most conceptually far-reaching lesson to be learned from nonlinear dynamical system theory in general, and the dynamics of CA in particular, is that *complex behavior need not have a complex dynamical origin*. Indeed, one of the principle motivations for studying such deceptively 'simple' systems, is to use their underlying simplicity to gain insight into more general nonlinear phenomena. We have already seen considerable phenomenological evidence that – despite arguably

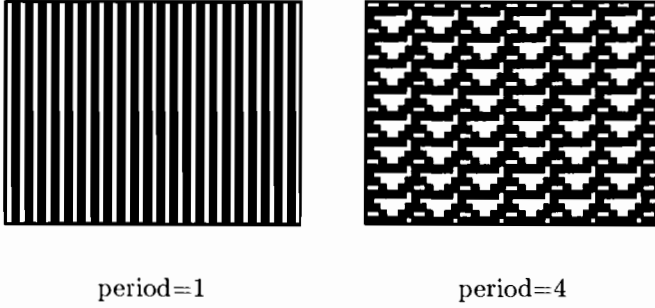


Fig. 3.28 Two periodic patterns for $k = 2$, $r = 1$ rule **R30**.

being among the simplest possible (nontrivial) dynamical systems that can be defined -- even one-dimensional CA display a spectacular variety of complex behavior.

We conclude our brief tour of one-dimensional CA by mentioning a few special properties of some selected one-dimensional rules. We will have occasion to refer back, more than once, to some of the behaviors discussed here, after the appropriate set of formal tools has been presented in later chapters.

3.1.4.1 The $k=2$, $r=1$ rule **R22**: Just How Complex Is It?

While none of the 256 possible radius $r = 1$ binary valued CA are believed to be capable of universal computation[†], the rule whose long time behavior has proven to be the most difficult to understand fully is rule **R22**:

$$\sigma_i(t+1) = \Phi[(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t))] = \begin{cases} 1 & \text{if } \sigma_{i-1}(t) + \sigma_i(t) + \sigma_{i+1}(t) = 1, \\ 0 & \text{else.} \end{cases} \quad (3.32)$$

A typical evolution of a disordered initial state under Φ is shown in figure 3.29. Apart from the irregularity in the distribution of the clear triangular regions that we have come, by now, to expect of the patterns of most class **c3** rules, **R22** appears at first sight to harbor no deeper ‘complexity’. Studies by Grassberger ([grass83], [grass84b]) and Zabolinsky [zabo88], however, have strongly suggested that very subtle long-range correlations lay hidden in this pattern. Their findings include:

1. The two-point spatial correlation function $C_2(r)$ (equation 3.26) does not decay exponentially with distance r , but appears instead to decay more slowly as $\exp(-\alpha\sqrt{r})$.

2. The decay of the *spatial block entropy*, h_N -- which gives the amount of information contained in a block of N contiguous site values $\sigma_1, \dots, \sigma_N$ needed to predict the value σ_{N+1} -- is considerably slower than $(\text{block-length})^{-1}$, and is therefore indicative of very long and complex correlations; we will come back to this point later in chapter 4, following our discussion of dynamical system theory.

[†]Rule **R110**, discussed below, may be an outside contender, however.

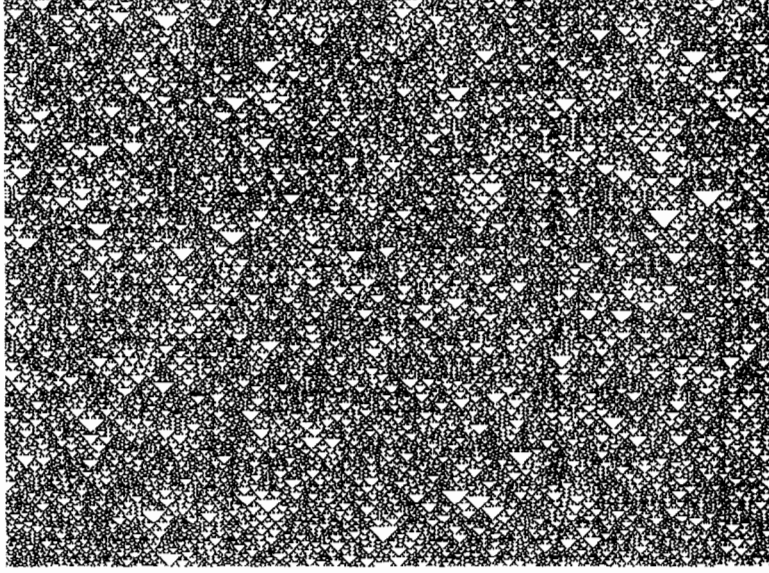


Fig. 3.29 Space-time pattern of one-dimensional elementary rule **R22**.

3. If the initial density of 1's, $\rho = \rho_1(t = 0)$, is thought of as being equivalent to the 'temperature' in a real magnetic system, $\rho = 0$ exhibits all of the properties of a critical parameter. For example, the decay of the deviation of the 'magnetization' $m(t) \equiv \frac{1}{N} \sum_i \sigma_i(t)$, from the final steady-state equilibrium value, $m(\infty) = 0.35096$ [grass84b], follows

$$|m(t) - m(\infty)| \propto e^{-\beta(\rho)t}, \quad \text{where } \beta(\rho) = 0.44\rho. \quad (3.33)$$

The fact that the decay becomes arbitrarily slow as $\rho \rightarrow 0$ indicates the presence of a critical point, $\rho = 0$. (Another example of critical-like behavior in a probabilistic system is given later in this subsection). A more detailed discussion of various critical-like properties of CA appears in chapter 7.

4. Define $\langle N_m \rangle$ to be the average number of *zero*-blocks of size m . Due to correlation effects, **R22** induces a greater number of large *zero*-blocks in the equilibrium state than typically appear in totally uncorrelated configurations having the same magnetization: $\langle M_m \rangle_{\text{R22}} \propto 0.75(3)^m$ compared to $\langle N_m \rangle_{\text{uncorr}} \propto 0.64904^m$, where both are Monte Carlo results obtained from 1340 independent samples of systems with 30,000 sites starting from an initial density of $\rho = 0.5$, and there is some uncertainty in the last digit of the coefficient calculated for **R22**. Zabolinsky [zabo88] has conjectured that due to some as-yet undiscovered 'hidden' property of rule **R22** it might be possible to prove exactly that $\langle N_m \rangle_{\text{R22}} \propto \left(\frac{3}{4}\right)^m$.

3.1.4.2 The $k=2, r=1$ rule R30: Just How Random Is It?

That neither complex nor random-like, behavior, need have a complex dynamical origin is well exemplified by the elementary one-dimensional class **c3** rule **R30**, studied extensively by Wolfram in [wolf84c]. It is defined explicitly by

$$\Phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)) = (\sigma_{i-1}(t) + \sigma_i(t) + \sigma_{i+1}(t) + \sigma_i(t)\sigma_{i+1}(t)) \bmod 2. \quad (3.34)$$

Consider, for example, the space-time pattern resulting from application of Φ to a single nonzero site value, shown in figure 3.30. We make the following observations:

1. The pattern consists of a curious mixture of regular behavior along the left-hand side and irregular behavior along the right-hand side, separated by a boundary moving towards the left at a 'speed' of approximately $\frac{1}{4}$ sites/sec.

2. The periodicity of the diagonal sequences on the left-hand side can be understood heuristically as follows. Any value situated at a distance d from the left-hand side boundary depends only on those values at distances $d' \leq d$; because of the single nonzero site value seeding, all other values on which it could depend are identically equal to zero. The diagonal sequences along the left-hand side (LHS) therefore follow an *effective* rule, Φ_{LHS} , which is a shifted version of equation 3.34:

$$\Phi_{\text{LHS}} = (\sigma_{i-2}(t) + \sigma_{i-1}(t) + \sigma_i(t) + \sigma_{i-1}(t)\sigma_i(t)) \bmod 2, \quad (3.35)$$

with boundary conditions setting two sites at one end to equal zero. Since all sites positioned within a distance d from the left-hand side edge therefore effectively evolve in time as though they were on a finite lattice of size ' d ', we expect the corresponding left-hand side diagonal time sequence to be periodic with period $\tau_d \leq 2^d$. In fact, it is observed that the actual periods of diagonal sequences along the left-hand side are of the form 2^j , with j increasing very slowly with d . The first few periods for small d are given by [wolf84c] $\tau_0 = \tau_1 = \tau_2 = 1, \tau_3 = 2, \tau_4 = 1, \tau_5 = \tau_6 = 2, \tau_7 = 1, \tau_8 = 4, \dots$

3. The effective rule for the right-hand side (RHS) diagonal pattern is similarly a *right-shifted* version of equation 3.34:

$$\Phi_{\text{RHS}} = (\sigma_i(t) + \sigma_{i+1}(t) + \sigma_{i+2}(t) + \sigma_{i+1}(t)\sigma_{i+2}(t)) \bmod 2, \quad (3.36)$$

with boundary conditions

$$\begin{cases} \sigma_{d-1}(t+1) &= \sigma_{d-1}(t) \oplus_2 \sigma_d(t), \\ \sigma_d(t+1) &= \sigma_d(t). \end{cases} \quad (3.37)$$

The periods of the right-hand side diagonal sequences are also found to be of the form $\tau_d = 2^j$, $j \leq d$, with

$$\tau_d \cong 2^{(d+1)/2}. \quad (3.38)$$

The first few values are given by [wolf84c] $\tau_0 = 1, \tau_1 = \tau_2 = 2, \tau_3 = 4, \tau_4 = \tau_5 = 8, \tau_6 = 16, \dots$

4. While all diagonal sequences must become periodic, those appearing closer to the vertical need not. For example, no periodicity has been detected in the vertical temporal sequence of the center values

$$\{\sigma_{\text{center}}(t = i)\}_{i=0}^n = \{1011100110001011001001110101110011101010110 \cdots\}, \quad (3.39)$$

for lengths $n \leq 2^{19}$ [wolf84c]. Moreover, this sequence of values has passed a barrage of statistical tests of randomness [wolf84c], strongly suggesting that it is in fact completely random. Systems having this intrinsic ability to generate randomness given regular, or non-random, input are called *autoplectic* systems [wolf84b].

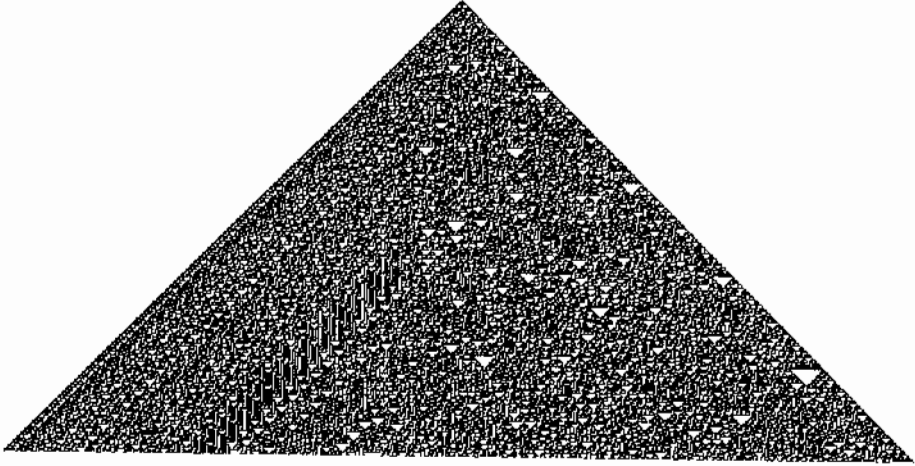


Fig. 3.30 Space-time pattern of one-dimensional elementary rule **R30**.

3.1.4.3 Critical-Like Behavior

A simple probabilistic radius $r = 1$ one-dimensional binary valued CA model exhibiting a behavior akin to a thermal phase-transition (but where ‘probability’ is substituted for ‘temperature’), was first studied by Grassberger, Krause and von der Twer [grass86b]. Instead of assigning a definite value, σ'_i , to each possible neighborhood configuration, $(\sigma_{i-1}, \sigma_i, \sigma_{i+1})$, the particular rule is defined by assigning a *probability*, $p(\sigma'_i = 1)$, that σ' equals ‘1’:

$$\begin{array}{cccccccc} \sigma_{i-1}\sigma_i\sigma_{i+1} : & 111 & 110 & 101 & 100 & 011 & 010 & 001 & 000 \\ \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ p(\sigma'_i = 1) : & 0 & p & 1 & 1 & p & 0 & 1 & 0 \end{array} \quad (3.40)$$

where $0 \leq p \leq 1$. Note that this rule is strictly deterministic whenever $p = 0$ (in which case it is equal to the elementary class **c2** rule **R50**) or $p = 1$ (in which case

it is equal to the class **c3** rule **R122**). The obvious question is how does rule **R50** turn into rule **R122** as the probability p is increased?

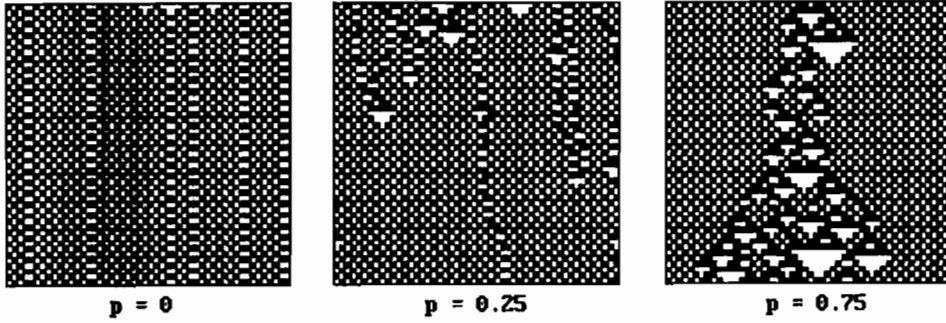


Fig. 3.31 Space-time patterns of probabilistic radius $r = 1$, $k = 2$ CA defined in equation 3.41 for $p = 0, 1/4$, and $3/4$; see text.

Figure 3.31 shows sample evolutions for $p = 0, 1/4$ and $3/4$. The space-time pattern for $p = 0$ rapidly settles into an ‘ordered state’ consisting of checkerboard-pattern domains, separated by two-site kinks; once formed, the kinks remain locked in place. As p is slowly increased, these kinks begin to undergo annihilating random walks, much like the ones we saw earlier in the evolution of (the deterministic) rule **R18**. Their density decreases like $\rho_{\text{kink}} \sim (pt)^{-1/2}$. Grassberger, *et.al.*, observed that, for $p > 0$, there is also a kink generating mechanism, *i.e.*,

$$\text{kink} \longrightarrow \text{kink} + (\text{kink} + \text{anti-kink}), \quad (3.41)$$

but that, for small enough p , it is overwhelmed by the number of annihilations. There exists a *critical* value, $p_c \sim 0.55$, however, such that for $p > p_c$, a single kink in an otherwise ordered initial state leads to a completely disordered state (see $p = 3/4 > p_c$ plot in figure 3.31). A similar critical-like transition exists between rules **R94** and rule **R22** [grass86b].

3.1.4.4 Particle-Like Behavior

Many rules give rise to persistent propagating particle-like structures. Because the final states in the evolution of all class **c2** rules are always cyclic (see figure 3.32), the simple particle-like structures they support can never interact with one another in an interesting manner. Class **c3** and **c4** rules, on the other hand, often support a large variety of different sized ‘particles’ moving with different ‘velocities’ and undergoing many complex ‘interactions’. We introduce a few such examples below.

k=2, r=1 Rule R110: Consider the elementary rule **R110**, a typical evolution of a disordered state under which is shown in figure 3.33. Just as the dynamics of rule **R18** was observed to give rise to a higher-level stochastic-like kink-dynamics (section 3.1.2), we see that the space-time pattern for rule **R1210** can be described either on the lower (or site) level – by explicitly reading off the values of individual

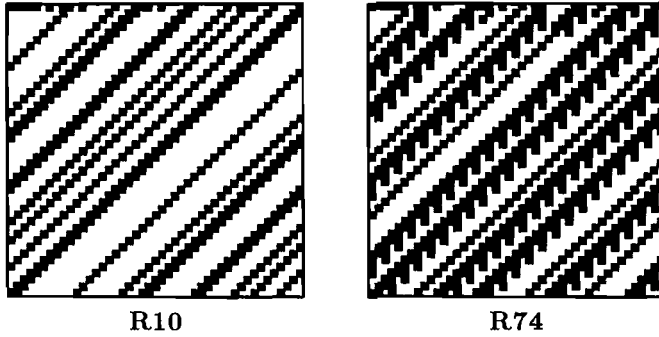


Fig. 3.32 Simple propagating structures supported by two elementary $k = 2$, $r = 1$ class **c2** rules.

sites – or in higher-level terms by noting that it is equally well represented as a *sea of particle-like structures superimposed on a periodic background*.

In fact, following a small initial transient period, temporal sections of the space-time pattern are always of the form

$$\dots \text{BBBBPBB} \dots \text{BB} \dots \text{BBBP}'\text{BB} \dots \text{BBBP}''\text{BBB} \dots, \quad (3.42)$$

where ‘B’ is state of the periodic background consisting of repetitions of the sequence ‘1001101111000’ (with spatial period $\pi_x = 14$ and temporal period $\pi_t = 7$), and the **P**’s represent ‘particles’, a few of which are tabulated below[†].

Particle	π_x	π_t
100011001110111111000	-6	12
00000	-4	15
1111000011000	-8	20
100011000	0	7
11101011000	2	10
111000	2	3

Although all of the ‘interactions’ are necessarily deterministic in nature, the enormous variety, and complexity, of possible particle-particle interactions reminds us once again that seemingly complex higher-level dynamics need not have a complex underlying dynamical origin. Indeed, had we been denied the rule (and not even been given any idea of a simple underlying dynamical mechanism) and given only the resulting space-time pattern, it is tempting to suppose that we would inevitably succumb to the traditional approach of experimental particle physics. We would set about systematically cataloging the various possible particle states and interactions, believing that our final tally somehow represents the fundamental dynamics of the system. We will be touching upon this theme many times throughout this book.

[†]From table 15 of the appendix in reference [wolf85c].

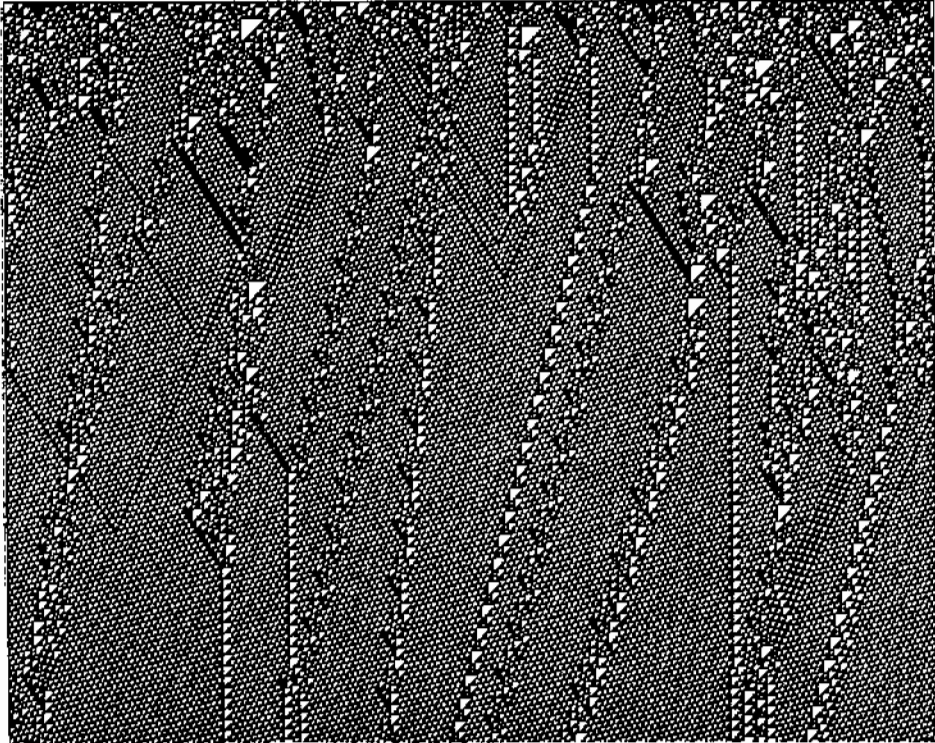


Fig. 3.33 Space-time pattern of one-dimensional elementary rule R110.

Class *c4* Rules, T20 ($r=2$) and T88 ($r=3$): It has been conjectured that *all generic class *c4* CA are capable of universal computation* [wolf85e]. With initial configurations specifying arbitrary algorithmic procedures, such systems can effectively evaluate any computable function and therefore mimic the action of any general purpose computer.

The simplest binary valued CA proven to be computation universal is John Conway's two-dimensional *Life* rule, about which we will have much to say later in this chapter. Many of the key ingredients necessary to prove universality, however, such as sets of propagating structures out of which analogs of conventional 'hardware' components (*i.e.*, *wires*, *gates* and *memory*) may be explicitly constructed, appear, at least in principle, to be supported by certain one-dimensional rules as well. The most basic component required is a mechanism for transporting localized packets of information from one part of the lattice to another; *i.e.*, *particle-like persistent propagating patterns*, whose presence is usually indicative of class *c4* behavior.

The totalistic $k=2$, $r=2$ rule **T20**, for example, defined by

$$\sigma_i(t+1) = \begin{cases} 1 & \text{if } \sum_{j=i-2}^{i+2} \sigma_j(t) = 2 \text{ or } 4 \\ 0 & \text{else,} \end{cases} \quad (3.43)$$

appears to possess many of the features necessary for universal computation. Two typical persistent structures, starting from initial states '10111011' and '1001111011', are shown in figure 3.34.

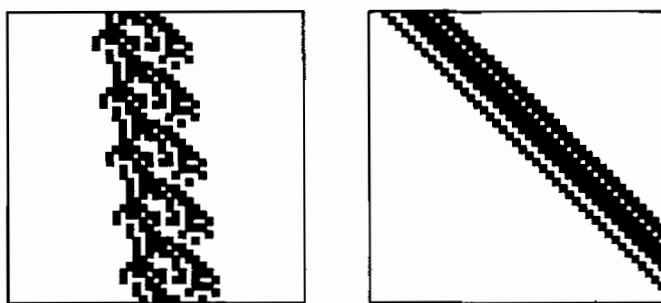


Fig. 3.34 Two particle-like patterns supported by the $k=2$, radius $r=2$ totalistic rule **T20**. The initial patterns are (a) '10111011' and (b) '1001111011'.

Examination of the evolution of all configurations with nonzero sites confined to a some finite region of N sites, reveals that the fraction of such configurations that generate persistent structures approaches 7% for large N and t (see figure 3.35).

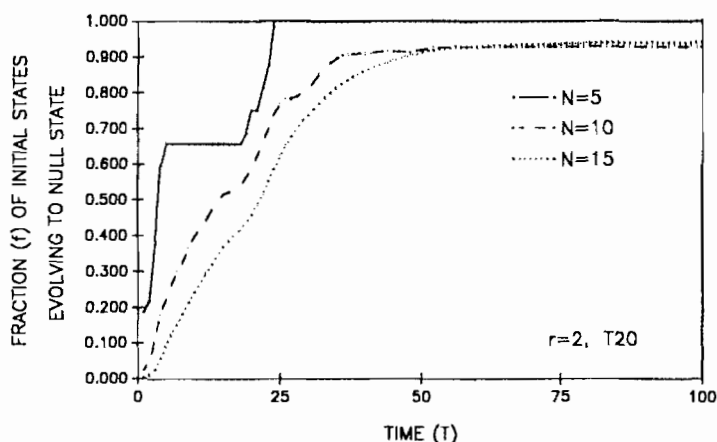


Fig. 3.35 Fraction of initial states evolving to the null state as a function of time for $r=2$ totalistic rule **T20**; see text.

Note also that the curves appear to approach a fixed, possibly universal, form for large N . Wolfram [wolf85e] speculates that at least some aspects of such curves may in fact be universal to all computationally universal systems.

Although the set of persistent structures supported by **T20** represent a significant fraction of those necessary to prove universality, they are not enough. The one missing element is something analogous to the *glider-gun* found in Conway's *Life* rule (see section 3.4.4), which acts as a clock by producing propagating structures at precisely timed regular intervals.

Such a clocklike object has been discovered by James K. Park in the evolution under the $k=2$, $r=3$ totalistic rule **T88**:

$$\sigma_i(t+1) = \begin{cases} 1 & \text{if } \sum_{j=i-3}^{i+3} \sigma_j(t) = 3, 4, \text{ or } 6 \\ 0 & \text{else,} \end{cases} \quad (3.44)$$

Park's glider gun, shown in figure 3.36, starts from the initial configuration $\bar{\Sigma}(t=0) = '\cdots 0011111111101100 \cdots'$ and generates either a left- or right- moving glider once every 238 iterations.

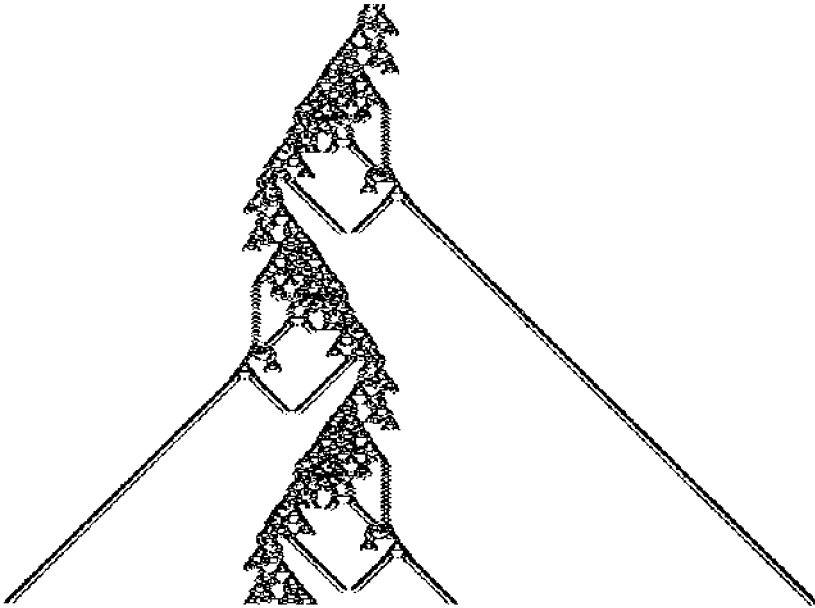


Fig. 3.36 Space-time pattern of $k=2$, $r=3$ totalistic rule **T88**: i.e. *Park's Glider Gun*.

Solitons: A mathematically appealing model of real particles is that of *solitons*. It is known that in a dispersive linear medium, a general wave form changes its shape as it moves. In a nonlinear system, however, shape-preserving *solitary* solutions exist.

The Korteweg-de Vries equation, for example,

$$\frac{\partial \phi}{\partial t} + \alpha \phi \frac{\partial \phi}{\partial x} + \frac{\partial^3 \phi}{\partial x^3} = 0, \quad \alpha = \text{constant}, \quad (3.45)$$

which is used to describe small-amplitude water waves, has the solitary wave solution

$$\phi(x, t) = \frac{3u}{\alpha} \operatorname{sech}^2 \{ \sqrt{u}(x - ut)/2 \}, \quad (3.46)$$

which moves with speed ‘ u ’. Solitary waves that preserve their shape even in collisions are called *solitons*.

In the evolutions of all of the rules we have discussed thus far, true soliton-like structures are actually very rare. Colliding particles (which, it is also worth pointing out, are for a given rule typically relatively few in number) either annihilate one-another completely or give rise to other particles that were not a part of the original collision; nondestructive collisions are extremely rare. Park, Steiglitz and Thurston [park86], however, have discovered an entire class of related CA rules called *Filter Automata* (FA) that support large numbers of soliton-like patterns.

Radius- r FA are defined in exactly the same way as conventional CA, except that the next time step of a given site is evaluated by using the *newly updated values* to either the right (or left) of the center site:

$$\sigma_i(t+1) = \Phi_{\text{FA}}(\sigma_{i-r}(t+1), \sigma_{i-r+1}(t+1), \dots, \sigma_{i-1}(t+1), \sigma_i(t), \dots, \sigma_{i+r}(t)). \quad (3.47)$$

A particular totalistic class of FA that have been found to support literally thousands of distinct solitons are called *parity-rule* FA (PFA), and are defined by

$$\sigma_i(t+1) = \begin{cases} 1 & \text{if } \left(\sum_{j=i-r}^{i-1} \sigma_j(t+1) + \sum_{j=i+1}^{i+r} \sigma_j(t) \right) \text{ is even but not zero} \\ 0 & \text{else.} \end{cases} \quad (3.48)$$

A typical evolution of a disordered state under a radius $r = 3$ parity-rule FA, showing a dissolution into, and subsequent soliton-like interaction between, several particles with different velocities, is shown in figure 3.37.

We note that no essential behavioral generality has been lost in assigning value dependence to newly updated values. By shifting the spatial axis and allowing for a values to be updated in a different order, it is in fact easy to show that any space-time pattern generated by an (r, k) FA can also be generated by an $(r' = r, k' = 2^{r+1})$ CA [park86]. Similarly, an $(r' = 2r, k')$ FA reproduces the space-time pattern of an arbitrary (r, k) CA, provided that each successive spatial pattern is displaced by r sites to the left with respect to the corresponding CA array.

Park, *et. al.*, make a number of interesting empirical observations about PFA. First, it is fairly easy to see that the position of the right-most ‘1’ in a given particle can never move further to the right; thus, all particles are either stationary or move left. Second, the maximum speed of a particle – defined as *displacement*, d ($=$ number of sites shifted to left before pattern begins repeating), divided by *period*,

π (= number of iterations before pattern repeats) is $r-1$, and is attained by the particle defined by $(r+1)$ consecutive 1's.

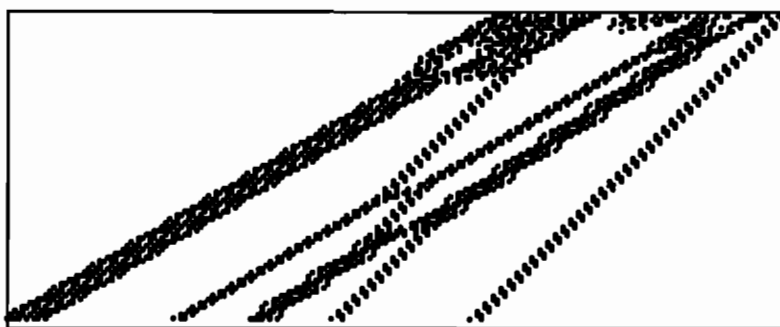


Fig. 3.37 Typical soliton-like evolution of the range $r = 3$ parity-rule filter automata, starting from an initially disordered state.

Particles may be indexed by a *canonical code*, defined to be the smallest binary number representing an intermediate state of a given particle. Empirically derived properties of particles with canonical codes with widths $w \leq 16$ evolving under a radius- r PFA rule, are summarized in table 3.4 [park86].

Radius (r)	# distinct Particles	Range of Speeds	# distinct d and π	Most Likely Speed	% of Collisions That are Soliton
2	8	0.0-1.0	6	1.0 (37.5%)	38.75%
3	198	0.333-2.0	24	1.333 (32.8%)	9.55%
4	682	0.667-3.0	23	2.333 (37.4%)	35.38%
5	6534	1.0-4.0	37	3.0 (36.6%)	45.20%
6	13109	1.333-5.0	26	4.0 (33.4%)	52.67%

Table 3.4 Properties of radius- r PFA particles with canonical codes with width $w \leq 16$.

Goldberg [goldc88], in a *tour-de-force*, not only rigorously proves virtually all of the observations made by Park, *et. al.* through computer simulation, but provides an almost complete mathematical description of PFA. Goldberg derives explicit formulae for speeds and periods of particles, sufficient conditions for soliton collisions, upper bounds on the number of possible particles, and, by using an intuitive definition of the 'energy' of a configuration, proves a number of general theorems. For example, defining 'small' particles to be those whose canonical code widths are less than or equal to $(r+1)$, Goldberg proves that collisions between such small particles are always soliton collisions. Perhaps the most significant result is the *soliton collision theorem*, which gives the duration of each possible collision, as well as the time shift between, and displacement of, each particle after the collision.

Goldberg points out, however, that despite any apparent similarity between PFA supported 'solitons' and the soliton solutions of differential equations such as the

KdV equation (equation 3.45), the nature of any deeper mathematical connection, if there is one, remains an intriguing open question.

3.1.4.5 Reversible Rules

As noted repeatedly in earlier sections, CA rules are generally irreversible; a given configuration typically has more than one predecessor. Although it is difficult to write down a reversible rule – for which each configuration has a unique predecessor – from scratch, there is a very simple way of turning an arbitrary (r, k) CA rule, ϕ , that is *first-order* in time into a *second-order* reversible rule, $\phi_{\mathcal{R}}$:[†]

$$\begin{aligned}\sigma_i(t+1) &= \phi_{\mathcal{R}}(\sigma_{i-r}(t), \dots, \sigma_{i+r}(t), \sigma_i(t-1)) \\ &= \phi(\sigma_{i-r}(t), \dots, \sigma_{i+r}(t)) \ominus_k \sigma_i(t-1),\end{aligned}\tag{3.49}$$

where ‘ $\ominus_k$ ’ is subtraction *modulo-k*. We shall call such rules *Fredkin-reversible*.[‡] We see that $\phi_{\mathcal{R}}$ is

1. *Reversible*: given an arbitrary, even irreversible, rule ϕ , we can uniquely solve for $\sigma_i(t-1)$ ($= \phi(\{\sigma_j(t)\}_{j=i-r}^{i+r}) \ominus_k \sigma_i(t+1)$),
2. *Time-reversal invariant*: the reverse sequence is obtained by inverting the last two configurations obtained in the forward direction and applying the *same* rule, $\phi_{\mathcal{R}}$.

Apart from their pedagogical value, reversible rules may be used to explore possible relationships between discrete dynamical systems and the dynamics of real mechanical systems, for which the microscopic laws are known to be time-reversal invariant. What sets such systems apart from continuous idealizations is their *exact reversibility*; discreteness assures us that computer simulations run for arbitrarily long times will never suffer from roundoff or truncation errors. As Toffoli points out, “...the results that one obtains have thus the force of *theorems* [toff84a].”

From an analytic point of view, the techniques of conventional thermodynamics, which describes systems whose microscopic dynamics is reversible, may be formally applied to reversible CA as well. We shall, in fact, follow this course in chapter 4.

Figures 3.38 and 3.39 show typical space-time patterns generated by a few $r = 1$ reversible rules starting from both simple and disordered initial states. Although analogs of the four generic classes of behavior may be discerned, there are important dynamical differences. The most important difference being the absence of *attractors*, since there can never be a merging of trajectories in a reversible system; for finite lattices this means that the state transition graph must consist exclusively of cyclic states. We make a few general observations.

[†]Although there is no specific reference to when this form was first used, it has been widely attributed to Fredkin (*Ex*: ([marg84], [vich84b]).

[‡]Note that an equivalent reversible rule that is *first-order* in time may be constructed in the usual way by using ‘effective’ site values $\tilde{\sigma} \in \{0, 1, \dots, k^2\}$.

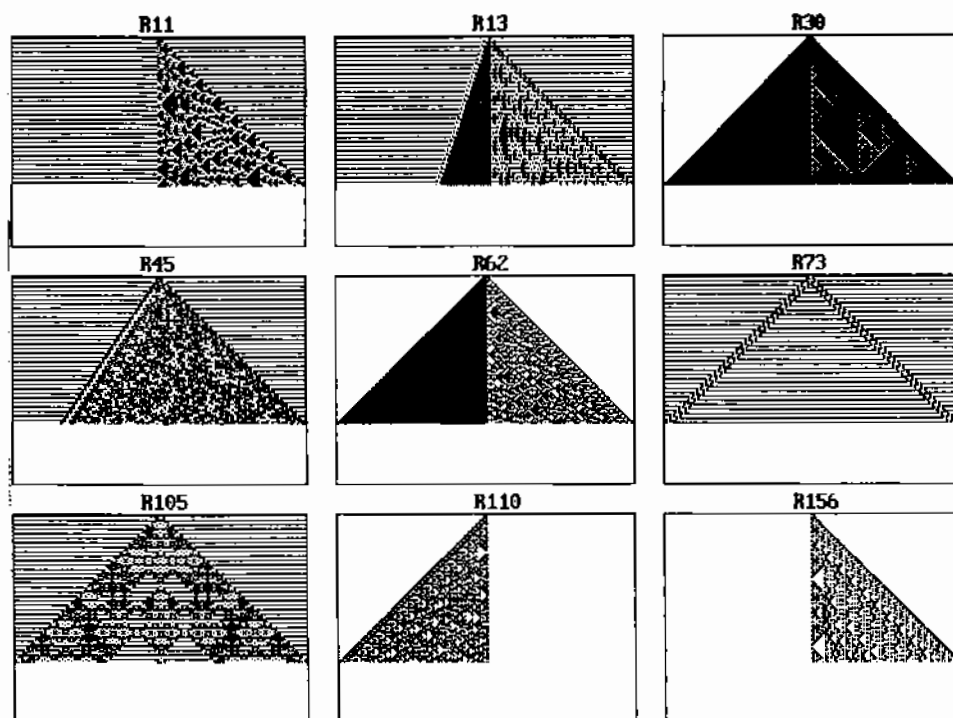


Fig. 3.38 Space-time patterns for a few one-dimensional $r = 1$ reversible rules starting from simple initial states.

As is generally true in mechanics, systems evolving under reversible rules must have as many conserved quantities as there are variables (*i.e.*, sites) describing the initial conditions. Reversible systems *remember* their initial state for arbitrarily long times since the clock can always be run backwards to recall it; *i.e.*, *there is a strict conservation of total information*. For example, we see that a few of the evolutions starting from a single nonzero site in figure 3.38 lead to very random looking patterns. Since these systems cannot have destroyed any of the ‘information’ contained in the simple initial state, what has really happened is that the initial information has simply diffused into many-cell correlations.[†] Any spatial correlations not present in the initial state can never spontaneously appear at a later time. ‘Self-organization’ may thus appear only in the guise of temporal correlations, and often becomes manifest as local ‘pockets’ of metastable order.

Do the conserved quantities of these systems lead to locally computable invariants analogous to classical mechanical energy? Margolus [marg84] gives an example of a local conservation law constraining cells to maintain a certain fixed relationship.

[†]We note, parenthetically, that such rules obviously make excellent *encryption* devices: a ‘message’ is suitably encoded as a binary string representing an initial state, and the system is then iterated repeatedly until all ‘obvious’ signs of the initial state are erased. Only if the rule is known can the successful reproduction of the original ‘message’ be assured by running the clock backwards.

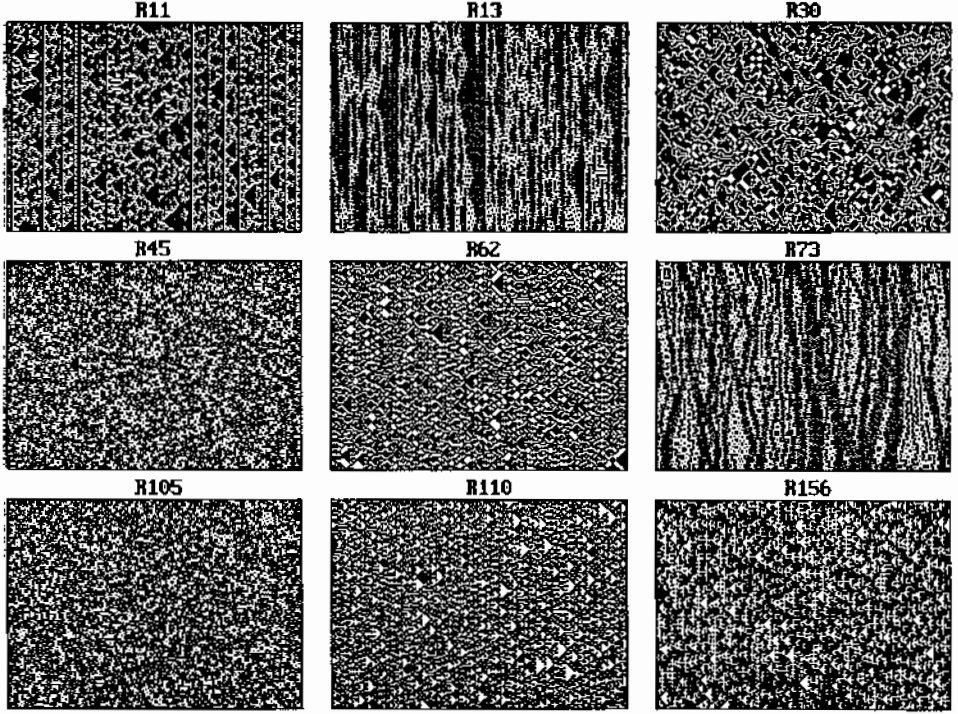


Fig. 3.39 Space-time patterns for a few one-dimensional $r = 1$ reversible rules starting from random initial states.

Consider rule **R129**, defined by

$$\phi(\sigma_{i-1}, \sigma_i, \sigma_{i+1}) = \begin{cases} 1 & \text{if } \sigma_{i-1} = \sigma_i = \sigma_{i+1}, \\ 0 & \text{else.} \end{cases} \quad (3.50)$$

If the global configurations, $\Sigma(t)$, $\Sigma(t+1)$, at times ' t ' and ' $t+1$ ', are of the form

$$\begin{aligned} \Sigma(t) &= \cdots \sigma_{i-1}(t), \sigma_i(t) = \alpha, \sigma_{i+1}(t) = \bar{\alpha}, \sigma_{i+2}(t) \cdots, \\ \Sigma(t+1) &= \cdots \sigma_{i-1}(t+1), \sigma_i(t+1) = \beta, \sigma_{i+1}(t+1) = \bar{\beta}, \sigma_{i+2}(t+1) \cdots, \end{aligned} \quad (3.51)$$

where $\alpha, \beta \in \{0, 1\}$ and $\bar{\alpha}, \bar{\beta}$ represent their binary complement, then an application of equation 3.49 gives

$$\Sigma(t+2) = \cdots \sigma_{i-1}(t+2), \sigma_i(t+2) = \alpha, \sigma_{i+1}(t+2) = \bar{\alpha}, \sigma_{i+2}(t+2) \cdots, \quad (3.52)$$

which is again of the same form.

We conclude that if the values at sites ' i ' and ' $i+1$ ' are initially complements of one another, they will forever remain being so. The evolution of these two sites is

thus effectively *decoupled* from the evolution of the global pattern.[†]

Consider now the dynamics of the active (*i.e.*, non-decoupled) part of the lattice. It is easy to see that the Fredkin-reversible form of **R129** conserves the number of initial state blocks of the form $\begin{pmatrix} \cdots \alpha \alpha \cdots \\ \cdots \beta \beta \cdots \end{pmatrix}$. This simple conservation law induces the propagation of local 3-cell *dislocations*, $\mathcal{D} \equiv (\alpha, \alpha, \alpha)$, defined to be a set of three contiguous equal valued sites sandwiched between sites with the same (but complementary) value: $\cdots \bar{\alpha} \mathcal{D} \bar{\alpha} \cdots$. Figure 3.40 shows a collision of two such *dislocations*.

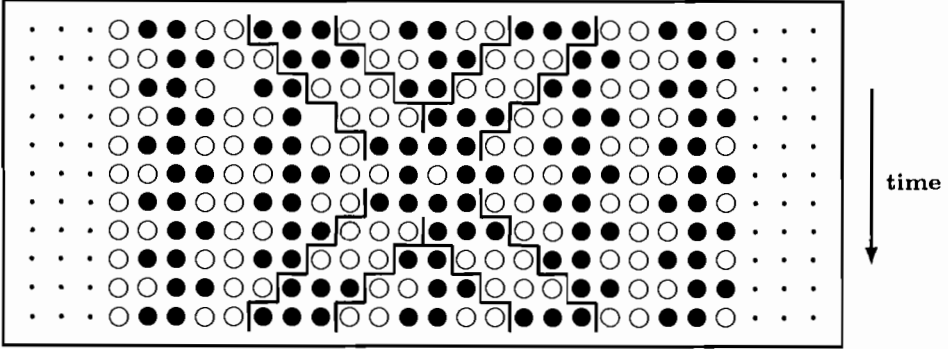


Fig. 3.40 Collision of two *dislocations* (shown between solid lines) during the evolution according to the Fredkin-reversible form of the rule **R129**.

We first observe that because the evolution is reversible, dislocations cannot annihilate one another in a collision (if we were to reverse time in such a case, the forward collision point would become a point of spontaneous creation). Margolus [marg84] point out, however, that, at every iteration step ' t ', the total number of blocks of the form

$$\begin{pmatrix} \cdots \alpha(t) \alpha(t) \cdots \\ \cdots \beta(t+1) \beta(t+1) \cdots \end{pmatrix} \quad (3.53)$$

plus the total number of blocks of the form

$$\begin{pmatrix} \cdots \delta(t) \delta(t) \cdots \\ \cdots \gamma(t+1) \gamma(t+1) \cdots \end{pmatrix}, \quad (3.54)$$

where $\alpha, \beta, \delta, \gamma \in \{0, 1\}$, is conserved. Since the first term counts the number of dislocation 'signals', it may be considered an analogue of *kinetic energy*; the second term, on the other hand, accounts for the disappearance of this kinetic energy during a collision, and may thus itself be considered an analogue of *potential energy*.

A formal analysis of the behavior of general reversible systems will be given in section 4.3. An explicit example of a two-dimensional reversible universal computer

[†]Note that were this an irreversible system, a similar finding that once complementarity is reached at an arbitrary time ' t ', it remains fixed for $t' \geq t$, *does not* permit to deduce that these sites must therefore also have been so related for all $t' < t$.

– the so-called *Billiard-Ball* model, introduced by Margolus [marg84] – is given in section 3.1.2.

3.2 Parameterizing the Space of CA Rules

We have already seen that except for only the simplest two state $r = 1$ CA, the set of possible transition rules is typically extremely large (see table 2.2). Moreover, there is no a-priori discernible order within that (largely undifferentiated) rule space. Although the existence of different behavioral patterns allows us, in principle, to partition the rule space into distinct regions such that all rules within a given region qualitatively obey the same dynamics – Wolfram’s classes **c1** through **c4**, for example – it would be better still if we could start with some natural ordering of the rule space (perhaps indexed by one or a few parameters), and quantitatively trace the behavioral changes as a function of that ordering. Note that it is not just a mere classification of rules that we are after; we seek a deeper understanding of the structure of the entire CA rule space. Two critical questions are

- *What is the underlying basis for the observed behavioral classes?*
- *What is the relationship between rule space partitions and differences in behavior?*

An important hierarchy of parameterization schemes based on successive refinements to a mean-field theoretic description, called *local structure theory*, has been developed by Gutowitz, *et. al.* ([guto87a], [guto87b], and [guto88]), and is discussed in detail in chapter five. Below we summarize results of what is essentially a *zeroth* order local structure theory developed by Langton [lang90].

3.2.1 Langton’s λ Parameter

Consider an arbitrary d dimensional, k state CA with neighborhood of size $\mathcal{N}$ and evolving in time according to the transition rule ϕ . Denoting the space of all possible rules for this CA by $\Phi_{k,\mathcal{N}}$, we recall that the number of such rules is $|\Phi_{k,\mathcal{N}}| = k^{k^{\mathcal{N}}}$.

Consider a parameter $\lambda(\phi)$ equal to the *fraction of entries in the rule table for ϕ that map to a non-zero value* [lang90]. Although it is a coarse measure, and not even necessarily the best one, it turns out that $\lambda(\phi)$ actually reveals a great deal about the internal structure of CA rule space, particularly for larger k and $\mathcal{N}$. We shall shortly see, for example, that as λ increases from 0 to 1, there is a distinct transition between periodic and chaotic rules. Although this transition is not sharp, in that there exists no unique λ at which the transition occurs (see below for discussion), it is nonetheless important because rules exhibiting the most complex behavior appear to be located precisely within this transition region. Packard [packard88], for example, has reported evidence that when CA rules are compelled to ‘evolve’ towards states in which they become increasingly well adept in performing specific

computational tasks, they tend naturally to drift towards rules in the transition region.

Defining $\aleph_0[\phi]$ to be the number of neighborhood configurations that map to $\sigma = 0$ under ϕ , and noting that there are a total of $k^{\mathcal{N}}$ possible neighborhood states, we see that $\lambda(\phi)$ is explicitly given by

$$\lambda(\phi) = 1 - \frac{\aleph_0[\phi]}{k^{\mathcal{N}}}. \quad (3.55)$$

Although the analogy is not perfect, this parameter can be thought of as a ‘temperature’ in statistical physics or as the degree of non-linearity in a dynamical system.

The idea now is to use λ to systematically sample, and study the behavior of, rules in the rule space $\Phi_{k,\mathcal{N}}$, starting with one-dimensional CA. The sections below follow Langton [lang90] and Li, et. al. [li90a].

3.2.2 Qualitative Overview of Behavior as a Function of λ

Consider the behavioral changes induced in a randomly chosen one-dimensional CA rule such that λ is successively and minimally incremented from 0 to 1. As an example, let us take $k = 4$ and $r = 2$ (i.e. neighborhood size $\mathcal{N} = 2r + 1$), and use a lattice of $N = 128$ sites with periodic boundary conditions. We summarize a typical sequence of induced behavioral changes:

$\lambda(\phi) \sim 0.00$ All activity dies within one time step; $\sigma_i \rightarrow 0$ for all ‘i’.

$\lambda(\phi) \sim 0.10$ A homogeneous fixed point is reached after a few time (1-5) time steps.

$\lambda(\phi) \sim 0.20$ Transient length increases to about 10 steps; periodic structures (with short periodicity) emerge.

$\lambda(\phi) \sim 0.25$ Transients length increases again; there are now three different possible outcomes of the dynamics, depending on the initial condition: a homogeneous fixed state, a heterogeneous fixed point consisting mostly of sites in a quiescent state σ_0 with a few other sites in another state, or a periodic state.

$\lambda(\phi) \sim 0.35$ Transient length grows significantly; a new kind of periodic structure with longer period appears, thereby increasing the spectrum of possible dynamical behaviors.

$\lambda(\phi) \sim 0.40$ Transient length increases to about 60 steps; periodic structures of period equal to about 40 steps appear.

$\lambda(\phi) \sim 0.45$ Transient length increases to about 1000 steps; periodic structures with periods in excess of 1000 steps appear.

$\lambda(\phi) \sim 0.50$ Transients are over 10000 steps.

$\lambda(\phi) \sim 0.55$ Transients become so long that they effectively represent the steady-state behavior; long-time dynamics is also essentially chaotic.

$\lambda(\phi) \sim 0.60$ Dynamics is chaotic; the number of transient steps necessary before the steady-state chaotic behavior appears decreases.

$\lambda(\phi) \sim 0.70$ Fully developed chaotic behavior appears after only about two time steps.

$\lambda(\phi) \sim 0.75$ The behavior is essentially random after only one time step.

We thus see that as λ is increased from 0.00 to 0.75 over the space of $k = 4$, $\mathcal{N} = 5$ rules, the behavior effectively changes from one of maximal order to maximal disorder with something resembling a *phase transition* taking place at intermediate values. Numerical simulations suggest several other general observations ([lang90], [li90a]):

- Transients grow exponentially fast near the transition ($\lambda_c \sim 1/2$); in the study of phase transitions in statistical physics this is known as *critical slowing down*.
- Dynamical behavior depends on lattice size N only for λ near λ_c ; transient length, for example, grows exponentially with N for $\lambda = \lambda_c$.
- As λ increases beyond λ_c , transient lengths decrease until, at $\lambda = 3/4$, they no longer show any dependence on lattice size.
- $\lambda = 3/4$ appears to represent a state of maximal disorder (as deduced from computing certain entropy and correlation measures; see next section).
- Rules for which λ is near λ_c appear to support propagating soliton structures, suggesting that the most complex rules (i.e. those belonging to Wolfram's class **c4**) lie within this transition region – λ for Conway's *Life* rule, for example, is equal to 0.273 and lies within the transition region for $k = 2$, $\mathcal{N} = 9$ two dimensional CA.

3.2.3 Quantitative Overview of Behavior as a Function of λ

In order to quantitatively trace behavior as a function of λ , it is clear that we need to look at statistical measures that distinguish between ordered and random behavior. To this end, consider the *spreading rates* of difference patterns and *entropy*.

3.2.3.1 Difference Pattern Spreading Rates

Recall that difference patterns are simply the space-time patterns of the difference between two evolutions of the same transition rule starting from two different starting configurations. For example, the value of the i^{th} site at time t of a difference pattern for a $k = 2$ global rule Φ and two different initial global states $\vec{\sigma}_1(0)$ and

$\vec{\sigma}_2(0)$, is defined by

$$\Delta_i(t) = \Phi^t[\vec{\sigma}_1(0)]_i \oplus_2 \Phi^t[\vec{\sigma}_2(0)]_i. \quad (3.56)$$

Provided that the limits exist, the *left* and *right* spreading rates – γ_{left} and γ_{right} , respectively – are then determined from

$$\begin{cases} \gamma_{\text{left}}(\vec{\sigma}_1(0), \vec{\sigma}_2(0)) &= \lim_{t, \tau \rightarrow \infty, t/\tau \rightarrow 0} \frac{i_{\min}(\tau) - i_{\min}(\tau + t)}{t - \tau}, \\ \gamma_{\text{right}}(\vec{\sigma}_1(0), \vec{\sigma}_2(0)) &= \lim_{t, \tau \rightarrow \infty, t/\tau \rightarrow 0} \frac{i_{\max}(\tau + 1) - i_{\max}(\tau)}{t - \tau}, \end{cases} \quad (3.57)$$

where $i_{\min}(t) = \min \{i \mid \Delta_i(t) = 1\}$ and $i_{\max}(t) = \max \{i \mid \Delta_i(t) = 1\}$. Although, according to this definition, the total difference pattern spreading rate, $\gamma \equiv \gamma_{\text{left}} + \gamma_{\text{right}}$, is an explicit function of $\vec{\sigma}_1(0)$ and $\vec{\sigma}_2(0)$, an average $\bar{\gamma}$ is in practice measured by averaging over many initial states.

Mean Field Estimate: It is easy to predict the value of $\bar{\gamma}$ from λ . Consider a one-dimensional $k = 2$, $r = 1$ CA evolving according to rule ϕ for which $\lambda(\phi) = \lambda$. The probability that two randomly chosen $(2r + 1)$ neighborhood blocks map to the same value is equal to $p_{\text{same}} = \lambda^2 + (1 - \lambda)^2$. The average left spreading rate of ϕ is then given by

$$\bar{\gamma}_{\text{left}} = \sum_{i=0}^{\infty} (r - i) \times (\text{probability that } \gamma_{\text{left}} = r - i). \quad (3.58)$$

Consider the contribution from the maximum spreading rate r . The probability that $\bar{\gamma}_{\text{left}} = r$ is equal to the probability that blocks $(\sigma_{i-r}, \dots, \sigma_{i+r-1}, 1)$ and $(\sigma_{i-r}, \dots, \sigma_{i+r-1}, 0)$ map to different values. This probability is equal to the probability that two randomly selected $(2r + 1)$ blocks map to different values: $1 - p_{\text{same}}$. Similarly, the probability that $\bar{\gamma}_{\text{left}} = r - 1$ is equal to the probability that $(\sigma_{i-r}, \dots, \sigma_{i+r-1}, 1)$ and $(\sigma_{i-r}, \dots, \sigma_{i+r-1}, 0)$ map to the same value ($= p_{\text{same}}$) *times* the probability that $(\sigma_{i-r}, \dots, \sigma_{i+r-2}, 1, \sigma_{i+r})$ and $(\sigma_{i-r}, \dots, \sigma_{i+r-2}, 0, \sigma_{i+r})$ map to different values ($= 1 - p_{\text{same}}$).

Accounting, in this way, for all contributions from $\gamma_{\text{left}} = 0$ to $\gamma_{\text{left}} = r$, and noting that $\bar{\gamma} = \bar{\gamma}_{\text{left}} + \bar{\gamma}_{\text{right}} = 2\bar{\gamma}_{\text{left}}$, we find that

$$\begin{aligned} \bar{\gamma} &= 2 \sum_{i=0}^{\infty} (r - i) p_{\text{same}}^i (1 - p_{\text{same}}), \\ &= 2 \left(r - \frac{p_{\text{same}}}{1 - p_{\text{same}}} \right), \\ &= \frac{(2r + 2)(\lambda - \lambda^2 - 1)}{\lambda(1 - \lambda)}. \end{aligned} \quad (3.59)$$

One immediate conclusion can be drawn from this expression. Defining a critical λ_c^γ to be the value of λ for which $\bar{\gamma}$ attains its first non-zero value, we can express λ_c^γ as a function of r by setting $\bar{\gamma}(\lambda_c^\gamma) = 0$ and solving for λ_c^γ :

$$\lambda_c^\gamma = \frac{1}{2} - \frac{1}{2} \sqrt{1 - \frac{2}{r+1}}. \quad (3.60)$$

Numerical Observations: Figure 3.41 shows a schematic plot[†] of $\bar{\gamma}$ versus $(\lambda - \lambda_c^{(2)})$, where $\lambda_c^{(2)}$ is defined as the value of λ for which $\bar{\gamma} = 2$ – this is a threshold value for $\bar{\gamma}$ above which we arbitrarily define a given rule to be *chaotic*. In the figure, the spreading rate is averaged over 200 $r = 7$ one-dimensional rules. Since different rules generally undergo a transition to chaos for different values of λ , a plot of $\bar{\gamma}$ versus $(\lambda - \lambda_c^{(2)})$ facilitates an examination of the typical behavior around the transition point.

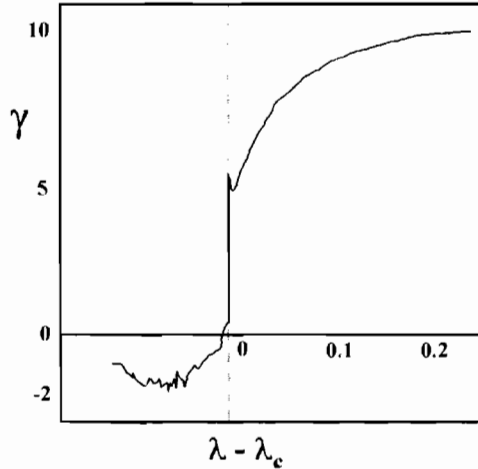


Fig. 3.41 Schematic form of a plot of $\bar{\gamma}$ versus $(\lambda - \lambda_c^{(2)})$; see text.

3.2.3.2 Entropy

We recall that the single-site entropy of a k state CA is defined by

$$H = - \sum_{i=0}^{k-1} p_i \log_2 p_i, \quad (3.61)$$

where p_i is the probability of $\sigma = i$ and $\log_2$ is the logarithm base two.

Mean Field Estimate: H may be estimated from $\lambda(\phi)$ in two steps: First, we find the steady-state probability of a given site having value zero. Let $p_0(t)$ be the

[†]Patterned after Li, et al's, figure 2 appearing in [li90a].

probability that a randomly selected site has $\sigma(t) = 0$. On the next time step, that site will remain equal to zero either if the neighborhood configuration is equal to zero (in which case $\sigma(t+1) = 0$ with probability one), or at least one site within the neighborhood is non-zero (in which case $\sigma(t+1) = 0$ with probability $(1 - \lambda(\phi))$). Since the probability that a neighborhood of size $\mathcal{N}$ contains all zeroes at time t is $p_0^{\mathcal{N}}(t)$, and the probability that it contains at least one non-zero site equals $1 - p_0^{\mathcal{N}}(t)$, we see that

$$p_0(t+1) = p_0^{\mathcal{N}}(t) + (1 - p_0^{\mathcal{N}}(t))(1 - \lambda(\phi)). \quad (3.62)$$

In particular, assuming that once the evolution has reached the steady state, $p_0 \neq p_0(t)$, p_0 must satisfy the equation

$$p_0 = p_0^{\mathcal{N}} + (1 - p_0^{\mathcal{N}})(1 - \lambda(\phi)). \quad (3.63)$$

Second, using $p_0 = p_0(\lambda)$ found as a solution to the above equation for a given λ , and assuming that all non-zero values appear equally often (i.e. that $p_i = (1 - p_0)/(k - 1)$ for $i = 1, \dots, k - 1$), we can estimate the entropy by computing

$$H = - \left[p_0(\lambda) \log_2 p_0(\lambda) + (1 - p_0(\lambda)) \log_2 \frac{1 - p_0(\lambda)}{k - 1} \right]. \quad (3.64)$$

As in the case of the spreading rate γ , we can again define a critical λ_c^H to be the value of λ for which H attains its first non-zero value. It is easy to see that λ_c^H is given by

$$\lambda_c^H = \frac{1}{\mathcal{N}} = \frac{1}{2r + 1}. \quad (3.65)$$

Numerical Observations: Figure 3.42 shows a schematic plot of H versus λ for $k = 8$ $\mathcal{N} = 5$ two dimensional CA. The lattice size is 64×64 with periodic boundary conditions. In the figure, the evolution of the single-site entropy is traced for four different transition events. In each case, for a given λ , a rule table consistent with that λ is randomly chosen and the system is made to evolve for 500 steps to allow transients to die out before H is measured.

Observe how in each of these four events, H is zero until, at some critical λ_c (which is different for different cases), H abruptly jumps to some higher value and thereafter proceeds relatively smoothly to its final maximum value $H_{\max} = \log_2(8) = 3$ at $\lambda = 7/8$. In statistical physics, such abrupt, discontinuous changes in entropy are representative of first-order phase transitions. Interestingly, an examination of a large number of such transition events reveals that there is a small percentage of smooth transitions, which are associated with a second-order phase transition [li90a].

In fact, the mean-field estimate for H , given by equation 3.64, predicts a second-order transition. While abrupt changes in entropy characterize sudden transitions between regions of periodic and chaotic rules, smooth changes in entropy as λ is increased instead suggest that the rule path sometimes passes through a region of

critical rules, which lie between periodic and chaotic rules. Because rules within this region may also possess arbitrarily long transients (see qualitative discussion above) and various statistical measures generally converge to their steady state values very weakly, it has been conjectured that this critical region in fact contains the class of rules capable of supporting universal computation ([lang90], [packard88]).

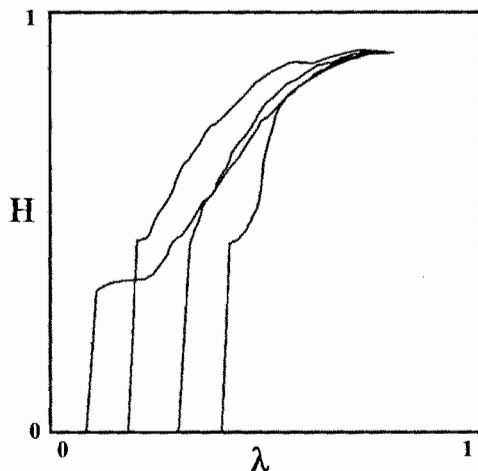


Fig. 3.42 Schematic plot of H versus λ for separate runs; see text.

3.2.4 Mutual Information

Mutual information, $\mathcal{I}_M$, effectively measures the degree to which two probability distributions – or, in the context of CA, two sites or blocks – are correlated. Given probability distributions p_i and p_j and the joint probability distribution p_{ij} , $\mathcal{I}_M$ is defined by:

$$\mathcal{I}_M = \sum_i \sum_j p_{ij} \log_2 \frac{p_{ij}}{p_i p_j}. \quad (3.66)$$

The distributions p_i and p_j can refer to the probability of either having k values on each of two separated sites or having k^B values on two separated blocks of sites. In either case, $\mathcal{I}_M$ measures correlation between the patterns generated at separate parts of the lattice: small $\mathcal{I}_M$ implies that sites (or blocks) are essentially uncorrelated and evolve in an effectively independent manner (such is the case for both periodic and chaotic rules); large $\mathcal{I}_M$, on the other hand, implies that sites (or blocks) are well correlated, and typically are found for complex rules according to which highly complex structures may evolve. Its ability to distinguish among the dominant types of behavior makes mutual information an important measure to use in isolating the transition from periodic to chaotic regimes.

Numerical experiments by Langton [lang90a] show once again that when $\mathcal{I}_M$ is plotted against λ , there is a region for small λ for which $\mathcal{I}_M$ is essentially zero, a critical λ at which $\mathcal{I}_M$ jumps to some moderate value followed by a slow decay as

λ increases from that point on. From the perspective of computation theory taken in his paper, Langton argues that it is the set of intermediate values of λ that are most important.

A particularly revealing plot in this regard, shown schematically in figure 3.43, is a graph of $\mathcal{I}_M$ versus H , where $\mathcal{I}_M$ is computed between a site and itself at the next iteration step and H is normalized to $H_{\max} = 1$.

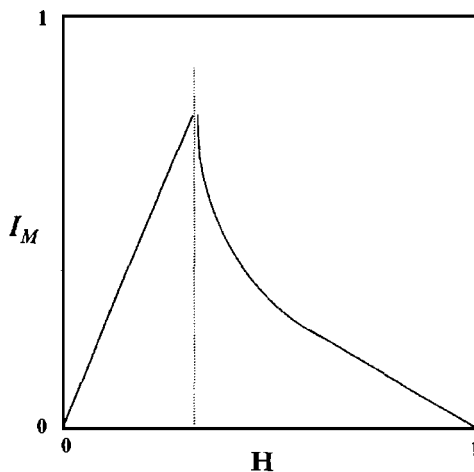


Fig. 3.43 Schematic form of a plot of mutual information $\mathcal{I}_M$ vs. average single-site entropy H .

Notice the sharp maximal value of $\mathcal{I}_M$ at a critical H_c (~ 0.32), suggesting that there exists an *optimal entropy* for which CAs yield large spatial and temporal correlations. Langton conjectures that this results from two competing requirements that must both be satisfied in order for an effective computational ability to exist: *information storage*, which involves lowering entropy, and *information transmission*, which involves increasing entropy.

It would appear that the tradeoffs between these two requirements are optimized at the phase transition. Langton also cites a very similar relationship found by Crutchfield [crutch90] between a measure of *machine complexity*[†] and the (per-symbol) entropy for the logistic map. The fact that the complexity/entropy relationship is so similar between two different classes of dynamical systems in turn suggests that what we are observing may be of fundamental importance: *complexity generically increases with randomness up until a phase transition is reached, beyond which further increases in randomness decrease complexity*. We will have many occasions to return to this basic idea.

[†]Specifically, the size of the minimal finite state machine that is required to recognize strings of 0's and 1's generated by the logistic map (chapter 6).

3.2.5 Discussion

Numerical investigations such as those outlined above provide useful hints about the generic structure of the CA rule space as parameterized by λ . As λ is increased from its minimal to maximal values, a path is traced in the rule space which starts in a periodic regime, passes through an intermediate transition region, and ends in a chaotic regime. The transition region is a complex subspace. Some parts of this region act as simple boundaries between periodic and chaotic rules, such that all paths passing through such boundaries yield abrupt first-order transition-like changes in statistical measures of the dynamics. These parts have essentially zero measure and hence harbor no rules within them. Other parts of the transition region have a finite measure and paths passing through them give rise to smooth second-order transition like changes in statistical measures.

Statistical quantities generally do not converge well at or near the second-order transition region. This has led Li, et. al. [Li90a] to suggest that the *width of the distribution of values of a given statistical measure* be used as a measure for ‘critical’ rules within this region. Using this measure, rules near the transition have wide distributions, while rules away from the transition have narrow distributions.

3.2.5.1 Large $\mathcal{N}$ Limit

Li et. al. [Li90a] show that as the local site neighborhood size $\mathcal{N}$ increases, the critical λ_c that separates periodic and chaotic regions decreases. In particular, $\lambda_c \rightarrow 0$ for $\mathcal{N} \rightarrow \infty$. We could have expected this, heuristically, since as the neighborhood size gets larger and larger, sites become increasingly sensitive to values of more distant sites, thus making chaotic dynamics more likely. From the mean-field predictions for λ_c given by equations 3.60 and 3.65, we in fact see that $\lambda_c(r) \sim \frac{1}{2r}$ for large r .

3.2.5.2 Large k Limit

Because the rule table can quickly become unmanageably large, it is difficult to run numerical simulations for the case where the number of values per site k is large. It is easy, however, to examine the case when $k = \infty$. Assuming that the lattice size is finite and that the system evolves for a finite time, the net effect of having an infinite number of symbols is that each site will continually attain new values. Since the rule table appropriate for a given λ is constructed randomly, the result is that such a system evolves as though it were a *probabilistic CA* with two symbols: zero and ‘other’. The zero neighborhood is mapped onto the zero state with probability one and all other states are mapped to ‘other’ with probability λ .

Numerical simulations of the $k = \infty$ case reveal a sharp phase transition at $\lambda_c = 0.27$ [wootter]. Simulations also suggest that the spread in values of entropy decreases with increasing k , and that the width of the transition region probably goes as $k^{-1/2}$ [woot90].

3.2.5.3 Complexity Resides in the Transition Region?

Perhaps the most interesting result to come out of these investigations is the strong likelihood that the most complex rules, those capable of supporting universal computation, are in fact located within the second-order transition region. There are at least three strong reasons for this:

(1) Class **c4** rules characteristically have long transients, propagating soliton-like structures, large correlation lengths, etc. These are all properties possessed by rules within the transition region.

(2) A fundamental property of universal computation is given by the *Halting theorem*, which states (see chapter 12) that it is in-principle impossible to decide whether or not a given computation will halt. While the ultimate fate of both periodic and chaotic rules, or those lying on either side of the transition region, is predictable, that of rules located within the transition region is not. Their behavior may eventually settle down to either periodicity or chaos but, because of the arbitrarily long transients, it may be effectively undecidable which of these two dynamical behaviors will eventually emerge.

(3) Effective computation requires both the storage and transmission of information. If correlations between separated sites are too small, the sites evolve essentially independently of one another and little or no transmission of information takes place. On the other hand, if the correlations are too strong, distant sites may cooperate so strongly so as to effectively mimic each others behavior; this, too, is not conducive to effective computation. It is only within the transition region that information can propagate freely over long distances without appreciable decay.

3.3 Dependence on Lattice Topology

In this section we examine the relationship between global dynamical properties of a CA system – as characterized, for example, by certain features of the state transition graph $G_{\mathcal{L}}$ – and the topology of the underlying lattice $\mathcal{L}$. To do so, we first introduce the notion of a *natural topology*, which effectively transforms the dynamical content of a CA system into a structure-based description. The natural topology of a system will subsequently be used in section 5.4.3 to generate explicit solutions for general systems whose site values are taken from finite fields of arbitrary size, directly linking behavioral characteristics with topological properties of $\mathcal{L}$. The numerical observations made in this section will help set the stage for that later analytical discussion. The discussion in this section is based on [ilach87].

3.3.1 Natural Topology

Consider a finite but structurally arbitrary lattice $\mathcal{L}$, with geometry completely specified by the $(N \times N)$ *adjacency matrix* $\mathbf{L}$:

$$(\mathbf{L})_{ij} = \begin{cases} 1 \longleftrightarrow & \text{'i' is linked to 'j'} \\ 0 \longleftrightarrow & \text{otherwise} \end{cases} \quad (3.67)$$

At each of N sites is a variable σ_i belonging to a finite field $\mathcal{F}[q = p^n]$ (p is a prime, n is any integer), so that a particular configuration is specified by the vector $\Sigma(t) \equiv (\sigma_1(t), \dots, \sigma_N(t))^T$.

Defining a distance function $d(i, j) \equiv \min_{paths} \{ \# \text{ of links } (i, j; \text{ path}) \}$ and a ' d '-size neighborhood of ' i ' as $\mathcal{N}_d(i) \equiv \{ 'k' \text{ such that } d(i, k) \leq d \}$, we wish to study the discrete time-evolution of $\Sigma(t)$ in which the site variables undergo transitions of the general form

$$\sigma_i(t+1) = \phi_{\mathcal{L}} \left[\sum_{j \in \mathcal{N}_d(i)} \sigma_j(t) \right], \quad (3.68)$$

where the subscript on ' ϕ ' is to emphasize that $\phi_{\mathcal{L}}$ acts on a particular lattice. Since there is no universally applicable *local* labeling procedure for sites in a random lattice $\mathcal{L}$, this is in fact the most general form possible. As always, $\phi_{\mathcal{L}} : \mathcal{Z} \rightarrow \mathcal{F}[q]$ is the same for all ' i ' and is defined explicitly by enumerating, for all $y \in \mathcal{F}[q]$, all possible values $x \in \mathcal{Z}$ for which $\phi_{\mathcal{L}}(x) = y$.

Given any lattice $\mathcal{L}$ and arbitrary transition rule ' $\phi_{\mathcal{L}}$ ' we define a *natural topology* $\mathcal{L}_{\phi}$:

$$(\mathbf{L}_{\phi})_{ij} = \begin{cases} 1 \longleftrightarrow & \sigma_i(t+1) \text{ depends on } \sigma_j(t) \text{ through } \phi_{\mathcal{L}} \\ 0 \longleftrightarrow & \text{otherwise,} \end{cases} \quad (3.69)$$

upon which the site transitions become strictly *local*:

$$\phi_{\mathcal{L}} \left[\sum_{j \in \mathcal{N}_d(i)} \sigma_j(t) \right] = \phi_{\mathcal{L}_{\phi}} \left[\sum_{j \in \mathcal{N}_{d=1}(i)} \sigma_j(t) \right]. \quad (3.70)$$

We are effectively transforming functional identity into topological information: *i.e.* different choices of rules correspond to different topologies and all rules are taken to be simple functions of local sums.

The general form of the global transition function may then be written

$$\Sigma(t+1) = \Phi[\mathbf{L}^* \cdot \Sigma(t)], \quad (3.71)$$

where $[\Phi(\mathbf{x})]_i = \phi(x_i)$, $x_i \equiv \mathbf{L}_{ij}^* \Sigma_j$ and the matrix product is taken over $\mathcal{Z}$. *Additive* rules are defined by $\phi(x) = x \pmod{q}$, so that our goal is to explore the dependence of the global dynamics of the system

$$\Sigma(t+1) = \mathbf{L} \cdot \Sigma(t) \quad (3.72)$$

on the topological features of the lattice represented by $(\mathbf{L})_{ij}$. Throughout this section, *outer-totalistic OT* rules will refer to loopless graphs ($\mathbf{L}_{ii} = 0$); *totalistic T* rules to graphs with loops ($\mathbf{L}_{ii} = 1$).

Figure 5.3 shows $\mathcal{L}^*$ for three different additive rules in 1-dim (*i.e.* $\mathcal{L} \equiv 1$ -dim topology). The dynamics may be equally well represented either as taking place entirely on a one-dimensional lattice but under three different rules, or obeying the same rule ($\equiv \oplus_q(\sigma_{neighbors})$) but defined on three different lattices. Having subsumed, in this way, the dynamical content of a given rule into the underlying

Rule	$r = 1$	$r = 2$	$r = 3$	Rule	$r = 1$	$r = 2$	$r = 3$
T: 4	2	2	2	T: 12	2	3	3
8	1	2	2	14	1	3	3
2	3	3	3	20	2	4	3
10	3	3	3	28	2	3	3
OT: 2	2	2	2	OT: 14	2	3	3
8	2	2	2	16	1	2	3
4	3	3	3	18	2	2	3
12	3	3	3	20	2	3	3

Table 3.5 Behavioral classes for *range- r* one-dimensional systems obeying a variety of **T** and **OT** rules. Rules whose behavioral classification *changes* with ' r ' are given at right.

natural topology, the fundamental question becomes: *What are the topological characteristics of $\mathcal{L}_\phi$ which determine the system's global dynamical behavior?*

That there generally exists a non-trivial relation between dynamics and the topology underlying that dynamics is easy to see. Figure 3.44, for example, shows the evolution of rule **T20** on a one-dimensional lattice with *ranges* $r = '1, 2$ and $3'$. We see that each of the three distinct topologies supports an entirely different *class* of behavior: *class-2* for $r = 1$, *class-4* for $r = 2$ and *class-3* for $r = 3$. Similarly, in figure 3.45, we see that although rule **T12** is definitely *class-3* for $r = '2, 3'$, it can induce *class-2* behavior on what may be considered to be *intermediate topologies*, defined by adding a certain fraction of $r = 3$ *vertices* to the initially pure $r = 2$ lattice. It is this apparently unresolved intermediate (or *transitional*) behavior that we study more closely in the remainder of this chapter. Table 3.5 gives the behavioral class range-dependence for a number of **T** and **OT** rules.

The following questions are of fundamental importance:

1. *Is there a more general behavioral classification scheme by which the intrinsic dynamical complexity of rules may be described?*

Behavioral classes of rules have been phenomenologically determined only for simple lattice topologies. Although there exists a general phraseology with which dynamics on more complicated structures can be rather loosely identified, there are presently no available formalisms providing a more general behavioral classification scheme. Moreover, aside from a few isolated studies of dynamics as a function of *size* of circuit graphs, questions dealing purely with topology – such as asking for the topological characteristics of lattices supporting the most complex dynamics – have yet to receive any sort of formal attention.

It is often the case, for example, that certain rules heretofore labeled *class-3* on range ' 2 ' or ' 3 ' one-dimensional lattices, in fact induce a substantially less complicated dynamics on most other *nearby* graphs. Similarly, graphs can be found for which apparently trivial *class-1* or ' 2 ' behavior turns into *class-3* dynamics upon addition or deletion of a single link. Two rules, ' $\mathcal{R}_1, \mathcal{R}_2$ ', showing the same simple dynamical behavior for a particular graph ' g ', but where $\mathcal{R}_1$ induces a large

variety of behaviors on graphs differing only slightly from $\mathbf{g}$ and $\mathcal{R}_2$ continues exhibiting simple dynamics, ought to be formally classified according to two different *complexity classes* (modulo the family of graphs close to $\mathbf{g}$). A more complete characterization of the generic behavioral complexity of a given rule ' ϕ ', is provided by the relative magnitudes of fluctuations in behavior for families of structurally similar topologies[†]. *Dynamical profiles* of rules across sequences of graphs defining such families, therefore, may prove to be useful to any concerted effort at establishing a more general behavioral classification scheme. Other important questions, answered partially below, include the following:

2. What does the set of possible state transition graph topologies for families of structurally similar graphs look like?

3. What is the dynamical response of a system to a sequence of systematically applied minimal topological deformations of a 1-dim lattice?

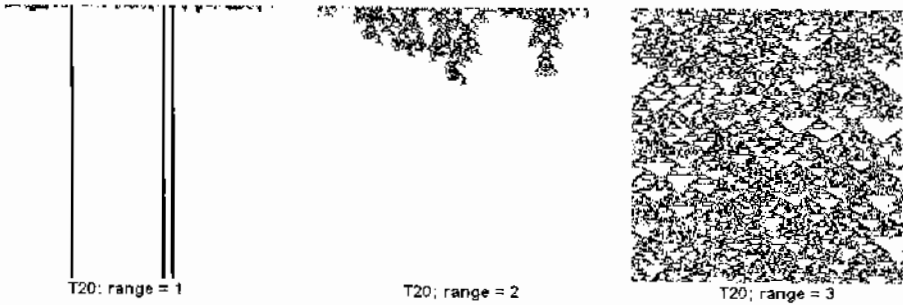


Fig. 3.44 Example of the *range dependent behavior* of rule **T20**: the system evolves as *class-2* for $r=1$, *class-4* for $r=2$ and *class-3* for $r=3$. The various possible intermediate (or *transitional*) behaviors can be studied by successively applying well-defined minimal topological deformations to the initial lattice.

3.3.2 Transitional Lattice Construction

The *dynamical profile* across a landscape of structurally similar topologies, starting from a *range-1* 1-dim lattice, is obtained by observing the global behavior for each graph in a sequence $\mathbf{G}_S \equiv \{\mathbf{g}_1, \mathbf{g}_2, \dots, \mathbf{g}_{N_{\max}}\}$, constructed as follows ($\mathcal{L}_r \equiv$ pure *range- r* graph):

1. $\mathbf{g}_1 \equiv$ ' $r=1$ ' one-dimensional lattice with linked endpoints ($\mathbf{L}_{1N} = \mathbf{L}_{N1}$).
2. Define the sequence ' $\mathbf{g}_2, \mathbf{g}_3, \dots, \mathbf{g}_{N+1}$ ' by randomly adding, *one by one*, each of the ' N ' edges linking vertices a distance $D=2$ apart in $\mathbf{g}_1$. Successive topologies ' $\mathbf{g}_i, \mathbf{g}_{i+1}$ ' thus differ in exactly one pair of linked vertices.
3. The sequence ' $\mathbf{g}_{(r-1)N+2}, \dots, \mathbf{g}_{rN+1}$ ', is similarly defined between $\mathcal{L}_r$ and $\mathcal{L}_{r+1}$ lattices, by successive additions of randomly selected edges linking vertices a dis-

[†]Defined as equal size graphs with topologies which differ by at most a few links.

tance $D=r$ apart in $\mathbf{g}_1$.

4. Since particular choices for intermediate link additions will generally yield *non-isomorphic* sequences of topologies, the typical intermediate dynamical behaviors are obtained by averaging each measure over the number N_g of such collections of graphs $\{\mathbf{g}_1, \mathbf{g}_2, \dots, \mathbf{g}_{r_{max}N+1}\}$.

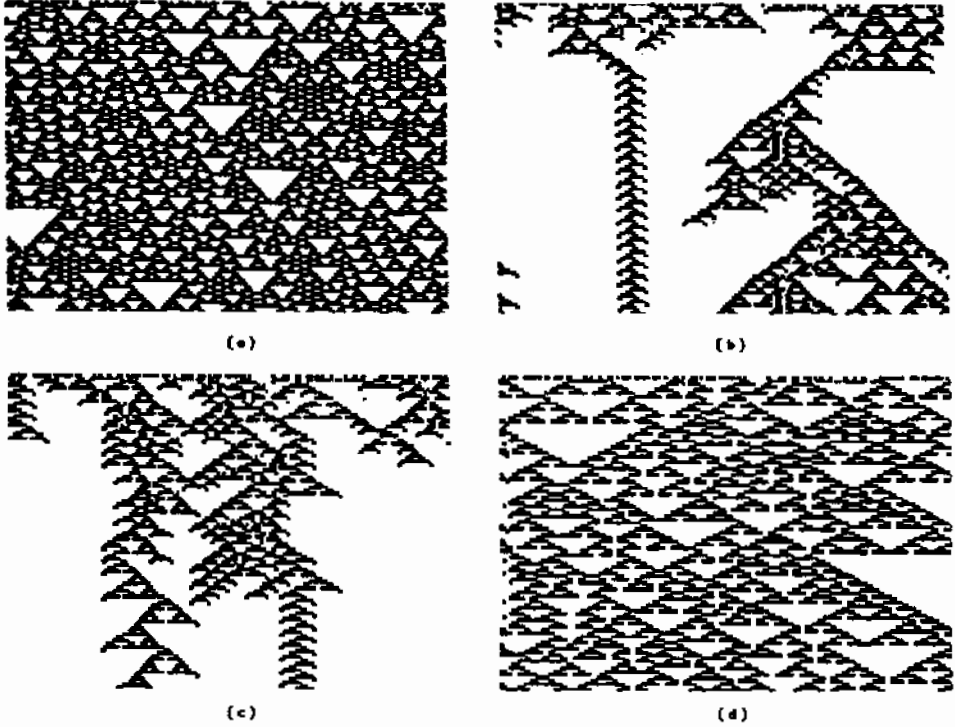


Fig. 3.45 Time evolution of rule **T12** on (a) $r=2$ lattice, (b,c) *intermediate* lattices, defined by populating an $r=2$ lattice with a fraction ' ρ ' of vertices that have '6' nearest-neighbors, with $\rho_b \sim 0.15$, $\rho_c \sim 0.30$, and (d) $r=3$. We see that the *class-3* behavior on the *pure range- r* graphs in (a) and (b) can become effectively *class-2* on certain intermediate (or hybrid) topologies.

In figures 3.46-3.49, which show dynamical profiles of various measures for sequences $\mathbf{G}_S$, $r_{max} = 3$ or 4, and the x -axis labels the number of edges added to $\mathbf{g}_1$. $\mathcal{L}_r$ lattices ($= \mathbf{g}_{(r-1)N+1}$) are denoted by dashed vertical lines, while vertical bars for each graph give the mean absolute deviation of measure ' m ': $\frac{1}{N_g} \sum_i |m_i - \bar{m}|$, where N_g is the total number of graph sequence samples. Measures include *cycle number* ($\equiv |C|$), *fraction of initial states* $\Sigma_0 \rightarrow 0$ ($\equiv f_0$), *mean transient time* ($\equiv \langle t \rangle$), *mean and maximal cycle lengths* ($\equiv \langle C \rangle$, C_{max}), *internal, external and dynamic complexities* ($\equiv S_I$, S_E , S_g).

The already established behavior of rules on one-dimensional lattices, will be la-

beled by $[cl_1 : cl_2 : cl_3]$, where $cl_i \equiv$ behavioral class on a *range- i* one-dimensional lattice.

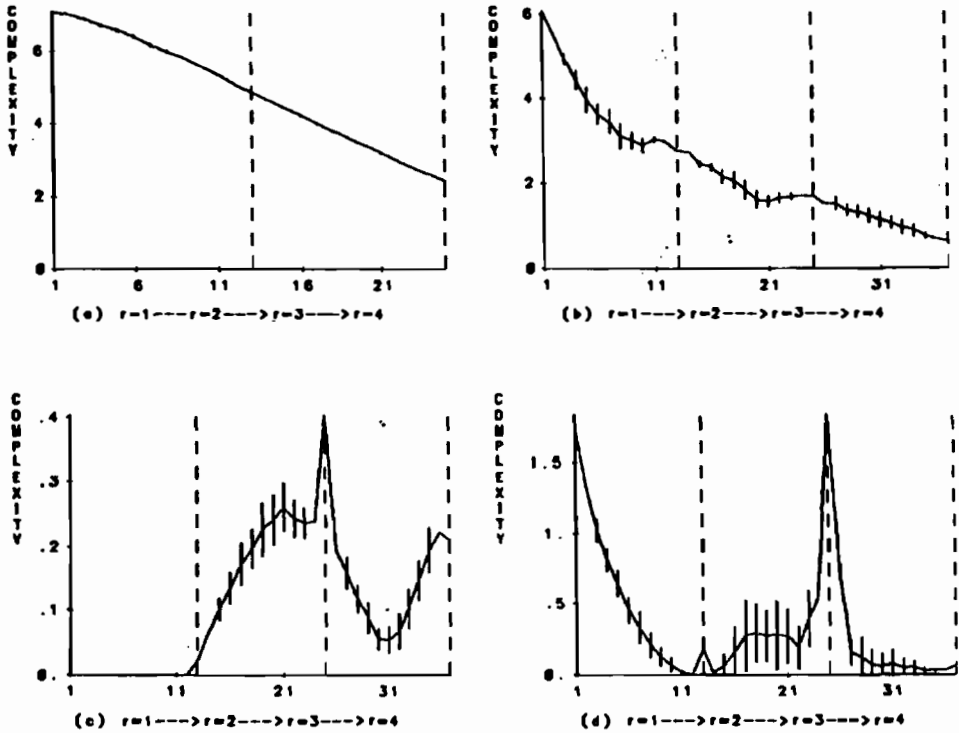


Fig. 3.46 *Dynamical profiles* for graph sequences G_S (defined in section 3.3.2), representing averages over N_g sequence samples. The x-axis labels each $g \in G_S$, dashed lines denote pure range- r topologies $\mathcal{L}_r$ with $g_1 \equiv$ 'range-1, 1-dim lattice' and vertical bars give the mean absolute deviations of a particular measure. Each system has *size* $N=12$, with N_g and *rules* $\mathcal{R}$ as follows: (a) $N_g = 50$, $\mathcal{R} = \text{OT10}$, (b) $N_g = 25$, $\mathcal{R} = \text{OT26}$, (c) $N_g = 50$, $\mathcal{R} = \text{T16}$, (d) $N_g = 50$, $\mathcal{R} = \text{T4}$.

3.3.3 [2 : 2 : 2] *Dynamical Profiles*

Figures 3.46-3.49 show typical profiles of several key dynamic measures for rules belonging to classes 1 and 2. Their behavior on $\mathcal{L}_r$ is known to consist of relatively short transient times leading to any number of cycles of short length.

Since there can be no meaningful global information exchange between distant sites, we can guess that these rules are effectively ignorant of the precise structure of a given graph. It is not surprising, therefore, to find that the relatively simple behavior occurs generally throughout the spectrum of structurally similar graphs and is not merely confined to $\mathcal{L}_r$ topologies.

Except for occasional bursts of irregularity when specific measures are particularly sensitive to the topology and may show unexpectedly large absolute deviations, range independent *class-2* rules generally possess *regular, predictable profiles* which are relatively insensitive to exact g_i topologies.

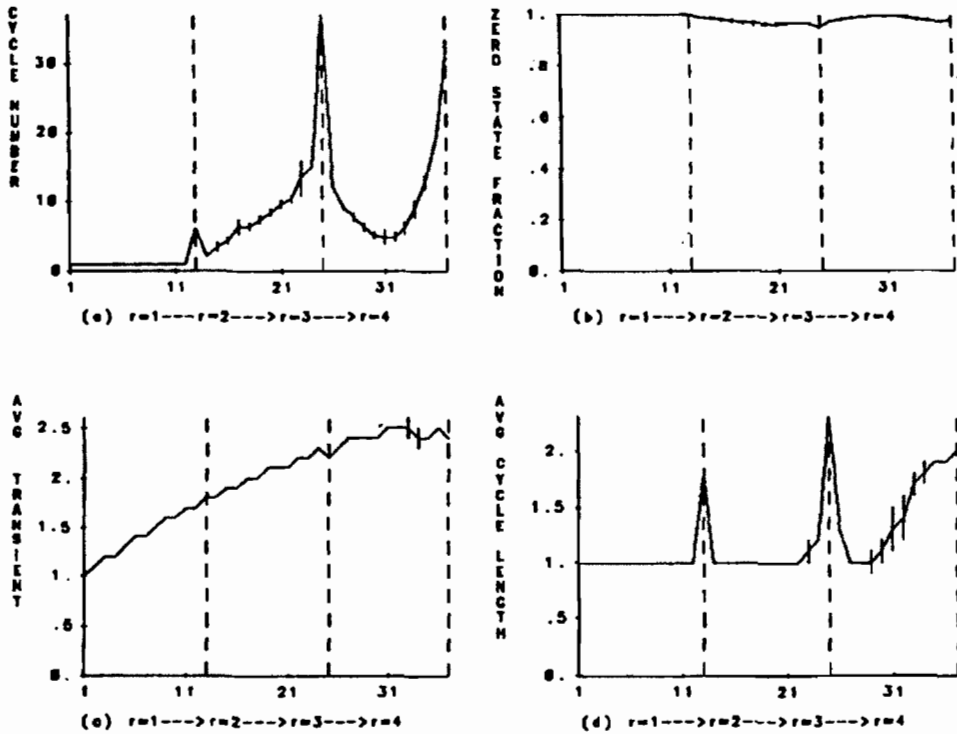


Fig. 3.47 Four additional dynamical measures for the system defined in figure 3.46-c: $N = 12$, $N_g = 50$ and $\mathcal{R} = \mathbf{T16}$. The zero state fraction refers to the fraction of initial states $\Sigma_0 \rightarrow 0$.

Despite this apparent simplicity, however, we nonetheless observe a rich variety of transitional behaviors. Compare the very smooth decay of $S_g^{\mathbf{OT10}}$ in figure 3.46-a), for example, to the much more complex behaviors of $S_g^{\mathbf{T16}}$ and $S_g^{\mathbf{T4}}$ in figures (3.46-c,d) (note that $\mathbf{T16}$ is *class-1* for $r=1$).

Note that the *form* of development of these systems from *left to right* remains approximately constant over the range of sizes sampled ($8 \leq N \leq 16$), which may therefore represent *characteristic signatures* of behavior by which specific rules evolving larger systems may be identified. It is clear that even at this relatively primitive level of behavioral complexity there nonetheless already exists an unexpected dynamic richness.

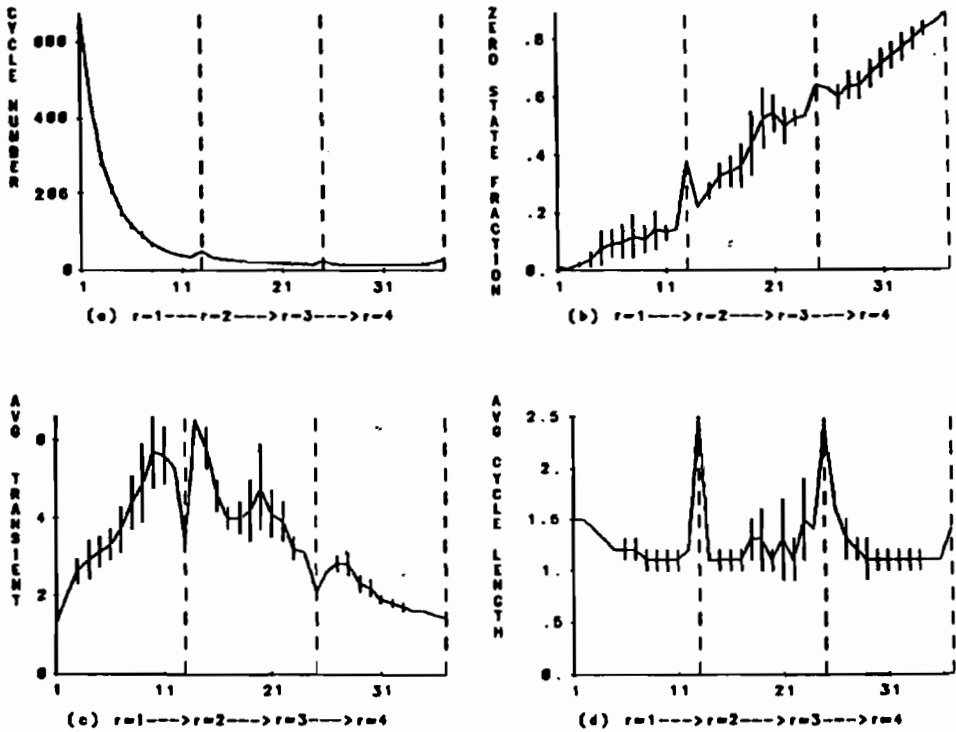


Fig. 3.48 Four additional measures for the system defined in figure 3.46-b: $N = 12$, $N_g = 25$ and $\mathcal{R} = \text{OT26}$.

Certain measures respond particularly strongly to the intrinsic structural symmetry of $\mathcal{L}_r$ lattices: *cycle number* ($\equiv |\mathcal{C}|$) enumeration, for example, *does not* identify two cycles all of whose states are related by a spatial translation. Specific profiles may, therefore, be interrupted by a series of pronounced peaks at $\mathbf{g}_i = \mathcal{L}_r$ (see figures (3.47-a,d), (3.48-d) and (3.49-a), for example).

Special behavior, however, is not necessarily restricted to $\mathcal{L}_r$, as certain *intermediate* topologies, such as the random $\mathbf{g}_i$ positioned roughly midway between $\mathcal{L}_2$ and $\mathcal{L}_3$ for which there is a relative minimum of S_g^{T16} in figure 3.46-c, are occasionally singled out.

3.3.4 [3 : 3 : 3] Dynamical Profiles

[3 : 3 : 3] profiles typically have the following characteristics:

1. There is a large range of individual profiles, most of which have complex structure. Knowing a given rule's behavior just on $\mathcal{L}_r$ lattices generally tells us very little about its generic dynamic properties: two rules having approximately the same measure values on $\mathcal{L}_r$ topologies, for example, often exhibit significantly different behaviors on surrounding graphs.

2. Although $[3 : 3 : 3]$ profiles are more sensitive to system size than those for $[2 : 2 : 2]$ rules, the essential characteristics of their general form appear to remain unchanged over the set of sizes sampled.

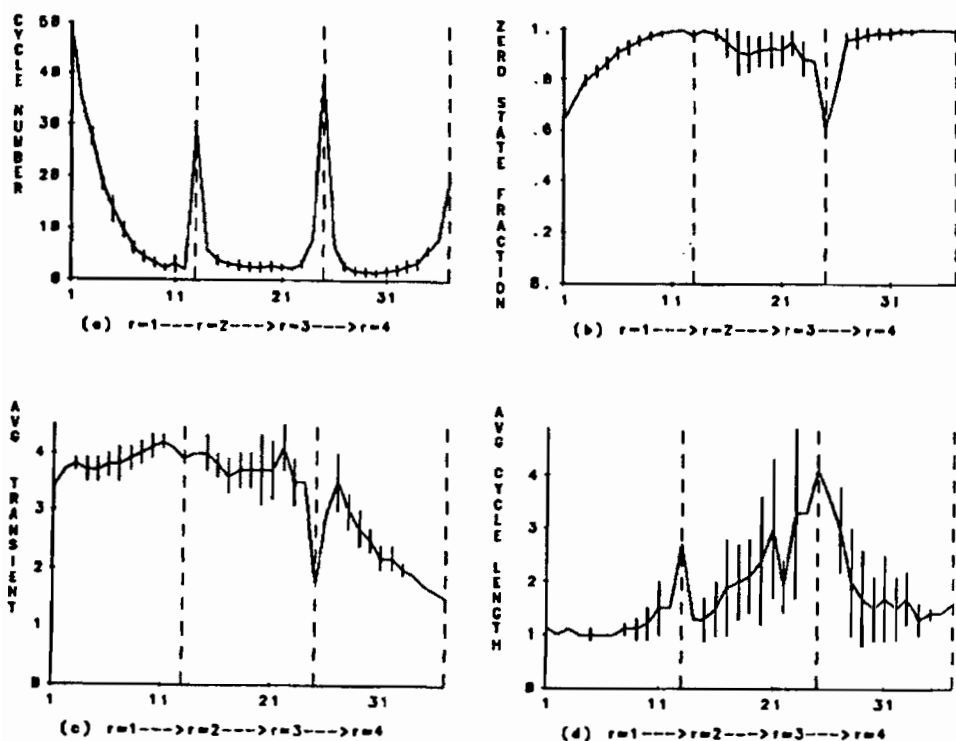


Fig. 3.49 Four additional measures for the system defined in figure 3.46-d: $N = 12$, $N_g = 50$ and $\mathcal{R} = \mathbf{T4}$.

3. There is a strong dependence on the exact lattice structure: intermediate topologies typically have large measure fluctuations.

4. *Minimal* and *maximal* values of particular measures typically occur for $\mathbf{g_i} = \mathcal{L}_r$.

5. If we *define* systems as being ‘complex’ or ‘chaotic’ by their having only small numbers of cycles with long periods, then, for most of the small size systems studied here, it is upon the intermediate topologies that the most complex dynamics takes place: when compared with the behaviors on surrounding graphs, dynamical complexity appears to be *inhibited* by $\mathcal{L}_r$ lattices.

3.3.5 Dynamical Profiles for Range Dependent Rules

A few *class-2* $\rightarrow$ *class-3* transitions are $\mathcal{L}_r$ -*symmetry* dependent. For example, while the observed behavior of certain rules on $\mathcal{L}_3$ may be different from $\mathcal{L}_2$, the dynamics on all *intermediate* and *succeeding* topologies may, in fact, remain of the

same class. The $\mathcal{L}_r$ behavior can in these cases be considered *anomalous* and does not truly represent the generic complexity of a specific rule.

Most transitions are indicative of a true behavioral change. Whether this change occurs spontaneously at a certain $\mathcal{L}_r$, at which point the dynamics is converted to a new class and maintained thereafter, or develops gradually for the intermediate topologies, appears to be an intrinsic property of the chosen rule.

3.3.6 Discussion

This section has focused on the evolution of the behavioral response of rules from pure *range- r* to *range- $r + 1$* 1-dimensional lattices. We have seen a few plots of certain global dynamic measures for sequences of structurally similar graphs, starting from a simple 1-dim lattice and including *range- $2, 3$ and 4* lattices upon which the dynamics is well cataloged. These plots provide a series of dynamic profiles with which a more complete specification of the intrinsic behaviors of rules can be made. *Class-3* rules evolving on a *range- r* topology, for example, can (depending on the size) display an apparently trivial dynamics; they are nonetheless distinguished from less *complex* rules by exhibiting strong behavioral variation on all nearby topologies. Because much of the generic behavior on pure *range- r* lattices actually stems from their intrinsic structural symmetries, a number of profiles display peaks or troughs at those topologies. We will continue our discussion of the CA dynamical dependence on the underlying lattice topology in section 5.4, where we examine this interesting question *analytically* for CA whose state space is a finite field.

3.4 Two-dimensional Systems

The formal study of CA really began not with the simpler one-dimensional systems discussed in the previous section but with von Neumann's work in the 1940's with self-reproducing two-dimensional CA [vonN66]. Such systems also gained considerable publicity (as well as notoriety!) in the 1970's with John Conway's introduction of his *Life* rule and its subsequent popularization by Martin Gardner in his *Scientific American* "Mathematical Games" department [gardner83] (see section 3.4.4).

We recall from section 2.2.2 that two dimensional CA may be defined on a variety of different lattices and can use many different neighborhood structures (see figure 3.50). The neighborhood structures are clearly related to the symmetries of the underlying lattice. If we restrict ourselves only to lattices that possess both rotational and translational symmetry about each site, for example, we see that we can define CA on *hexagonal* (i.e. 3-neighbor), *square* (i.e. 4-neighbor) or *triangular* (i.e. 6-neighbor) lattices. The most commonly studied square (or so-called *Euclidean*) lattice neighborhoods include the *von-Neumann* neighborhood, consisting of the four site horizontally and vertically adjacent to the center site of interest, and the *Moore* neighborhood, consisting of all eight sites immediately adjacent to the

Rule Type	<i>von-Neumann</i>	<i>Moore</i>	<i>Hexagonal</i>
General	$4 \cdot 10^9$	10^{154}	$3 \cdot 10^{38}$
Reflection symmetric	$2 \cdot 10^7$	$5 \cdot 10^{86}$	10^{22}
Rotation symmetric	4096	10^{42}	$2 \cdot 10^{19}$
Completely symmetric	4096	$5 \cdot 10^{30}$	$3 \cdot 10^8$
Outer-Totalistic	1024	$3 \cdot 10^5$	16384
Totalistic	32	512	128

Table 3.6 Numbers of possible rules of various types for $k = 2$ two-dimensional CA with specified neighborhood structures.

center site. Their explicit forms are given as follows:

$$\left\{ \begin{array}{l} \text{von-Neumann: } \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i,j}^{(t)}, \sigma_{i-1,j}^{(t)}, \sigma_{i+1,j}^{(t)}, \sigma_{i,j-1}^{(t)}, \sigma_{i,j+1}^{(t)}) \\ \text{Moore: } \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i-1,j-1}^{(t)}, \sigma_{i,j-1}^{(t)}, \sigma_{i+1,j-1}^{(t)}, \sigma_{i-1,j}^{(t)}, \sigma_{i,j}^{(t)}, \\ \sigma_{i+1,j}^{(t)}, \sigma_{i-1,j+1}^{(t)}, \sigma_{i,j+1}^{(t)}, \sigma_{i+1,j+1}^{(t)}) \end{array} \right. \quad (3.73)$$

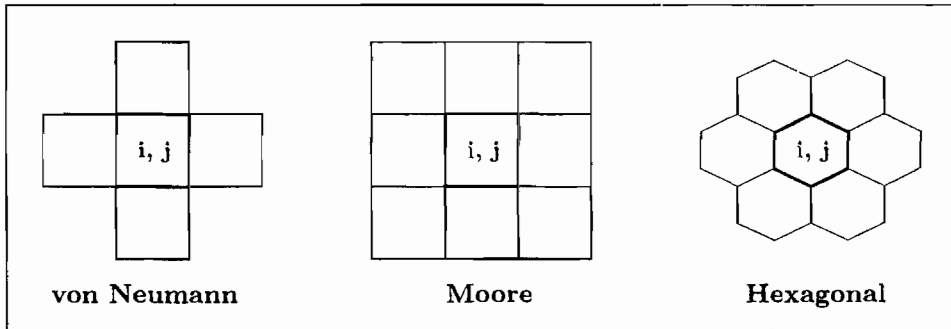


Fig. 3.50 A few examples of possible two-dimensional neighborhoods of site ' i, j '.

Triangular and hexagonal lattices (which, along with the *von-Neumann* neighborhood, may be considered as special cases of the nine-neighbor *Moore* neighborhood), can also be used. *Totalistic* (T), *outer-totalistic* (OT), and *additive* rules are defined exactly as in the one-dimensional case, while *legal* rules may now be generalized to include rotation, reflection, and completely symmetric rules. The various numbers of such two-dimensional rules, for $k = 2$, are given in table 3.6. It is clear from this table that, unless a sufficient number of restrictions are placed upon the rules, it is in general a hopelessly impossible task to even contemplate an exhaustive analysis of all possible rules for a given lattice and neighborhood structure.

The description and overview of (mostly generic) two-dimensional systems given in this section focuses mainly on T- and OT- type rules. For the *von-Neumann*

neighborhood, for example, these rules are defined as follows:

$$\left\{ \begin{array}{ll} \text{Totalistic:} & \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i,j}^{(t)} + \sigma_{i-1,j}^{(t)} + \sigma_{i+1,j}^{(t)} + \sigma_{i,j-1}^{(t)} + \sigma_{i,j+1}^{(t)}) \\ \text{Outer-Totalistic:} & \sigma_{i,j}^{(t+1)} = \phi(\sigma_{i,j}^{(t)}, \sigma_{i-1,j}^{(t)} + \sigma_{i+1,j}^{(t)} + \sigma_{i,j-1}^{(t)} + \sigma_{i,j+1}^{(t)}). \end{array} \right. \quad (3.74)$$

It turns out, rather fortuitously, that if the desire is to merely obtain an overview of the general types of possible two-dimensional behaviors, then focusing only on **T**- and **OT**- type rules is not really a restriction, as the set of all possible behaviors is well represented. Having said that, we should be quick to point out that if the desire is instead to study either a class of CA systems with a special set of behavioral characteristics or to find an appropriate CA model for a real physical system, specific rules and/or lattice connectivities and neighborhoods will have to be invented. For our brief introductory look in this section at generic two-dimensional behavior, however, we will be content to restrict ourselves (for the most part) to commentary on **T**- and **OT**- type rules.

Generalizing the **T** and **OT** rule-codes given for one-dimensional systems in equations 2.38 and 2.39 (see section 2.2.1), respectively, k -state two-dimensional **T** and **OT** rules can be conveniently specified by the rule codes **T** $[\phi_{\text{tot}}]$ and **OT** $[\phi_{\text{out-tot}}]$, given by

$$\left\{ \begin{array}{ll} \mathbf{T}[\phi_{\text{tot}}] & = \sum_{0 \leq n \leq |\mathcal{N}_{ij}|} \phi_{\text{tot}}(n) k^n, \\ \mathbf{OT}[\phi_{\text{out-tot}}] & = \sum_{\substack{0 \leq n \leq |\mathcal{N}_{ij}|-1 \\ 0 \leq \alpha \leq k}} \phi_{\text{out-tot}}(\alpha, n) k^{\alpha+kn}, \end{array} \right. \quad (3.75)$$

where $|\mathcal{N}_{ij}|$ is the number of sites in the neighborhood of site (i, j) . The totalistic rule $\phi_{\text{tot}} : \sigma_{i,j}^{(t)} \rightarrow \sigma_{i,j}^{(t+1)} = \sum_{\sigma \in \mathcal{N}_{ij}} \sigma_{i,j}^{(t)} \text{ modulo } 2$, as defined on the von-Neumann neighborhood, for example, can be more concisely labeled by the code **T42**. Similarly, Conway's infamous *Life*-game CA (see section 3.4.4) is defined by the code **OT224**.

The extension of generic CA systems to two dimensions is significant for two reasons: first, the extension brings with it the appearance of many new phenomena involving behaviors of the boundaries of, and interfaces between, two-dimensional patterns that have no simple analogs in one-dimensional systems. Secondly, two-dimensional dynamics make it an easy (sometimes *trivial*) task to compare the time behavior of such CA systems to that of real physical systems. Indeed, as we shall see in later sections, models for dendritic crystal growth, chemical reaction-diffusion systems and a direct simulation of turbulent fluid flow patterns are in fact specific instances of 2D CA rules and lattices.

In this brief overview section we follow closely Packard and Wolfram's exploratory study [packard85], which the interested reader should consult for more details.

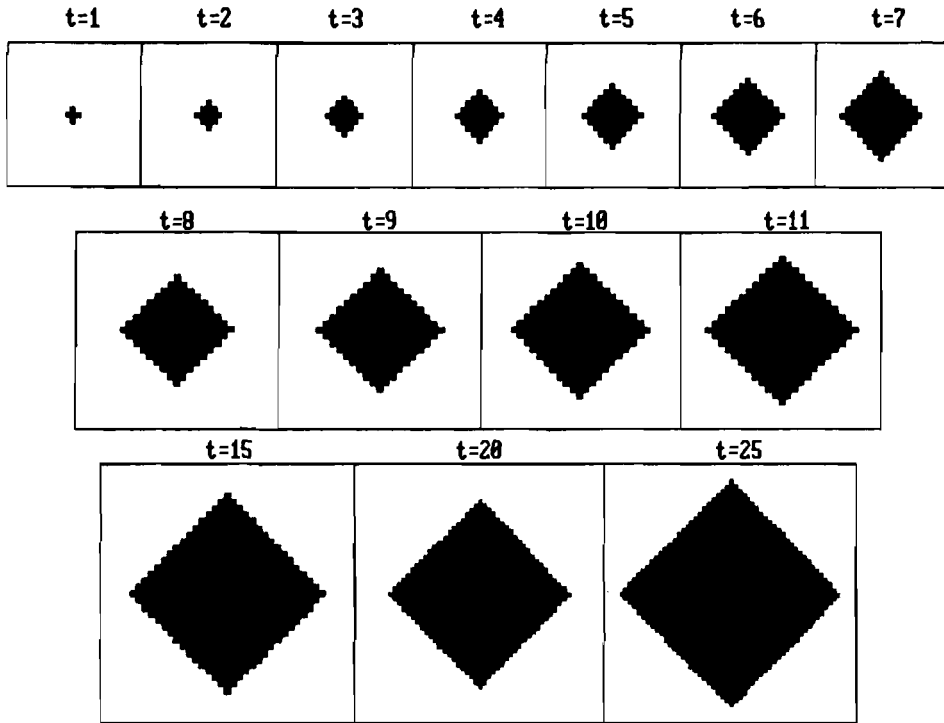


Fig. 3.51 A few Snapshots of two-dimensional von-Neumann neighborhood totalistic rule $\sum = 1, 2, 3, 4 \rightarrow 1$.

3.4.1 Simple Seeds

As with our earlier discussion of one-dimensional systems we begin by looking at the binary (i.e. $k = 2$) patterns that emerge from simple seeds, by starting off our CA systems with at most a few non-zero sites. Figures 3.51-3.57 show some typical examples of such patterns. In each figure, the evolution starts from a single non-zero site at the center of either a 4-neighbor *von-Neumann* or 8-neighbor *Moore* lattice. Snapshot views of the entire lattice are shown for times $1 \leq t \leq 25$.[†]

[†]Note that for times $15 \leq t \leq 25$, successively greater portions of the underlying lattice are actually included within the spatial 'windows' (enclosed within the outlined squares) corresponding to a given time, but that these windows are not drawn to scale. The square for $t = 15$, for example, shows only the sites $14 \leq i, j \leq 52$; the square for $t = 20$ shows only the sites $6 \leq i, j \leq 60$ and the square for $t = 25$ shows only the sites $5 \leq i, j \leq 61$. The actual lattice is of size 67×67 .

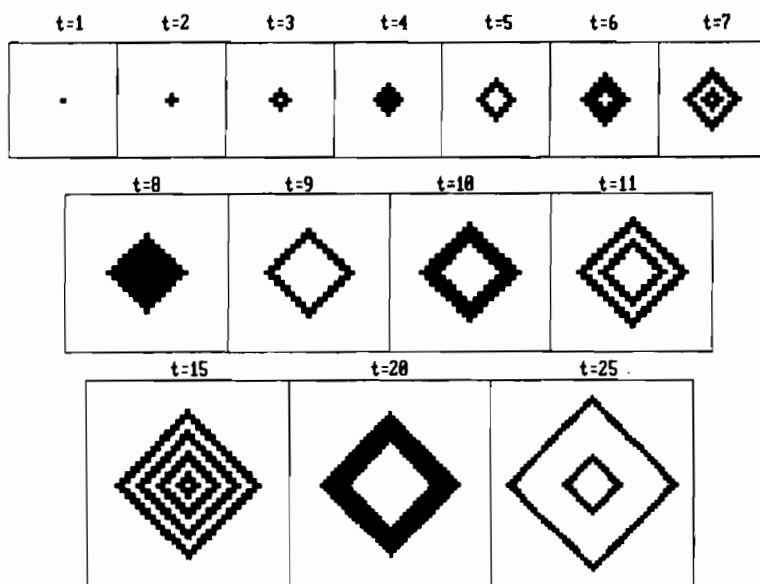


Fig. 3.52 A few Snapshots of two-dimensional von-Neumann neighborhood totalistic rule $\sum = 1, 2, 3, 4 \rightarrow 1$.

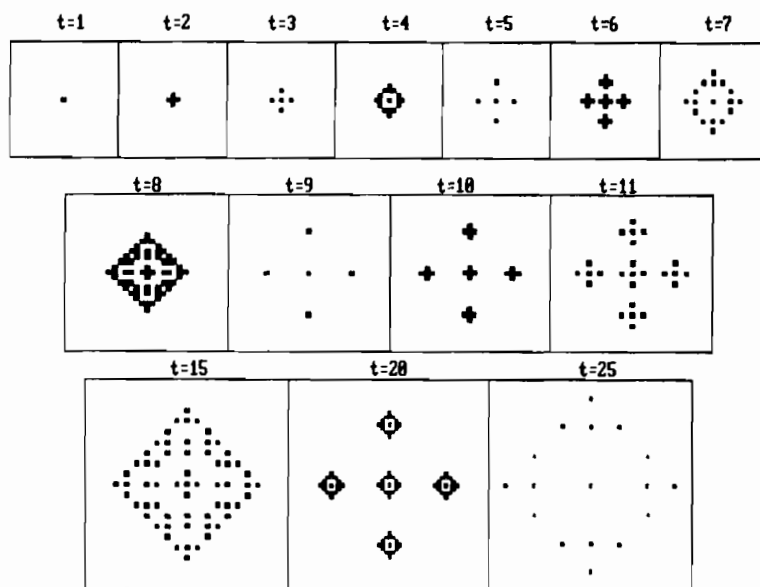


Fig. 3.53 A few Snapshots of two-dimensional Moore neighborhood totalistic rule $\sum = 1, 2, 3, 4 \rightarrow 1$.

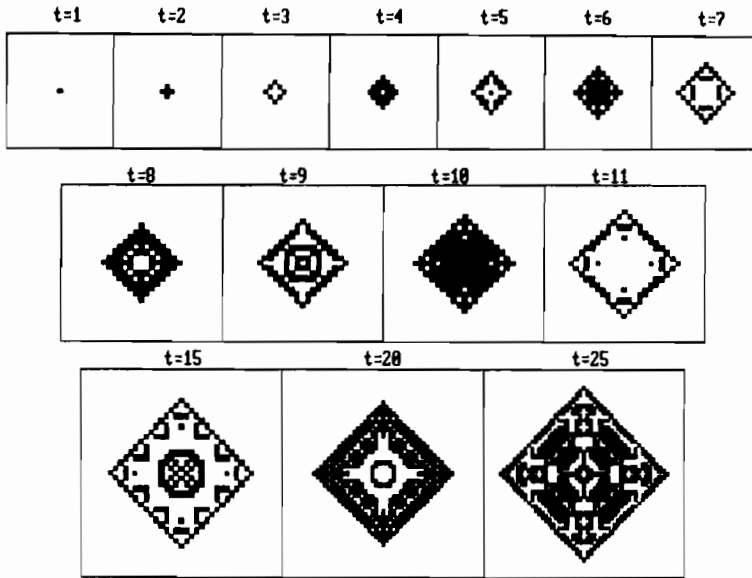


Fig. 3.54 A few Snapshots of two-dimensional von-Neumann neighborhood outer-totalistic rule $\sum_0 = 1, 2, 3, 4 \rightarrow 1$, $\sum_1 = 0, 2 \rightarrow 1$.

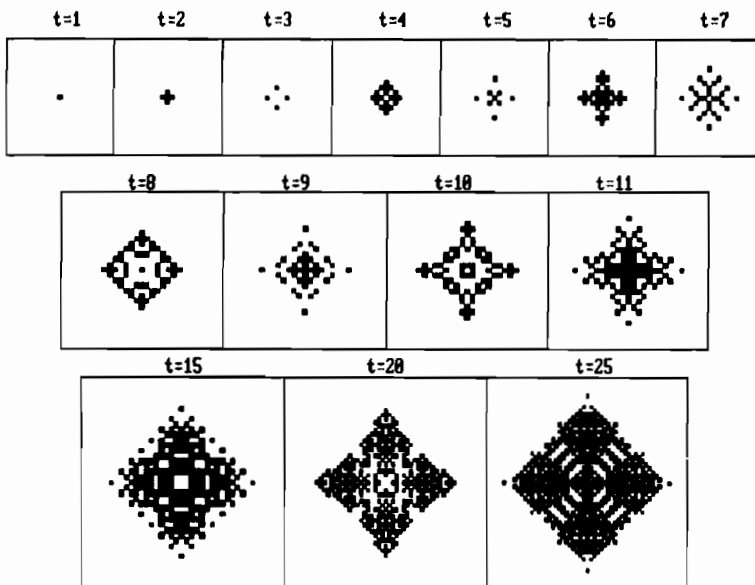


Fig. 3.55 A few Snapshots of two-dimensional von-Neumann neighborhood totalistic rule $\sum = 1, 3, 4 \rightarrow 1$.

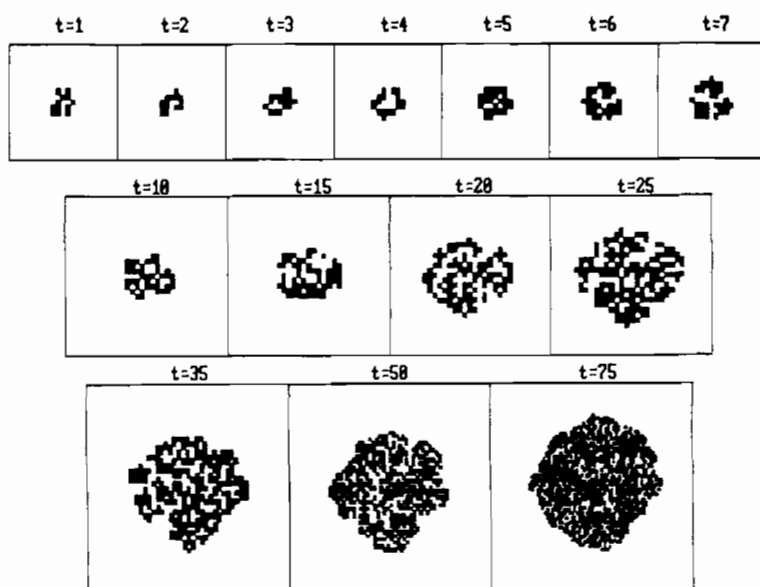


Fig. 3.56 A few Snapshots of two-dimensional Moore neighborhood outer-totalistic rule $\sum_0 = 3, 6, 7 \rightarrow 1$, $\sum_1 = 2, 3, 4, 6, 8 \rightarrow 1$.

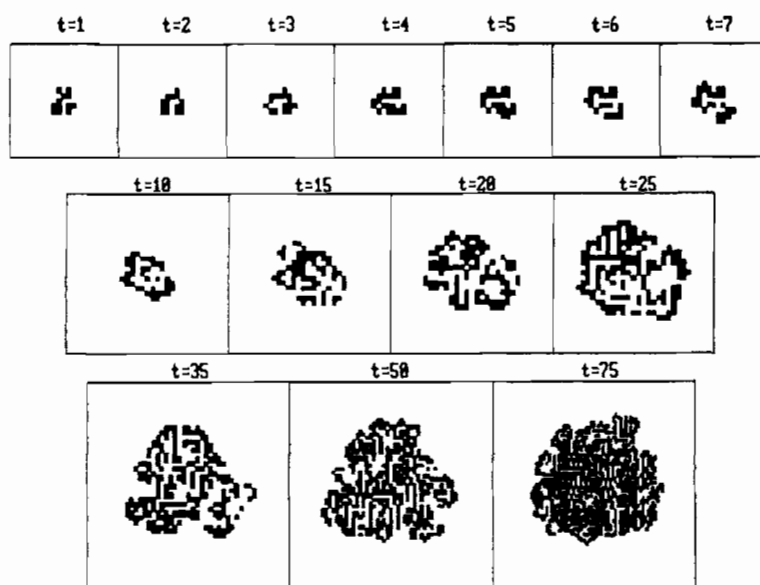


Fig. 3.57 A few Snapshots of two-dimensional Moore neighborhood outer-totalistic rule $\sum_0 = 3 \rightarrow 1$, $\sum_1 = 2, 3, 4 \rightarrow 1$.

3.4.2 Random Seeds

Figures 3.58 and 3.59 show some typical space-time patterns of two-dimensional rules starting from random initial states. The figures show snapshots of runs taken at times $t = 1, 5, 10, 25, 50$ and a cross-sectional view of the y -axis sites taken along an arbitrarily selected x site value for all times $t = 1$ through $t = 50$.

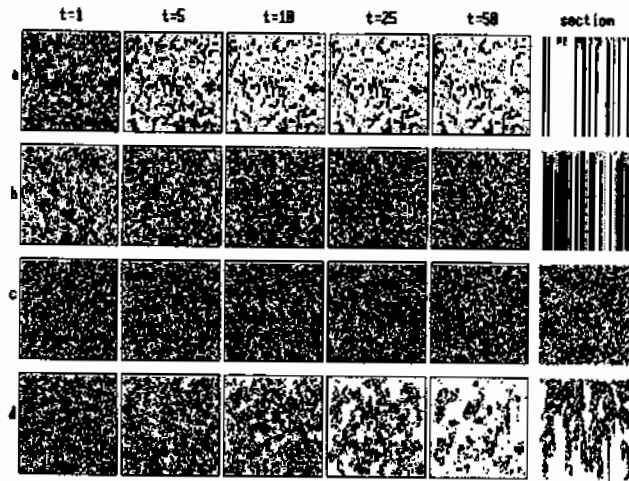


Fig. 3.58 Snapshots of four two-dimensional von-Neumann neighborhood outer-totalistic rules: (a) $(\sum_0 = 0, 3; \sum_1 = 0, 2, 3 \rightarrow 1)$, (b) $(\sum_0 = 0, 4; \sum_1 = 2, 3, 4 \rightarrow 1)$, (c) $(\sum_0 = 1, 3; \sum_1 = 0, 2, 4 \rightarrow 1)$, and (d) $(\sum_0 = 2, 4; \sum_1 = 1, 3, 5 \rightarrow 1)$.

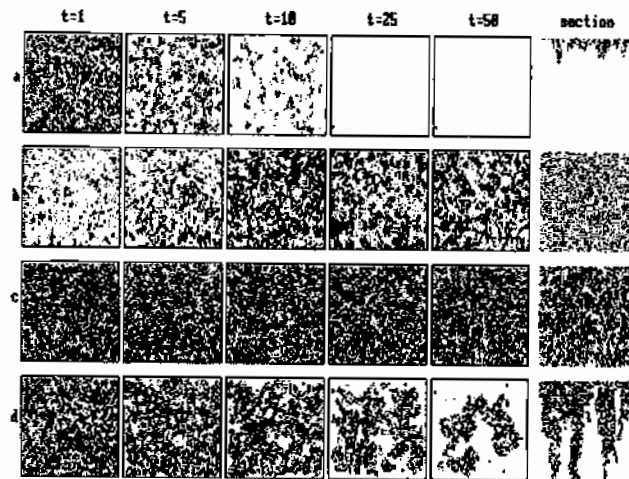


Fig. 3.59 Snapshots of four two-dimensional Moore neighborhood outer-totalistic rules: (a) $(\sum_0 = 3, 5; \sum_1 = 3, 6, 7 \rightarrow 1)$, (b) $(\sum_0 = 1, 2, 7; \sum_1 = 2 \rightarrow 1)$, (c) $(\sum_0 = 2, 5, 7, 8; \sum_1 = 2, 4, 5 \rightarrow 1)$, and (d) $(\sum_0 = 3, 4; \sum_1 = 3, 6, 8 \rightarrow 1)$.

3.4.3 Voting Rules

Voting rules are rules that update center-site values according to the “popularity” of the values found in their local neighborhood. Each site in the neighborhood is given one “vote” as to whether to update the center-site with a particular value, and the center-site is given the voted-on value on the next time step only if the number of votes exceeds some threshold. Confining our attention to binary (i.e. $\sigma = 0$ or 1) systems, voting rules are therefore of the general form

$$\sigma(t+1) = \begin{cases} 1 & \text{if } \sum_{\sigma_j \in \mathcal{N}(i)} \sigma_j \geq \tau, \\ 0 & \text{else,} \end{cases} \quad (3.76)$$

where τ is the threshold and $\mathcal{N}(i)$ is the neighborhood around site i .

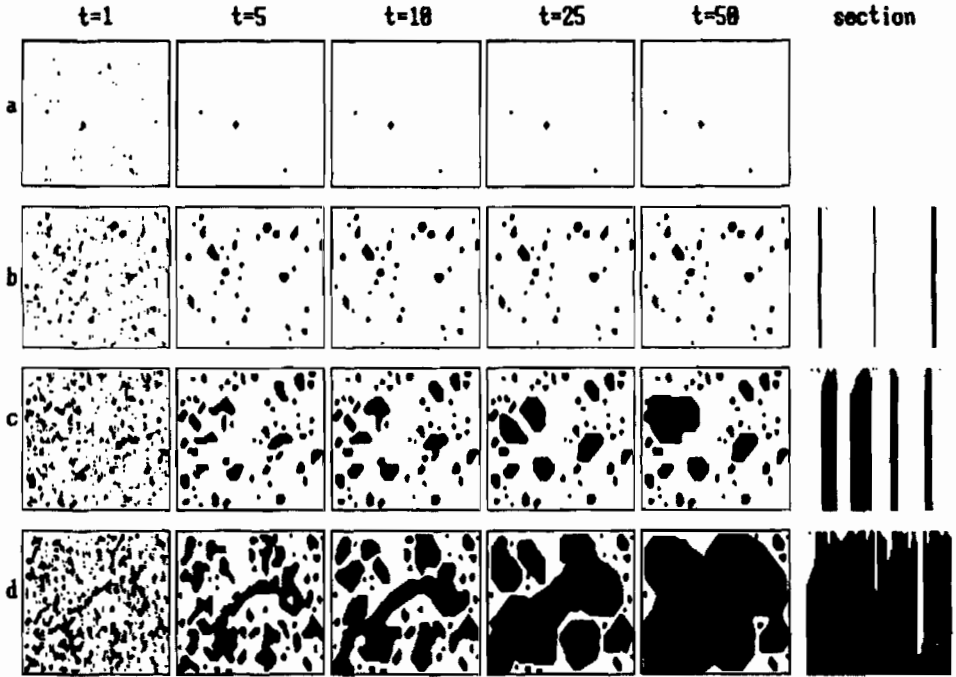


Fig. 3.60 Some snapshots of the evolution of an 8-neighbor Moore neighborhood voting rule $\sum \geq 4$; the initial densities are (a) $\rho = 0.1$, (b) $\rho = 0.15$, (c) $\rho = 0.25$ and (d) $\rho = 0.3$.

Although the first detailed observations of the behavior of such rules were made in a series of papers by Vichniac in the middle 1980's ([vich84], [vich86a], and [vich88]), voting rules are but a special case of the threshold-rules used in neural-networks, dating back to McCulloch and Pitts' original (c.1943) neuron [mccul43]. An important theoretical tool used for studying these systems is the *Lyapunov* (or *Energy*) function ([goles81], [goles85]), and will be discussed in section 5.5.

Modifying Vichniac's [vich84] original notation only slightly, we will refer to a general voting rule of the form given in equation 3.76 by writing $\chi\tau$, where

$X = V, V', M$, or M' if $\mathcal{N}$ is the von Neumann, von Neumann with center-site excluded, Moore or Moore with center-site excluded neighborhoods, respectively.

Of particular interest is the long-term behavior of voting-rule systems, which turns out to very strongly depend on the initial density of sites with value $\sigma = 1$ ($= \rho$). While all such systems eventually become either stable or oscillate with period-two,[†] they approach this final state via one of two different mechanisms: either through a *percolation* or *nucleation* process. Figure 3.60 shows a few snapshots of a Moore-neighborhood voting rule $\sum \geq 4$ for $\rho = 0.1, 0.15, 0.25$ and 0.3 .

3.4.3.1 Percolating Rules

If the sites of a lattice are randomly colored either black (with probability p_{black} or white (with probability $p_{\text{white}} = 1 - p_{\text{black}}$) then there exists a *percolation threshold* p_c , such that if, say, $p_{\text{black}} < p_c$, the lattice consists of isolated clusters of black sites immersed in a white ‘sea’, and if $p_{\text{black}} > p_c$, a connected black structure *percolates* (i.e. spans) the entire lattice.

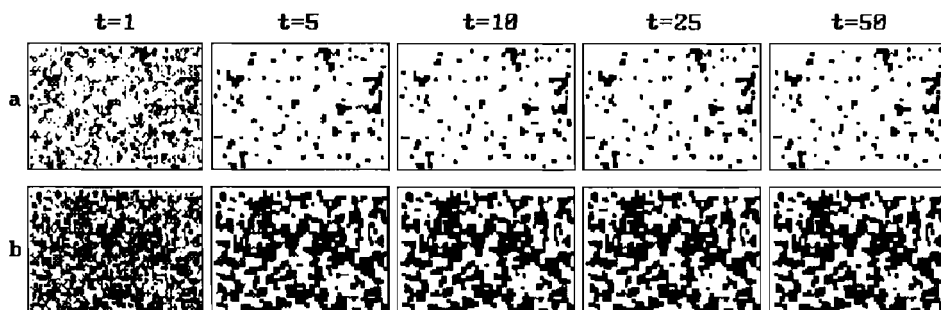


Fig. 3.61 Some snapshots of the evolution of a 5-neighbor von Neumann neighborhood *percolating* voting rule $V3$; the initial densities are (a) $\rho = 0.35 < \rho_c$ and (b) $\rho = 0.50 = \rho_c$.

Voting rule systems approaching their final state through percolation display much of this same behavior. There is a critical initial density, ρ_c , such that for $\rho > \rho_c$, a connected network of $\sigma = 1$ valued sites ‘percolates’ through the lattice. If $\rho < \rho_c$, on the other hand, a similar $\sigma = 0$ valued lattice-spanning structure percolates through the lattice. In either case, the set of sites with the *minority* value consists of a disconnected sea of isolated islands, and a finite number of islands persist to the system’s final state as long as the initial density $\rho > 0$.

Figure 3.61 shows a few steps in the contrasting evolutions of the percolating voting-rule system $V3$ when $\rho < \rho_c$ and $\rho \sim \rho_c$.

3.4.3.2 Nucleating Rules

‘Nucleation’ is a term that naturally arises in the study of dynamical critical phenomena, which is concerned not so much with the equilibrium properties of a sys-

[†]That these are the *only* two possible fates of voting-rule systems is due to a theorem by Goles [goles85]; it is discussed in chapter 5.

tem, but with the effects of *fluctuations about that equilibrium* (such as determining how quickly equilibrium is reestablished once the system is perturbed away from it). Suppose, for example, that a fluid is enclosed in a sealed container, its temperature T is sufficiently high and its mean density ρ is sufficiently low that the system exists in a disordered vapor phase. If the temperature is quickly lowered (or *quenched*) below the liquid-vapor coexistence temperature $T_c(\rho)$, small droplets of liquid will begin appearing. If ρ differs greatly from the critical density ρ_c , the emerging droplets will occupy only a very small fraction of the available volume. This kind of phase separation is called *nucleation*. In the special case when the system is prepared at its critical density, the same quench gives rise to different type phase separation called *spinodal decomposition*; in this case, the quench gives rise to two phases having roughly equal volumes.

Similarly, in the study of crystals, nucleation is a fluctuation phenomenon by which a new crystal phase begins growing. A new phase begins growing in a given medium when the appropriate thermodynamic variables (such as temperature, pressure, etc.) have strayed sufficiently far from their equilibrium values. There appears to be a critical “embryo size” for nucleation to occur: particles that are larger than this critical size tend to continue growing, whereas smaller particles have a tendency to dissolve. Note that nucleation exhibits some of the typical universal behavior near the critical point. For example, the radius of the emerging droplets grows as a power of time after the quench [vich86b].

Some CA voting rule systems undergo a very similar nucleation-like process. In the such systems, the approach to the asymptotic state is effectively determined by the convex-hull forming nature of the rules. That is to say, rules of this kind are such that the growth of local clusters proceeds by the filling in of all concavities in the cluster’s structure. Growth stops only when the convex-hull surrounding an original cluster structure is entirely filled. Larger clusters may form when two or more smaller clusters merge while filling in their own concavities.

Figure 3.62 shows how two rectangular convex-hulls may merge in a system evolving according to the 4-neighbor (excluded center-site) von Neumann neighborhood voting rule $V'2$:

$$\sigma(t+1) = \begin{cases} 1 & \text{if } \sum_{j \in \mathcal{N}'(i)} \sigma_j \geq 2, \\ 0 & \text{else.} \end{cases} \quad (3.77)$$

The solid L-shaped pattern on the bottom-left will fill its convex-hull (denoted by the thin dashed lines extending the pattern above and to the right) and eventually merge with the upper-right pattern’s own convex-hull (indicated by thin dashed lines extending that pattern below and to its right). Once merged, the two initially separated patterns will form a single cluster filling the larger convex hull (indicated by the thick dashed lines surrounding the two patterns). This newly formed larger cluster may itself merge with other clusters until either no more clusters remain to be met or the lattice becomes completely filled by this process.

Whether this cluster-merging continues on forever depends critically on the ini-

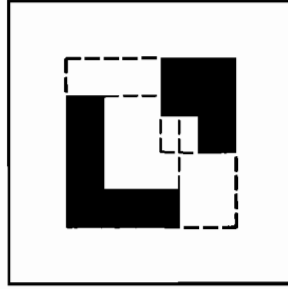


Fig. 3.62 An example of overlapping convex-hulls in the 4-site (center-site excluded) von Neumann neighborhood voting rule with threshold = 2; see equation 3.77.

tial density, ρ . For $\rho < \rho_c \sim 0.133$ [vich84], for example, the convex hulls generally stop growing before they have had a chance to merge and the final state consists of isolated convex-hull islands immersed in an ocean of $\sigma = 0$ sites. For $\rho > \rho_c$, on the other hand, all of the convex hulls initially randomly distributed throughout the lattice eventually fully merge, so that the final state consists entirely of $\sigma = 1$ sites.

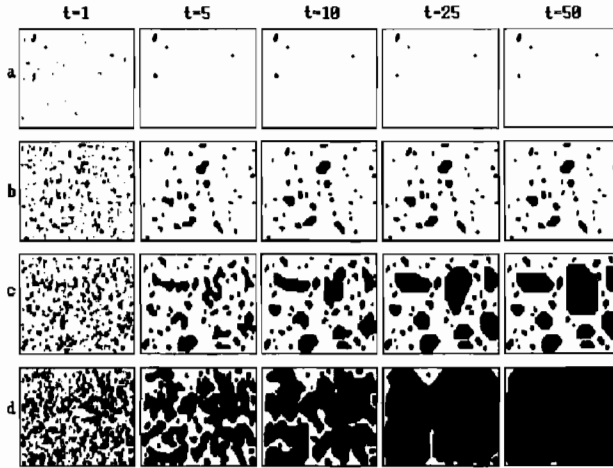


Fig. 3.63 Some snapshots of the evolution of a 9-neighbor Moore neighborhood voting rule *M4*. Initial states are random with probability($\sigma = 1$) equal to (a) 0.1, (b) 0.225, (c) 0.275 and (d) 0.35. The critical density for this system is $\rho_c \sim 0.250$; see text.

A similar behavior is obtained in the full 9-neighbor Moore neighborhood rule *M4*:

$$\sigma(t+1) = \begin{cases} 1 & \text{if } \sum_{j \in \mathcal{N}(i)} \sigma_j \geq 4, \\ 0 & \text{else,} \end{cases} \quad (3.78)$$

but with $\rho_c \sim 0.250$ and a more fluid-like nucleation [vich86a] due to smoother truncated-octagon convex-hulls; see figure 3.63.

Table 3.7 lists the critical density and type of process for several von Neumann and Moore neighborhood rules. In the first and fourth columns, the rules are defined by the fractions (m/n) , which specify a threshold of m $\sigma = 1$ sites out of a total of n possible votes. The table entries for ρ_c are taken from published results [vich84] using the CAM-6 hardware simulator [marg87]; whether some or all of these values can be determined analytically remains an open problem.

von Neumann Neighborhood			Moore Neighborhood		
Rule (m/n)	ρ_c	Process	Rule (m/n)	ρ_c	Type
1/4	> 0	nucleation	3/8	> 0	nucleation
2/4	0.133	nucleation	4/8	0.333	nucleation
1/5	> 0	nucleation	3/9	> 0	nucleation
2/5	0.0822	nucleation	4/9	0.250	nucleation
3/5	1/2	percolation	5/9	1/2	percolation

Table 3.7 Critical densities ρ_c and types of processes for a few selected voting rules defined on von Neumann and Moore neighborhoods.

Notice that $\rho_c = 1/2$ exactly for both the von Neumann neighborhood 3/5 rule and Moore neighborhood 5/9 rule. This simple result follows immediately from the $0 \leftrightarrow 1$ symmetry of these *simple majority* rules. A simple majority rule is one in which the total possible number of votes is evenly split between yes ($\sigma = 1$) and no ($\sigma = 0$) votes, and can obviously exist only if the neighborhood size is *odd*.

Infinite Systems: The ultimate fate of infinite systems, in the infinite time limit, is quite different from their finite cousins. In particular, the fate of infinite systems does not depend on the initial density of $\sigma = 1$ sites. In the thermodynamic limit, there will always exist, with probability one, some convex cluster large enough to grow without limit. As $t \rightarrow \infty$, the system thus tends to $\rho \rightarrow 1$ for all nonzero initial densities. What was the critical density for finite systems, ρ_c , now becomes a *spinodal* point separating an unstable phase for $\sigma = 0$ sites for $\rho > \rho_c$ from a *metastable* phase in which $\sigma = 0$ and $\sigma = 1$ sites coexist. For systems in the metastable phase, even the smallest perturbation can induce a cluster that will grow forever.

3.4.3.3 Variations on a Theme

There are a number of simple variations on the basic voting-rule theme. One class of closely-related rules, called “twisted” voting rules [vich86a], is formed by interchanging neighboring slots in the rule-table. For example, the twisted form of the 9 neighbor voting rule *M5* is given by

$$\sigma(t+1) = \begin{cases} 1 & \text{if } \sum_{j \in \mathcal{N}(i)} = 4 \text{ or } \sum_{j \in \mathcal{N}(i)} \geq 6, \\ 0 & \text{else.} \end{cases} \quad (3.79)$$

This simple flipping of two rule-table entries encourages a continual reshuffling between 0 and 1 domains at the boundary, where the majority is marginal; the “frustration” that exists at the boundary effectively prevents the system from ever settling into a stable or simple oscillatory state. The result is a gradual *annealing* to ever smoother boundary layers, a process that Vichniac [vich86b] has likened to a dynamical optimization since the evolution tends to steadily decrease the length of the domain boundaries.[†] Figure 3.64 shows some steps in the evolution of the twisted voting-rule defined above, but these few static pictures simply cannot do justice to the continual undulations of the boundary.

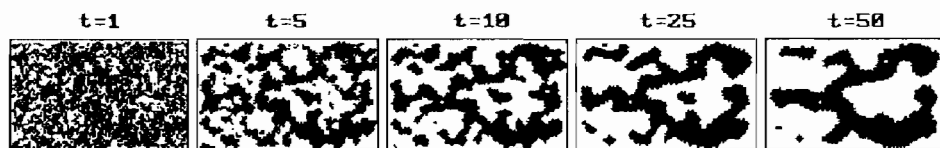


Fig. 3.64 Some snapshots of the evolution of a “twisted” form of the 9-neighbor voting rule $M5$ (see equation 3.79); the initial density $\rho = 0.50$.

Toffoli and Margolus [toff86] point out that what appears on the macroscopic scale is a good simulation of *surface tension*, in which the boundaries behave as though they are stretched membranes exerting a pull proportional to their curvature. Vichniac adds that the behavior of such “twisted” majority rules actually simulates the Allen-Cahn equation of surface tension rather accurately:

$$v_r(P) = -\alpha\kappa(P), \quad (3.80)$$

where $v_r(P)$ is the normal velocity at point P , $\kappa(P)$ is the curvature at P and α is the coefficient of surface tension. That apparent conflict in measuring curvature – which is a local variable but ostensibly needs global information to compute – by a local rule, is resolved by a continual exchange of the information necessary to compute curvature between far-separated sites via Conway-*Life*-like ‘particles’ moving along the boundary [vich88]. As a result, the behavior of each site appears, over time, to have been responded to many more sites than just those in its immediate local neighborhood.

Other variations of the basic voting rule may involve adding small “impurities” or perturbations to otherwise very regular initial conditions, or adding some anisotropies to the vote-counting by, for example, changing the sign of some vote entries. The latter variants typically leads to the creation of metamagnetic structures [vich84].

[†]Unlike conventional simulated annealing, however, in which a system is gradually cooled from a finite temperature and great care must be taken that the system always remains close to equilibrium at all intermediate temperatures, we here *start* at zero temperature.

3.4.4 Conway's Life Rule

Perhaps the single most studied (and joyfully played with)[†] rule – certainly the most famous – is the two-dimensional Moore neighborhood binary-valued CA invented by John H. Conway, and popularized extensively by Martin Gardner in his “Mathematical Games” column in *Scientific American* in the early 1970's ([gardner70], [gardner71], [gardner78]).

Conway, aware of Fredkin's and Ulam's rules defined in the preceding section, wanted to create a rule that would be both as simple to write down and as difficult to predict the behavior of as possible. To this end, Conway concentrated on meeting the following three criteria:

1. There should not exist simple initial patterns that *obviously* grow without limit; it should be difficult to prove that an arbitrary pattern grows forever.
2. There should exist simple patterns that give the *appearance* of growing forever; not all simple initial states should immediately yield trivial final states.
3. There should exist simple patterns that evolve for many iterations before settling into a simple (either stable or oscillatory) final state.

After a great deal of experimentation with many different rules, Conway finally settled on to what is arguably the single-most interesting elementary two-dimensional rule living on a regular lattice (we will shortly define what is meant by ‘interesting’). That this rule has demonstrated such remarkable ‘staying-power’, and continues to surprise and inspire those who ‘play’ with it, is a testament to Conway's deep mathematical intuition.

3.4.4.1 Definition of Life

Displaying no obvious hints as to the truly extraordinary behavioral complexity which dramatically emerges from it, the *Game-of-Life* is deceptively simple to state. Calling cells with value $\sigma = 1$, *alive*, and those with $\sigma = 0$, *dead*, the following definition makes obvious *Life*'s relation to ‘real’ population growth and decay:

$$\left\{ \begin{array}{ll} \text{BIRTH:} & \text{a previously dead cell comes alive if exactly 3 neighbors are alive} \\ \text{DEATH:} & \text{isolated living cells with no more than one live neighbor die;} \\ & \text{those with more than three neighbors die of overcrowding} \\ \text{SURVIVAL:} & \text{living cells with 2 or 3 neighbors survive} \end{array} \right. \quad (3.81)$$

More formally, *Life* is an outer-totalistic (code **OT224**) $k = 2$ rule defined on

[†]At the height of *Life*'s original popularity, *Time* magazine proclaimed in 1974 [time74] that “...millions of dollars in valuable computer time may have already been wasted by the game's growing horde of fanatics.”

the two-dimensional *Moore* neighborhood:

$$\begin{aligned}\sigma_{i,j}(t+1) &= \phi_{\text{LIFE}}[\sigma(t) \in \mathcal{N}_{\text{Moore}}] \\ &= \begin{cases} \sigma_{i,j}(t), & \text{if } \sum_{\sigma \in \mathcal{N}_{\text{Moore}}} \sigma(t) = 2, \\ 1, & \text{if } \sum_{\sigma \in \mathcal{N}_{\text{Moore}}} \sigma(t) = 3, \\ 0, & \text{otherwise,} \end{cases} \end{aligned} \quad (3.82)$$

where $\sum_{\sigma \in \mathcal{N}_{\text{Moore}}} \sigma$ is a sum over all values in the *Moore* neighborhood of a given center site, $\sigma_{i,j}$.

3.4.4.2 What's so Special About Life?

It's probable, given a large enough Life space, initially in a random state, that after a long time, intelligent self-reproducing animals will emerge and populate some parts of the space.

– John H. Conway (1970)

A remarkable, but (at first sight, at least) naively unimpressive, feature of this rule is its class **c4**-like ability to give rise to complex ordered patterns out of an initially disordered state, or *primordial soup*. In figure 3.65, for example, which provides a few snapshot views of the evolution of four different random initial states taken during the first 50 iterations, we see evidence of the same typically class **c4**-like behavior that we have already seen so much of in one-dimensional systems. What distinguishes this system from all of the previous ones that we have studied, however, and makes this rule truly remarkable, is that *Life* has been proven to be capable of *universal computation*.

Although the formal meaning of this statement will be discussed greater detail a bit later in this section, its profound implication is just as easy to appreciate informally. By virtue of being a universal computer, a proper selection of initial conditions can ensure that *Life* can be made to carry out arbitrary algorithmic procedures – i.e., *Life can serve as a general purpose computer!*

Given any mathematical conjecture, $\mathcal{C}$, for example, a finite initial *Life* pattern, Σ_0 , can be found such that $\Phi_{\text{LIFE}}^N[\Sigma_0] = \vec{0}$, for some finite step N , if and only if the conjecture $\mathcal{C}$ is true.

Note that the really interesting thing here is not so much that *Life* can itself be used in place of a standard digital computer to compute $\sqrt{2}$ or a fast-fourier-transform, but what the fact that it can do so *in principle* implies about its latent dynamical complexity. Since, as we shall see, there are fundamental limits on the *predictability* of universal computers – the famous *Halting Theorem*, for example, asserts that there cannot exist a general algorithm for predicting when a computer will *halt* its execution of a given program – the same limits must apply to the general evolution of *Life*.

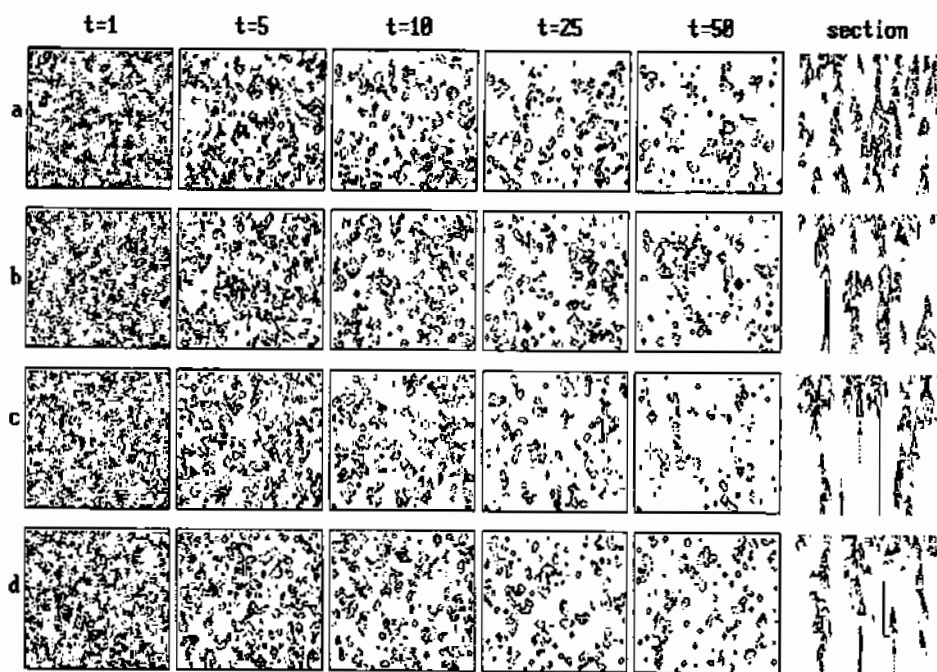


Fig. 3.65 Some snapshots of Conway's *Life* rule; see text.

Translated to *Life*'s terms, this means that one cannot, in general, tell whether a particular starting configuration will eventually die out. *There is no short-cut route to the final outcome of Life's evolution*; the best that can in principle be hoped for is to sit back and patiently await *Life*'s own final outcome. Since *Life* is able to carry out any and all computations that a conventional computer is able to, it can therefore be said that, in this sense, this rather unremarkable seeming rule is actually capable of displaying arbitrarily complicated behavior!

Indeed, upon observing the seemingly unlimited complexity and variety of *Life*'s evolving patterns, it becomes almost impossible to refrain from imagining, along with Conway, that, were the game really to be played on an infinite lattice, there must surely arise true living 'life-forms', perhaps themselves evolving into more complex, possibly sentient, 'organisms'.

Our much more modest and immediate goal in the present section is to provide a brief glimpse of *Life*'s well documented zoology, before setting-the-stage for our later discussion and proof (outlined in section 3.4.5) of its universality.

3.4.4.3 *Life's Zoology*

Since its conception in 1970, the temporal fates of literally thousands of various initial configurations have been analyzed and cataloged. As always, the obvious way to start is by asking what happens to simple seeds.

Simple Seeds and Stable Patterns: First, because live cells survive only if surrounded by 2 or 3 other live cells and dead cells become alive only if surrounded by exactly three live cells, initial states consisting of either *single* or *neighboring* live cells immediately yield the null state. Survival in *Life* therefore requires a minimum of three live cells. Figures 3.66 and 3.67 show the fates of all starting configurations consisting of *three* and *four* live cells.

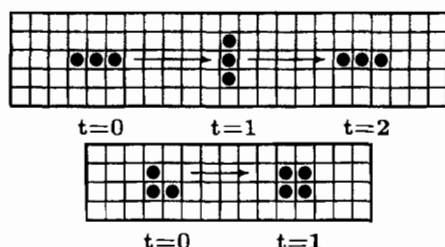


Fig. 3.66 The simple fates of the two three *live-cell* initial states.

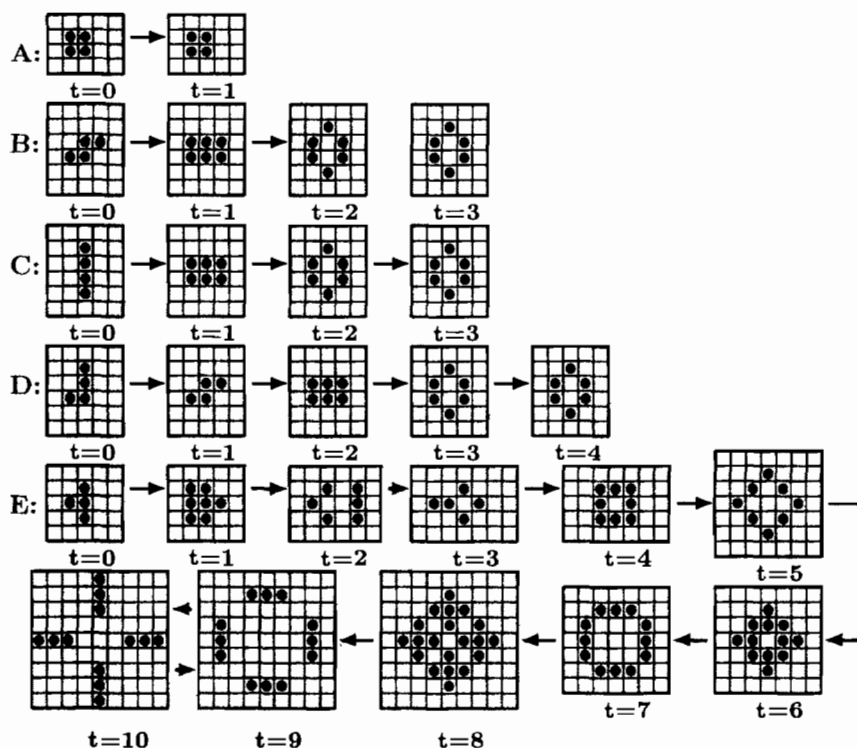


Fig. 3.67 Fates of each of the five possible *four-live cell* initial states. The bottom most state (E) terminates in a period-2 state (at times $t = 9$ and $t = 10$).

The final states of these simple patterns are but a few of the known stable or (small period) oscillatory patterns that have been observed. Figure 3.68 shows all known stable patterns consisting of eight *live* cells or less, while figure 3.69 provides a sampling of a few common period-2 oscillators. Many more patterns with widely differing periods are also known. It is worth noting that the eventual appearance of any of these live-cell clusters does not depend on having simple initial configurations; each of them is in fact a frequent remnant of a *primordial soup* origin.

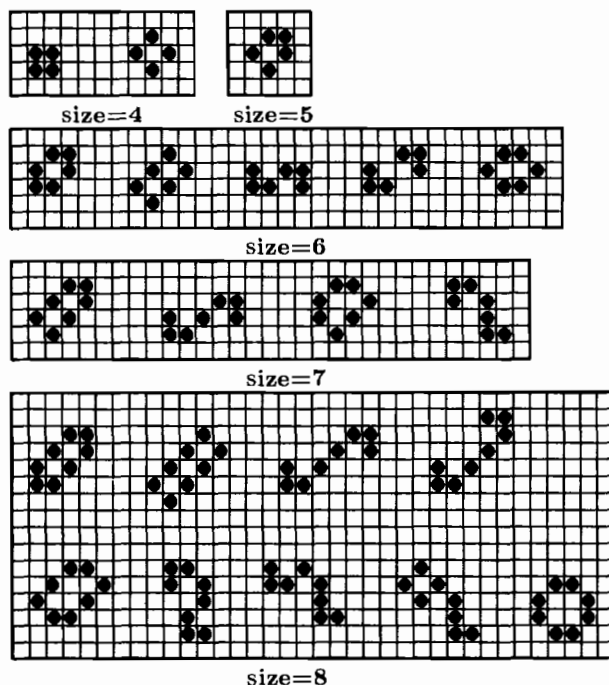


Fig. 3.68 All known stable patterns with eight *live* cells or less.

Of the 12 possible initial states with 5 live cells, 5 yield the null state within $t = 4$ steps, 2 yield a stable state and four lead to the same period two oscillator marking the end of the evolution of state **E** in figure 3.67. In marked contrast to this rather benign behavior, however, the remaining 5-cell pattern – called the *R-pentamino* – evolves in a considerably more dramatic fashion.

From figure 3.70, we see that the *R-pentamino* is in fact wildly unstable, expanding outward and continually undergoing change while scattering various bits



Fig. 3.69 A sampling of period-two patterns under Conway's *Life* rule.

of 'debris' in all directions. This continues for 1103 iterations steps (a portion of the final pattern of which appears in figure 3.71), marking a time beyond which all of the various local patterns remain forever isolated and noninteracting. Apart from providing a dramatic illustration of the latent complexity of even very simple patterns, the significance of this evolution actually lies in what is *not* shown (because it would appear off-page) in the state appearing at time=1103: namely, the emergence of an oscillatory and propagating pattern known as the *glider*.

Gliders: In Conway's own words [berk82], "When we first tracked the *R-pentamino* ... some guy suddenly said "Come over here, there's a piece that's walking!" We came over and found figure..." 3.72.

This remarkable five *live-cell* pattern is called a *glider* because after two iteration steps it produces a pattern that is both diagonally displaced by one site and reflected in a diagonal line – i.e., patterns separated by two steps are related by a *glide reflection*. In this way, the original pattern is reproduced in a diagonally displaced position every four iterations.

Spaceships: It turns out that, despite being common remnants of a *primordial* origin, there are only four distinct moving and self-replicating figures (see figure 3.73). They are individually referred to as *spaceships* of varying 'weight' classes, with the glider being designated the *featherweight* because it consists of the fewest *live-cells*. Unlike the *glider*, however, the *lightweight*, *middleweight*, and *heavyweight* spaceships are merely horizontally (not diagonally) displaced. Moreover, their shifted replicated patterns are adjoined by transient 'sparks' that immediately vanish on the next time step.

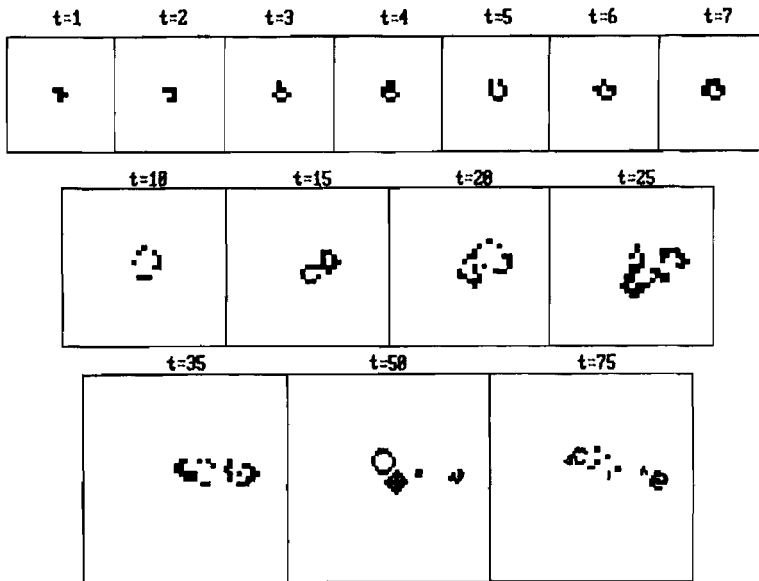


Fig. 3.70 Some snapshots of the *R-pentomino* pattern; see text.

Flotillas: Although each spaceship of a particular weight class is a simple generalization of the next lower weight class, spaceships with more than *six live-cells* along the bottom row become unstable. These heavier spaceships may move forward only if *escorted* by a suitable combination – or *flotilla* of smaller weight class spaceships. Conway discovered that arbitrarily heavy spaceships may be escorted in this fashion. It is noted in passing that flotillas are artificially ‘engineered’ patterns and do not appear to arise naturally by *Life* itself.

Glider Shuttle: Another interesting combination of distinct patterns is what is for obvious reasons called a *shuttle glider* (see figure 3.74). It consists of a single glider and two identical and stationary but oscillatory 12 *live-cell* patterns. The net effect is that the glider continually shuffles its way from one to the other of these larger patterns.

Garden-of-Eden Configurations: We recall that *Garden-of-Eden* configurations are those that can arise only as initial states. A crude counting argument suffices to show that there must exist at least one such ‘parentless’ *Life* configuration: consider a $(5n - 2)$ by $(5n - 2)$ square, whose parent, if it exists, can come only from the surrounding $5n$ by $5n$ square. Since any one of the component 5×5 squares may, if they are empty, be replaced with another 5×5 square with a single *live-cell* in its center without affecting the state on the next time step, there are a total of $(2^{25} - 1)^{n^2}$ possible ‘parent’ states within the $5n \times 5n$ square. On the other hand, we know that there are only a total of $2^{(5n-2)^2}$ possible ‘offspring’ states within the $(5n - 2)$ by $(5n - 2)$ square. We conclude that if

$$(2^{25} - 1)^{n^2} < 25n^2 - 20n + 4,$$

then one of the states within the $(5n - 2)$ by $(5n - 2)$ square will have no parent. This happens for $n = 465163200$, so that a garden-of-eden configuration must exist within a 2325816000 by 2325816000 square. Tighter bounds on the size of the minimal square within which a garden-of-Eden state must exist can of course be obtained with more careful counting. The first explicit example was discovered by Roger Banks in 1971, and is contained within a 9×33 rectangle. It is shown in figure 3.75.

Eaters: A fascinating structure with the ability to destroy, or *eat*, nearby patterns without damaging the integrity of its own form, is called the *eater*. Figure 3.76, for example, shows how an *eater* kills a glider in four time steps and repairs itself in the process. When two *eaters* are made to attack each other, they produce an oscillating pattern in which each takes a ‘bite’ out of the other and quickly repairs itself before taking another bite. Although not everything can be successfully eaten by this pattern (simple 2×2 stable patterns of live cells – called *blocks*, for example, are indigestible), the number of digestible patterns is impressively large. Indeed, in a way to be made clear later, this ‘pattern-killing’ ability makes *eaters* an important ingredient in the proof of *Life*’s universality.

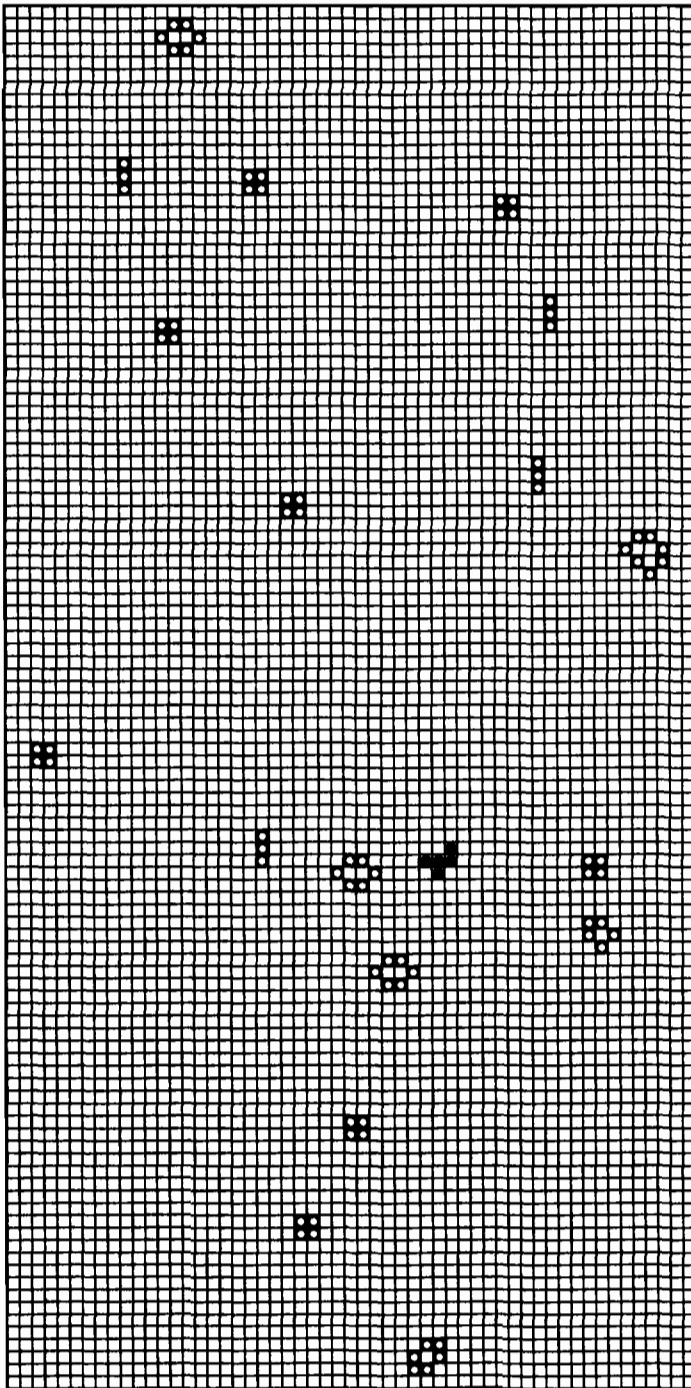


Fig. 3.71 The '*R*'-pentomino's period-two configuration (open circles) reached at time $t=1103$; six *gliders* are also produced but are beyond range. The original *R*-pentamino pattern is shown in solid black.

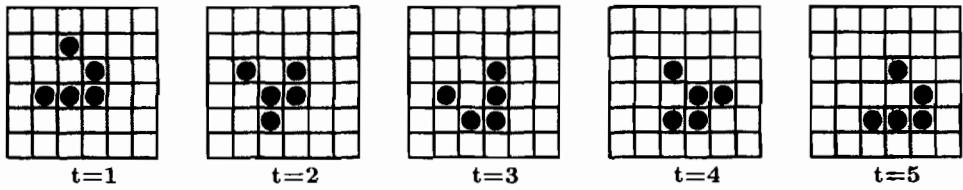


Fig. 3.72 The glider pattern evolving under Φ_{LIFE} .

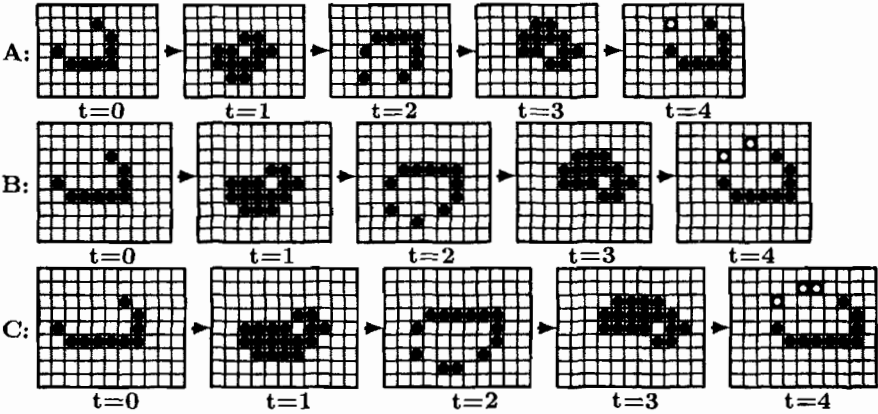


Fig. 3.73 Motion of *lightweight* (A), *mediumweight* (B) and *heavyweight* (C) 'spaceships'. The open circles represent 'sparks' that vanish at the next time step. Patterns with a greater number of live cells along the bottom are unstable.

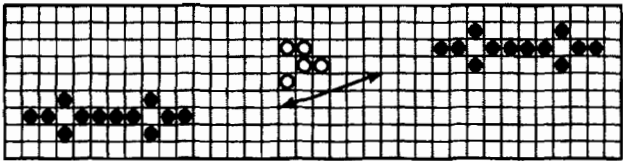
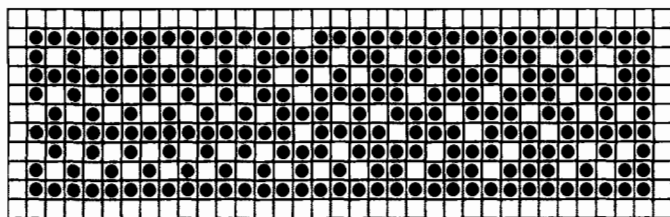
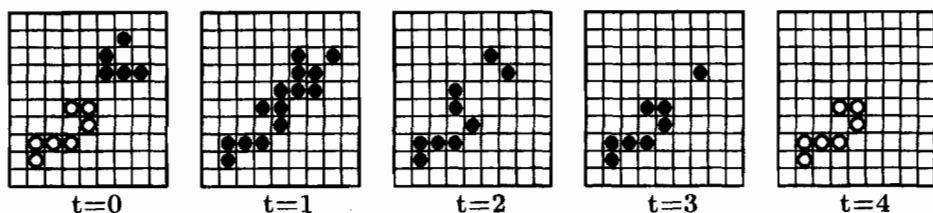


Fig. 3.74 Glider Shuttle.

Glider-Glider Collisions: A critical element in the proof of *Life's* universality will turn out to be the ability to manufacture all of the necessary ingredients out of nothing but glider-glider collisions. As hinted by figure 3.77, which shows the results of four different two-glider collisions, the results are surprisingly diverse. In fact, some careful counting shows that, in all, 73 distinct two-glider collisions are possible. An extraordinary result of a *thirteen* glider collision will be presented below.

Puffer Trains, Guns and Breeders: Conway originally conjectured that *no pattern can grow without limit*, offering 50\$ to the first person who either proved

Fig. 3.75 A *Garden-of-Eden* configuration.Fig. 3.76 An *eater* (open circles at $t=0$) devours a *glider*.

or disproved this claim. Needless to say, the task at first appeared to be more than a little daunting: (1) scarcely little can be directly inferred from the formal rules themselves, and (2) given that a particular configuration is painstakingly tracked for even several million steps, there is no guarantee that it will not in fact stabilize after a million more.

Despite these difficulties, however, the prize was won within a year of its announcement by a group of MIT students working for the *Artificial Intelligence Project*.[†] After a great deal of experimentation, the group stumbled upon an oscillatory configuration that periodically produced a new glider; they had discovered a *glider gun*. Since each emerging glider adds 5 live cells to the global population, the configuration obviously grows without limit.

After collecting their prize, the members of this MIT group had made an even more remarkable discovery. They found that the glider gun itself can be manufactured out of a 13-glider collision, a few snapshots of the evolution of which are shown in figure 3.79 Emerging at $t=75$ and starting at $t=100$, the glider gun henceforth spews out a glider once every 30 steps.

Alternative means of achieving unlimited growth include (1) the generation of propagating patterns that leave some form of *debris* in their wake as – otherwise intact and essentially unchanging – they wander across the lattice and (2) the creation of evolving patterns whose rate of growth actually increases with their age. The former class of patterns are known as *puffer trains* (two simple examples

[†]The group consisted of Robert April, Michael Beeler, R. William Gosper, Jr., Richard Howell, Rich Schroepel and Michael Speciner.

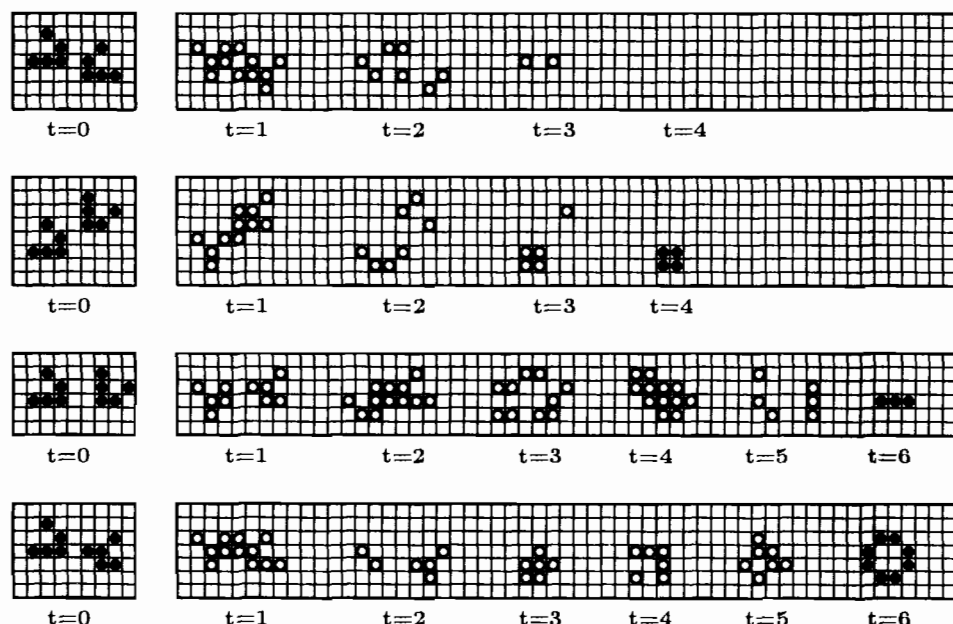


Fig. 3.77 A variety of *glider-glider* collisions.

of which are shown in figure 3.78), while the latter are called *breeders* and are arguably among the most fascinating of all of the known *Life* patterns to watch develop. Breeders consist of a flotilla of ten special puffer trains which produce two backward waves of gliders (with period 32) and a pair of blocks (with period 64). The flotilla is carefully arranged so that the emitted gliders crash to form glider guns along the axis of the flotilla's forward motion. As the flotilla moves forward, the firing rate of the ever increasing number of glider guns left in its wake increases without limit.

3.4.4.4 Ingredients for Universality

All of the basic ingredients necessary for a proof of *Life*'s universality (an outline of which appears in section 3.4.5, following a more formal discussion of computation theory) have already been presented in this section. As we shall see, the proof consists essentially of showing that all of the necessary building blocks of a conventional computer can be built out of *Life*'s patterns. In this way, given a pattern representing an arbitrary 'program', the pattern representing a 'computer' will carry out the instructions of the program and produce the desired result, itself expressed in terms of a *Life* pattern. Numerical calculations, for example, might involve final patterns consisting of a requisite number of gliders in a particular area of the lattice.

The proof proceeds from the observation that each of the four essential 'primitive' elements for computation – namely, the *storage* (requiring an internal memory), *transmission* (requiring an internal clock and wires), and *processing* (requiring

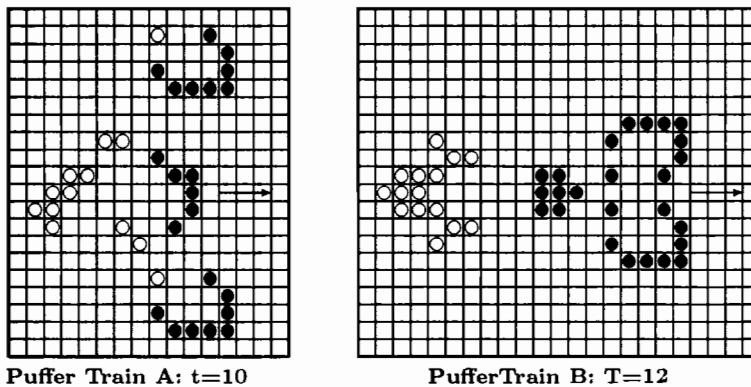


Fig. 3.78 Two *puffer trains* (solid circles) shown with their ‘exhaust’ (open circles) after 10 and 12 iteration steps, respectively.

AND, OR, and NOT gates) of information – can be implemented by the evolution of appropriate *Life* patterns. Indeed, it will be shown that the circuitry of any computer can actually be constructed out of nothing but *gliders*, *glider-guns*, *blocks* and *eaters*!

3.4.5 Sketch of a Proof that Conway’s Life-rule is Universal

Perhaps the simplest way to prove that a system is capable of universal computation – certainly the most straightforward way – is to show that the system in question is formally equivalent to another system that has already been proven to be a universal computer. In this section we sketch a proof of the computational universality of Conway’s *Life*-rule by explicitly constructing dynamical equivalents of all of the computational ingredients required by a conventional digital computer.

While the precise design of a computer may be complex, its basic ingredients, or set of primitive computational elements, are relatively simple and few in number. In addition to having some form of *bit-stream signals* to work with, we need conduits, or *wires*, for those signals; we need to be able to somehow route those signals, such as by redirection (for example, turning a signal through a 90 deg turn) or sending multiple copies of a given bit-stream into different directions; we need an internal system clock, or *timer*, to introduce any necessary delays in building circuits; we need a (potentially infinite) memory, a requirement that can also be met with a finite *sized* memory but one that can store arbitrarily large numbers [minsky67]; and we need a set of universal logic gates, such as **NOT**, **AND** and **OR**, from which all other logical functions and operations can be obtained. Once it can be shown that a given system supports these computational primitives, the construction of the actual working circuitry of a conventional computer effectively becomes little more than a formal (albeit, exhausting) exercise in symbol/block building. We therefore confine ourselves to showing how to construct the required set of computational primitives.

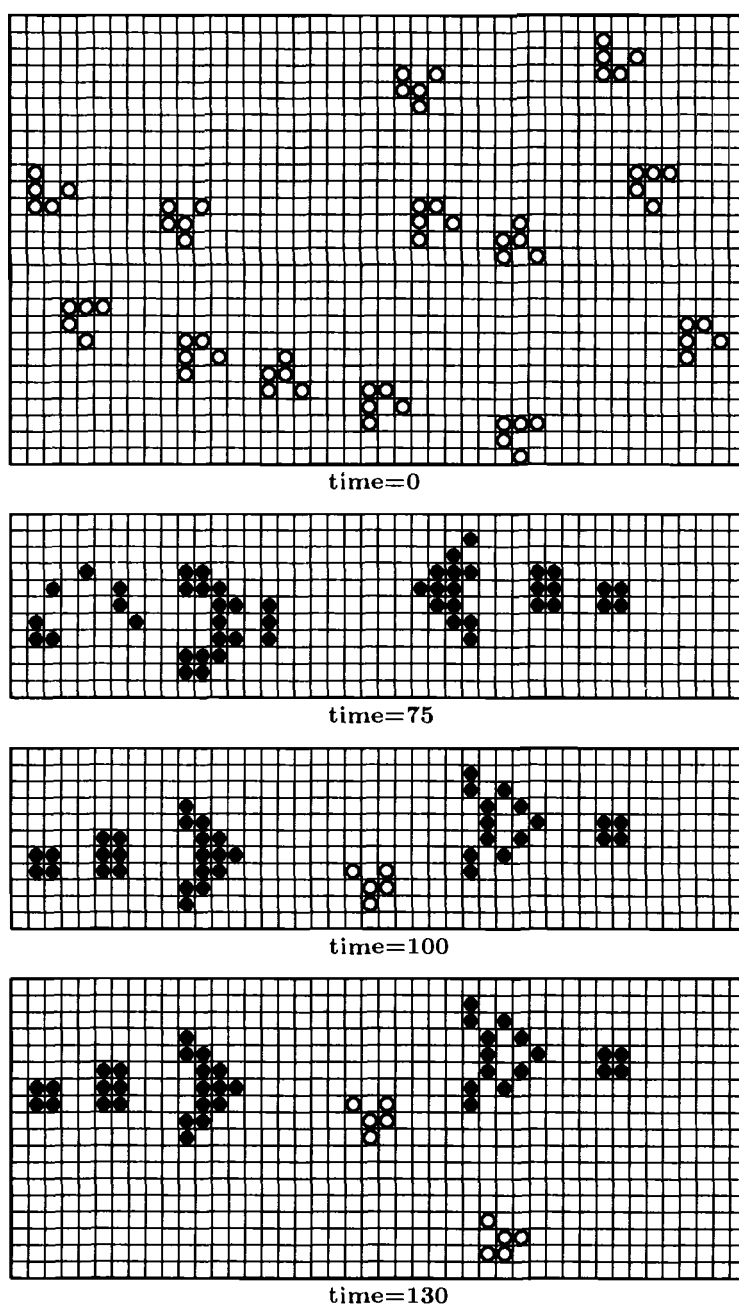


Fig. 3.79 A thirteen glider collision at $t = 0$ produces a period $p = 30$ glider-gun at $t = 75$, generating a glider once each period.

The original proof appears in Berkelamp, Conway and Guy's mathematical game opus [berk82]; other discussions may be found in Langton's thesis [lang92c] and the book by Poundstone [pound85]. Before proceeding with this section, the reader may also want to refamiliarize himself with the 'zoology' of *Life*'s patterns, including *gliders* and *glider-guns* by referring back to section 3.3.4.

3.4.5.1 *Bits* $\iff$ *Gliders*

We begin by postulating the obvious equivalence between, on the one hand, electrical pulses and bits of a pulse-stream signal in physical computers and, on the other hand, gliders and glider-streams in Conway's *Life*-rule CA. In *Life*, we will interpret the presence or absence of an individual glider in a well-defined (i.e. well-timed) slot of a glider-stream as denoting the corresponding bit value in a physical pulse-stream signal. That is to say, we will interpret a glider's *presence* as denoting the fact that the corresponding 'bin' in the physical pulse-stream has bit value 1, and a glider's *absence* as denoting a bit-value 0.

We already know that *glider-guns* can create a steady stream of gliders. Since glider-guns produce gliders once every 30 iteration steps (with the distance between gliders being exactly $7\frac{1}{2}$ lattice-sites), however, two or more glider-streams moving on mutually intersecting courses cannot cross without interfering with one another. Since, in order to build circuits, we clearly desire non-interacting glider-streams, the next step is to produce a *thin-glider-gun* to create glider-streams of arbitrarily long periods.

3.4.5.2 *Thin Glider Gun*

The thin-glider-gun is relatively easy to construct and depends on only four basic constructs: (1) a basic period-30 *glider-gun*, (2) an *eater*, (3) a glider-glider annihilation reaction, and (4) a *kickback* reaction. The first two constructs are familiar from our general discussion of the *Life* rule. We recall from that discussion that the *eater* is so-called because it has the ability to essentially 'eat' patterns that impinge on it without damaging the integrity of its own form (see figure 3.80). Glider-glider annihilations are also nothing new; we have already seen examples of mutually annihilating glider-glider collisions. The last construct is new and consists of two gliders set on a 90 deg intersect course (see $t = 0$ in figure 3.80). In this kickback-reaction, the two gliders undergo a process whereby, at time $t = 6$, one of the original gliders disappears and the other emerges out of the *reaction-zone* shifted in space by half a diagonal lattice position and moving in the reversed direction.

Figure 3.81 shows how these four basic constructs can be used to create a new *thin-glider-gun* that produces a stream of gliders with arbitrarily large spacing between them. In the figure, the symbols **E**, **G** and **K** as short-hand notation for *eaters*, *glider-guns* and *kickback-reactions*, respectively.

The thin-glider-gun uses two parallel but oppositely directed glider stream outputs of conventional glider-guns. A single glider also shuttles between those two glider-streams. The timing is such that whenever the shuttling glider collides with

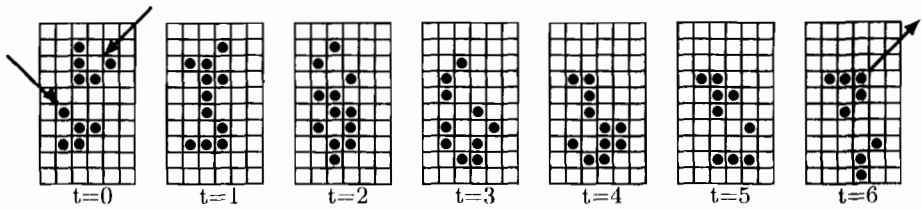


Fig. 3.80 Kickback reaction in Conway's Life-rule.

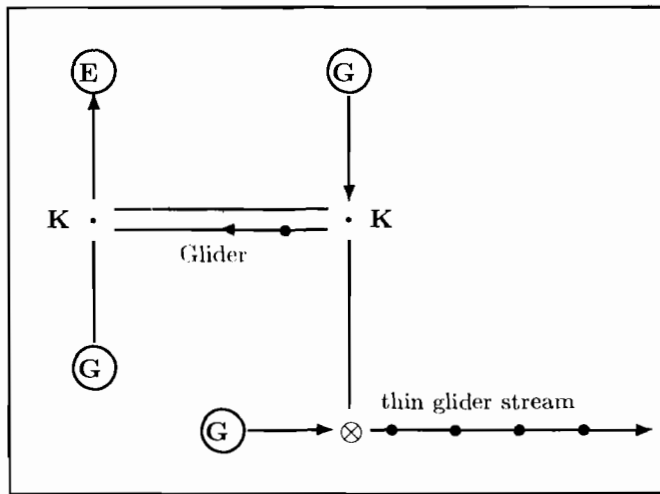


Fig. 3.81 Schematic for a Thin Glider Gun; E = eater (see figure 3.76), G = glider-gun (see figure 3.79) and K = kickback reaction.

a glider stream it undergoes a kickback-reaction; i.e. it annihilates the glider in the glider-stream and is itself shifted slightly upward and reversed in direction. A kickback-reaction with the glider-stream on the right shifts the shuttling-glider downward to complete the closed-loop.

While the upward glider-stream on the left-hand-side is not needed, and is annihilated by an eater, the downward stream on the right-hand-side is fed into a mutually annihilating reaction with a third glider-stream shown at the bottom of figure 3.81. Since every n^{th} glider on the downward stream is annihilated by the single glider shuttling back and forth between kickback-reactions on the left and right, the resulting glider stream that finally emerges out of the thin-glider-gun consists of a *thinned* set of gliders spaced $30n$ steps apart. In order to get the right phase-timing, n must be divisible by four, but can be arbitrarily large. In this way we can therefore construct glider-streams with gliders spaced arbitrarily far apart.

3.4.5.3 Logic Gates

Let us now use the preceding constructs to build a set of universal logic gates: **NOT**, **AND** and **OR** (see figure 3.82).

The **OR** gate is the easiest to construct; in fact, it has already been introduced as an element of the thin-glider-gun circuit. Referring to figure 3.82-a, we assume that input A is some *coded* glider-stream. Once in the gate, all of the gliders in this input stream annihilate once they collide with gliders in an uncoded glider-stream produced by a thin-glider-gun. The only gliders that emerge from the **NOT** gate are those that were in the original thin-glider-gun stream and were not annihilated by gliders in A; i.e. a particular 'slot' of the output stream contains a glider if and only if the corresponding 'slot' in A did *not*.

In the **AND** gate (figure 3.82-b), two input streams, A and B, enter the gate in parallel. Gliders from a glider-gun move on a perpendicular course and into an eater, with the timing such that the collisions between gliders in this glider-stream and those in the two inputs are mutual-annihilations. Provided that the gliders in A are *delayed* in time by an amount equal to the distance between the two annihilation reactions (see below), it should be evident from the figure that a glider makes it into the output stream if and only if *both* of the corresponding 'slots' in A and B contain gliders. The operation of the **OR** gate, the schematic of which is shown in figure 3.82-c, proceeds in a similar fashion.

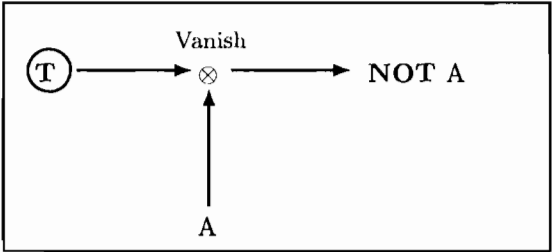
3.4.5.4 Time Delays

It was mentioned above that in order for the **AND** gate shown in figure 3.82-b to operate properly, the gliders in input A must be *delayed* by a time equal to the distance between the two annihilation reactions. The same is true of the operation of the **OR** gate, shown in figure 3.82-c.

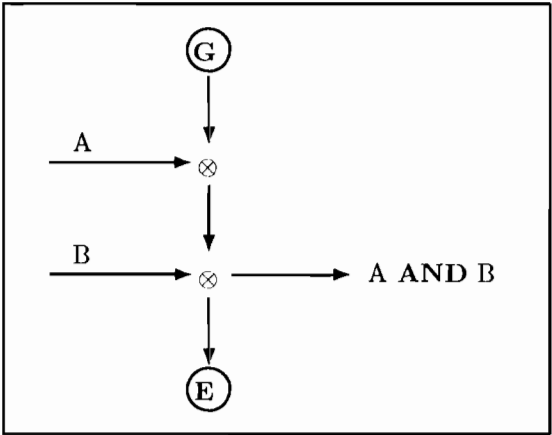
Signal time-delays are easily constructed out of **NOT** gates. The idea is to simply build a detour consisting of as many steps as needed for the delay, and then routing the signal-stream back to its original course. Figure 3.83 shows the schematic for one such delay using four **NOT** gates. The first **NOT** negates the input stream and detours it by 90 deg. The second gate restores the content of the original signal and detours it by another 90 deg. The third and fourth **NOT** gates repeat the process, so that the final outcome is that the original signal emerges from the circuit along the same direction as it came in but delayed in time by however long it took to progress along the detour. Other configurations of **NOT** gates can delay and reroute signals by 180 deg and/or shift them into parallel paths. No combination of **NOT** gates, however, can be made to turn a stream sideways (i.e. rotate it by 90 deg). Fortunately, this capability comes *free-of-charge* with Conway's glider-stream copying circuit.

3.4.5.5 A Glider-Stream Copier

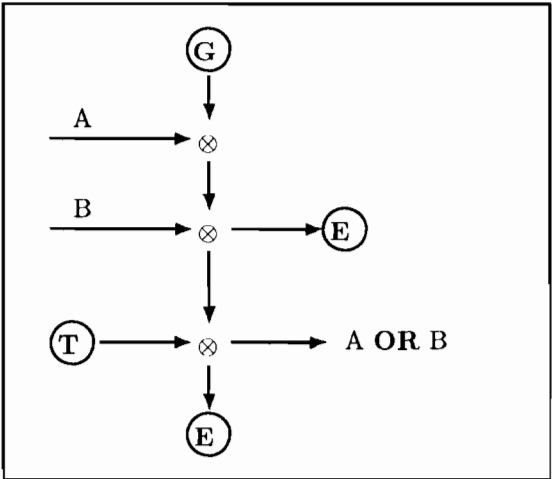
It would be an essentially impossible task to construct any useful computational circuits without being able to route multiple copies of signal streams. The set of



(a) NOT Gate



(b) AND Gate



(c) OR Gate

Fig. 3.82 Schematic representations of NOT, AND and OR gates; E = eater (see figure 3.76), G = glider-gun (see figure 3.79) and T = thin glider-gun (see figure 3.81).

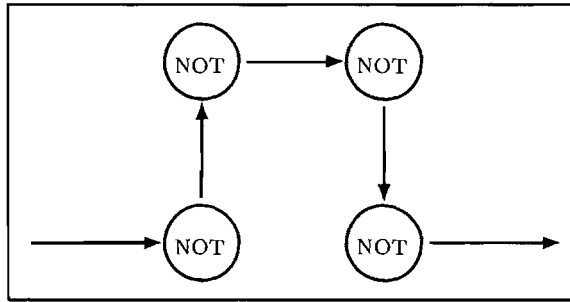


Fig. 3.83 Schematic of a time-delay circuit using four **NOT** gates.

tools that we have defined thus far allow us only to re-route single glider streams into parallel directions of motion (i.e. with the re-routed signals being offset by either 0deg or ± 180 deg from their original direction); there exists as yet no provision either for offsetting the direction of a given signal by 90deg or for making copies of a signal. One of the simplest circuits that solves *both* of these problems is due to Conway and is shown in figure 3.84.

Conway's circuit uses the kickback reaction to send gliders back into their own signal-stream. Suppose we have a factor 4 thin-glider-gun, i.e. that an *uncoded* data-stream consists of the string '11111...' and that a glider passes a given point along the the direction of its motion every $4 \times 30 = 120$ time steps. Suppose, also, that the *coded* signal-stream has been *thinned* by another factor of 10. That is say, suppose that the *nine* period-120 glider-bit positions are always empty ($= 0$), and it is only the *tenth* glider-bit position that may or may not contain an encoded glider-bit. For example, the coded signal '011' would be thinned to a glider-stream representation given by '000000000000000000010000000001'. In the figure, we have indicated the value of this tenth glider-bit position with a question-mark, '?'.

Conway's circuit functions as follows. The input data stream that is to be copied enters an **OR** gate located at the top-left. The other input to the **OR** gate is the output of a (likewise, factor 40) thin-glider-gun but whose glider-stream is such that the ninth glider-bit position *always* contains a glider. The **OR** gate combines these two signals to produce an output consisting of a glider-stream that always has the same glider-bit set as does the original coded signal and always contains a glider in the ninth position; it is represented by the string '000000001?'.

Now consider what happens when this string encounters a kickback-reaction. If $? = 1$, it will 'kick-back' the first glider in the downward '111...' stream, creating a pile-up collision. While the coded glider is itself annihilated, however, the glider behind it in the ninth position will pass through the kickback-reaction region unaffected. The output is the string '0000000010'. If $? = 0$, the first glider in the string '111...' will pass through unaffected, but the ninth glider behind the coded glider-bit position will kick-back the next glider in the '111...' stream. The output stream therefore contains no gliders and is given by '0000000000'. In short, if the coded glider-bit position contains a glider bit '?', the output of the kickback-reaction is

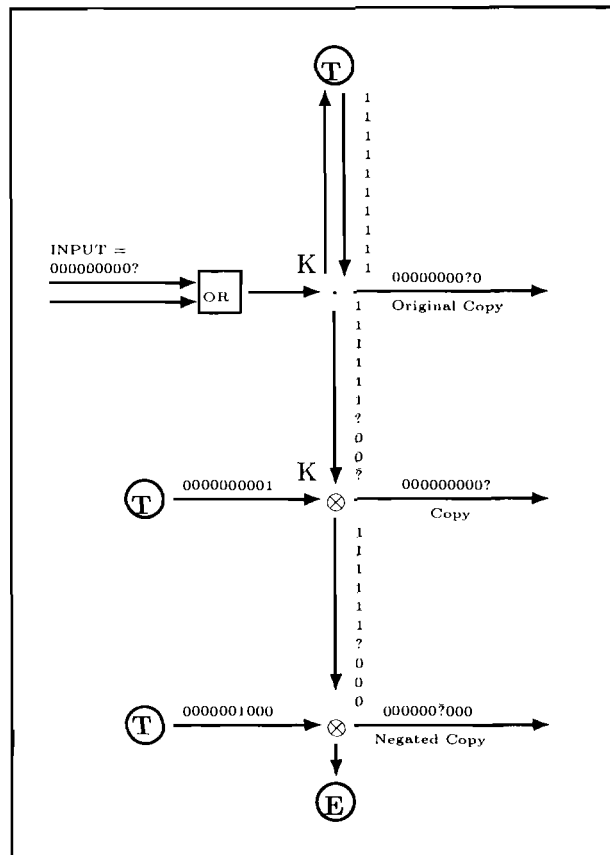


Fig. 3.84 A schematic representation of a *glider-stream copier*. E = eater, T = *thin-glider-gun* and K = kickback reaction.

given by '00000000?0'; i.e. it contains the same information as the original signal but the coded glider bit is delayed by one position.

Consider what happens to the downward moving '111...' glider-stream after it enters the kickback-reaction region. It is easy to see that the kickback-reaction itself always removes exactly three gliders. If the coded-string that enters the kickback region contains a glider in the tenth position ($? = 1$), then the kickback reaction strips the first three gliders off of the downward stream; if the coded-string that enters the kickback region does not contain a glider in the tenth position ($? = 0$), then the leading glider of the downward stream is left alone but the next three gliders are stripped off by the kickback reaction. Schematically, the output is given by '11111?00?', where $\bar{?} \equiv \text{NOT}(?)$.

This downward moving stream next collides with a transverse thinned glider-stream consisting of all empty glider-bit positions except for the tenth, which always contains a glider. The output stream on the right can therefore have a glider only in

this last position, and only when the $\bar{?}$ position in the downward stream is empty. In other words, the leading position of the output at right is **NOT**[**NOT** (?)]=?, so that the output is a perfect replica of the original coded glider-stream: '000000000?'. We leave it to the reader to show that a collision between the downward output of this collision, '111111?000' and a transverse thinned signal '0000001000' essentially produces a *negated* copy of the original signal, '000000?000'.

Conway's circuit therefore has a total of three outputs: one is an exact replica, another is a faithful copy but with the information-carrying glider-bits shifted by one position, and the third a negated copy of the original signal and with the information-carrying glider-bits shifted by three positions. Notice that all three outputs remain *parallel* to the direction of motion of the original signal. Since we already know from our discussion of **NOT** gates that a *negated* copy of signal can be re-routed by 90 deg, we now see how to use Conway's basic signal copying circuit to re-route a signal itself by 90 deg. We merely use two *eaters* to capture and annihilate the top two (faithful copy) outputs and insert a **NOT** gate at the bottom to negate and re-route the negated copy output.

3.4.5.6 Memory Storage

The only ingredient in the proof of *Life*'s universality that we have not yet discussed is *memory storage*. While a *finite* memory is fairly easy to implement with wires and logic gates – for example, glider-stream-encoded information can be made to circulate around a memory circuit contained within the computer – the construction of an *arbitrarily large* memory requires a bit more work.

A universal Turing machine uses an arbitrarily long tape as a potentially infinite memory storage device. Instead, for his proof, Conway used Minsky's idea that a potentially infinite memory can also be obtained by storing arbitrarily large numbers in memory registers. The idea is sketched in figure 3.85.

Using Berkelamp, *et. al.*'s *Fermat's theorem* example [berk82], suppose our *Life* computer was asked to compute the quantities $x^n + y^n$ and z^n for all quadruples (x, y, z, n) and then stop when it had found a quadruple satisfying $x^n + y^n = z^n$. A simple way of keeping track of the inevitably large numbers the computer will be forced to try, is to use stable *blocks* as value markers in an auxiliary memory storage register. The distance of the block in a given register with respect to an arbitrarily designated 0-level defines the quantity stored in that register. In figure 3.85, for example, registers A, B, C and D contain the "numbers" 2, 5, 0 and 4, respectively.

Register memory works in the following way. Suppose register x contains a block at "location" N . In order for the computer to "read" this value, it must perform the loop

$$\begin{cases} \text{decrease contents of register } x \text{ by } 1 \\ \text{test to see if contents of register } x = 0 \end{cases} \quad (3.83)$$

until the contents of register x is equal to zero. The number of internal "clock-ticks"

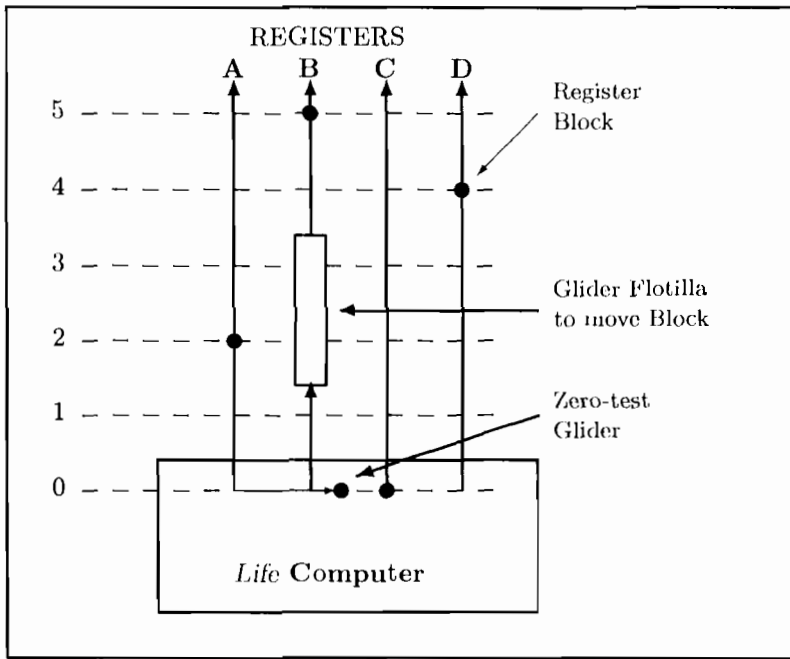


Fig. 3.85 A schematic representation of an auxiliary memory storage circuit.

required to decrease the distance of the given block from the zero-level then yields the desired register memory “value.” Conway showed that all of the required block movements – including the ability to “push” blocks upwards in a register to “store” a given value and to “pull” blocks down to “read” already stored values – could be accomplished by a suitable flotilla of gliders. While there does not exist any single glider-block collision capable of displacing a block by one lattice-site, it may be shown that ten gliders can be coerced into moving a block by one diagonal lattice site (see [berk82] for a sketch of the resulting collisions).

We will not discuss the only remaining issue that the astute reader has no doubt already recognized to be absent from the preceding discussion; namely, how do we manage to keep our flotilla of gliders moving up and down parallel paths only a few lattice sites apart? Since each glider must, at some time, have been produced by a glider-gun, each of which clearly takes up some non-trivial amount of space on the lattice, would not the output of one glider-gun have to effectively *shoot-through* another closely-spaced glider-gun? The answer lies in a clever scheme called *side-tracking* which we invite the reader to either re-invent for himself or read about in either [berk82] or [pound85].

Having demonstrated, by construction, that each of the computational elements required of a conventional digital computer for its own computation – namely, (1) digital bit-stream signals, (2) wires, (3) redirection circuits, (4) an internal system clock, (5) a (potentially infinite) memory, and (6) a set of universal logic gates

(NOT, AND and OR) – is supported by *Life's* dynamics, we have thus proven that *Life* is universal. Indeed, from the above discussion, it is clear that the circuitry of any *Life*-based computer can be built entirely out of gliders, glider-guns, eaters and blocks. ■

3.4.6 Three-dimensional Life?

Bayes, in a series of papers, ([bayes87a], [bayes87b], [bayes88], [bayes90], and [bayes91]) has searched for three-dimensional analogs of Conway's *Life*-rule that are "worthy of the name" [dewd87].

Bayes considers two types of three-dimensional lattices: (1) a generic three-dimensional Euclidean cubic lattice where each site has 26 neighbors, and (2) a three-dimensional generalization of the two-dimensional hexagonal grid, or a hexahedral tessellation in which a given site has a total of 12 neighbors that line up in four intersecting hexagons. On the cubic lattice, site values are updated according to

$$\sigma_{i,j,k}^{(t+1)} = \phi[\overbrace{\sigma_{i-1,j-1,k-1}^{(t)}, \dots, \sigma_{i,j,k}^{(t)}, \dots, \sigma_{i+1,j+1,k+1}^{(t)}}^{27 \text{ terms}}], \quad (3.84)$$

The hexahedral tessellation presents more of a problem because of its nonorthogonality. Bayes [bayes87b] suggests two update schemes, both based on situating the sites on a cubic lattice: (1) update according to

$$\sigma_{i,j,k}^{(t+1)} = \phi[\sigma_{i,j,k}^{(t)}, \sigma_{i-1,j,k-1}^{(t)}, \sigma_{i,j+1,k-1}^{(t)}, \sigma_{i+1,j,k-1}^{(t)}, \sigma_{i,j+1,k}^{(t)}, \sigma_{i+1,j,k}^{(t)}, \sigma_{i,j-1,k}^{(t)}, \sigma_{i-1,j,k}^{(t)}, \sigma_{i+1,j+1,k}^{(t)}, \sigma_{i,j-1,k+1}^{(t)}, \sigma_{i-1,j,k+1}^{(t)}], \quad (3.85)$$

in which case the universe is shaped like a rhombohedron and some adjustments must be made to fit it properly onto a rectangular shaped computer display (see [prest84]), or (2) update according to

$$\sigma_{i,j,k}^{(t+1)} = \phi[\sigma_{i,j,k}^{(t)}, \sigma_{i+1,j-1,k+1}^{(t)}, \sigma_{i+1,j+1,k+1}^{(t)}, \sigma_{i-1,j,k+1}^{(t)}, \sigma_{i-1,j-1,k-1}^{(t)}, \dots, \sigma_{i,j+2,k}^{(t)}, \sigma_{i,j-2,k}^{(t)}, \sigma_{i+2,j-1,k}^{(t)}, \sigma_{i+2,j+1,k}^{(t)}, \sigma_{i-2,j-1,k}^{(t)}, \sigma_{i-2,j+1,k}^{(t)}], \quad (3.86)$$

in which case alternate locations and alternate rows are left vacant in the (i, j) planes, but the universe otherwise remains approximately "cubic" in appearance. Another way of picturing the second lattice type is as a collection of densely packed spheres [bayes87a].

Although, for either lattice, the iterative application of the update rules themselves is straightforward, the visualization of the time evolution of patterns is complicated by the fact that not all sites can be seen at one time.

Before we summarize Bayes' results, we should discuss briefly what the behavior of a *Life*-like rule "worthy of the name" ought to look like, or what we can expect it to look like. While the original two-dimensional *Life*-game was introduced in the last section formally as an outer-totalistic code **OT224** rule, it is much more convenient to define it in terms of the sizes of two environments: a *survival environment* E , and

a fertility environment F, E , where $0 \leq E_l \leq E \leq E_u \leq 26$, is the number of living neighbors that must surround a given site if that site is to remain living at the next time step. F , where $0 \leq F_l \leq F \leq F_u \leq 26$, is the number of living neighbors that must surround a dead site if that site is to become living on the next time step. Two-dimensional *Life* is then defined as the 4-tuple $\Phi = (E_l E_u F_l F_u) = (2333)$.

Consider the cubic lattice. Since there are $26 + 25 + \dots + 1 = 351$ pairs of survival parameters (E_l, E_u) with $E_l \leq E_u$, and an equal number of fertility parameter pairs (F_l, F_u) , there are a total of $351^2 = 123,201$ possible rules satisfying this template in three dimensions. In the case of the hexahedral tessellation, there are $(13 + 12 + \dots + 1)^2 = 8281$ rules of this type.

Bayes' searches for three-dimensional *Life*-like behavior in rules conforming to this basic template. While there is nothing sacred about this particular template -- and one is of course free to search among all 2^{13} possible nearest-neighbor rules on the hexahedral tessellation and all 2^{27} rules on the cubic lattice, not to mention expanding the search to next-nearest neighbors and so on -- there is an unmistakable elegance to two-dimensional *Life*'s sheer simplicity that we intuitively expect to be carried over into higher dimensions.

Bayes' search criteria for "worthy" three-dimensional rules consist of two basic requirements [bayes87a]: all rules of the form $\Phi = (E_l E_u F_l F_u)$ are said to describe a "game of *Life*" if and only if (1) a *glider* is naturally formed when Φ is applied to random configurations (or a *primordial soup* [bayes87a]) and (2) all random configurations exhibit, under Φ , bounded growth. These criteria are not so much formal characterizations of what makes two-dimensional *Life* so special as heuristic guides for what to look for in potential three-dimensional analogs.

Consider the cubic lattice. While Bayes' starts off with what appears to still be a rather large set of rules in which to search for *Life*-like behavior, he immediately makes two simplifying observations [bayes87a]. One is that any rule $\Phi = (E_l E_u F_l F_u)$ where $F_l \geq 10$ cannot support a glider. The other is that any rule $\Phi = (E_l E_u F_l F_u)$ where $F_l \leq 4$ cannot induce unlimited growth. The first observation follows from the fact that the number of living sites on any plane that is adjacent to a dead site is bounded above by 9. Therefore, if Φ is of the form $(E_l E_u 10 F_u)$, the surface of any cluster of live sites cannot propagate. To see the second point, just seed the lattice with a cluster of four neighboring living sites. Similar reasoning shows that, in the case of the hexahedral tessellation, any "worthy" rule must be of the form $(E_l E_u 33)$.

The search technique consists of initializing the center $7 \times 7 \times 7$ portion of a $23 \times 23 \times 23$ three-dimensional universe randomly with 20% live sites and simply waiting for a glider to appear. The search for gliders can be partially automated by monitoring the *signature* of patterns that hit an edge of the $23 \times 23 \times 23$ universe.

The signature, S , of a pattern, $\mathcal{P}$, is, for the cubic lattice, the 53-tuple,

$$S(\mathcal{P}) = \{A_{26} A_{25} \dots A_0 \diamond D_1 D_2 \dots D_{26}\}, \quad (3.87)$$

where A_i is the total number of live sites in $\mathcal{P}$ that have exactly i live neighbors and D_j is the total number of dead sites in the vicinity of $\mathcal{P}$ that have exactly j

live neighbors. An important, and easily proven, property of S , for a given pattern, is invariance under a change of orientation; i.e. a glider has the same signature no matter what direction it is moving in.[†] Other useful properties are discussed in [bayes87b]. An analogous 25-tuple signature can also be defined for the hexahedral tessellation.

After exhaustive simulations, Bayes' has found only three rules on the cubic lattice ($\Phi = (4555)$, $\Phi = (5766)$, $\Phi = (5655)$) and two rules on the hexahedral tessellation ($\Phi = (3333)$ and $\Phi = (4633)$) that can arguably be called "worthy of the name" ([bayes87a], [bayes90] and [bayes91]). We follow Bayes' nomenclature in calling these rules, respectively, *Life-4555*, *Life-5766*, *Life-5655*, *Life-3333* and *Life-4633*.

Figure 3.86 shows the initial states of the four known gliders for the cubic lattice. Note that the second of the two gliders shown for *Life-5766* and the only one found thus far for *Life-5655* appear to be considerably rarer than the other two gliders. The glider for *Life-4555* typically appears once every 5000 simulation runs. Bayes reports that *Life-5766*'s second glider is about 2000 times rarer than the first [bayes90]. The glider for *Life-5655* is rarer still. In fact, Bayes has found that the only way to produce *Life-5655*'s glider in a "reasonable" time is to impose the same kind of symmetry (namely, reflection in a plane parallel to one of the coordinate planes; say, $z = 0$) that one might expect of a glider for this rule on the primordial soup states themselves.

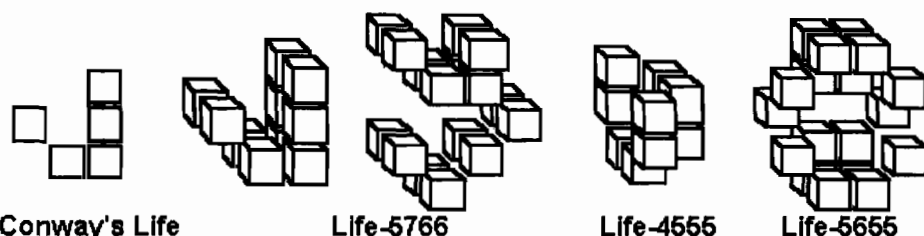


Fig. 3.86 Initial states of gliders for Conway's two-dimensional *Life* and *Life 5766*, *Life 4555* and *Life 5655* for the cubic lattice. Note that two (and the only two known) gliders are shown for *Life-5766*.

Bayes reports that, if such a symmetry is *not* imposed, no gliders appear even after running several million experiments. He guesses that 20 – 500 million runs would be needed to produce even one glider. However, *with* the reflection symmetry imposed on the primordial states, Bayes reports finding seven gliders after 30 million runs [bayes91]. It is also interesting to note that if the same kind of symmetry is imposed on initial states for *Life-4555* and *Life-5766*, the gliders for those two rules appear about 30 to 100 times more frequently than for non-symmetric initial states.

Of the three rules for the cubic lattice, *Life-5766* appears most *Life*-like, with many of the two-dimensional rule's patterns having analogs within *Life-5766*'s three-

[†]Note that calculating the signature of a pattern does not introduce any additional steps during a simulation, as all neighboring values must be checked anyway.

dimensional universe (see subsection below). The first of the two known gliders for this rule, for example, consists of two back-to-back copies of the original Conway-rule glider. *Life-4555* exhibits a large number of small stable (and typically symmetric) oscillating configurations, but its behavior has much less in common with that of Conway's rule than *Life-5766*. However, since *Life-4555* also typically undergoes longer transient periods than *Life-5766*, it may have more of a chance for something interesting to evolve during the intermediate time steps, leading Bayes to suggest that ultimately *Life-4555* may prove to be the more interesting rule [bayes87a].

An important general difference between the behavior of Conway's two dimensional *Life* and any "worthy" three-dimensional rule is the size of the remaining residue of live sites after a long transient. While Conway's rule typically leaves about 5% of the lattice sites in the $\sigma = 1$ state, only 0.05% to 0.1% are left living in the three-dimensional universe. This may be part of the reason why no three-dimensional analog of the two-dimensional *Life's* glider-gun has yet been found for any three-dimensional rule. Recall that a glider-gun is a pattern of live sites that periodically spews forth gliders. If any of the "worthy" three-dimensional rules are also universal computers (as is two-dimensional *Life*; see section 3.3.4), the glider-gun would play a critical role in the "proof" of that capability. There is also no evidence of the prolific "zoo" of exotic patterns (spaceships, flotillas, shuttles, puffer trains and many others) known to populate the two-dimensional *Life* universe. This may again be a consequence, in part, of the relatively rapid convergence of three-dimensional patterns when compared to their two-dimensional counterparts. In Conway's *Life*, there is typically a much longer period of time during which "interesting" patterns can emerge.

3.4.6.1 *Analogs of Conway "Objects" in 3D*

We have already alluded to patterns that evolve under Conway's original two-dimensional rule as either having or not having "analogs" in three-dimensions. We now make this notion of "analogous" more precise.

Assume we are on a cubic lattice. Define a *Conway object* as any pattern of live sites that emerges during Conway's *Life*. Without loss of generality, we may suppose that the two-dimensional pattern lives on the $z = 0$ plane of the cubic lattice.

Next, introduce two primitive concepts [bayes87a]. (1) An *expansion*, $\mathcal{E}(C)$, of a Conway object $C \equiv \{(x_i, y_i, z = 0)\}$, which is a three-dimensional pattern, P , formed by copying all live cells of that object onto an adjacent plane, so that $\mathcal{E}(C) = \{(x_i, y_i, z = 0), (x_i, y_i, z = 1)\}$. (2) A *projection* of a three-dimensional *Life* object into two dimensions, which exists if and only if (i) all of its live sites lie in two adjacent planes (say $z = 0$ and $z = 1$), and (ii) all pairs of sites, $(x_i, y_i, 0)$ and $(x_i, y_i, 1)$ are either both live or both dead.

A *three-dimensional analog of a Conway object* is then defined to be an expansion such that, when subjected to the appropriate three-dimensional *Life*-rule, yields after each and every generation a projection that is identical to the original Conway object for the same iteration step under Conway's original two-dimensional

rule.

Consider *Life-5766*. By comparing the number of neighbors and the status of two-dimensional *Life*'s and *Life-5766*'s sites, it is easy to show that a Conway object has an analog under *Life-5766* if and only if the Conway object satisfies the following two properties at each subsequent iteration step [bayes87a]: (1) no dead site in the neighborhood of the object can have six live neighbors, and (2) a live site cannot have five neighbors. One can show, by the same reasoning, that of all possible three-dimensional rules of the form $\Phi = (E_l E_u F_l F_u)$, *Life-5766* is the one most analogous to Conway's original rule. In contrast, one can show that for *Life-4555*, any Conway object that changes from one iteration step to the next has no analog in three dimensions. The "universes" of *Life-5766* and *Life-4555* are therefore fundamentally very different.

Appendix: Color Plates

We conclude this chapter with a few illustrative color plates. Simple B&W graphics are sufficient for viewing CA only in the special case when sites take on one of two values. In all other cases, color is indispensable for visualizing the behavior of the system. The plates were produced using the freely available CA software packages *MCell*, *Cellab* and *WinCA*. See **Appendix A: CA Research Tools** for a description of these programs and links to web sites from which they can be downloaded

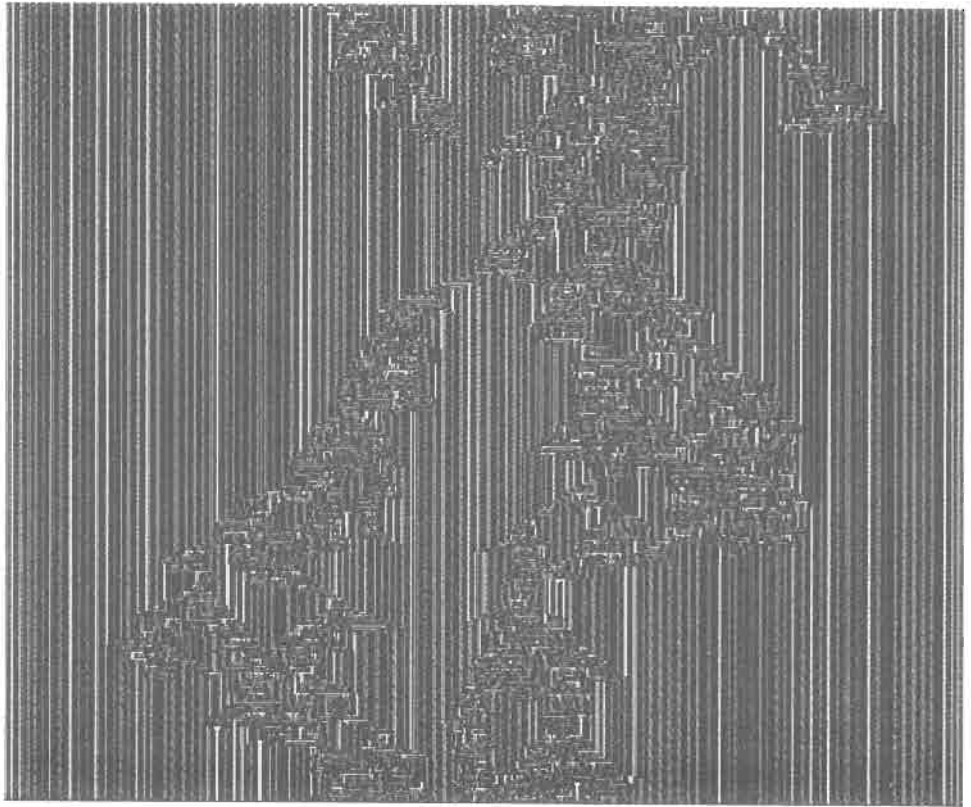


Plate 1. A space-time plot of a Wolfram class-4 one-dimensional $k = 10$ (i.e. 10 state), radius $r = 6$ totalistic CA rule.

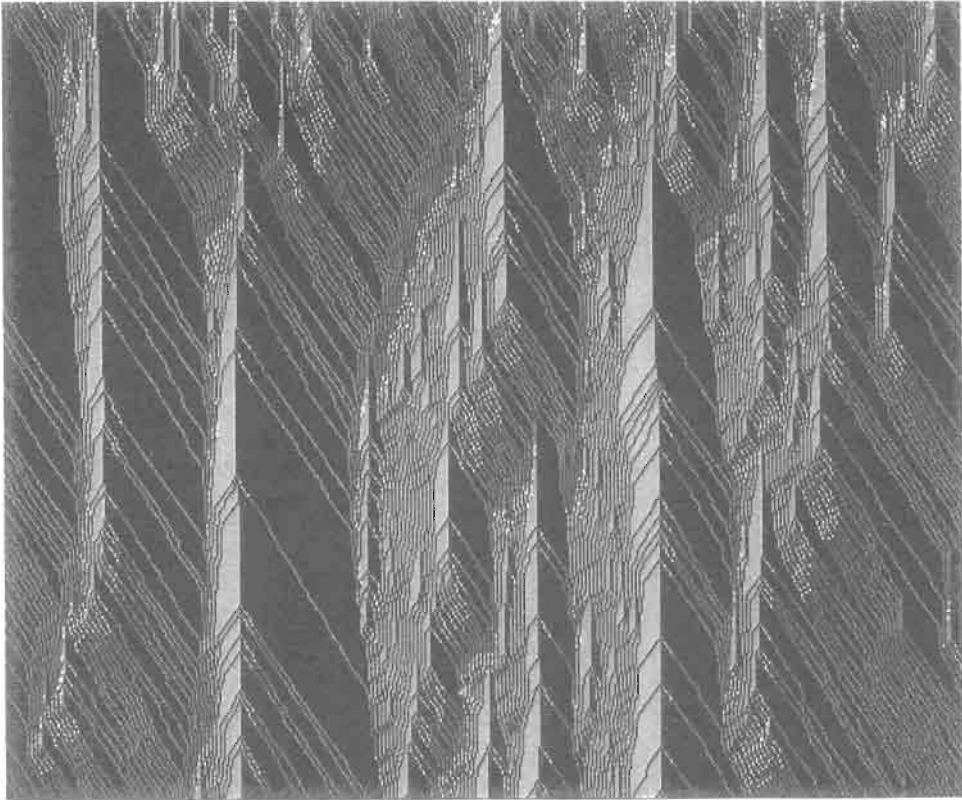


Plate 2. A space-time plot of a probabilistic *Traffic CA* rule. According to this rule (defined by David Griffeath; see <http://psoup.math.wisc.edu/>), traffic moves to the right, so the only possible transitions are of the form 10 to 01 at some pair of adjacent sites. Four parameters govern all transitions (synchronously in time): acceleration, braking, congestion and free-flow driving.

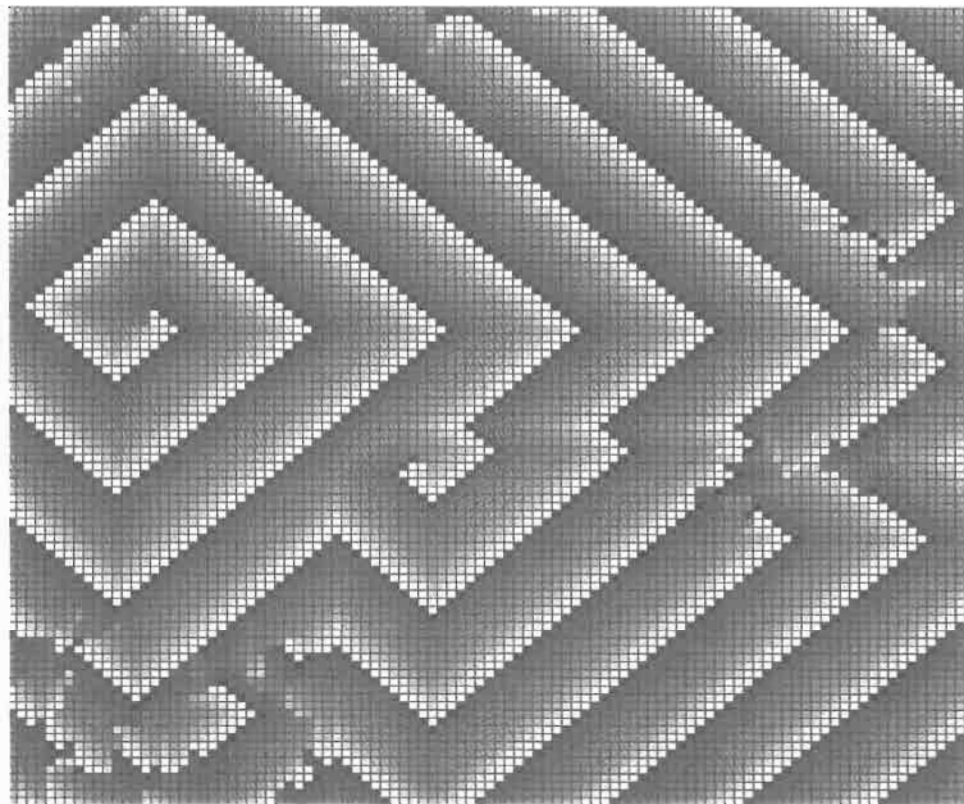


Plate 3. A snapshot of a *Cyclic Cellular Automata* (CCA) rule, which is a typical representative of a class of CA rules first introduced by David Griffeath (see <http://psoup.math.wisc.edu/kitchen.html>). In this example, 14 colors are arranged cyclically. Each color advances to the next, with the last color cycling back to 0. Each update of a site's color advances that color by 1 if there are at least a threshold number of sites of the next color within that site's neighbourhood. The example shown in this figure uses the 4-neighbor von Neumann neighbourhood. See Chapter 8.

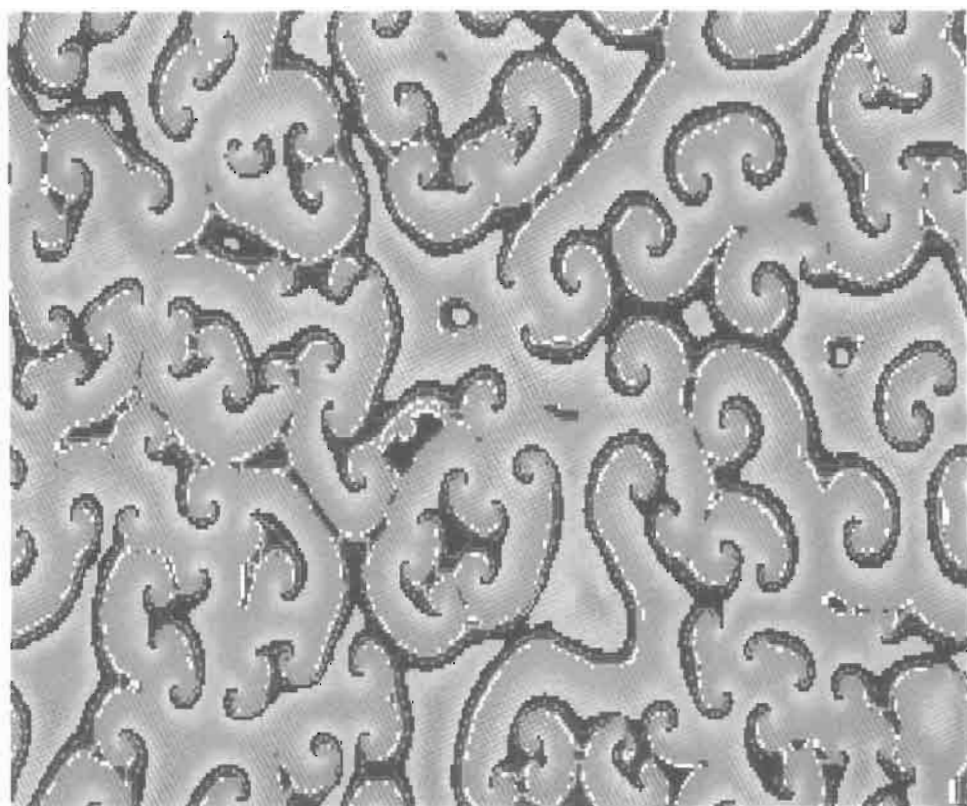


Plate 4. A snapshot of the *Hodgepodge* CA. The Hodgepodge rule, introduced by Gerhardt and Schuster [gerh89], is characterized by its self-organized spiral structures and is a crude model of a famous oscillating chemical reaction-diffusion system called the *Belousov-Zhabotinskii* reaction. See Chapter 8.

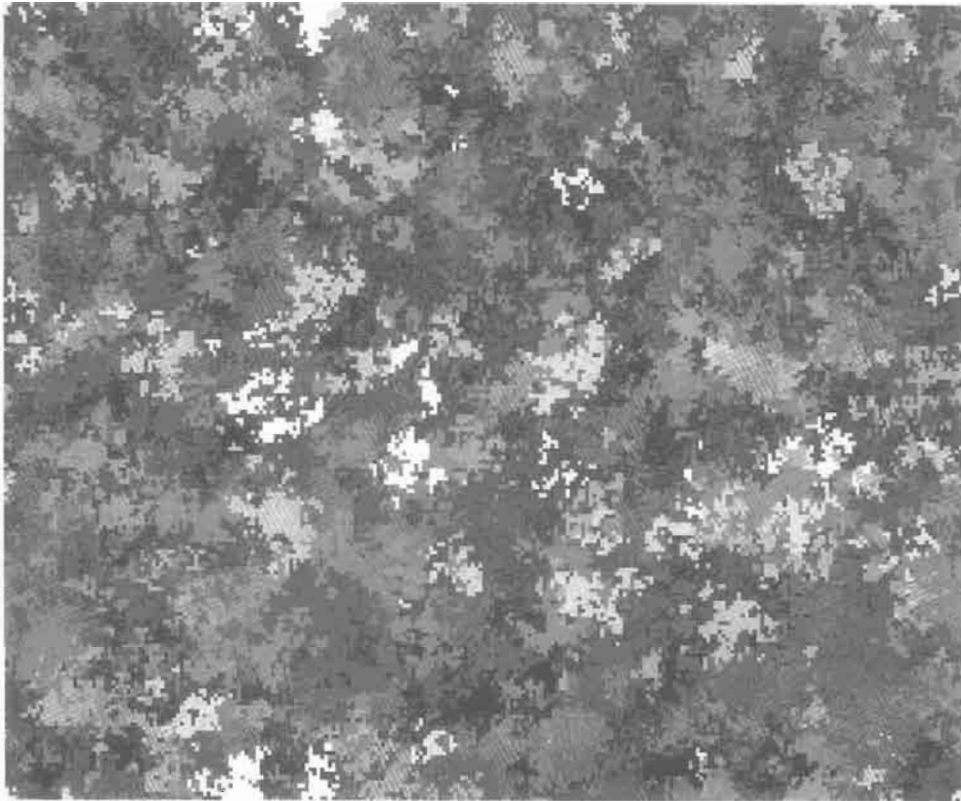


Plate 5. A snapshot of David Griffeath's *Stepping Stone* CA. The rule is defined as follows. First, choose a number between 0 and 1 to set the update probability ρ for all sites. For each site i , generate a random number $0 < p_i < 1$ at each time step. If $p_i > \rho$, change the color of the site to that of one of its (four nearest) neighbors selected at random. In effect, the *Stepping Stone* rule has each site randomly eat one of its neighbors. See <http://psoup.math.wisc.edu/>.

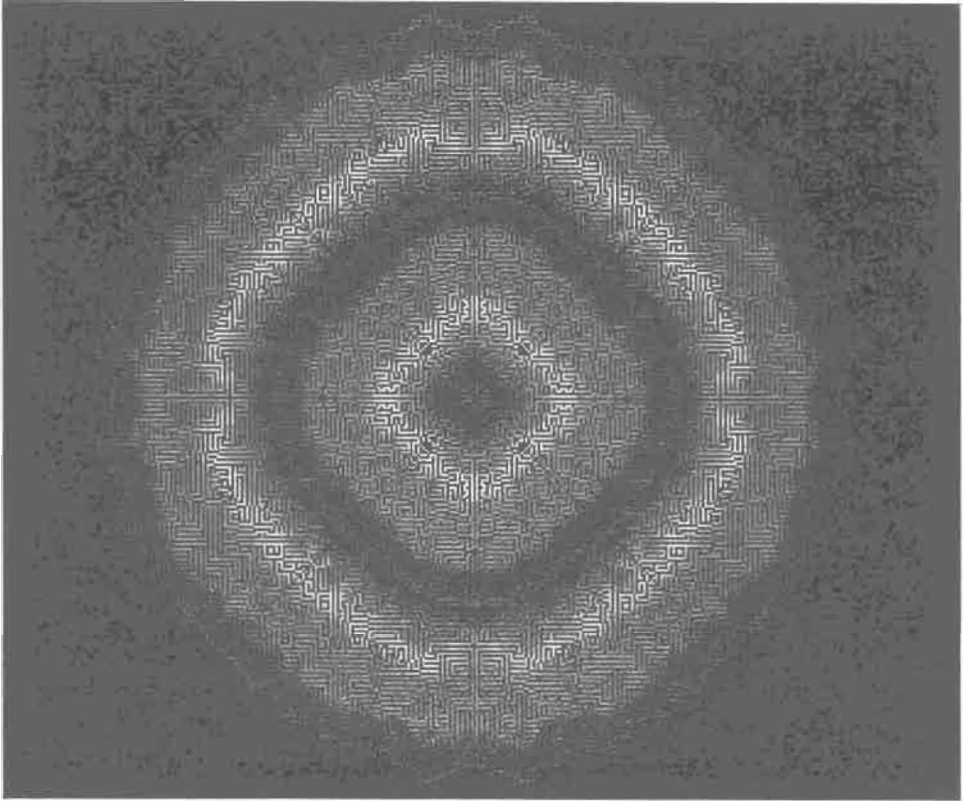


Plate 6. Packard and Wolfram have conjectured that certain slowly spreading CA growth rules might produce isotropic growth [packard85]. The question is whether local parallel dynamics can compensate for the obvious anisotropy of the underlying lattice. The CA shown here suggests that its limiting shape may indeed be very close to circular.

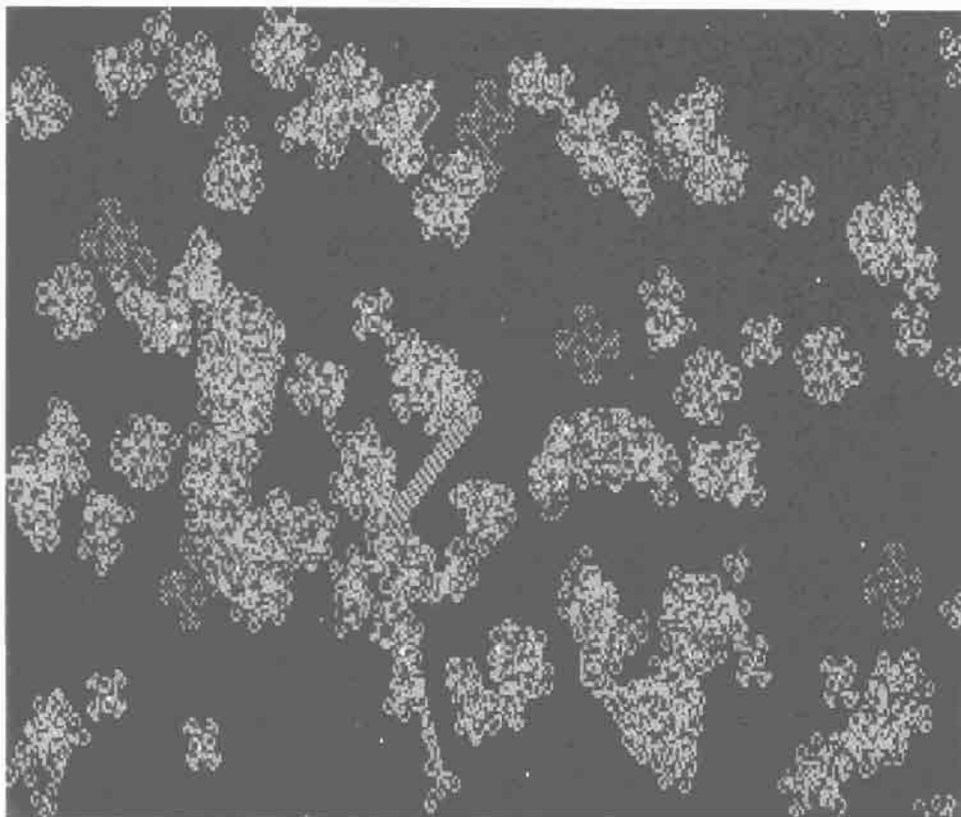


Plate 7. A snapshot of Brian Silverman's *Brain* CA [sil87]. Brain has three states: 0, 1, and 2. If a site is in state 1, it enters state 2. If a site is in state 2, it enters state 0. If a site is in state 0, it counts how many of its eight nearest neighbors are on. If exactly two of them are on, the site turns on. When viewed in real-time on a computer screen, *Brain* displays a very rich behavioral repertoire.

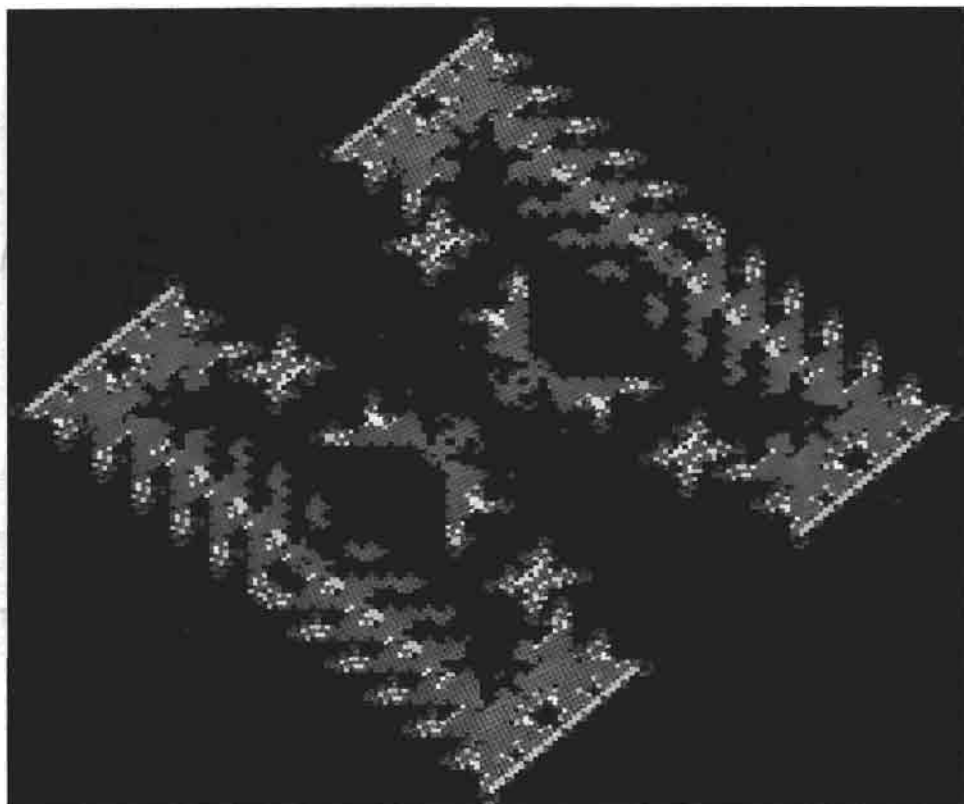


Plate 8. A snapshot of Rudy Rucker's *Faders* CA. Each site contains a live state, a dead state or any one of 127 refractory states. A dead site requires exactly two firing neighbors to get turned on. A firing site keeps firing if it has exactly two firing neighbors. When a site leaves the firing state it goes into a sequence of refractory states. See Rucker's site for additional details: <http://www.mathcs.sjsu.edu/faculty/rucker/>.

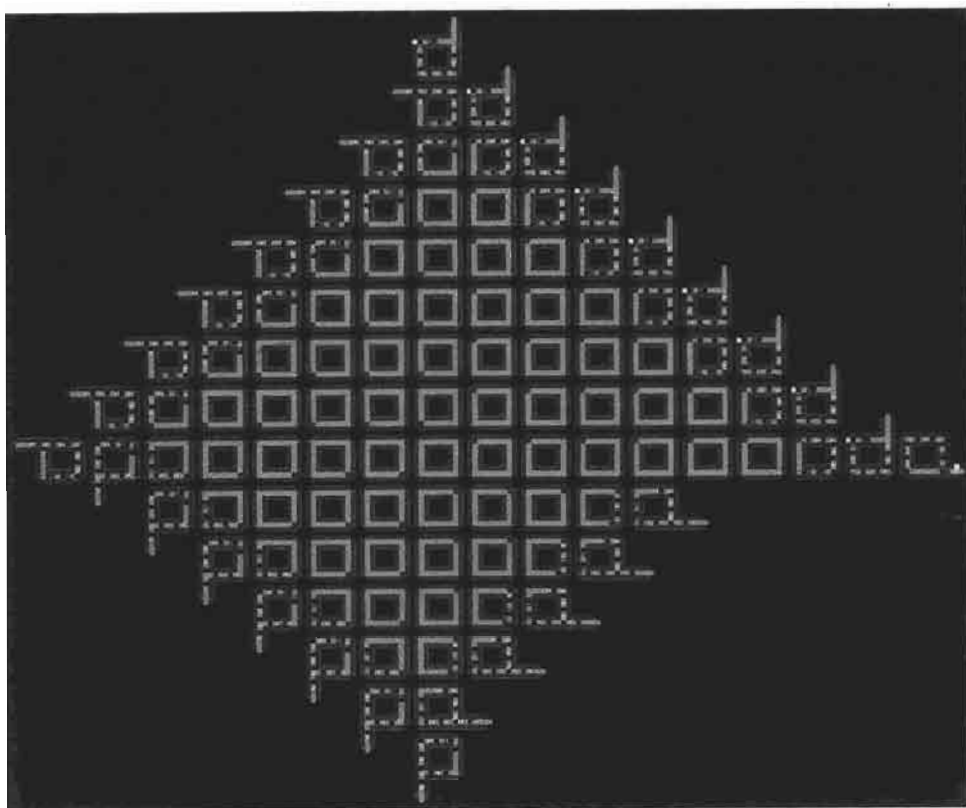


Plate 9. Langton's self-reproducing *Loop*. Consider a two-dimensional array of sites, where each site $\sigma_{i,j} \in \{0, 1, \dots, 7\}$ and evolves according to a four-neighbor von Neumann neighborhood rule. Each of the eight states has a specific function to perform. The state $\sigma = 0$, for example, represents the quiescent state; states $\sigma = 1$ and $\sigma = 2$ are used to guide the signal, where $\sigma = 1$ is itself an element of the data path while $\sigma = 2$ forms a protective *wall* around the signal as it propagates. The remaining five states $3 \leq \sigma \leq 7$ represent the signal, where an individual signal consists of a string of any number of these five states followed by the state $\sigma = 0$. See Chapter 11.

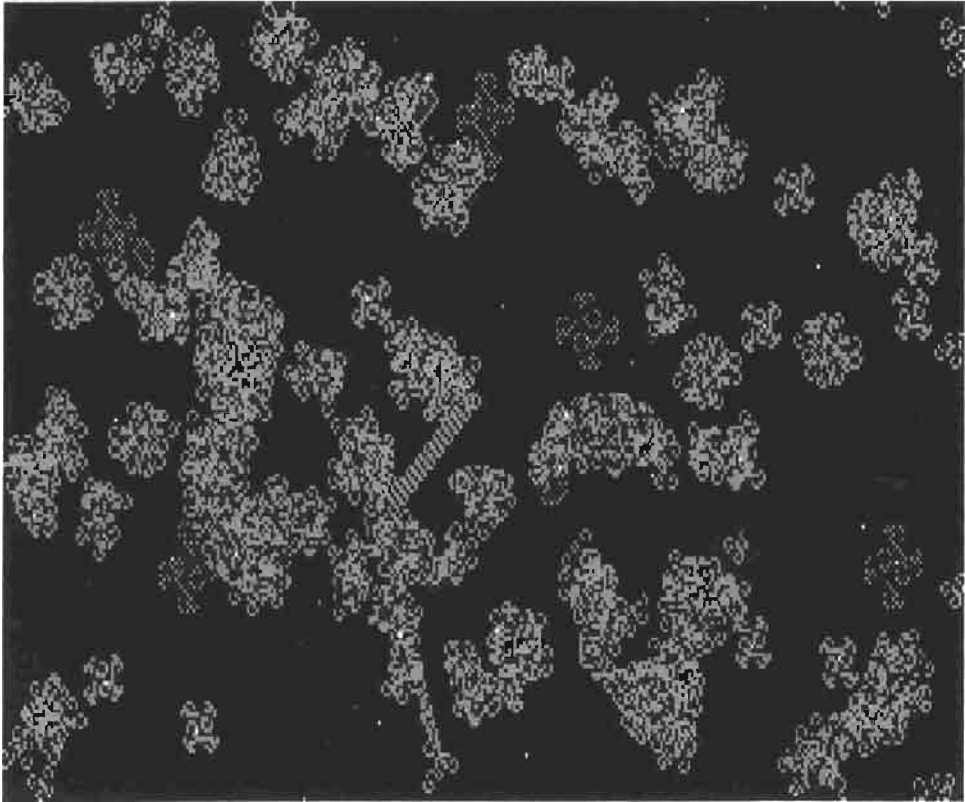


Plate 10. A snapshot of Langton's Vants CA [lang86]. Vants (whose number is conserved) live on a two-dimensional Euclidean lattice and can move in any of four directions (E,W,N,S). Each site is either empty or contains different types of food. How a vant moves through the lattice depends on its color. Each vant looks at the site it is about to move into, moves into it, changes the color of that site according to the food previously stored there, and changes direction. If a vant enters an empty site it continues to move straight ahead. If two or more vants enter the same site, they continue with their respective motions as though the site was unoccupied by other vants (i.e. there is no explicit vant-vant interaction at any site). See Chapter 11 for additional details.

Chapter 4

Dynamical Systems Theory Approach

In the previous chapter, the generic behavior of CA was analyzed in a purely *experimental* fashion. Typical dynamical behaviors were observed through explicit computer simulation of the evolution of various initial configurations according to selected CA rules. Except for a heuristic extraction of some exactly computable properties of a few selected rules, no formal behavioral analysis was attempted. Apart from attaining a formal analytical understanding of the temporal behavior of CA rules (which, though deep for particular classes of rules such as additive rules, does not always extend easily to more general classes and is often limited to relatively simple lattice geometries; see chapter 5), a great deal of insight into the behavior of general rules may be achieved by using existing tools in either (i) *dynamical system theory* or (ii) *the theory of information processing systems*. In this chapter, the former approach is taken. A variety of computational tools are borrowed from the theory of continuous dynamical systems to help provide a more quantitative characterization of the CA behavior discussed in the previous chapter. A number of important ideas are also introduced from the study of *chaos* to illustrate the general issues of computability and predictability. We begin this chapter by briefly surveying continuous dynamical system theory, concentrating mostly on the terminology specific to, and methods developed for analyzing, nonlinear systems. We emphasize that the goal is not to completely cover this enormous field – indeed, whole volumes have been written about most of the terms that will be only briefly defined here – but rather to introduce the ideas and terminology that will be of use to us in our study of the dynamics of CA. Among the many excellent review articles and texts on nonlinear dynamics we recommend the ones by Rasband [rasb90], Schuster [schush88], Devaney [devan86], Iooss, *et al.* [iooss83] and Pietgen *et al.* [peit92]. Nonlinear time series analysis is covered in depth by Kantz and Schreiber [kantz97]. A review of regular and irregular motion in classical Hamiltonian systems is given by Tabor [tabor89]. There are also several good collections of reprints of many landmark papers dealing specifically with chaos – see [bai84], [bai87], [bai88] and [cvit84].

4.1 Dynamical System Theory

Without immersing ourselves in mathematical rigor, we define a *dynamical system* – from a physicist’s perspective – as being any physical system that evolves in time according to some well-defined rule. To be somewhat more specific, a general continuous dynamical system satisfies the following two properties:

1. Its state is completely defined at all times by the values of N variables, $\{x_1(t), x_2(t), \dots, x_N(t)\}$, where $x_i(t)$ represent any physical quantity of interest (position, velocity, temperature, *etc.*). The abstract space in which these variables ‘live’ is called the *phase space* Γ .
2. Its temporal evolution is specified by an autonomous system of N , possibly coupled, ordinary first-order differential equations:*

$$\begin{cases} \frac{dx_1}{dt} &= F_1(x_1, x_2, \dots, x_N; \alpha_1, \alpha_2, \dots, \alpha_M), \\ \frac{dx_2}{dt} &= F_2(x_1, x_2, \dots, x_N; \alpha_1, \alpha_2, \dots, \alpha_M), \\ \vdots &\vdots \\ \frac{dx_N}{dt} &= F_N(x_1, x_2, \dots, x_N; \alpha_1, \alpha_2, \dots, \alpha_M). \end{cases} \quad (4.1)$$

where $\{\alpha_1, \alpha_2, \dots, \alpha_M\}$ are a set of M *control parameters*, representing any external parameters by which the intrinsic evolution may be modified. The temporal evolution of a point $\mathbf{x}(t)$ traces out a *trajectory* (or *orbit*) of the system in Γ . The system is called either *linear* or *nonlinear*, depending on whether $\mathbf{F}$ is linear or nonlinear.

Once the initial state $\mathbf{x}(t = 0)$ of the system is specified, future states, $\mathbf{x}(t)$, are uniquely defined for all times ‘ t ’. Moreover, the uniqueness theorem of the solutions of ordinary differential equations guarantees that trajectories originating from different initial points never intersect.

4.1.1 Discrete-time Poincaré Maps

A convenient method for visualizing continuous trajectories is to construct an equivalent discrete-time mapping by a periodic ‘stroboscopic’ sampling of points along a trajectory. One way of accomplishing this is by the so-called Poincaré map (or surface-of-section) method (see figure 4.1). In general, an $(N - 1)$ -dimensional surface-of-section $S \subset \Gamma$ is chosen, and we consider the sequence of successive intersections of the flow $\mathbf{x}(t)$ with S , $\{\mathcal{I}_1, \mathcal{I}_2, \dots, \mathcal{I}_n, \dots\}$. Introducing a system

*By *autonomous* we mean that $F_i \neq F_i(t)$. This is not really a restriction since any non-autonomous system can always be transformed into an autonomous one by the addition of extra variables. Similarly, an N^{th} -order differential system can always be transformed to a first order one by introducing additional variables.

of coordinates, $\{y_1, y_2, \dots, y_{N-1}\}$, on $\mathcal{S}$ and representing the intersections $\mathcal{I}_i$ by coordinates $(y_{i,1}, y_{i,2}, \dots, y_{i,N-1})$, the differential system defined by equations 4.2 is then replaced by the discrete-time Poincaré mapping

$$\begin{cases} y'_{i,1} &= G_1(y_{i,1}, y_{i,2}, \dots, y_{i,N-1}; \alpha_1, \alpha_2, \dots, \alpha_M), \\ y'_{i,2} &= G_2(y_{i,1}, y_{i,2}, \dots, y_{i,N-1}; \alpha_1, \alpha_2, \dots, \alpha_M), \\ \vdots &\vdots \\ y'_{i,N-1} &= G_{N-1}(y_{i,1}, y_{i,2}, \dots, y_{i,N-1}; \alpha_1, \alpha_2, \dots, \alpha_M). \end{cases} \quad (4.2)$$

Poincaré maps of this form have the obvious advantage of being much simpler to study than their differential-equation counterparts, without sacrificing any of the essential behavioral properties. They may also be studied as generic systems to help abstract behaviors of more complicated systems.

4.1.2 Phase Space Volumes

Consider a small rectangular volume element $\Delta V(\mathbf{x}_0, t) = \prod_{i=1}^N \Delta x_i(\mathbf{x}_0, t)$, around the point $\mathbf{x}_0$, where $\Delta x_i(\mathbf{x}_0, t) = (\partial x_i / \partial x_{i,0}) \Delta x_{i,0}$. The rate of change of ΔV is then determined to be

$$\begin{aligned} \Lambda(\mathbf{x}) &= \frac{1}{\Delta V} \frac{\partial(\Delta V)}{\partial t} = \sum_{i=1}^N \frac{1}{\Delta x_i} \frac{\partial(\Delta x_i)}{\partial t}, \\ &= \sum_{i=1}^N \frac{1}{\Delta x_i} \frac{\partial}{\partial x_{i,0}} \left\{ \frac{\partial x_i}{\partial t} \Delta x_{i,0} \right\}, \\ &\rightarrow \Lambda = \sum_{i=1}^N \frac{\partial F_i}{\partial x_i} = \text{div } \mathbf{F}, \end{aligned} \quad (4.3)$$

where the instantaneous rate of change, Λ has been obtained by using $(\partial x_i / \partial t) \rightarrow dx_i / dt = F_i$ and evaluating the resulting expression at $t = 0$. In the case of discrete-time Poincaré maps of the form $\mathbf{x}_{n+1} = \mathbf{G}(\mathbf{x}_n)$, Λ is effectively given by the absolute value of the *Jacobian*,

$$\Lambda = |\mathcal{J}| = \left| \det \left(\frac{\partial G_i}{\partial x_j} \right) \right|. \quad (4.4)$$

In this case, $\Lambda <, =, > 0$ corresponds to $|\mathcal{J}| <, =, > 1$.

Assuming that the motion in the phase space is bounded, we know that volumes cannot, on average, expand; i.e., that $\Lambda \not> 0$. On the other hand, the set of possible behaviors of systems for which $\Lambda < 0$ is different from those for which $\Lambda = 0$. A brief overview of each of these two fundamental types of dynamical systems is given in the remaining paragraphs of this section; more detailed discussions, with examples, follow in sections 4.1.1 and 4.1.2.

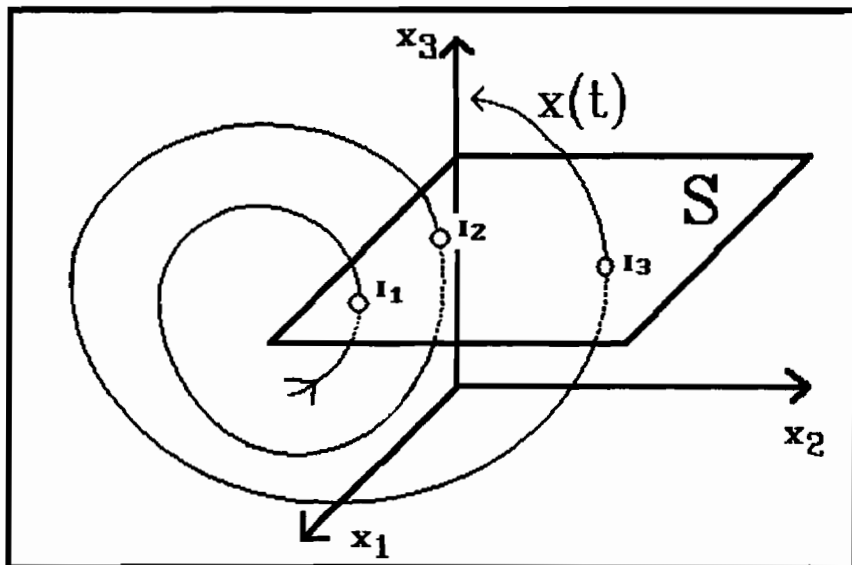


Fig. 4.1 Poincaré section; see text.

Dissipative Systems ($\Lambda < 0$)

Dissipative systems – whether described as continuous flows or Poincaré maps – are characterized by the presence of some sort of ‘internal friction’ that tends to contract phase space volume elements. They are roughly analogous to *irreversible* CA systems. Contraction in phase space allows such systems to approach a subset of the phase space, $\mathcal{A} \subset \Gamma$, called an *attractor*, as $t \rightarrow \infty$. Although there is no universally accepted definition of an attractor, it is intuitively reasonable to demand that it satisfy the following three properties ([ruelle71], [eckman81]):

- (i) *Invariance* – $\mathcal{A}$ is invariant under the map F : $F\mathcal{A} = \mathcal{A}$.
- (ii) *Attractivity* – there is an open neighborhood $\mathcal{B}$ containing $\mathcal{A}$ such that all points $\mathbf{x}(t) \in \mathcal{B} \rightarrow \mathcal{A}$ as $t \rightarrow \infty$. The set of initial points $\mathbf{x}_i^*(t=0)$ such that $\mathbf{x}_i^*(t)$ approaches $\mathcal{A}$ is called the *basin of attraction* of $\mathcal{A}$.
- (iii) *Irreducibility* – $\mathcal{A}$ cannot be partitioned into two nonoverlapping invariant and attracting pieces. A more technical demand is that of *topological transitivity*: there must exist a point $\mathbf{x}^* \in \mathcal{A}$ such that for all $\mathbf{x} \in \mathcal{A}$ there exists a positive time T such that $\mathbf{x}^*(T)$ is arbitrarily close to $\mathbf{x}$ ([ruelle71], [devan86]).

The simplest possible attractor is a *fixed point*, for which all trajectories starting from the appropriate basin-of-attraction eventually converge onto a single point. For linear dissipative dynamical systems, fixed-point attractors are in fact the *only* possible type of attractor. Non-linear systems, on the other hand, harbor a much richer spectrum of attractor-types. For example, in addition to fixed-points, there may exist periodic attractors such as *limit cycles* for two-dimensional flows or *doubly periodic orbits* for three-dimensional flows. There is also an intriguing class of attractors that have a very complicated geometric structure called *strange attractors* [ruelle80].

Strange Attractors: The motion on strange attractors exhibits many of the properties normally associated with completely random or *chaotic* behavior, despite being well-defined at all times and fully deterministic. More formally, a strange attractor $\mathcal{S}$ is an attractor (meaning that it satisfies properties (i)-(iii) above) that also displays *sensitivity to initial conditions*. In the case of a one-dimensional map, $x_{n+1} = f(x_n)$, for example, this means that there exists a $\delta > 0$ such that for all $x \in \mathcal{S}$ and any open neighborhood U of x , there exists $x' \in U$ such that $|f^n(x) - f^n(x')| > \delta$. The basic idea, to which we will return many times, is that initially close points become exponentially separated for sufficiently long times. This has the important consequence that while the behavior of each initial point may be accurately followed for short times, prediction of long time behavior of trajectories lying on strange attractors becomes effectively impossible. Strange attractors also frequently exhibit a self-similar or Cantor-set-like structure, and are characterized by non-integer Hausdorff dimension (see section 2.1.1). Examples of strange attractors are given in section 4.1.1.

Conservative Systems ($\Lambda = 0$)

In contrast to dissipative dynamical systems, conservative systems preserve phase-space volumes and hence cannot display any attracting regions in phase space; there can be no fixed points, no limit cycles and no strange attractors. There can nonetheless be *chaotic* motion in the sense that points along particular trajectories may show sensitivity to initial conditions. A familiar example of a conservative system from classical mechanics is that of a *Hamiltonian* system.

Hamiltonian Systems: A Hamiltonian system is characterized by an even number of dimensions $N = 2n$ (= *number of degrees of freedom*), with variables conventionally labeled as $\{q_i\}_{i=1}^n$ (representing canonical positions) and $\{p_i\}_{i=1}^n$ (representing canonical momenta). The system is completely specified by the *Hamiltonian* function $\mathcal{H}(\{q_i\}, \{p_i\})$, which determines the time evolution of the canonical variables according to

$$\begin{cases} \frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \\ \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}, \end{cases} \quad i = 1, 2, \dots, n. \quad (4.5)$$

The assertion that Hamiltonian flows preserve phase-space volumes is known as *Louville's Theorem*, and is easily verified from equation 4.3 by using the Hamiltonian equations 4.5:

$$\Lambda = \sum_{i=1}^n \left\{ \frac{\partial}{\partial q_i} \left(\frac{dq_i}{dt} \right) + \frac{\partial}{\partial p_i} \left(\frac{dp_i}{dt} \right) \right\} = \sum_{i=1}^n \left\{ \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_i} - \frac{\partial^2 \mathcal{H}}{\partial p_i \partial q_i} \right\} = 0. \quad (4.6)$$

If $\mathcal{H} \neq \mathcal{H}(t)$ then equations 4.5 also show that

$$\frac{d\mathcal{H}}{dt} = \sum_{i=1}^n \left\{ \frac{\partial \mathcal{H}}{\partial q_i} \frac{dq_i}{dt} + \frac{\partial \mathcal{H}}{\partial p_i} \frac{dp_i}{dt} \right\} + \frac{\partial \mathcal{H}}{\partial t} = 0. \quad (4.7)$$

Thus, as long as $\mathcal{H}$ is not an explicit function of time, it remains a conserved quantity. Typically, $\mathcal{H}$ is just the total energy of the system and equation 4.7 is just a statement of *conservation of energy*. For one-degree-of-freedom systems, this one constant – or *integral* – of the motion in fact suffices to completely solve for the behavior of the system; we simply ‘integrate’ the equations of motion. The picture becomes considerably more complicated for systems with $n > 1$ degrees of freedom.

Analogously to the one-degree-of-freedom case, *complete integrability* for systems with n degrees of freedom means that there exist n independent integrals of the motion, $\{I_1(\{q_i\}, \{p_i\}), I_2(\{q_i\}, \{p_i\}), \dots, I_n(\{q_i\}, \{p_i\})\}$, such that $dI_i/dt = 0$, $i = 1, 2, \dots, n$. Even if the dynamics of such completely integrable systems is explicitly nonlinear, the resulting behavior will nonetheless be smooth in all regions of phase space. Completely integrable systems may also be thought of being essentially analogous to *reversible* CA, for which, as we have commented earlier (see the end of section 3.1.4), there are as many ‘constants’ of the motion as there are sites in the lattice. The behavior of nonintegrable Hamiltonian systems, on the other hand, may include features of deterministic chaos. We will go into a bit more detail on issues of integrability in section 4.1.2 below.

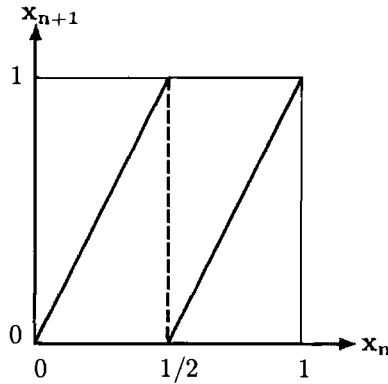
4.1.3 A Generic Chaotic System — The Bernoulli Shift Map

Despite bearing no direct relation to any physical dynamical system, the one-dimensional discrete-time piecewise linear *Bernoulli Shift* map nonetheless displays many of the key mechanisms leading to deterministic chaos. The map is defined by (see figure 4.2):

$$x_{n+1} = f(x_n) \equiv 2x_n \pmod{1}, \quad 0 < x_0 < 1.^\dagger \quad (4.8)$$

We are interested in the properties of the sequence of values x_0 , $x_1 = f(x_0)$, $x_2 = f(x_1) = f^2(x_0), \dots$ – or *orbit* of x_0 – generated by successive applications of the Bernoulli shift to the initial point, x_0 .

[†]By $\pmod{1}$ we mean that $x \pmod{1} = x - \text{Integer}(x)$.

Fig. 4.2 The Bernoulli Shift map: $x_{n+1} = 2x_n \bmod 2$.

It turns out that the most convenient representation for the initial point, x_0 , is as a binary decimal. That is, we write

$$\begin{aligned} x_0 &= \sum_{i=1}^{\infty} \alpha_i 2^{-i} = \frac{a_1}{2} + \frac{a_2}{4} + \cdots, \\ &\equiv 0.\alpha_1\alpha_2\alpha_3\cdots, \end{aligned} \quad (4.9)$$

where $\alpha_i \in \{0, 1\}$ for all ' i '.[†] For example, the binary expansion of $1/3 = 0/2 + 1/2^2 + 0/2^3 + 1/2^4 + \cdots = 0.0101\overline{01}$, where $\overline{01}$ means that the sequence '01' is repeated *ad-infinitum*. A simple procedure for obtaining expansions for arbitrary rationals $r \equiv p/q$, where p and q are integers, is given below; expansions for irrational numbers may be obtained by first finding a suitably close rational approximation (Ex: $\pi - 3 \sim 4703/33215 = 0.001001000011$, which is correct to 12 binary decimal places).

This binary decimal representation of x_0 should make obvious the reason why this map is named the Bernoulli *shift*. If $x_0 < 1/2$, then $a_1 = 0$; if $x_0 > 1/2$ then $a_1 = 1$. Thus

$$\begin{aligned} x_1 = f(x_0) &= \begin{cases} 2x_0 & \text{if } a_1 = 0, \\ 2x_0 - 1 & \text{if } a_1 = 1, \end{cases} \\ &= 0.\alpha_2\alpha_3\alpha_4\cdots. \end{aligned} \quad (4.10)$$

In other words, a single application of the map f to the point x_0 discards the first digit and *shifts to the left* all of the remaining digits in the binary decimal expansion of x_0 . In this way, the n^{th} iterate is given by $x_n = \alpha_{n+1}\alpha_{n+2}\cdots$.

[†]It is not difficult to show that such binary expansions – in fact expansions to an arbitrary base $b > 1$ – are complete in the unit interval; see I. Niven, "Irrational Numbers", *The Carus Mathematical Monographs* 11 (1956).

What of the properties of the actual orbit of x_0 ? Since f effectively ‘reads off’ the digits in the binary expansion of x_0 , the properties of the orbit depend on whether x_0 is itself *rational* or *irrational*.

x_0 is Rational: Suppose that x_0 is rational. This means that x_0 is of the form p/q , where p and q are both integers. Recalling from chapter 2.1.1 that the set of rational numbers, $\mathcal{Q}$, is *countable*, we can immediately show that the total *length* in the interval $[0, 1]$ occupied by $\mathcal{Q}$, $L_{\mathcal{Q}}$, equals zero: label the rationals by the integers $1, 2, \dots$, and place a one-dimensional ‘disk’ of width $\delta_n = \epsilon/2^n$ around the n^{th} rational. The total length occupied by this set is then $L_{\mathcal{Q}} = \sum_{i=1}^{\infty} \delta_n = \epsilon$, which goes to zero as epsilon is made arbitrarily small. Next, we know that, as a subset of $[0, 1]$, $\mathcal{Q}$ is *dense*; i.e., given any two real numbers $r_1, r_2 \in [0, 1]$, there are infinitely many rationals r with $r_1 < r < r_2$. Finally, we show, by construction, that every $r = (p/q) \in \mathcal{Q}$ has a periodic binary decimal expansion: Multiplying r by 2, and writing the result in the form

$$2 \frac{p}{q} = [2 \frac{p}{q}] + \frac{p_1}{q}, \quad (4.11)$$

where $[x]$ is the integer part of x and p_1/q is the remainder, we get the first digit, $\alpha_1 = [2p/q]$. The second digit, α_2 , is obtained by repeating the expansion for p_1/q :

$$2 \frac{p_1}{q} = [2 \frac{p_1}{q}] + \frac{p_2}{q}, \quad (4.12)$$

so that $\alpha_2 = [2p_1/q]$. We now observe that because there can be at most q different possibilities for p_i , *one of the p_i must repeat for some $i \leq q$* . The binary decimal expansion of r must therefore be of the form

$$r = \alpha_1 \alpha_2 \cdots \alpha_{i^*} \underbrace{\alpha_{i^*+1} \alpha_{i^*+2} \cdots \alpha_{i^*+n}}_{\text{period-}n \text{ string}} \underbrace{\alpha_{i^*+1} \alpha_{i^*+2} \cdots \alpha_{i^*+n}}_{\text{repeat \# 1}} \underbrace{\alpha_{i^*+1} \alpha_{i^*+2} \cdots \alpha_{i^*+n}}_{\text{repeat \# 2}} \cdots, \quad (4.13)$$

where the expansion begins repeating, with period $\pi = n$, after the $(i^*)^{\text{th}}$ digit. Conversely, it is easy to show that if a binary decimal expansion is periodic, then the expansion represents a rational number. Orbits for rational x_0 are thus both *periodic* and *dense* in the unit interval.

x_0 is Irrational: Using the same argument as given above, orbits for irrational x_0 must be *nonperiodic*, with the attractor in this case being the entire interval. Because any finite sequence of digits appears infinitely many times within the binary decimal representation of almost all irrational numbers in $[0, 1]$ (all except for a set of measure zero), the orbit of almost all irrationals approaches *any* $x \in [0, 1]$ to within a distance $\epsilon \ll 1$ an infinite number of times; i.e., the Bernoulli shift is *ergodic*.

We began this section by asserting that this simple map is often used to illustrate many of the fundamental concepts associated with chaos and computability. Four such concepts are introduced below:

1. *Stability.* Chaotic attractors may be distinguished from regular, or nonchaotic, attractors by being unstable with respect to small perturbations to the initial conditions; this property is frequently referred to as simply a *sensitivity to initial conditions*.[†] In the present example, suppose that two points, x_0 and x'_0 , differ only in the n^{th} place of their respective binary decimal expansions. By the time we have taken n iterates of each initial point, the difference between their evolved values, $|f^n(x_0) - f^n(x'_0)|$, will be expressed in the first digit; *i.e.*, *arbitrarily small initial 'errors', are exponentially magnified*. If $|x_0 - x'_0| \sim \epsilon = 10^{-31}$, for example, their respective orbits would differ by order ~ 1 by the 100^{th} iterate. Physically, we know that any measurement will have an arbitrarily small, but inevitably finite, error associated with it. In systematically magnifying these errors, nonlinear maps such as the Bernoulli shift effectively transform the information originating on microscopic length scales to a form that is macroscopically observable.

2. *Predictability.* Exponential divergence of orbits places a severe restriction on the predictability of the system. If the initial point x_0 is known only to within an 'error' δx_0 , for example, we know that this error will grow to $\delta x_n = \exp\{n \ln 2\} \delta x_0 \pmod{1}$ by the n^{th} iteration. The *relaxation time*, τ_r , to a statistical equilibrium – defined as the number of iterations required before we reach a state of total ignorance as to the location of the orbit point within the unit interval $[0, 1]$; *i.e.*, $\tau_r = \min(n)$ such that $\delta x_n \sim 1$ – is therefore given by

$$\tau_r \sim \frac{-\ln |\delta x_0|}{\ln 2}. \quad (4.14)$$

For all times $t > \tau_r$, the initial and final states of the system will be *causally disconnected*.

3. *Deterministic Randomness.* On the one hand, equation 4.8 is a trivial linear difference equation possessing an equally as trivial solution for each initial point x_0 : $x_n = 2^n x_0 \pmod{1}$. Once an initial point is chosen, the future iterates are determined uniquely. As such, this simple system is an intrinsically deterministic one. On the other hand, look again at the binary decimal expansion of a randomly selected x_0 . This expansion can also be thought of as a particular semi-infinite sequence of coin tosses,

$$\begin{aligned} x_0 &= . \quad 0 \quad 1 \quad 1 \quad 0 \quad 1 \quad \dots \\ &\quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \downarrow \\ &= . \quad T \quad H \quad H \quad T \quad H \quad \dots, \end{aligned} \quad (4.15)$$

in which each '1' represents *heads* and each '0' represents *tails*. In this way, the set of all binary decimal expansions of $0 < x_0 < 1$ may be regarded as being *identical to the set of all possible sequences of random coin tosses*. Put another way, if we are merely reading off a string of digits coming out of some 'black-box', there is no

[†]Note that while all Bernoulli-shift orbits are generically *unstable* in this sense, only those originating from irrational x_0 are *chaotic*.

way of telling whether this block-box is generating the outcome by flipping a non-biased coin or is in fact implementing the Bernoulli shift for some precisely known initial point. Arbitrarily selected x_0 will therefore generate, in a strictly deterministic manner, a random sequence of iterates, $x_0, x_1, x_2, \dots$. Notice, however, that the Bernoulli-shift generated ‘randomness’ is of an altogether different form from that observed for the temporal sequence of center-site values for the elementary CA rule **R30** (see section 3.1.4). While the CA system generates random sequences from manifestly nonrandom simple initial seeds, the Bernoulli-shift effectively unravels the randomness that is already present in the initial state. Moreover, we should hasten to point out, that despite being assured, with probability one, that a randomly selected x_0 will be *irrational* (by virtue of the fact that rationals only occupy a space of measure zero, as shown above), we are at the same time limited in a practical computational sense to always working with finite, and therefore *rational*, approximations of x_0 . We turn to the consequences of this fact in the third point below.

4. *Computability.* While we are free to formally represent an arbitrary point x by the infinite expansion defined by equation 4.9, we are limited in practice to being able to work only with the finite expansion, $x = \sum_{i=1}^N \alpha_i/2^i$. Conversely, any sequence of coin tossings must also necessarily be finite in duration and therefore defines only a rational number. Given this restriction, in what sense may it then be said that chaotic orbits are computable? When implemented on a computer, for example, a single application of the Bernoulli map is realized by a left shift of one bit followed by an insertion of a zero as the rightmost bit. Since any x_0 is stored as finite-bit computer ‘word’, the result is that all x_0 are eventually mapped to the (stable fixed point) $x^* = 0$:

$$\begin{array}{rcccccccc}
 x_0 & = & 0 & . & \alpha_1 & \alpha_2 & \alpha_3 & \cdots & \alpha_{N-1} & \alpha_N, \\
 x_1 & = & 0 & . & \alpha_2 & \alpha_3 & \alpha_4 & \cdots & \alpha_N & 0, \\
 x_2 & = & 0 & . & \alpha_3 & \alpha_4 & \alpha_5 & \cdots & 0 & 0, \\
 \vdots & & & & & \vdots & & & \vdots & \\
 x_N & = & 0 & . & 0 & 0 & 0 & 0 & 0 & 0.
 \end{array} \tag{4.16}$$

All of the points of a finite length orbit, $x_0, x_1, \dots, x_n$, may be assured of having at least N -bit accuracy by computing x_0 to $(N + n)$ -bits. A number ‘ x ’ is said to be *computable* (or *Turing computable*[‡]), if its expansion coefficients α_i may be *algorithmically generated to arbitrarily high order*. Thus, so long as the initial point x_0 is itself a computable irrational number, its orbit will be chaotic and computable; as we shall see in chapter 6, however, there are many more *noncomputable* irrationals than computable ones!

[‡]The general theory of computability, particularly how it relates to general CA systems, is discussed at some length in chapter 6.

4.1.4 Dissipative Systems

“Not only in research, but also in the everyday world of politics and economics, we would all be better off if more people realized that simple dynamical systems do not necessarily lead to simple dynamical behavior” – R.M. May

So concludes Robert M. May his now famous 1976 *Nature* review article [may76] of what was then known about the behavior of first-order difference equations of the form

$$\mathbf{x}_{n+1} = \mathbf{F}(\mathbf{x}_n). \quad (4.17)$$

In many ways, May’s sentiment echoes the basic philosophy behind the study of CA, the elementary versions of which, as we have seen, are among the simplest conceivable dynamical systems. There are indeed many parallels and similarities between the behaviors of discrete-time dissipative dynamical systems and generic irreversible CA, not the least of which is the ability of both to give rise to enormously complicated behavior in an attractive fashion. In the subsections below, we introduce a variety of concepts and terminology in the context of two prototypical discrete-time mapping systems: the one-dimensional *Logistic* map, and the two-dimensional *Hénon* map.

4.1.4.1 The Logistic Map

Just as the *Bernoulli* map provides important insights into some of the fundamental properties of dynamical chaos, the *Logistic* map is arguably the simplest (continuous and differentiable) nonlinear system that captures most of the key mechanisms responsible for producing dynamical chaos. Indeed, the Logistic map appears to capture much of the essence of a whole class of real-world phenomena, including that of the transition to turbulence in fluid flows. Although the study of its behavior dates back at least forty years, and includes such distinguished theorists as Ulam and von Neumann [ulam52], Metropolis and Stein [metro73], and May [may76], the most profound series of revelations was no doubt obtained by Mitchell Feigenbaum in 1975, culminating in his universality theory ([feig78], [feig79]).[†] Feigenbaum observed that the ‘route to chaos’ as found in the logistic map in fact occurs (apart from a few mild technical restrictions) in *all first-order difference equations* $x_{n+1} = f(x_n)$, where the function $f(x)$ (after a suitable rescaling) has a single maximum on the unit interval $[0, 1]$. Moreover, the transition to chaos is characterized by a scaling behavior governed by universal constants whose value depends only on the *order* of the maximum of $f(x)$. The subsections below provide an overview of the behavior of this simple dynamical system.

[†]It is ironic that such an intensely computational mathematical science as chaos theory owes much of its modern origin to calculations that were performed not on a large mainframe computer but rather a simple programmable pocket calculator, a Hewlett-Packard HP-65! Feigenbaum would explain years later that had the series of intermediate calculations not been carried out sufficiently *slowly*, it is likely that most of the key observations would have been missed [feig80a].

Definition: The Logistic map is defined by

$$x_{n+1} = f_{\alpha}(x_n) = \alpha x_n(1 - x_n), \quad x_0 \in \{0, 1\}, \quad 0 < \alpha \leq 4. \quad (4.18)$$

As long as the single control parameter, α , is less than or equal to four, the orbit of any point $x_0 \in (0, 1)$ remains bounded on the unit interval. Notice also, that like the Bernoulli map, this map is *noninvertible*; there are two antecedents, x_n and x'_n , for each point x_{n+1} . We now want to study the behavior of orbits as a function of the parameter α . That the behavior of this map strongly depends on the value of α is easily appreciated from figure 4.3, which shows sample evolutions for $\alpha = 0.5, 2.5, 3.3, 4$.

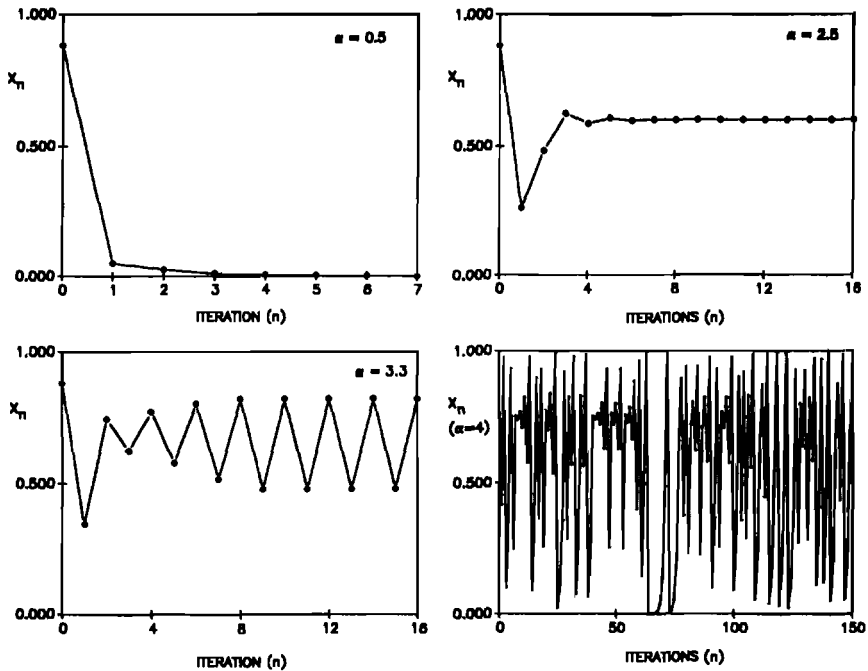


Fig. 4.3 x_n versus iteration n for four different values of α for the logistic map: (a) $\alpha = 0.5$, (b) $\alpha = 2.5$, (c) $\alpha = 3.3$ and (d) $\alpha = 4$; see text.

Fixed Point Solutions: We begin by asking whether there are any values of α for which the system has fixed points. Solving the fixed-point equation

$$x^* = f_{\alpha}(x^*) = \alpha x^*(1 - x^*), \quad (4.19)$$

we indeed find two such points: $x^* = x_{(0)}^* = 0$ and $x^* = x_{(1)}^* = (\alpha - 1)/\alpha$. In order for $x_{(1)}^*$ to be in the unit interval, we must have that $\alpha \geq 1$. What of the stability of these two points? As we have already seen in the case of the Bernoulli map, the divergence of initially closeby points is a crucial issue in the analysis of the dynamical behavior.

Given a fixed point, x^* , the subsequent evolution of a nearby point, $x^{*'} = x^* + \epsilon$,

where $\epsilon \ll 1$, may be determined by substituting $x_n = x^* + \epsilon_n$ and $x_{n+1} = x^* + \epsilon_{n+1}$ into equation 4.18 and leaving only the terms that are linear in ϵ_n and ϵ_{n+1} :

$$\epsilon_{n+1} = \alpha(1 - 2x^*)\epsilon_n + \mathcal{O}(\epsilon_n^2). \quad (4.20)$$

We find that, regardless of the initial point x_0 , the deviations from the fixed point $x_{(0)}^*$ decrease exponentially fast for all $\alpha < 1$; i.e., all points $x_0 \in (0, 1)$ are *attracted to the fixed point* $x^* = 0$: $\lim_{n \rightarrow \infty} x_n = 0$.

At the critical value $\alpha = \alpha_1 = 1$, however, $x_{(0)}^*$ becomes *unstable* and the α -dependent fixed point $x_{(1)}^*$ becomes stable. This exchange of stability between two fixed points of a map is known as a *transcritical bifurcation*. By using the same linear-stability analysis as above, we see that $x_{(1)}^*$ remains stable if $-1 < \alpha(1 - x_{(1)}^*) < 1$, or for all α such that $1 < \alpha < 3$. Something more interesting happens at $\alpha = 3$.

Period-2 Limit Cycle: At the second critical value, $\alpha = \alpha_2 = 3$, $x_{(1)}^*$ itself becomes unstable and is replaced by a stable *attracting period-2 limit cycle*, $\{x_{(2)}^1, x_{(2)}^2\}$. This new bifurcation – called the *pitchfork bifurcation* – is shown schematically in figure 4.4 below.

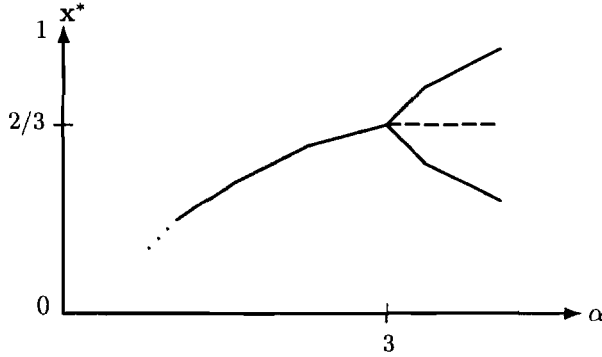


Fig. 4.4 A schematic representation of the *pitchfork bifurcation*: a stable fixed point bifurcates into a period-2 limit cycle plus an unstable fixed point.

The points $x_{(2)}^1$ and $x_{(2)}^2$ are each fixed points of the doubly iterated map, $f^2(x)$:

$$\begin{aligned} x^* &= f(f(x^*)), \\ &= \alpha^2(x^*(1 - x^*)[1 - \alpha x^*(1 - x^*)]), \\ &= \alpha^3 x^* \left(x^* - \left(1 - \frac{1}{\alpha}\right) \right) \left\{ x^{*2} - \left(1 + \frac{1}{\alpha}\right) x^* + \frac{1}{\alpha} \left(1 + \frac{1}{\alpha}\right) \right\}. \end{aligned} \quad (4.21)$$

Neglecting the two previous, and now unstable, fixed point solutions $x^* = 0$ and

$x^* = 1 - 1/\alpha$, the new stable period-2 solution is given by

$$\begin{aligned} x_{(2)}^1 &= \frac{1}{2\alpha} \left(1 + \alpha + \sqrt{\alpha^2 - 2\alpha - 3} \right), \\ x_{(2)}^2 &= \frac{1}{2\alpha} \left(1 + \alpha - \sqrt{\alpha^2 - 2\alpha - 3} \right). \end{aligned} \quad (4.22)$$

Noting that the derivative $f^{2'}(x_{(2)}^i) = f'(x_{(2)}^1)f'(x_{(2)}^2)$, $i = 1, 2$, we find that the period-2 solution is stable as long as $|\alpha^2(1 - 2x_{(2)}^1)(1 - 2x_{(2)}^2)| < 1$, or

$$\alpha_2 = 3 < \alpha < \alpha_3 = 1 + \sqrt{6}. \quad (4.23)$$

At $\alpha_3 = 1 + \sqrt{6}$ we again have a simultaneous loss of stability for the period-2 set $\{x_{(2)}^1, x_{(2)}^2\}$ and a bifurcation to a 4-cycle.

Period- n Limit Cycles: As α increases, the system undergoes an infinite sequence of successive period-doublings via pitchfork bifurcations. In general,

- a stable period- 2^{n-1} limit cycle exists for all α such that $\alpha_{n-1} < \alpha < \alpha_n$,
- at the n^{th} critical value of α , α_n , all points of the 2^{n-1} -cycle simultaneously become unstable via pitchfork bifurcations in $f_\alpha^{2^n} = [f_\alpha^{2^{n-1}}]^2$, leading to a new stable period- 2^n cycle for $\alpha_n < \alpha < \alpha_{n+1}$.

While the period of the limit-cycles approaches infinity as $n \rightarrow \infty$, the distance between successive critical α 's rapidly decreases:

$$\left\{ \begin{array}{ll} \alpha_1 = 3.0 & \alpha_6 = 3.56969 \dots \\ \alpha_2 = 3.44949 \dots & \alpha_7 = 3.56989 \dots \\ \alpha_3 = 3.54409 \dots & \alpha_8 = 3.56993 \dots \\ \alpha_4 = 3.56441 \dots & \vdots \\ \alpha_5 = 3.56876 \dots & \alpha_\infty = 3.5699456 \dots \end{array} \right. \quad (4.24)$$

What does the orbit look like for α_∞ ? It is an infinite (and therefore aperiodic) self-similar point set with fractal dimensionality, $D_{\text{fractal}} \sim 0.5388$ [grass86c].[‡] Figure 4.5 shows the first six stages in the Cantor-set like construction.

Note that while the attractor for α_∞ is a fractal, it is not a *chaotic* attractor, since initially neighboring points do not undergo the same kind of exponential divergence that we observed earlier in the Bernoulli map.

[‡]We recall that the fractal dimension, $D_{\text{fractal}}(A)$, of a set A , is defined by

$$D_{\text{fractal}}(A) = \lim_{\epsilon \rightarrow 0} \frac{\ln N(A, \epsilon)}{\ln (1/\epsilon)},$$

where $N(A, \epsilon)$ is the smallest number of ϵ -balls needed to cover the set A (see section 2.1.1).



Fig. 4.5 Sets of stable attractors for the first six critical values of α . Note the self-similarity between the boxed subpattern for α_6 and the entire pattern for α_4 appearing two lines above. A Cantor-set-like fractal pattern appears in the limit $\alpha_n \rightarrow \infty$.

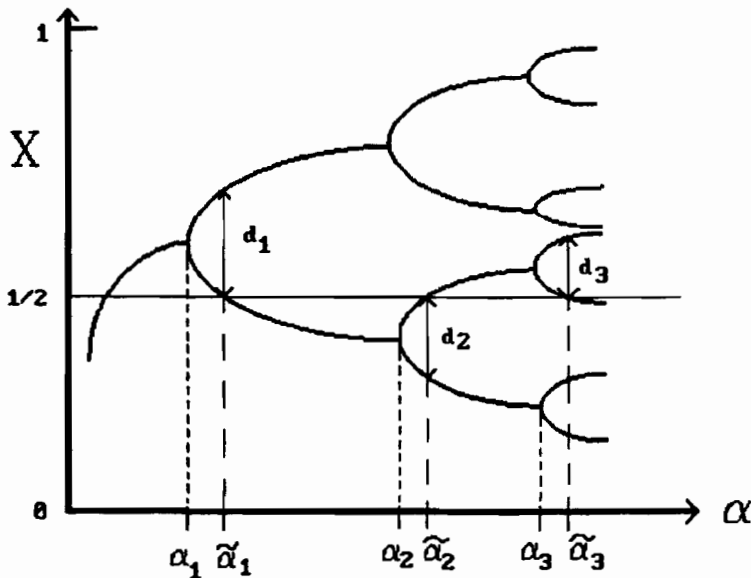


Fig. 4.6 An illustration of some parameters describing pitchfork bifurcations used to define *universality*; see text.

Universality: Feigenbaum's remarkable discovery consisted of the following two quantitative observations (see figure 4.6):

1. *Critical Parameter Convergence:* Feigenbaum's found that the convergence rate of the critical parameters, α_n , is in fact *geometric*; i.e., the α_n scale as $\alpha_n = \alpha_\infty - c \delta^{-n}$, where $n \gg 1$ and 'c' and ' δ ' are constants. A little calculation shows

that

$$\delta \equiv \lim_{n \rightarrow \infty} \frac{\alpha_n - \alpha_{n-1}}{\alpha_{n+1} - \alpha_n} = 4.6692016091 \dots \quad (4.25)$$

This first universal *Feigenbaum constant*, δ , describes the geometric convergence of critical parameters, α_n , for all one-dimensional maps $x_{n+1} = f(x_n)$, where $f(x)$ has a single locally quadratic maximum on $[0, 1]$.[†] For example, while the set of critical α 's, $\alpha'_1, \alpha'_2, \dots, \alpha'_\infty$, calculated for the system defined by $x_{n+1} = \alpha \sin \pi x_n$, will be distinct from the set of α 's computed above for the Logistic equation ($\alpha'_\infty \sim 0.892$), their geometric convergence to α'_∞ is determined by the same Feigenbaum constant, δ .

2. Scaling of Pitchfork-branch Splittings: We define a *supercycle* to be a cycle, $\{x_i^*\}$, such that $\prod_{i=1}^{2^n} f'(x_i^*) = 0$. In particular, since $f'_\alpha(x) = 0$ only when $x = 1/2$, we know that the point $x = 1/2$ must always be an element of a supercycle. Define d_n to be the smallest distance between $x = 1/2$ and the nearest other point on the same 2^n -supercycle:

$$d_n \equiv f_{\tilde{\alpha}_n}^{2^{n-1}}\left(\frac{1}{2}\right) - \frac{1}{2}, \quad (4.26)$$

where $\tilde{\alpha}_n$ defines the new n^{th} critical value of α , $\alpha_n < \tilde{\alpha}_n < \alpha_{n+1}$, at which $x = 1/2$ becomes an element of the 2^n -cycle. Feigenbaum's second observation was that the relative scale of successive splittings at $\tilde{\alpha}_1, \tilde{\alpha}_2, \dots$ approaches another universal constant, Δ :

$$\Delta \equiv \lim_{n \rightarrow \infty} \frac{d_n}{d_{n+1}} = 2.5029078750 \dots \quad (4.27)$$

We should note that the convergence rate of $\tilde{\alpha}$ follows the same form as for α_n : $\tilde{\alpha}_n - \tilde{\alpha}_\infty = c'\delta^{-n}$, where δ is the same as above and $\tilde{\alpha}_\infty = \alpha_\infty$.

Behavior for $\alpha > \alpha_\infty$: What happens for $\alpha > \alpha_\infty$? The simple answer is that the logistic map exhibits a transition to chaos, with a variety of different attractors for $\alpha_\infty < \alpha \leq 4$ exhibiting exponential divergence of nearby points. To leave it at that, however, would surely be a great disservice to the extraordinarily beautiful manner in which this transition takes place.

An overview is provided by figure 4.7: plot (a) shows the numerically determined attractor sets for all $2.9 < \alpha \leq 4$; plot (b) – lest it be thought that the ‘white’ regions in plot (a) are artifacts of the printing process – shows a blowup view of the windowed region within one of those wide white bands in plot (a). The general behavior is summarized as follows:

1. The attracting sets for many – but not all – $\alpha > \alpha_\infty$ are aperiodic and chaotic on various subintervals of $[0, 1]$.

[†]The technical condition that has to be met is that the so-called *Schwarzian* derivative of $f(x)$, $f'_S \equiv (f'''(x)/f'(x)) - \frac{3}{2}(f''(x)/f'(x))^2$, must be negative on $[0, 1]$.

2. As α increases, the chaotic intervals merge together by *inverse bifurcations* obeying the same δ , Δ scalings as in the $\alpha < \alpha_\infty$ region, until the attracting set becomes distributed over the entire unit interval at $\alpha = 4$.

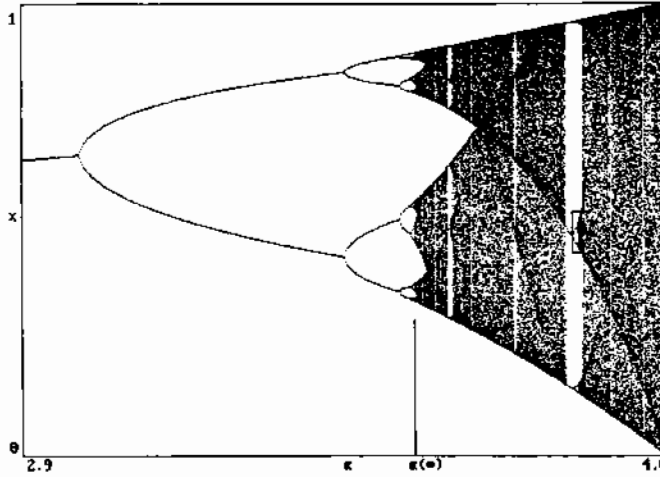


Fig. 4.7(a) Attractor set of the logistic map for $2.9 < \alpha \leq 4$; see text.

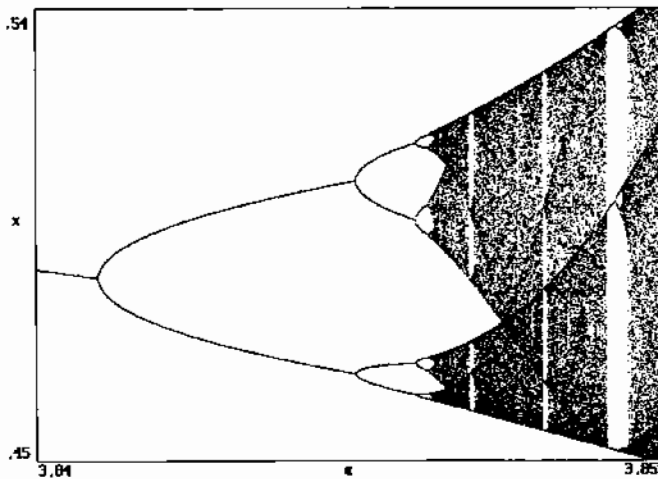


Fig. 4.7(b) Attractor set of the logistic map for $3.840 < \alpha < 3.855$; i.e. a *blowup* of the boxed region shown on the right hand side of figure 4.7(a).

3. There are a large number of 'windows' of finite width within which the attracting set is a stable periodic cycle; chaotic and periodic regions are in fact densely interwoven. The largest window – a snapshot of which is shown in figure 4.7-(b) – corresponds to a stable 3-cycle and spans the width $3.8284 \dots < \alpha < 3.8415 \dots$.

4. The periodic windows harbor m -cycles, $m = 3, 5, 6, \dots$, that undergo period doubling bifurcations, $m \rightarrow 2m \rightarrow 4m \rightarrow \dots$, at a set of critical parameters, $\hat{\alpha}_1, \hat{\alpha}_2, \dots$, that again scale as $\hat{\alpha}_n = \hat{\alpha}_\infty - \hat{c} \delta^{-n}$, with the same universal δ that appears in equation 4.25.

5. Other periodic windows harbor period *triplings*, *quadruplings*, etc., occurring at different sets of $\{\hat{\alpha}_i\}$, but all of which scale in the familiar fashion (albeit with different universal $\hat{\delta} \neq \delta$).

6. Although a rigorous mathematical analysis of the $\alpha_\infty < \alpha < 4$ region is at best very difficult to come by, it turns out that we have already discussed much of the most chaotic behavior, which occurs at $\alpha = 4$ and covers the entire unit interval. A simple change of variables suffices to show that the behavior of the logistic equation at $\alpha = 4$ is effectively identical to that of the Bernoulli map, the properties of which were discussed at some length in the preceding section. Define θ_n , $0 < \theta_n < 1$, by $x_n \equiv \frac{1}{2}(1 - \cos 2\pi\theta_n)$, and substitute this expression into equation 4.18: $x_{n+1} = 4x_n(1 - x_n) \implies$

$$\begin{aligned} \frac{1}{2}(1 - \cos 2\pi\theta_{n+1}) &= 4 \cdot \frac{1}{2}(1 - \cos 2\pi\theta_n) \cdot \frac{1}{2}(1 + \cos 2\pi\theta_n), \\ \sin^2 \pi\theta_{n+1} &= 1 - \cos^2 2\pi\theta_n = \sin^2 2\pi\theta_n, \\ \theta_{n+1} &= 2\theta_n \pmod{1}. \end{aligned} \quad (4.28)$$

The discussion of the randomness of the Bernoulli map iterates therefore applies equally well to the behavior of the $\alpha = 4$ attractor set of the logistic equation.

4.1.4.2 Hénon Map

A simple two-dimensional analogue of the logistic equation, introduced by Hénon in 1976 [hénon76], is defined by

$$\begin{cases} x_{n+1} &= 1 - \alpha x_n^2 + y^n, \\ y_{n+1} &= \beta x_n. \end{cases} \quad (4.29)$$

The Jacobian of this mapping is given by

$$\mathcal{J} = \begin{vmatrix} \partial x_{n+1}/\partial x_n & \partial x_{n+1}/\partial y_n \\ \partial y_{n+1}/\partial x_n & \partial y_{n+1}/\partial y_n \end{vmatrix} = \begin{vmatrix} -2\alpha x_n & 1 \\ \beta & 0 \end{vmatrix} = -\beta, \quad (4.30)$$

so that while α controls the extent of the *nonlinearity*, β controls the degree of *dissipation*. Note that, unlike the logistic map, the Hénon map is *invertible*. Non-invertibility is necessary for chaos in one-dimensional maps; it is not so for higher-dimensions.

Generally, the sequence of points, $(x_0, y_0), (x_1, y_1), \dots, (x_i, y_i), \dots$, either diverges to infinity (for x_0 large) or settles onto an attractor (for (x_0, y_0) near the origin). An analysis similar to the one performed earlier for the logistic equation may be carried out here to determine the behavior of the map as a function of α

and β . For example, the fixed points are easily found to be

$$\begin{cases} x_{\pm}^* &= \frac{1}{2\alpha} \left\{ -(1-\beta) \pm \sqrt{(1-\beta)^2 + 4\alpha} \right\}, \\ y_{\pm}^* &= \beta x_{\pm}^*, \end{cases} \quad (4.31)$$

where the point $(x_-^*, \beta x_-^*)$ is always *unstable* and $(x_+^*, \beta x_+^*)$ becomes unstable for $\alpha > \frac{3}{4}(1-\beta)^2$.

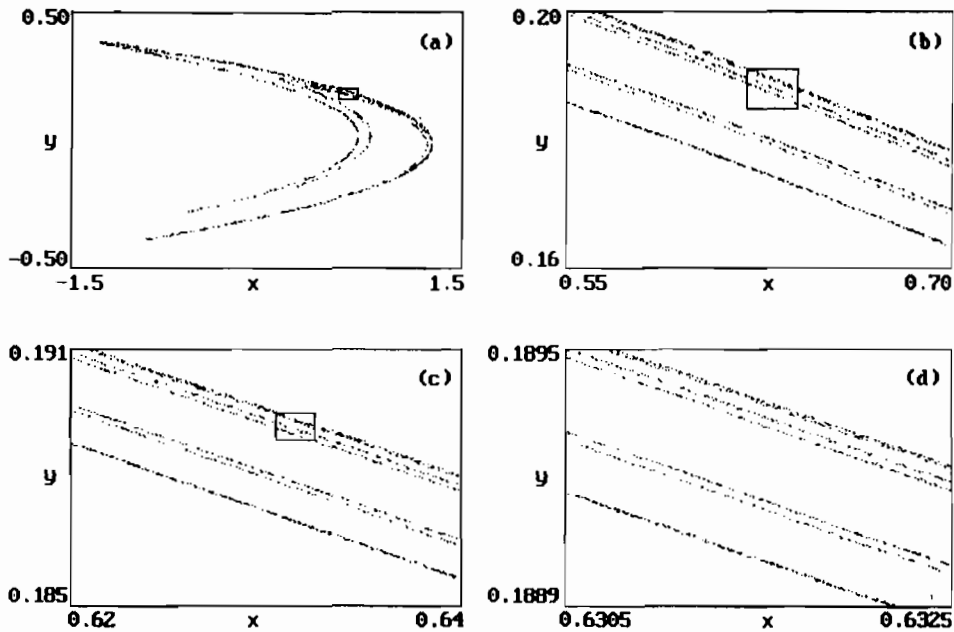


Fig. 4.8 Four snapshots of the Hénon attractor for $\alpha = 1.4$ and $\beta = 0.3$. Plots (b), (c) and (d) provide enlargements of the small window regions shown in plots (a), (b) and (c), respectively; see text.

For $\beta = 3/10$, both fixed points become unstable for $\alpha = \alpha_1 = 0.3675$ and a *two-cycle* is born. At $\alpha = \alpha_2 = 0.9125$ the two-cycle attractor becomes unstable and a *four-cycle* is born. As α is increased further, the system undergoes period-bifurcations obeying the same Feigenbaum constants found to describe the period doublings in logistic equation:

n	period (2^n)	α_n	$(\alpha_n - \alpha_{n-1})/(\alpha_{n+1} - \alpha_n)$
1	2	0.3675	-
2	4	0.9125	4.844
3	8	1.026	4.3269
4	16	1.051	4.696
5	32	1.056536	4.636
6	64	1.05773083	4.7748
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\rightarrow \infty$	$\rightarrow \infty$	1.0580489...	$\delta = 4.6694 \dots$

Figure 4.8 shows four snapshot views of the structure of the *Hénon strange attractor* for $\alpha = 1.4$ and $\beta = 0.3$. In the figure, plots (b), (c) and (d) provide enlargements of the small window regions shown in plots (a), (b) and (c), respectively. The attractor possesses two noteworthy properties:

1. *Exponential divergence of nearby trajectories (i.e., strangeness)*. Just as global space-time CA patterns must be allowed to slowly emerge over many iteration steps before becoming ‘recognizable’ and have a characteristic appearance that is often difficult if not impossible to predict beforehand from a knowledge of the CA rule alone, so too do strange attractors slowly, and in a highly irregular manner, form on a computer screen. While individual points jump around in an apparently haphazard fashion, it is only after several hundred have been plotted that the outline of the underlying attractor becomes clear. Numerical experiments confirm that the dynamics on this attractor are indeed chaotic.

2. *Self-Similarity*. What is most obvious from comparing the sequence of magnifications of an isolated section of the Hénon attractor as shown figure 4.8, is its transverse self-similarity, or its Cantor-set-like structure. Since the map is area-contracting, the attracting set must have zero area (just as the classical Cantor-set has zero length); its Hausdorff dimension is nonintegral, however, which is a characteristic feature of fractals ($D_{\text{fractal}} \sim 1.26$, see sections 2.1.1 and 4.4). Moreover, although this may not be clear from the figure, the Hénon attractor has an *inhomogeneous* structure. That is to say, the probabilities, p_i , for a point of the attractor to be in the i^{th} band in plots (b), (c) or (d), are *all different*. The important general problem of finding appropriate geometrical and statistical characterizations of strange attractors is discussed in section 4.4.

Other Examples of Two Dimensional Strange Attractors

David Ruelle concludes his popular 1980 review of strange attractors that appeared in *The Mathematical Intelligencer* [ruelle80] with this eloquent passage on the often strikingly beautiful patterns weaved by strange attractors: “*I have not spoken of the esthetic appeal of strange attractors. These systems of curves, these clouds of points suggest sometimes fireworks or galaxies, sometimes strange and disquieting vegetal proliferations. A realm lies here to explore and harmonies to discover.*”

Both to give more of a feeling for the enormous variety of strange attractors that is to be found among the the uncountably many possible nonlinear systems, and to have a point of reference for our discussion of *strange-attractor*-like behaviors in CA systems, we conclude this section with four additional examples of two dimensional strange attractors. Figure 4.9 shows plots for the following four systems:

$$\left\{ \begin{array}{l} x_{n+1} = \alpha y_n / (1 + y_n^{10}) + \beta x_n \\ y_{n+1} = x_n \\ \alpha = 1.8, \beta = 0.385 \end{array} \right\} \longleftrightarrow \text{figure 4.9-(a)} \quad (4.32)$$

$$\left\{ \begin{array}{l} x_{n+1} = \alpha x_n (1 - x_n - y_n) \\ y_{n+1} = \beta x_n y_n \\ \alpha = \beta = 3.43 \end{array} \right\} \longleftrightarrow \text{figure 4.9-(b)} \quad (4.33)$$

$$\left\{ \begin{array}{l} x_{n+1} = x_n \exp\{\alpha(1 - x_n/10) - \beta y_n\} \\ y_{n+1} = x_n(1 - \exp\{-\beta y_n\}) \\ \alpha = 2.53, \beta = 0.52 \end{array} \right\} \longleftrightarrow \text{figure 4.9-(c)} \quad (4.34)$$

$$\left\{ \begin{array}{l} x_{n+1} = z \cdot \cos(2\pi x_n) \\ y_{n+1} = z \cdot \sin(2\pi y_n) \\ z \equiv \frac{1}{2} (1 + (\alpha x_n - y_n)/(1 + \alpha)) \quad \alpha \approx 2.1 \end{array} \right\} \longleftrightarrow \text{figure 4.9-(d)} \quad (4.35)$$

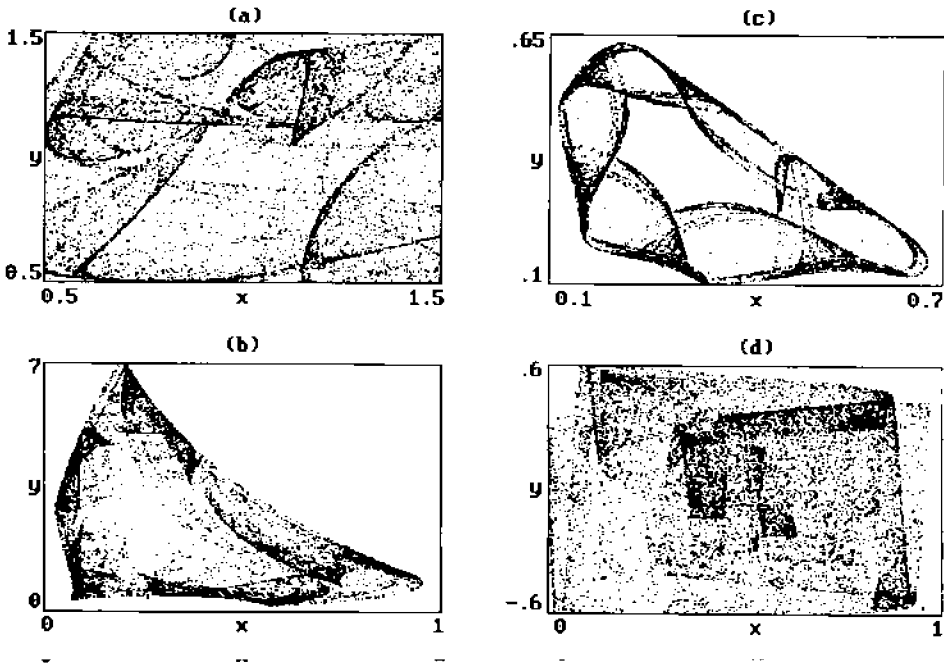


Fig. 4.9 Snapshots of strange attractors defined by the expressions appearing in equation 4.32.

4.1.5 Conservative Systems

"...these intersections form a kind of net, web, or infinitely tight mesh; neither of the two curves can ever cross itself, but must fold back on itself in a very complex way in order to cross the links of the web infinitely many times. One is struck with the complexity of this figure that I am not even attempting to draw. Nothing can give us a better idea of the complexity of the three-body problem." - H. Poincaré (1899)

The quote is from the third volume of Henri Poincaré's *New Methods of Celestial Mechanics*, and is a description of his discovery of *homoclinic orbits* (see below) in the restricted three-body problem.[†] It is also one of the earliest recorded formal observations that very complicated behavior may be found even in seemingly simple classical Hamiltonian systems. Although Hamiltonian (or conservative) chaos often involves fractal-like phase-space structures, the fractal character is of an altogether different kind from that arising in dissipative systems. An important common thread in the analysis of motion in either kind of dynamical system, however, is that of the *stability* of orbits.

In our earlier overview of dynamical systems (see section 4.1), we stated that while dissipative continuous systems are roughly analogous to irreversible CA, reversible CA are analogous to completely integrable Hamiltonian systems. What of the connection between the class of nonintegrable Hamiltonian systems and CA? This still largely unexplored question goes right to the heart of the problem of finding a general connection between continuous and fully discrete dynamical systems. Despite the many apparent similarities, there remain fundamental differences. For example, while *Noether's Theorem* describes an intimate relationship between the existence of integrals of the motion and symmetries of a given continuous system, no such analogue has yet been found for CA. We begin this section with a brief discussion of integrability in Hamiltonian systems.

4.1.5.1 Integrability

We recall that the motion of an n -degree-of-freedom system defined by the Hamiltonian function $\mathcal{H} = \mathcal{H}(q_1, q_2, \dots, q_n; p_1, p_2, \dots, p_n)$, is given by

$$\begin{cases} \frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \\ \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}, \end{cases} \quad i = 1, 2, \dots, n. \quad (4.36)$$

A change of variables, from $(\{q_i\}, \{p_i\})$ to $(\{Q_i\}, \{P_i\})$, is called a *canonical transformation*, if the transformed equations of motion have the same form as that given in equation 4.36, but with $\mathcal{H} \rightarrow \tilde{\mathcal{H}} = \tilde{\mathcal{H}}(\{Q_i\}, \{P_i\})$. In particular, if there exists a canonical transformation such that $\tilde{\mathcal{H}} = \tilde{\mathcal{H}}(P_1, P_2, \dots, P_n)$ only, then the equations

[†]The restricted 3-body problem is defined as the motion of 3 point masses under the effect of their mutual inverse-square attraction with the following three restrictions: (1) mass $m_3 = 0$, (2) m_1 and m_2 undergo circular orbits about their center-of-mass, and (3) m_3 moves in the orbital plane of masses m_1 and m_2 . This deceptively simple system has been shown to contain chaotic orbits; see M. Hénon, *Bull. Astron.* 3 (1966) fasc. 1, 57 and fasc. 2, 49.

of motion for the transformed system may be integrated immediately, yielding

$$\begin{cases} \frac{dQ_i}{dt} = \frac{\partial \mathcal{H}}{\partial P_i} = \omega_i(P_1, P_2, \dots, P_n) \longrightarrow Q_i(t) = \omega_i t + Q_i(0), \\ \frac{dP_i}{dt} = -\frac{\partial \mathcal{H}}{\partial Q_i} = 0 \longrightarrow P_i(t) = P_i(0). \end{cases} \quad (4.37)$$

Such systems are called *integrable*. Expressed in terms of the ‘old variables’, we have the following $N = 2n$ integrals-of-motion:

$$\begin{cases} I_i = Q_i(q_1(t), q_2(t), \dots, q_n(t); p_1(t), p_2(t), \dots, p_n(t)), \quad i = 1, 2, \dots, n \\ I_i = P_i(q_1(t), q_2(t), \dots, q_n(t); p_1(t), p_2(t), \dots, p_n(t)), \quad i = n+1, \dots, 2n. \end{cases} \quad (4.38)$$

Harmonic Oscillator: The simplest example of an integrable system is the harmonic oscillator, with Hamiltonian $\mathcal{H} = \frac{1}{2}(p^2 + \omega^2 q^2)$. Using the canonical transformation

$$\begin{cases} q \rightarrow \sqrt{\frac{2p}{\omega}} \sin Q, \\ p \rightarrow \sqrt{2\omega P} \cos Q, \end{cases} \quad (4.39)$$

$\mathcal{H} \rightarrow \tilde{\mathcal{H}} = \omega P \implies P(t) = P(0), \quad Q(t) = \omega t + Q(0)$. The first integral of the motion, in terms of the original variables, is thus $I = q^2 + p^2$, which tells us that the trajectories of the system lie on circles $q^2 + p^2 = r^2$, where r^2 is proportional to the energy of the oscillator and is fixed by $q(0)$ and $p(0)$.

Comparing the solution to this simple example with the equations above, it should not surprise us to learn that the general behavior of integrable systems is very similar to that of n uncoupled oscillators. As we have just seen, the motion for $n = 1$ is circular with constant angular velocity; *i.e.*, it is periodic. For $n = 2$, there are two radii (given by $P_1(0)$ and $P_2(0)$) with angular velocities ω_1 and ω_2 , so that the motion is confined to a two-dimensional *torus*. If the ratio ω_1/ω_2 is rational, the trajectory will be a periodic one; if the ratio of angular velocities is irrational, on the other hand, the motion can no longer be periodic and the resulting so-called *quasi-periodic* trajectory winds around the surface of the torus, densely filling it as it does so.

There are two obvious questions concerning integrable systems:

1. How large a fraction of the space of Hamiltonian systems is taken up by integrable systems?
2. How does the general behavior of an integrable system, $\mathcal{H}_0$, change as a small nonintegrable component, $\alpha\mathcal{H}_1$ (where α is some small control parameter), is added?

The answer to the first question is given by *Seigel’s theorem*, which asserts

that, if $n > 2$, it is extremely rare for a Hamiltonian system to be integrable.[†] Indeed, omitting only a minor technical qualification, it turns out that nonintegrable Hamiltonians are *dense in the space of all analytic Hamiltonians*; they usually cannot even be *approximated* by a sequence of integrable systems.

A sweeping answer to the second question is that the phase space of *all non-integrable* Hamiltonians must contain chaotic regions.[‡] The particular manner in which these chaotic regions arise – or, more precisely, the manner in which integrable ‘regularity’ is *lost* – is given by the celebrated *Kolmogorov-Arnold-Moser* (KAM) *theorem* ([arnold78], [licht83]).

KAM Theorem: The KAM theorem states that as long as the following three conditions are satisfied...

1. The perturbation term, $\alpha\mathcal{H}_1$, is sufficiently small
2. The angular frequencies, $\omega_i(\mathbf{P})$, obey the nonresonance condition, $\det \frac{\partial(\omega_1, \omega_2, \dots, \omega_n)}{\partial(P_1, P_2, \dots, P_n)} \neq 0$.
3. The frequencies $\omega_i(\mathbf{P})$ are *sufficiently irrational*:

$$|\omega(\mathbf{P}) \cdot \mathbf{I}| \geq c/|\mathbf{I}|^{N+1}, \quad c > 0, \quad \forall N \text{ dimensional integer vectors } \mathbf{I}, \quad (4.40)$$

...the motion of the system remains confined to an n -torus (except possibly for a set of initial conditions of measure zero).

Although the n -tori (conventionally called *KAM-tori* or *KAM surfaces*) may be distorted versions of the curves appearing for the integrable Hamiltonian $\mathcal{H}_0$ alone, the qualitative nature of the motion remains the same. Initial conditions starting from the exceptional set result in trajectories that wander freely over the energy surface (defined by $\mathcal{H} = \text{constant}$).

What happens when the perturbation gets large enough to violate the conditions of the KAM theorem? Since it would take us too far afield to provide a complete description of the manner in which the resulting Hamiltonian form of chaos sets in as more and more KAM-tori disintegrate, we will content ourselves with a heuristic outline. Details may be obtained from the sources cited in the introduction to this chapter. We begin by discussing the stability of fixed points in the phase-space portraits of integrable systems.

4.1.5.2 Phase Portraits and Stability

Consider a simple plane pendulum, defined by the Hamiltonian $\mathcal{H}(p_\theta, \theta) = p_\theta^2/(2ml^2) - mgl \cos \theta$, where ‘ m ’ is the pendulum mass at the end of a length- l arm, and $p_\theta \equiv ml^2(d\theta/dt)$. The Hamiltonian equations 4.36 yield the well-known equation of motion $d^2\theta/dt^2 + (g/l) \sin \theta = 0$, which allows us to solve for $\theta(t)$ and $\frac{d\theta}{dt}(t)$ for

[†]See C.L.Seigel, *Ann. Math.* **42** (1941) 806-822 and **128** (1954) 144-170.

[‡]See N.N.Nehoroshev, *Usp. Mat. Nauk.* **32** (1977) 6.

any time ' t ' given the initial values $\theta(0)$ and $\frac{d\theta}{dt}(0)$. In particular, since the energy is an integral of the motion, the behavior of the system may be represented in the ' $\theta - \frac{d\theta}{dt}$ ' phase-plane by plotting the contours of *constant-energy* (see figure 4.10).

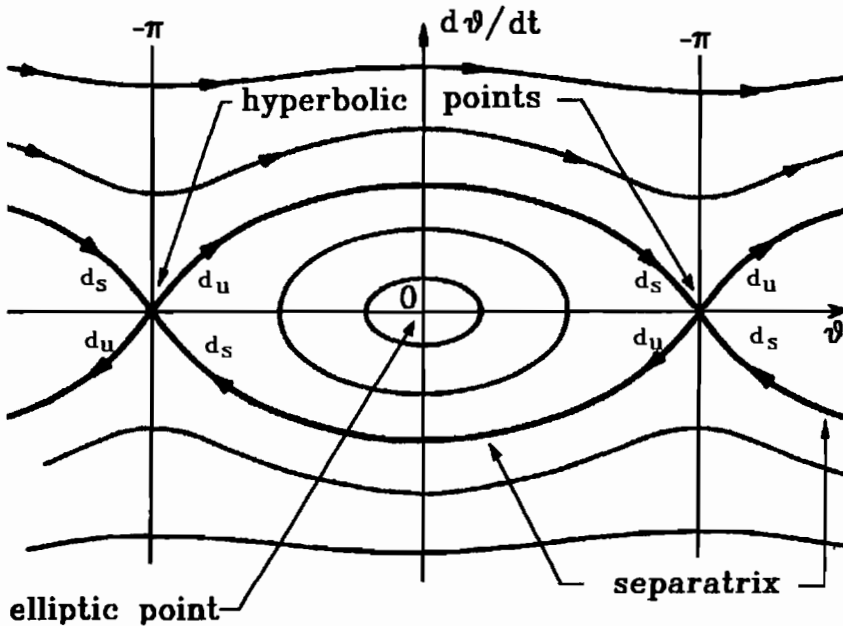


Fig. 4.10 $\theta - \frac{d\theta}{dt}$ phase-plane contours of equal energy; see text.

We see that the phase-plane is broken up into a sequence of fixed points and a series of both open and closed constant-energy curves. The origin ($\theta = \frac{d\theta}{dt} = 0$) and its periodic equivalents ($\theta = \pm 2\pi n$, $\frac{d\theta}{dt} = 0$), are *stable fixed points* (or *elliptic points*), corresponding to a pendulum that is pointing straight down and is at rest. An elliptic point is called 'stable' because the pendulum responds to small perturbations by oscillating about the elliptic point. The points ($\theta = \pm(2n + 1)\pi$, $\frac{d\theta}{dt} = 0$), on the other hand, are *unstable fixed points* (or *hyperbolic points*), and also correspond to the pendulum being at rest but now in an inverted position. In contrast to elliptic points, these fixed points are unstable because the smallest perturbation causes the pendulum to move away from them. The curve connecting the points $(-\pi, 0)$ and $(\pi, 0)$, and their periodic equivalents, is called the *separatrix*, and divides the phase-plane into three distinct regions: *periodic oscillation* near the central elliptic point, and *unbounded rotation* in which θ either increases (for $\frac{d\theta}{dt} > 0$) or decreases (for $\frac{d\theta}{dt} < 0$). Notice that the separatrix leaves one hyperbolic point along an unstable direction, d_u (corresponding to the outgoing arrow) and enters another along a stable direction, d_s (corresponding to an ingoing arrow).

Nesting of KAM-tori: For two-degree-of-freedom system, the KAM theorem states that for sufficiently weak perturbations, all sufficiently irrational KAM-tori are pre-

served under the perturbation.[†] If the frequency ratio, ω_1/ω_2 , is rational, then the original KAM-torus decomposes into smaller and smaller tori in a manner consistent with the *Poincaré-Birkhoff theorem*[†]. Specifically, each KAM-torus is replaced by an even number of new fixed-points, one half of which are elliptic and the other hyperbolic. In the small areas around the new elliptic fixed points, however, there exist smaller rational KAM-tori which themselves must therefore decompose in the exactly the same manner. This process is repeated, *ad infinitum*, and thus gives rise to a self-similar, or fractal-like, nesting of KAM-tori.

Chaos and Homoclinic Points: It is the behavior of separatrices resulting from perturbations of rational KAM-tori that is mainly responsible for the emergence of chaos around hyperbolic points. If the system is nonintegrable, a trajectory starting on an unstable separatrix branch need no longer either *exactly* come back to the same hyperbolic fixed point or *exactly* reach the next such point in the cycle. Fixed-point intersections between these branches in figure 4.10 generalizes to intersections at non-fixed-points between stable and unstable manifolds; such intersection points are called *homoclinic points*. Chaos arises because between each homoclinic point and its neighboring hyperbolic fixed point there *must exist an infinite number of, densely interwoven, other homoclinic points* ([iooss83], [licht83]). Because of these extremely complex networks woven by the stable and unstable manifolds, orbits in these regions of phase space exhibit the telltale sign of chaos; namely, sensitivity to initial conditions. Recalling the self-similar nesting of KAM-tori (see paragraph above), we are left with the picture that regular and irregular motion in conservative systems is densely interwoven in a fractal-like manner. In the next section we discuss a map that serves as a paradigm for conservative chaos.

4.1.5.3 Prototypical Hamiltonian Mapping — Standard Map

Just as the logistic map provides a useful model for many of the fundamental routes-to-chaos in dissipative dynamical systems, the so-called *Standard Map* serves much the same purpose for a certain class of conservative systems. Specifically, it is a generic model of the response of nonlinear oscillators to periodic perturbations; it has been used to study systems ranging from simple ‘kicked’ rotators to the motion of charged particles in toroidal magnetic fields to electrons moving in highly excited hydrogen atoms in the presence of intense electromagnetic fields.[§] We begin by

[†]‘Sufficiently irrational’ tori here means those tori whose frequency ratio ω_1/ω_2 is such that

$$\left| \frac{\omega_1}{\omega_2} - \frac{a}{b} \right| \geq \frac{k}{|b|^{2+\beta}}$$

for all integers a, b and some $0 < \beta < 1/2$, and where $c > 0$ [iooss83].

[†]Original reference: G.D.Birkhoff, “Nouvelles Recherches Sur les Systems Dynamiques”, *Mem. Pont. Acad. Sci. Novi Lyncae* **1** (1935) 85.

[§]See (1) G.M.Zaslavsky and B.V.Chirikov, “Stochastic instabilities in nonlinear oscillations”, *Sov. Phys. Usp.* **14** (1972) 549, (2) B.V.Chirikov, “A universal instability of many oscillator systems”, *Physics Reports* **52** (1979) 265, and (3) G.Casati, B.V.Chirikov, D.L.Shepelyansky and

discussing how a general two-dimensional area-preserving discrete-time map may be derived from a Hamiltonian.

Two-dimensional Area-Preserving Maps: Consider a Hamiltonian of the form

$$\mathcal{H}(q, p) = \frac{p^2}{2} + V(q)\delta_T, \quad (4.41)$$

where $\delta_T \equiv \sum_{i=-\infty}^{\infty} \delta(i - t/T) = 1 + 2 \sum_{i=1}^{\infty} \cos(2\pi nt/T)$ is a periodic delta-function of period T . Physically, this Hamiltonian defines a system which undergoes free translation at all times except for times $t = nT$, $n = 1, 2, \dots$, during which it experiences an impulsive force due to a potential $V(q)$.

The equations of motion are given by

$$\begin{cases} \frac{dq}{dt} = \frac{\partial \mathcal{H}}{\partial p} = p, \\ \frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial q} = -\frac{\partial V}{\partial q} \delta_T. \end{cases} \quad (4.42)$$

Letting q_n and p_n be the values of q and p just prior to the n^{th} delta-function impulse, equations 4.42 may be integrated to yield the mapping

$$\begin{cases} p_{n+1} = p_n - T \left(\frac{\partial V}{\partial q} \right) \Big|_{q=q_n}, \\ q_{n+1} = q_n + Tp_{n+1}. \end{cases} \quad (4.43)$$

Since the absolute value of the jacobian $\mathcal{J} = \partial(q_{n+1}, p_{n+1})/\partial(q_n, p_n) = 1$, we see that this discrete-time map is indeed area-preserving.

The Standard Map: The Standard map may be derived from equations 4.43 by setting $T = 1$ and substituting the potential $V(q) = -(\frac{\alpha}{2\pi}) \cos(2\pi q)$:

$$\begin{cases} p_{n+1} = p_n + \alpha \sin(2\pi q_n) \pmod{1}, \\ q_{n+1} = q_n + p_{n+1} \pmod{1}. \end{cases} \quad (4.44)$$

It is customary to put both variables on the unit torus; that is, q and p are taken to be periodic variables with period equal to one. The sole control parameter, α , determines the extent of the nonlinearity. As α increases, there is a dramatic transition between regular smooth orbits and trajectories that are almost completely chaotic.

Figure 4.11 shows sample trajectories starting from various initial conditions for four different values of α . (Keep in mind that these are *not plots of attractors*; each trajectory is unique to a particular starting position on the unit torus). For $\alpha = 0$,

the standard map takes the form

$$\begin{cases} p_{n+1} = p_n & (\text{mod } 1), \\ q_{n+1} = q_n + p_{n+1} & (\text{mod } 1), \end{cases} \quad (4.45)$$

and is thus clearly ‘integrable’. The motion in this case is regular since the orbits are just straight lines that wrap around the unit torus in the q -direction. If p_0 is rational, then the set of iterates of q is a periodic cycle; if p_0 is irrational, then the dynamics is quasi-periodic and the set of iterates will, for almost all initial q_0 , trace out an orbit that fills out a solid line.

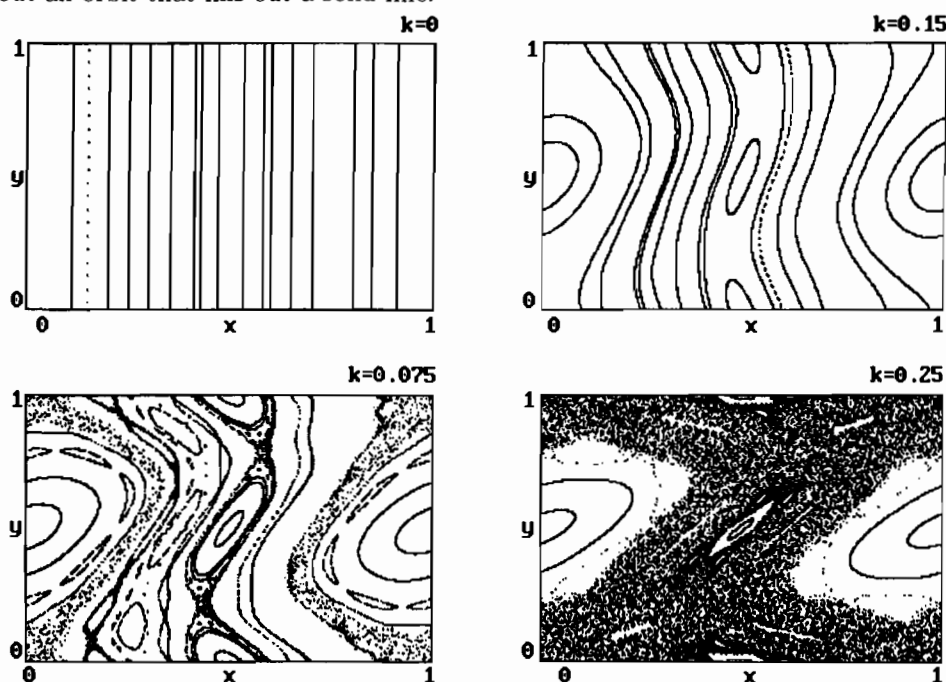


Fig. 4.11 Sample trajectories of the *Standard Map* for various initial conditions for four different values of α : (a) $\alpha = 0$, (b) $\alpha = 0.15$, (c) $\alpha = 0.075$ and $\alpha = 0.25$; see text.

As α is increased to $\alpha = 0.075$, we see that most orbits retain their ‘regularity’, in that they still lie on smooth – albeit crooked – curves. We also see the appearance of three elliptical islands around the points $(0, 1/2)$, $(1/2, 0)$ and $(1/2, 1/2)$. A variety of elliptic island ‘chains’ corresponding to periods of different lengths begin appearing at $\alpha = 0.15$. Although irregular orbits begin appearing as well, there remain a sufficient number of regular trajectories to confine this ‘chaos’ to isolated regions of the phase space. Notice that chaotic orbits do not lie on smooth curves, but instead wander around whole areas in the phase space, the size of which grows as α increases. It is worth emphasizing that the chaotic ‘bands’ – such as the one running from the left- to the right- hand side of the plot for $\alpha = 0.15$, for example – represent a *single* trajectory for a specific initial point. For $\alpha = 0.25$, a single

such chaotic orbit in fact fills more than half of the available phase space.

Recall that the KAM theorem states that as long as a nonlinear perturbation to an integrable system – such as that represented by the nonzero α term added to the ‘integrable’ system defined by equations 4.45 – is sufficiently small, most trajectories will continue to lie on smooth KAM-curves.

As figure 4.11 shows, these KAM curves survive for relatively large values of $\alpha \sim 0.15$. Wherever they are found, they constitute impenetrable ‘barriers’ that chaotic orbits are not permitted to cross.[¶] As their number dwindles with increasing α , however, an increasingly large fraction of phase space is taken up by chaotic orbits. The last KAM-curve to disintegrate is the one whose frequency ratio is the ‘most irrational’ – $\omega_1\omega_2 = (\sqrt{5} - 1)/2$. McKay has shown that this last confining KAM-curve decays into a complex self-similar curve called a *cantorus*, which shows both scaling behavior and universality. Single chaotic orbits leak through the ‘gaps’ in this cantorus to finally fill large areas of the phase space. The critical value, α_c , for which this global chaos appears has been numerically estimated as $\alpha_c \sim 0.15464058$. For $\alpha \gg \alpha_c$, a single orbit would (almost) fill the entire phase space.[†]

4.2 Symbolic Dynamics

The ‘coarse-grained’ representation of dynamical orbits as discrete-symbol sequences is called the method of *symbolic dynamics*. As long as the essential features of the evolution are retained in the transcription, the ‘simpler’ symbolic dynamical system may be studied to gain insight into various questions about the original dynamical system. Introduced in the 1930’s as a part of the abstract topological theory of dynamical systems[‡], symbolic dynamics today offers a powerful and rigorous mathematical tool with which to analyze chaotic behavior. While much of the well-developed mathematical theory is beyond the scope of this book, we will present enough of the basic theory to motivate our discussion of its connection to CA. Excellent detailed surveys may be found in [alek81][§] and [bai84]; discussions of applications to one-dimensional maps and ‘noisy’ chaos are given in [crutch82] and [crutch83].

[¶]This is strictly true only for two-dimensional area-preserving maps; in dimensions $N \geq 4$, chaotic orbits may ‘leak’ through KAM surfaces by a process called *Arnold diffusion* (see [licht83]).

[†]There would always remain regular – albeit infinitesimally small – regions near periodic points.

[‡]M. Morse and G.A.Hedlund, *American Jour. Math.*, **60** (1938) 815.

[§]That the use of symbolic dynamics to study the behavior of complex or chaotic systems in fact heralds a new epoch in physics was boldly suggested by Joseph Ford in the foreword to this *Physics Reports* review. Ford writes, “Just as in that earlier period [referring to 1922, when *The Physical Review* had published a review of Hilbert Space Operator Algebra] physicists will shortly be faced with the arduous task of learning some new mathematics... For make no mistake about it, the following review heralds a new epoch. Despite its modest avoidance of sweeping claims, its theorems point like arrows toward the physics of the second half of the twentieth century. ”

4.2.1 Basic Theory

Consider, once again, a one-dimensional discrete-time map

$$x_{n+1} = f(x_n), \quad x \in [0, 1]. \quad (4.46)$$

Having a complete description of the dynamics of $f : [0, 1] \rightarrow [0, 1]$ is equivalent to knowing all orbits $\mathcal{X}(x_0) \equiv \{x_0, x_1, x_2, \dots\}$ for all initial points x_0 . An n^{th} -order coarse-grained description of the same dynamics may be obtained by (i) partitioning the unit interval into n (not necessarily equal sized) bins, each of which is labeled with a symbol $\beta_i \in \{0, 1, \dots, n-1\}$, and (ii) replacing each point, $x_i \in \mathcal{X}(x_0)$, of an orbit by the symbol β_i , corresponding to the bin in which that point is situated:

$$\mathcal{X}(x_0) \equiv \{x_0, x_1, x_2, \dots\} \longrightarrow \mathcal{B}(x_0) \equiv \{\beta_0, \beta_1, \beta_2, \dots\}, \quad (4.47)$$

where (for the case of equal sized bins)

$$\beta_i = \begin{cases} 0 & \text{if } 0 \leq x_i < 1/n, \\ 1 & \text{if } 1/n \leq x_i < 2/n, \\ \vdots & \vdots \\ n-1 & \text{if } (n-1)/n \leq x_i \leq 1 \end{cases} \quad (4.48)$$

The time evolution of the function ‘ f ’ is thus replaced by a sequence of discrete symbols labeling the bins visited by each point of the orbit. Because of the coarse-graining of the phase space, however, detailed knowledge of the actual orbits is generally lost; *i.e.* many different orbits may yield the same symbolic sequence. Different state-space partitionings also generally give rise to different symbolic representations.

In the space of all possible symbol sequences, $\Gamma \equiv \{\mathcal{B} = \{\beta_0, \beta_1, \dots\}\}$, the *admissible* sequences under mapping ‘ f ’, $\Gamma_f \subseteq \Gamma$, are those for which $x_i = f^i(x_0) \in \beta_i$. Γ is made into a metric space as follows: let $\mathcal{B}_1 = \{\beta_0^{(1)}, \beta_1^{(1)}, \dots\}$ and $\mathcal{B}_2 = \{\beta_0^{(2)}, \beta_1^{(2)}, \dots\}$, and define the distance between $\mathcal{B}_1$ and $\mathcal{B}_2$ to be

$$\partial(\mathcal{B}_1, \mathcal{B}_2) \equiv \sum_{i=0}^{\infty} \frac{|\beta_i^{(1)} - \beta_i^{(2)}|}{n^i}. \quad (4.49)$$

Next, we introduce the *shift* mapping, γ , which truncates the first orbit symbol and shifts all other symbols one place to the left:

$$\gamma\{\beta_0, \beta_1, \beta_2, \dots\} = \{\beta_1, \beta_2, \beta_3, \dots\}. \quad (4.50)$$

It is easy to check that $\gamma : \Gamma \rightarrow \Gamma$ is continuous under the metric ‘ ∂ ’.

The dynamical system $\{\Gamma_f, \gamma\}$, consisting of the set of admissible sequences under ‘ f ’ and the shift map, γ , is the n^{th} -order symbolic dynamical system induced by ‘ f ’. The power of the method resides in the following – provided that the

dynamical system defined by 'f' is ergodic, the following diagram commutes:

$$\begin{array}{ccc} [0, 1] & \xrightarrow{f} & [0, 1] \\ \mathcal{B} \downarrow & & \downarrow \mathcal{B} \\ \Gamma_f & \xrightarrow{\gamma} & \Gamma_f \end{array}$$

In this way, $\mathcal{B}$ preserves the essential dynamical properties of 'f' by preserving orbits; i.e., $\gamma^n \circ \mathcal{B}(x) = \mathcal{B} \circ f^n(x)$. In particular, there is a one-to-one correspondence between repeating symbol sequences in Γ and periodic orbits of 'f'.

We have already encountered a simple example of a 2-bin coarse-graining in our discussion of the Bernoulli map, $x_{n+1} = 2x_n \pmod{1}$ (see section 4.1.1). There, individual points of orbits were replaced by a back and forth hopping between two bins. Note that in this case, however, the mapping $\mathcal{X}(x_0) \equiv \{x_0, x_1, x_2, \dots\} \rightarrow \mathcal{B}(x_0) \equiv \{\beta_0, \beta_1, \beta_2, \dots\}$ is *exact*, since to each $\mathcal{B}(x_0)$ there corresponds a unique orbit.

Universality in Unimodal Maps: A seminal work on the 2-symbol dynamics of one-dimensional unimodal mappings[¶] due to Metropolis, Stein & Stein [metro73]. Specifically, they studied the iterates of various mappings within periodic windows, labeling the attractor sequences by strings of the form $RLLRL \dots$, where R and L indicate whether $f^n(x_0)$ falls to the right or left of x_0 , respectively. Each periodic sequence therefore corresponds to a unique finite length *word* made up of R 's and L 's.

What Metropolis, *et.al.* found was that it is possible to compile a 'dictionary' of admissible words so that there is a correspondence between the placement of the word within the dictionary and the position of a particular period along the control parameter axis. Moreover, this ordering of symbol sequences is universal for all unimodal maps with a differentiable maximum; it *does not* depend on the nature of the maximum (quadratic, cubic, *etc.*), as does Feigenbaum's scaling universality discussed earlier for the logistic map. Table 4.1 (taken from [metro73]) gives a listing of the universal symbol sequences, up to period 7, for the three maps $f_1(x) = \alpha x(1-x)$, $f_2(x) = \alpha' \sin \pi x$ and $f_3(x) = \alpha'' y(3-3y+y^2)$, where $y \equiv 3x(1-x)$.

As should have been made plausible by the above discussion, symbolic dynamics provides an intuitive conceptual 'bridge' between continuous and discrete dynamical systems. On the one hand, except for the fact that the coarse-grained discrete dynamics of symbolic systems is typically *nonlocal* in character (see the following section), symbolic dynamical systems are essentially *CA-in-disguise*. On the other hand, by exploiting the fundamental CA property of continuity in the Cantor-set topology under the metric defined by equation 4.49, real-valued representations of CA dynamics may be readily obtained. We discuss these two alternative points of

[¶]Mapping of the form $x_{n+1} = f_\alpha(x_n)$, where α is an arbitrary control parameter and the function $f : [0, 1] \rightarrow [0, 1]$ is (i) continuously differentiable, (ii) has a single maximum at $x = 1/2$, and (iii) is monotonic for $0 \leq x \leq 1/2$ and $1/2 < x \leq 1$.

Period	Universal Sequence	α in $f_1(x)$	α' in $f_2(x)$	α'' in $f_3(x)$
2	R	3.2360680	0.7777338	0.9325336
4	RLR	3.4985617	0.8463822	0.9764613
6	RLRRR	3.6275575	0.8811406	0.985107
7	RLRRRR	3.7017692	0.9004906	0.9955132
5	RLRR	3.7389149	0.9109230	0.9990381
7	RLRRLR	3.7742142	0.9213346	1.0024311
3	RL	3.8318741	0.9390431	1.0073533
6	RLLRL	3.8445688	0.9435875	1.0083134
7	RLLRLR	3.8860459	0.9568445	1.0111617
5	RLLR	3.9057065	0.9633656	1.0123766
7	RLLRRR	3.9221934	0.9687826	1.0132699
6	RLLRR	3.9375364	0.9735656	1.0140237
7	RLLRRL	3.9510322	0.9782512	1.0146450
4	RLL	3.9602701	0.9820353	1.0149542
7	RLLLRL	3.9689769	0.9857811	1.0152122
6	RLLLRL	3.9777664	0.9892022	1.0154974
7	RLLLRR	3.9847476	0.9919145	1.0156711
5	RLLL	3.9902670	0.9944717	1.0157727
7	RLLLLR	3.9945378	0.9966609	1.0158320
6	RLLLL	3.9975831	0.9982647	1.0158621
7	RLLLLL	3.9993971	0.9994507	1.0158718

Table 4.1 Listing of universal symbol sequences, up to period 7, for the three unimodal maps $f_1(x) = \alpha x(1 - x)$, $f_2(x) = \alpha' \sin \pi x$ and $f_3(x) = \alpha'' y(3 - 3y + y^2)$, where $y \equiv 3x(1 - x)$; taken from [metro73].

view in the following two sections.

4.2.2 CA-like Representation of Real-valued Maps

We have seen above that the space of all possible sequences, Γ , is effectively metrized by mapping an entire orbit $\mathcal{X}(x_0)$ onto a single n -ary fraction

$$\mathcal{X}(x_0) \longrightarrow \Phi_n(x_0) = \sum_{i=1}^{\infty} \frac{\beta_i}{n^i}, \quad (4.51)$$

where $n > 1$ and β_i is defined in equation 4.48. This idea can be generalized as follows.

Consider an arbitrary one-dimensional system, $x_{i+1} = f_\alpha(x_i)$, where $f : [0, 1] \rightarrow [0, 1]$ and α is some fixed parameter. Expand x_{i+1} , x_i and α in the same manner

as shown in equation 4.51:

$$\left\{ \begin{array}{l} x_{i+1} = \sum_{j=1}^{N(i+1)} \beta_j(i+1)/n^j, \\ x_i = \sum_{j=1}^{N(i)} \beta_j(i)/n^j, \\ \alpha = \sum_{j=-N'}^{N'} \epsilon_j/n^j, \end{array} \right. \quad (4.52)$$

where $\beta_j(i+1)$, $\beta_j(i)$, $\epsilon_j \in \{0, 1, \dots, n-1\}$ and $N(i+1)$, $N(i)$ and N' are the 'precisions' of x_{i+1} , x_i and α , respectively. The map ' f ' is in this way replaced by an algorithm for the computation of $\{\beta_j(i+1)\}$ in terms of the sets $\{\beta_j(i)\}$ and $\{\epsilon_j\}$. The base-2 decimal expansion coefficients for the Bernoulli map, for example, yield the simple CA rule $\alpha_j(i+1) = \alpha_{j+1}(i)$. Thinking of ' j ' as a lattice index, however, the specification of $\beta_j(i+1)$ typically involves values $\beta_k(i)$, where $|j-k| \gg 1$; in other words, the induced CA-like integer map is usually nonlocal. Additional material on integer-maps of this form may be found in [mccau86], [mccau88] and [mccau93].

4.2.3 Real-valued Representation of CA Evolution

A partial analogy between the dynamics of CA and the behaviors of continuous dynamical systems may be obtained by exploiting a fundamental property of CA systems; namely, *continuity in the Cantor-set Topology*. We recall from section 2.2.1 that the collection of all one-dimensional configurations, or the CA phase space, $\Gamma \equiv \Sigma^{\mathcal{Z}}$, where $\Sigma = \{0, 1, \dots, k\} \ni \sigma$ and $\mathcal{Z}$ is the set of integers by which each site of the lattice is indexed, is a compact metric space homeomorphic to the Cantor set under the metric

$$\partial(\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}) = \sum_{i=-\infty}^{\infty} k^{-|i|} |\vec{\sigma}^{(1)} - \vec{\sigma}^{(2)}|, \quad \vec{\sigma}^{(1)}, \vec{\sigma}^{(2)} \in \Gamma. \quad (4.53)$$

This Cantor set may be explicitly visualized in the n -dimensional euclidean space $\mathcal{R}^n$ by defining a mapping $\psi : \Gamma \rightarrow \mathcal{R}^n$ ([grass83] and [pack1]). The j^{th} coordinate of the resulting vector $\psi(\vec{\sigma})$ is given by:

$$[\psi(\vec{\sigma})]_j = \sum_{s_j \in \mathcal{Z}} \frac{\vec{\sigma}_{s_j}}{k^{|s_j|}}, \quad (4.54)$$

where s_j is any monotonically increasing (or decreasing) subset of $\mathcal{Z}$ corresponding to the j^{th} coordinate.

Consider, for example, the case when $k = 2$ and $n = 2$. We then have the mapping $\psi : \{0, 1\}^{\mathcal{Z}} \rightarrow (x, y)$, where $0 < x < 1$ and $0 < y < 1$ are both real

and may be regarded as being the base-ten equivalents of two semi-infinite binary decimal strings of site values:

$$\begin{aligned} x &= (0.\sigma_0\sigma_1\sigma_2\cdots)_{10}, \\ y &= (0.\sigma_{-1}\sigma_{-2}\sigma_{-3}\cdots)_{10}. \end{aligned} \quad (4.55)$$

Using $s_1 = \{0, 1, 2, \dots\}$ and $s_2 = \{-1, -2, -3, \dots\}$ in equation 4.54, the explicit expansions for x and y appear as follows:

$$\begin{aligned} x &= \sum_{i=0}^{\infty} \frac{\sigma_i}{2^{i+1}} = \frac{\sigma_0}{2} + \frac{\sigma_1}{4} + \frac{\sigma_2}{8} + \cdots, \\ y &= \sum_{i=0}^{\infty} \frac{\sigma_{-i-1}}{2^{i+1}} = \frac{\sigma_{-1}}{2} + \frac{\sigma_{-2}}{4} + \frac{\sigma_{-3}}{8} + \cdots. \end{aligned} \quad (4.56)$$

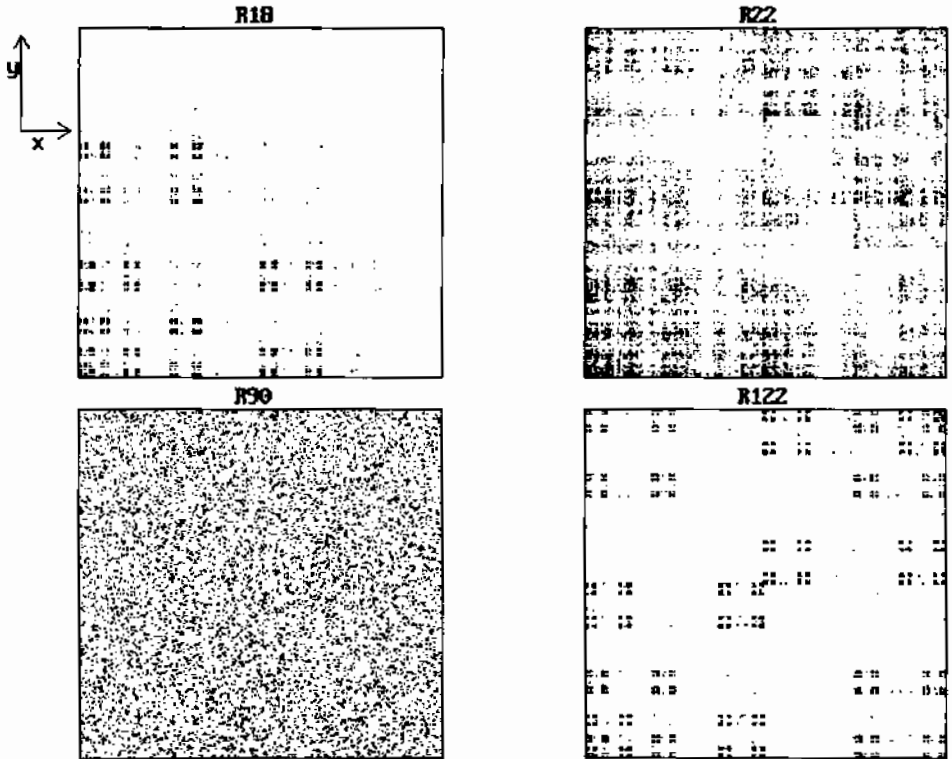


Fig. 4.12 x versus y for x and y as defined in equation 4.53. Patterns are plotted for elementary rules **R18**, **R22**, **R90** and **R122**; see text.

The time evolution of the discrete-valued CA rule, $\Phi : \Gamma \rightarrow \Gamma$, is thus converted into a two-dimensional continuous-valued discrete-time map, $\Psi : (x_t, y_t) \rightarrow (x_{y+1}, y_{y+1})$. This 'continuous' form clearly facilitates comparisons between the long-time behaviors of CA and their two-dimensional mapping counter-

parts.

Figure 4.12 shows sample ‘ x vs y ’ plots obtained in this manner for a few elementary CA rules. Note that the patterns for nonlinear rules such as **R18**, **R22**, and **122** appear to possess a characteristic fractal-like structure reminiscent of the strange attractors appearing in continuous systems shown earlier. We will comment on the nature of this similarity a bit later on in this chapter.

4.3 Lyapunov Characteristic Exponents

As we have seen, a fundamental property of chaotic motion is *sensitivity to small changes to initial conditions*. Initially closely separated starting conditions evolving along regular dynamical trajectories diverge only linearly in time; a chaotic evolution, on the other hand, leads to an exponential divergence in time. *Lyapunov characteristic exponents* quantify this divergence – for both conservative and dissipative systems – by measuring the mean rate of exponential divergence of initially neighboring trajectories.

4.3.1 Continuous Flows

Consider a general n -dimensional dynamical system defined by the differential equations

$$\frac{dx_i}{dt} = F_i(x_1, \dots, x_n), \quad i = 1, 2, \dots, n. \quad (4.57)$$

We want to examine the relative behaviors of the two neighboring phase space trajectories, $\mathbf{x}^*(t)$ and $\mathbf{x}(t)$, starting from the initial conditions $\mathbf{x}^*(0)$ and $\mathbf{x}(0) = \mathbf{x}^*(0) + \delta\mathbf{x}(0)$, respectively. The time evolution of their separation, $\delta\mathbf{x}(t)$, may be approximated by linearizing the equations about the ‘reference’ trajectory, $\mathbf{x}^*(t)$:

$$\frac{d(\delta x_i)}{dt} = \sum_{j=1}^n \delta x_j \left(\frac{\partial F_i}{\partial x_j} \right) \Big|_{\mathbf{x}=\mathbf{x}^*(t)}, \quad (4.58)$$

where $\delta x_i(t)$ is the i^{th} component of the difference vector $\mathbf{x}(t) - \mathbf{x}^*(t)$.

The mean rate of exponential divergence between $\mathbf{x}^*$ and $\mathbf{x}(t)$ is defined by

$$\lambda(\mathbf{x}(0)) = \lim_{\substack{t \rightarrow \infty \\ \mathcal{D}(0) \rightarrow 0}} \left(\frac{1}{t} \right) \ln \left(\frac{\mathcal{D}(t)}{\mathcal{D}(0)} \right), \quad (4.59)$$

where the Euclidean norm

$$\mathcal{D}(t) \equiv \sqrt{\sum_{i=1}^n \delta x_i^2(t)} \quad (4.60)$$

measures the divergence of the two nearby trajectories.

It can be shown that λ both exists and is finite. Moreover, we can always find a set of n tangent-space basis vectors, $\hat{e}_i$ ($i = 1, \dots, n$), such that $\delta \mathbf{x} = (\delta x_1, \dots, \delta x_n) = \sum_{i=1}^n a_i \hat{e}_i$. The divergence (or contraction) along a given basis direction, $\hat{e}_i$, is then measured by the i^{th} *Lyapunov characteristic exponent*, λ_i . These n (possibly nondistinct) exponents are usually ordered by size according to $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$.

For regular motion, $\mathcal{D}(t)$ grows only linearly with time, so that the exponents are all zero. On the other hand, because chaotic flows are characterized by exponential divergences of initial nearby trajectories, a characteristic signature of such flows is the existence of at least one positive Lyapunov exponent.

Phase-Space Volume Expansion

Lyapunov exponents can also be used to predict the mean expansion rate of a volume, $\delta V(t) = \delta x_1(t) \cdots \delta x_n(t)$ in the phase space, Γ :

$$\lambda_\Gamma = \sum_{i=1}^n \lambda_i = \text{div } \mathbf{F}. \quad (4.61)$$

Since $V(t) = V(0)$ for all times 't' in conservative systems, $\lambda_\Gamma = 0$. The presence of attractors in dissipative systems, on the other hand, implies that the available phase space volume is contracting, and thus that $\lambda_\Gamma < 0$. Since chaotic motion (either in conservative or dissipative systems) yields $\lambda_1 > 0$, this therefore also means that, in dissipative systems, the phase space volume is both expanding along certain directions and contracting along others.

Attractor Classification

It has been suggested that the *signature*, $\mathcal{S} \equiv (\text{sign}(\lambda_1), \text{sign}(\lambda_2), \dots, \text{sign}(\lambda_n))$, of the Lyapunov exponents may be used to provide a qualitative characterization of of attractors for dissipative flows. Among the possibilities for $n = 4$, for example, we have the following:

$$\begin{array}{ll} (-, -, -, -) & \longrightarrow \text{fixed point,} \\ (0, -, -, -) & \longrightarrow \text{limit cycle,} \\ (0, 0, -, -) & \longrightarrow \text{quasiperiodic motion on torus,} \\ (+, 0, -, -) & \longrightarrow \text{chaos,} \\ (+, +, 0, -) & \longrightarrow \text{chaos} \end{array} \quad (4.62)$$

Moreover, since the signature changes as the control parameters are varied, $\mathcal{S}$ also provides a classification of the qualitative transitions between types of attractors.

Numerical Computation

Except for simple cases, it is generally a nontrivial task to compute the Lyapunov exponents of a flow. In trying to estimate $\lambda(\mathbf{x}(0))$ in equation 4.59, for example, the exponentially increasing norm, $\mathcal{D}(t)$, may lead to computer overflow problems.

There are nonetheless a variety of sophisticated techniques available; we will content ourselves with mentioning the *pullback* method introduced by Benettin, *et.al.*[†], which is frequently used to obtain estimates for the largest characteristic exponent, λ_1 .[‡]

Pullback Technique: The technique consists of (i) normalizing the initial norm, $\mathcal{D}(0)$, to unity, (ii) measuring the trajectory divergence for all times $t < \delta t$, where δt is some small interval, and (iii) renormalizing the norm at $t = \delta t$ back to unity to prevent overflow catastrophes. This procedure yields a sequence of values, $d_i = \|\delta \mathbf{x}^{(i)}(\delta t)\|$, where $\delta \mathbf{x}^{(i)}(0) = \delta \mathbf{x}^{(i-1)}(\delta t)/d_i$ and $\delta \mathbf{x}^{(i)}(\delta t)$ is computed by integrating equation 4.58 along the trajectory from $\mathbf{x}(n \delta t)$ to $\mathbf{x}((n+1)\delta t)$, with initial condition $\delta \mathbf{x}^{(i)}(0)$. By analogy with equation 4.59, we define

$$\lambda_n = \frac{1}{n} \sum_{i=1}^n \ln d_i. \quad (4.63)$$

For δt that is not too large, it can be shown that the $n \rightarrow \infty$ limit exists, is independent of δt , and that $\lim_{n \rightarrow \infty} \lambda_n = \lambda_1$.

4.3.2 n-Dimensional Discrete Maps

The case of multidimensional discrete-time mappings of the form

$$\mathbf{x}_{i+1} = \mathbf{F}(\mathbf{x}_i), \quad i = 1, \dots, n \quad (4.64)$$

is handled in essentially the same manner as for flows; we can, in fact, obtain the $\lambda_{\text{discrete}}$ from equation 4.59 merely by replacing 't' by 'n'. An alternative method is to once again consider the tangent map

$$\begin{aligned} \delta \mathbf{x}_{i+1} &= \mathbf{T}_i \delta \mathbf{x}_i, \\ &= (\mathbf{T}_i \mathbf{T}_{i-1} \cdots \mathbf{T}_0) \mathbf{x}_0, \end{aligned} \quad (4.65)$$

where $\mathbf{T}_i \equiv (\partial \mathbf{F} / \partial \mathbf{x})|_{\mathbf{x}=\mathbf{x}_i}$, is the linearization of $\mathbf{F}$ at the point $\mathbf{x}_i$. The n Lyapunov exponents are then given by

$$\lambda_j = \lim_{i \rightarrow \infty} \ln |\alpha_j(i)|, \quad j = 1, 2, \dots, n, \quad (4.66)$$

where $\{\alpha_j(i)\}$, are the eigenvalues of the matrix

$$\mathcal{T}_i \equiv (\mathbf{T}_i \mathbf{T}_{i-1} \cdots \mathbf{T}_0)^{1/i}. \quad (4.67)$$

[†]G. Benettin, L. Galgani, and J.M. Strelcyn, "Kolmogorov entropy and numerical experiments", *Phys. Rev. A* **14** (1976) 2338.

[‡]For the slightly trickier problem of determining *all* of the exponents, see G. Benettin, L. Galgani, A. Giorgilli and J.M. Strelcyn, "Lyapunov characteristic exponents for smooth dynamical systems and for Hamiltonian systems; a method for computing all of them", *Meccanica* **15** (1980) 9.

Equation 4.65 takes a particularly simple form for one-dimensional maps, $x_{i+1} = f(x_i)$:

$$\lambda = \lim_{i \rightarrow \infty} \frac{1}{i} \sum_{j=0}^{i-1} \ln |f'(x_j)|. \quad (4.68)$$

The criterion for one-dimensional chaos is then specified succinctly by[†]

$$\begin{cases} \lambda > 0 & \longleftrightarrow \text{chaotic motion,} \\ \lambda \leq 0 & \longleftrightarrow \text{regular motion.} \end{cases} \quad (4.69)$$

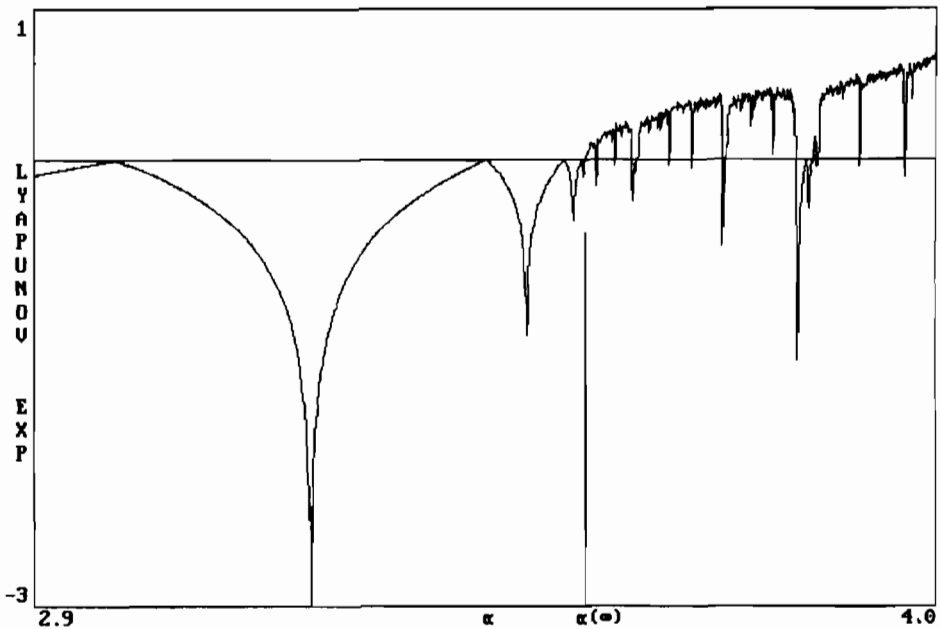


Fig. 4.13 *Lyapunov exponent versus α for $2.9 \leq \alpha \leq 4$ for the logistic equation; see text.*

EXAMPLES: (1) *Bernoulli map.* $x_{n+1} = 2x_n \pmod{1}$. Except for the point $x = 1/2$, $|f'(x)| = 2$. Applying equation 4.68, we find that $\lambda = \ln 2$, verifying the chaotic nature of the orbits of almost all initial points.

(2) *Logistic map.* $x_{n+1} = \alpha x_n(1 - x_n)$. A straightforward formal application of equation 4.68 gives

$$\lambda = \lim_{i \rightarrow \infty} \frac{\alpha}{i} \sum_{j=0}^{i-1} \ln |(1 - 2x_j)|.$$

Figure 4.13 shows a numerically obtained plot of λ vs. α for $2.9 \leq \alpha \leq 4$.[†] Consistent with our earlier observations of the behavior of this map, we see that (1) $\lambda \leq 0$ for all

[†]This plot is obtained by smoothing over 1100 equally spaced points ($\delta\alpha \sim 0.001$), with each point representing an average over 10,000 iterations.

$\alpha < \alpha_\infty$, (2) $\lambda > 0$ for most $\alpha > \alpha_\infty$, and (3) that there are multiple windows in the chaotic regime for which λ dips down below zero and the attractor thus becomes periodic. Finally, we note that Feigenbaum's ubiquitous universal constant δ shows up even here: it can be shown that near α_∞ , $\lambda \sim |\alpha - \alpha_\infty|^\eta$, where $\eta = \log 2 / \log \delta$.

4.3.3 Information-Theoretic Interpretation

As defined above, the Lyapunov exponents effectively determine the degree of 'chaos' that exists in a dynamical system by measuring the rate of the exponential divergence of initially closely neighboring trajectories. An alternative, and, from the point of view of CA theory, perhaps more 'fundamental' interpretation of their numeric content, is an information-theoretic one. It is, in fact, not hard to see that Lyapunov exponents are very closely related to the *rate of information loss in a dynamical system* (this point will be made more precise during our discussion of entropy in the next section).

Consider, for example, a one-dimensional interval $[0, 1]$, that is partitioned into n equal sized bins. Assuming that a point x_0 is equally likely to fall into any one of these bins, learning which bin in fact contains x_0 therefore constitutes an *information gain*

$$I_0 = - \sum_{i=1}^n \frac{1}{n} \log_2 \frac{1}{n} = \log_2 n, \quad (4.70)$$

where $\log_2$ is the logarithm to the base 2 (see section 2.1.2). Now consider a simple linear one-dimensional map $f(x) = \alpha \cdot x$, where $x \in [0, 1]$ and $\alpha > 1$. By changing the length of the interval, and thereby decreasing the effective resolution, by a factor $\alpha = |f'(0)|$, a single application of the map $f(x)$ results in an effective *information loss*

$$\begin{aligned} \delta I &= I_1 - I_0, \\ &= - \sum_{i=1}^{n/\alpha} \frac{\alpha}{n} \log_2 \frac{\alpha}{n} + \sum_{i=1}^n \frac{1}{n} \log_2 \frac{1}{n}, \\ &= - \log_2 |f'(0)|. \end{aligned} \quad (4.71)$$

Generalizing to the case when $|f'(x)|$ depends on position, and averaging over a large number of iterations, we obtain the following expression for the mean information loss:

$$\begin{aligned} \langle \delta I \rangle &= - \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^{N-1} \log_2 |f'(x_i)|, \\ &= \lambda / \log 2, \end{aligned} \quad (4.72)$$

where the latter expression is obtained by direct comparison with equation 4.68, defining the one-dimensional Lyapunov exponent, λ . We thus see that, in one dimension, λ measures the average loss of information about the position of a point in $[0, 1]$ after one iteration.

4.3.4 CA Analogs

The formalism for computing Lyapunov exponents for continuous dynamical systems that was introduced in the last section can also be used, with only minor modifications, for determining exponents for CA as well. The major modification involves replacing the Euclidean norm, $\mathcal{D}(t)$ – used for measuring the divergence of two nearby trajectories (see equation 4.60) – by the Cantor-set metric, $\partial(t)$:

$$\partial(t) = \sum_{i=-\infty}^{\infty} k^{-|i|} |\bar{\sigma}^{(1)}(t) - \bar{\sigma}^{(2)}(t)|, \quad (4.73)$$

where $\bar{\sigma}^{(i)}(t)$ are CA configurations at time ‘ t ’ (see section 4.2.3). Packard [pack1] has used a technique based on the *pullback* method discussed earlier to estimate Lyapunov characteristic exponents for a variety of elementary CA rules. An alternative, and simpler method, however, is to directly measure the time rate of change of two closely neighboring trajectories.

We recall from section 3.1.2 that a *difference pattern* is a space-time pattern of the difference between two evolutions of the same rule starting from two different initial states. For $k = 2$ CA rules Φ , for example, the value of the i^{th} site on the n^{th} step of the difference pattern is given by

$$\Delta_i(n) = \Phi^n[\sigma_1(0)]_i \ominus_2 \Phi^n[\sigma_2(0)]_i, \quad (4.74)$$

where $[\sigma_1(0)]_i$ and $[\sigma_2(0)]_i$ are the i^{th} -site values of the first and second starting configurations. By analogy to measuring the divergence of arbitrarily closely neighboring trajectories in continuous systems, we are in this case particularly interested in the case when the values of $\sigma_1(0)$ and $\sigma_2(0)$ differ only at a *single site*.

The CA analogs of Lyapunov exponents are the *left* ($=\lambda_L$) and *right* ($=\lambda_R$) *slopes of the difference pattern between two configurations differing at one site*. λ_L and λ_R thus measure the average rate of information transmission to the left and right of the lattice. If the sole differing site is located at $i = 0$, λ_L and λ_R are defined by

$$\begin{cases} \lambda_R = \lim_{t \rightarrow \infty} \frac{j_{\max}(t)}{t}, & j > 0 \\ \lambda_L = \lim_{t \rightarrow \infty} \frac{-j_{\max}(t)}{t}, & j < 0, \end{cases} \quad (4.75)$$

where $j_{\max}(t)$ is the furthest lattice-site from $i = 0$ for which the value of the difference pattern, $\Delta_{j_{\max}}(t) > 0$ at time ‘ t ’. Notice that *linearly* growing difference patterns ($j_{\max}(t) \sim \lambda t$, for large ‘ t ’), imply *exponential divergence* of the real numbers representing nearby configurations (see section 4.2.3). The table below (taken

from table six of reference [wolf86b]) gives a the values of λ_L and λ_R for a few selected elementary CA rules (interactions between initially far-separated particle-like structures produced by rule **R110** – see section 3.1.4 – complicate the measurement for this rule).

Rule	class	λ_L	λ_R
R29	2	0	0
R50	2	0	0
R45	3	~ 0.172	1
R54	3	~ 0.533	~ 0.533
R22	3	~ 0.766	~ 0.766
R90	3	1	1
R110	4	$.26 - .5$	$-.27 - 0$

Recognizing that the information transmission is often both *nonuniform* (since the left and right ‘fronts’ do not always propagate outward from the perturbation with a single well-defined velocity), and *dependent on choice of initial states*, one can instead define maximal and minimal average propagation speeds, $\lambda^{(\max)}$ and $\lambda^{(\min)}$, respectively. Letting the i^{th} lattice site be the center of a single ‘perturbation’ to the initial state, we define [wolf86d]

$$G_{i,j}(t) \equiv \begin{array}{l} \text{probability that } \sigma_j \text{ changes at time 't'} \\ \text{if } \sigma_i \text{ is changed at } t = 0. \end{array} \quad (4.76)$$

In giving the response of the system to an ‘impulse’ change to the initial configuration, $G_{i,j}(t)$ may thus be considered as being the *Green Function* for CA. If $j > i$, $\lambda_R^{(\max)}$ and $\lambda_R^{(\min)}$ are defined by

$$\begin{cases} G > 0 & \text{for almost all } j - i < \lambda_R^{(\min)}t, \\ G = 0 & \text{for almost all } j - i > \lambda_R^{(\max)}t, \end{cases} \quad (4.77)$$

with a similar definition of $\lambda_L^{(\max)}$ and $\lambda_L^{(\min)}$ for $j < i$.

4.4 Invariant Measures

An important statistical characterization of long-term motion is provided by the *invariant measure* (also called the *invariant distribution*, or simply the *probability distribution*) of a mapping $M : x \rightarrow f(x)$, $\rho_M(\vec{x})$. $\rho_M(\vec{x})$ satisfies two conditions:

$$\begin{cases} \int \rho_M(\vec{x}) d^n x = 1 & \longleftrightarrow \rho_M(\vec{x}) \text{ is a probability measure,} \\ \rho_M(\vec{x}) = \rho_M(M^{-1}\vec{x}) & \longleftrightarrow \rho_M(\vec{x}) \text{ is measure preserving.} \end{cases} \quad (4.78)$$

Although, in general, there may be many distinct invariant measures, we can single out one particular equilibrium measure by demanding that the *spatial average over the distribution for (almost) all initial points x_0 be equal to the temporal average over the trajectory, $\{x_0, x_1, x_2, \dots\}$.*

If f is the logistic map, for example, and $0 < \alpha < \alpha_\infty$, then

$$\rho_M(x) = \frac{1}{N} \sum_{i=1}^N \delta(x - x_i^*), \quad (4.79)$$

where $N = 2^n$ is the number of stable fixed points, and $\delta(x)$ is the Kronecker delta. Except for a set of measure zero, all initial points x_0 lead to this steady-state invariant distribution. A unique distribution exists for all $\alpha > \alpha_\infty$ as well, except that in this case it may be discontinuous and nonzero over finite sub-intervals of $[0, 1]$.

In general, $\rho_M(x)$ is defined by

$$\rho_M(x) \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=0}^N \delta(x - f(x_i)). \quad (4.80)$$

If $\rho_M(x)$ is independent of x_0 then the system is said to be *ergodic*. In this case, various temporal averages over some function $h(x)$ may be conveniently rewritten as spatial averages over $\rho_M(x)$:

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=0}^N h(x_i) \equiv \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=0}^N h(f(x_i)) = \int \rho_M(x) h(x) dx. \quad (4.81)$$

For example, the time average definition of the Lyapunov exponent for one-dimensional maps, $\lambda = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=0}^N \ln |f'(x_i)|$ (which is often difficult to calculate in practice), may instead be directly obtained by computing the spatial (or phase-space) average, $\lambda = \int \rho_M(x) \ln |f'(x)| dx$.

Frobenius-Perron Construction

The time evolution of an arbitrary density $\rho_{t=0}(x)$ may be obtained from equation 4.80 as follows. The Kronecker-delta function, $\delta(x - x_0)$, evolves into the function $\delta(x - f(x_0))$ after one step. Rewriting this in the form

$$\delta(x - f(x_0)) = \int \delta(x - f(y)) \delta(x_0 - y) dy, \quad (4.82)$$

and generalizing to an arbitrary density, $\rho_t(x)$, results in the *Frobenius-Perron* equation

$$\rho_{t+1}(x) = \int \delta(x - f(y)) \rho_t(y) dy. \quad (4.83)$$

The invariant distribution, $\rho(x)$, is a fixed point of this equation:

$$\rho(x) = \int \delta(x - f(y)) \rho(y) dy. \quad (4.84)$$

In practice, an initial guess, $\rho_0(x)$, is made and successive approximations to $\rho(x)$ are obtained by iterating equation 4.83.

Note that $\rho(x)$ is *invariant under invertible coordinate transforms*; i.e., if x is transformed to a new coordinate, $\bar{x} = h(x)$, where $h' \neq 0$, then $\bar{\rho}(\bar{x}) d\bar{x} = \rho(x) dx$.

EXAMPLES: (1) *Bernoulli map.* We recall that the Bernoulli map, defined by $x_{n+1} = 2x_n \pmod{1}$, has a two-valued inverse: $x_n = x_{n+1}/2$ and $x_n = (x_{n+1} + 1)/2$ both map to the point x_{n+1} . Rewriting $\delta(x - f(y))$ as

$$\delta(x - f(y)) = \frac{1}{|f'(x_a)|} \delta(y - x_a) + \frac{1}{|f'(x_b)|} \delta(y - x_b),$$

where $f(x_a) = f(x_b) = x$ and $|f'(x)| = 2$, $\rho_t(x)$ is given by

$$\rho_t(x) = \sum_{i=0}^{2^t-1} \frac{\rho_0((x+i)/2^t)}{2^t}.$$

In particular, setting $x_i = (x+i)/2^t$ and $\delta x_i = 1/2^t$, we see that

$$\rho_t(X) = \sum_{i=0}^{2^t-1} \delta x_i \rho_0(x_i) \xrightarrow{t \rightarrow \infty} \int_0^1 \rho_0(x) dx = 1.$$

(2) *Logistic Map.* The functional equation 4.84 in this case becomes

$$\rho(x) = \frac{\rho\left(\frac{1}{2} - \frac{1}{2}\sqrt{1-x}\right) + \rho\left(\frac{1}{2} + \frac{1}{2}\sqrt{1-x}\right)}{4\sqrt{1-x}}$$

The invariant density is given by $\rho(x) = \{\pi\sqrt{x(1-x)}\}^{-1}$, as is easily verified by substitution.

While there is, at present, no known CA analogue of a Frobenius-Perron construction, a systematic n^{th} -order approximation to the invariant probability distributions for CA systems is readily obtainable from the *local structure theory* (LST), developed by Gutowitz, *et.al.* [guto87a]; LST is discussed in some detail in section 5.3.

4.5 Entropies and Dimensions

4.5.1 Continuous Dynamical Systems

The typical strategy employed in studying the behavior of nonlinear dissipative dynamical systems consists of first identifying all of the periodic solutions of the system, followed by a detailed characterization of the chaotic motion on the attractors.

The task of finding and classifying periodic solutions is in principle a straightforward one; if a formal mathematical analysis proves too difficult, one may always

resort to simple numerical analysis, provided that the periods involved are not excessively long. Two computational tools that help in verifying that a solution is not simply periodic, are the *power spectrum* (see section 4.1.), and the *Lyapunov Characteristic Exponents* (which, we recall, quantify the magnitude of the exponential divergence of initially neighboring trajectories – see section 4.1.). Neither of these tools, however, provides enough structural or statistical information to be of much help in distinguishing among different strange attractors. Such information is instead provided by various sets of dimensions and entropies.

Since the phase space of a dissipative dynamical system contracts with time, we know that, in the long time limit, $t \rightarrow \infty$, the motion will be confined to some fixed attractor, $\mathcal{A}$. Moreover, because of the contraction, the dimension, D , of $\mathcal{A}$, must be *lower* than that of the actual phase space. While D adds little information in the case of a nonchaotic attractor (we know immediately, and trivially, for example, that all fixed-points have $D = 0$, limit cycles have $D = 1$, 2-tori have $D = 2$, etc.), it is of significant interest for strange attractors, whose dimension is typically non-integer valued. Three of the most common measures of D are the *fractal dimension*, *information dimension* and *correlation dimension*.

4.5.1.1 Fractal Dimension, D_F

The fractal dimension was introduced earlier in section 2.1.1. If the minimum number of d -dimensional boxes of side ϵ needed to cover the attractor $\mathcal{A}$, $N(\epsilon)$, scales as

$$N(\epsilon) \propto \epsilon^\alpha \quad (4.85)$$

for some constant α , that constant is called the *fractal dimension* (sometimes referred to as the *Kolmogorov capacity*, or just *capacity*) of $\mathcal{A}$. In other words,

$$D_F = \lim_{\epsilon \rightarrow 0} \frac{\ln[N(\epsilon)]}{\ln(1/\epsilon)}. \quad (4.86)$$

Since $N(\epsilon) \approx D_F \log(1/\epsilon)$, D_F essentially tells us *how much information is needed to specify the location of $\mathcal{A}$ to within a specified accuracy, ϵ* . In practice, one obtains values of $N(\epsilon)$ for a variety of ϵ 's and estimates D_F from the slope of a plot of $\ln(N(\epsilon))$ versus $\ln(1/\epsilon)$.

Notice that while D_F clearly depends on the *metric* properties of the space in which the attractor, $\mathcal{A}$, is embedded – and thus provides some *structural* information about $\mathcal{A}$ – it does not take into account any structural inhomogeneities in the $\mathcal{A}$. In particular, since the box ‘bookkeeping’ only keeps track of whether or not an overlap exists between a given box and $\mathcal{A}$, the individual frequencies with which each box is visited are ignored. This oversight is corrected for by the so-called information dimension, which depends on the probability measure on $\mathcal{A}$.

4.5.1.2 Information Dimension, D_I

As above, we partition the d -dimensional phase-space into boxes of volume ϵ^d . The probability of finding a point of an attractor $\mathcal{A}$ in box number ' i ' ($i = 1, 2, \dots, \mathcal{B}(\epsilon)$), is

$$p_i(\epsilon) = \frac{N_i(\epsilon)}{N(\epsilon)}, \quad (4.87)$$

where $N_i(\epsilon)$ is the number of points in the i^{th} box and $N(\epsilon)$ is the total number of non-empty boxes. $p_i(\epsilon)$ is thus the relative frequency with which the i^{th} box is visited.

The amount of information required to specify the state of the system to within an accuracy ' ϵ ' (or, equivalently, the information gain in making a measurement that is uncertain by an amount ' ϵ '), is given by

$$I(\epsilon) = - \sum_{i=1}^{N(\epsilon)} p_i(\epsilon) \ln p_i(\epsilon). \quad (4.88)$$

The *information dimension*, D_I , of an attractor $\mathcal{A}$ is then defined to be

$$D_I = \lim_{\epsilon \rightarrow 0} \frac{I(\epsilon)}{\ln(1/\epsilon)}. \quad (4.89)$$

Notice that if $\mathcal{A}$ is contained in a *single* box, b_i , then $p_i(\epsilon) = \delta_{ij} \frac{1}{N(\epsilon)} \Rightarrow I = 0$. On the other hand, if each box is visited equally often *i.e.*, if $p_i(\epsilon) = 1/N(\epsilon)$, for all ' i ' – then $I(\epsilon) = \ln[N(\epsilon)] \Rightarrow D_I = D_F$. For unequal probabilities, $I(\epsilon) < \ln[N(\epsilon)]$, so that, in general, $D_I \leq D_F$.

4.5.1.3 Correlation Dimension, D_C

Let $\mathcal{S}_{\mathcal{A}} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$, where $\mathbf{x}_i \in \mathcal{R}^n$, be a set of points lying on the attractor $\mathcal{A}$. The *correlation integral* of $\mathcal{S}_{\mathcal{A}}$ is defined to be

$$C(\epsilon) = \lim_{N \rightarrow \infty} \frac{1}{N^2} \sum_{\substack{i,j=1 \\ i \neq j}}^N \theta(\epsilon - |\mathbf{x}_i - \mathbf{x}_j|), \quad (4.90)$$

where $\theta(x)$ is the Heaviside function:

$$\theta(x) = \begin{cases} 1 & \text{if } x > 0, \\ 0 & \text{if } x \leq 0. \end{cases} \quad (4.91)$$

The summation in $C(\epsilon)$ thus gives the total number of pairs of points, ' $\mathbf{x}_i, \mathbf{x}_j$ ', whose distance $|\mathbf{x}_i - \mathbf{x}_j|$ is less than or equal to ϵ .

As ϵ decreases, $C(\epsilon)$ behaves as $C(\epsilon) \sim \epsilon^{D_C}$, so that the *correlation dimension*, D_C , is given by

$$D_C = \lim_{\epsilon \rightarrow 0} \frac{\ln(C(\epsilon))}{\ln(\epsilon)}. \quad (4.92)$$

Grassberger and Procaccia [grass83] show that $0 \leq D_C \leq D_I$, where D_I is the information dimension defined in equation 4.89.

4.5.1.4 Generalized Fractal Dimensions

The three dimensions introduced above, D_F , D_I and D_C , are actually three members of an (uncountably infinite) hierarchy of generalized fractal dimensions introduced by Hentschel and Procaccia [hent83]. The hierarchy is defined by generalizing the information function $I(\epsilon)$ (equation 4.88) used in defining D_I to the ν^{th} -order Rényi information function, $I_\nu(\epsilon)$:

$$I_\nu(\epsilon) \equiv \frac{1}{1-\nu} \ln \sum_{i=1}^{N(\epsilon)} p_i^\nu(\epsilon), \quad \nu \geq 0, \quad (4.93)$$

where $p_i(\epsilon)$ is, as above, the probability of finding a point of an attractor, $\mathcal{A}$, in box number ' i ' ($i = 1, 2, \dots, \mathcal{B}(\epsilon)$).

Using this generalized information we get the ν^{th} -order generalization of D_I (equation 4.89), D_ν :

$$D_\nu = \lim_{\epsilon \rightarrow 0} \frac{I_\nu(\epsilon)}{\ln(1/\epsilon)}. \quad (4.94)$$

It can be shown that D_ν is a non-decreasing function of ' ν ' [hent83]; *i.e.* that

$$D_\nu \leq D_{\nu'} \quad \text{for all } \nu, \nu' \quad \text{such that } \nu \geq \nu'. \quad (4.95)$$

$\nu \rightarrow 0$: For the case $\nu = 0$, we have that

$$\begin{aligned} p_i^{\nu \rightarrow 0} &= \begin{cases} 1 & \text{if } p_i \neq 0, \\ 0 & \text{if } p_i = 0, \end{cases} \\ \Rightarrow \sum_{i=1}^{N(\epsilon)} p_i^{\nu \rightarrow 0} &= \text{the number of boxes containing a piece of } \mathcal{A} = N(\epsilon). \end{aligned} \quad (4.96)$$

Thus, $D_0 = \lim_{\epsilon \rightarrow 0} \ln \left(\sum_{i=1}^{N(\epsilon)} 1 \right) / \ln(1/\epsilon) = \lim_{\epsilon \rightarrow 0} \ln [N(\epsilon)] / \ln(1/\epsilon) = D_F$.

$\nu \rightarrow 1$: By rewriting D_ν as

$$D_\nu = \frac{1}{1-\nu} \lim_{\epsilon \rightarrow 0} \frac{\ln [\sum_i p_i \exp(\nu-1) \ln p_i]}{\ln(1/\epsilon)}, \quad (4.97)$$

we find that $D_{\nu \rightarrow 1} = \lim_{\epsilon \rightarrow 0} I(\epsilon) / \ln(1/\epsilon) = D_I$, where $I(\epsilon)$ is given by equation 4.88.

$\nu \rightarrow 2$: Since

$$\begin{aligned}
 \sum_{i=1}^{N(\epsilon)} p_i^2(\epsilon) &= \text{probability that two points on } \mathcal{A} \text{ occupy same } \epsilon^d \text{ box} \\
 &\sim \text{probability that the distance between two points on} \\
 &\quad \text{the attractor is less than or equal to } \epsilon' \\
 &= \lim_{N \rightarrow \infty} \frac{1}{N^2} \{ \# \text{ of pairs 'ij' whose distance } |\mathbf{x}_i - \mathbf{y}_j| \leq \epsilon \} \\
 &= \frac{1}{N^2} \sum_{\substack{i,j=1 \\ i \neq j}}^N \theta(\epsilon - |\mathbf{x}_i - \mathbf{x}_j|), \\
 &= C(\epsilon) \text{ (see equation 4.90)}
 \end{aligned} \tag{4.98}$$

we see that $D_2 = \lim_{\epsilon \rightarrow 0} \left(\ln \sum_{i=1}^{N(\epsilon)} p_i^2(\epsilon) \right) / \ln(1/\epsilon) = \lim_{\epsilon \rightarrow 0} \ln[C(\epsilon)] / \ln(1/\epsilon) = D_C$.

The table below gives a few selected values of D_ν for the logistic and Henon map attractors:

Map	D_0	D_1	D_2	D_∞
logistic ($\alpha = 4$)	1	1	1	1
logistic ($\alpha = \alpha_\infty$)	0.538	0.537	0.500	0.394
Hénon ($\alpha = 1.4, \beta = 0.3$)	1.26	–	1.21	–

We should hasten to point out that a straightforward application of a *box-counting* algorithm to compute D_ν for even small ν becomes extremely time-consuming if the dimension of the original phase space $n \geq 2$. There are, however, a variety of alternative computational schemes available that make this task a much less daunting one ([bai87], [bai88]).

Lyapunov Dimension: An interesting attempt to link a purely *static* property of an attractor, $\mathcal{A}$ – as embodied by its fractal dimension, D_F – to a *dynamic* property, as expressed by its set of Lyapunov characteristic exponents, λ_i , was first made by Kaplan and Yorke in 1979 [kaplan79]. Defining the *Lyapunov dimension*, D_L to be

$$D_L = j + \frac{\sum_{i=1}^j \lambda_i}{|\lambda_{j+1}|}, \tag{4.99}$$

where ‘ j ’ denotes the largest λ such that $\sum_{i=1}^j \lambda_i \geq 0$, the *Kaplan-Yorke Conjecture* is that $D_F = D_L$. Although the equality appears to be rigorously true only for completely homogeneous attractors, it is often approximately satisfied by inhomogeneous attractors as well. Because the calculation of λ_i is a relatively easy one, this simple relation has proven to be useful for obtaining quick characterizations of fractal attractors.

Kolmogorov-Sinai Entropy

The discussion has so far focused exclusively on the amount of information gained from a single 'snap-shot' view of an attractor, $\mathcal{A}$. A useful alternative viewpoint is provided by asking about the *rate of information gain per unit time* achieved in observing the system over a period of time. If the dynamics are simple, the asymptotic information gain is zero since new measurements provide no new information; if the system is behaving chaotically, on the other hand, new measurements are constantly needed in order to update our knowledge of the system. The *Kolmogorov-Sinai Entropy* (or *metric entropy*), K , gives an upper bound on this information acquisition rate.[†]

To define K , we again partition a d -dimensional phase space into boxes of volume ϵ^d , $\{b_1, b_2, \dots, b_N\}$. We assume that the state of the system is measured in intervals of $\Delta t = \tau$ units, and define $p(b_1, b_2, \dots, b_N)$ to be the joint probability that $\mathbf{x}(t = 0) \in b_1$, $\mathbf{x}(t = \tau) \in b_2$, ..., and $\mathbf{x}(t = N\tau) \in b_N$. The Shannon information, $\mathcal{I}_N$, stored in this string is then given by

$$\mathcal{I}_N = - \sum_{b_1, b_2, \dots, b_N} p(b_1, b_2, \dots, b_N) \ln p(b_1, b_2, \dots, b_N). \quad (4.100)$$

Given the *a-priori* probabilities, $p(b_1, b_2, \dots, b_N)$, $\mathcal{I}_N$ gives the information needed to specify the location of $\mathcal{A}$ with accuracy ϵ . The additional information needed to predict which box $\mathbf{x}(t = (N+1)\tau)$ will be in, given $\mathcal{I}_N$, is given by $\mathcal{I}_{N+1} - \mathcal{I}_N$, which is therefore a measure of our information gain about the state of the system from time $t = N\tau$ to $t = (N+1)\tau$. The Kolmogorov-Sinai Entropy is the average rate of this information gain:

$$\begin{aligned} K &= \lim_{\substack{\tau \rightarrow 0 \\ \epsilon \rightarrow 0 \\ M \rightarrow \infty}} \frac{1}{M\tau} \sum_{N=0}^{M-1} (\mathcal{I}_{N+1} - \mathcal{I}_N), \\ &= - \lim_{\substack{\tau \rightarrow 0 \\ \epsilon \rightarrow 0 \\ M \rightarrow \infty}} \frac{1}{M\tau} \sum_{b_1, b_2, \dots, b_{M-1}} p(b_1, b_2, \dots, b_{M-1}) \ln p(b_1, b_2, \dots, b_{M-1}). \end{aligned} \quad (4.101)$$

It is easy to see that $K = 0$ for regular trajectories, while completely random motion yields $K = \infty$. Deterministic chaotic motion, on the other hand, results in K being both finite and positive.

The above definition may be generalized to ν^{th} -order form just as $D_F = D_0$ was generalized to D_ν in equation 4.94:

$$K_\nu = - \lim_{\substack{\tau \rightarrow 0 \\ \epsilon \rightarrow 0 \\ M \rightarrow \infty}} \frac{1}{M\tau} \frac{1}{\nu-1} \sum_{b_1, b_2, \dots, b_{M-1}} p(b_1, b_2, \dots, b_{M-1}) \ln p^\nu(b_1, b_2, \dots, b_{M-1}). \quad (4.102)$$

It follows that $K_1 = K$ and that $K_\nu < K_{\nu'}$ for all $\nu > \nu'$.

Recalling our earlier discussion of the information-theoretic interpretation of

[†]See A. Kolmogorov, *Dokl. Akad. Nauk SSSR* **124** (1959) 754, Ya.G.Sinai, *Dokl. Akad. Nauk SSSR* **124** (1959) 768.

the Lyapunov characteristic exponents (see section 4.3.3), we should perhaps not be surprised to learn that metric entropy and Lyapunov exponents are related. For one-dimensional maps, K is in fact equal to the positive Lyapunov exponent; in higher dimensions, K is equal to the averaged sum of the positive Lyapunov exponents:[†] $K = \int \rho(\mathbf{x}) \sum_i \lambda_i^+$, where $\rho(\mathbf{x})$ is the invariant distribution function.

4.5.2 CA Systems

We have previously seen that the set of all possible infinite configurations, or CA phase space, forms a Cantor set, and that the CA evolution itself may be viewed as a continuous mapping on this Cantor set. As such, virtually all of the definitions of dimensions and entropies introduced above to characterize chaotic dynamics in continuous systems, may – with only a few interpretive and notational changes – be used in identical fashion to characterize the evolution of CA. There are thus CA analogs of fractal dimension, information dimension, Kolmogorov-Sinai entropy, *etc.*. Variations arise from using finite versus infinite lattices and considering purely spatial site-value sequences, purely temporal sequences or full space-time patches. We begin by recalling the definitions for both the spatial *set* and spatial *measure* entropies for finite lattices (see section 3.1.3).

Spatial Set Entropy: The global set entropy, $S_{\text{set}}(t)$, of a spatial sequence of site-values on a finite one-dimensional lattice at time ‘ t ’ is defined by

$$S_{\text{set}}^{(x)}(t) = \frac{1}{N} \log_k N^{(x)}(t), \quad (4.103)$$

where N is the lattice size, $\log_k$ is the logarithm to base- k , and $N^{(x)}(t)$ is the total number of possible configurations that may be reached at time ‘ t ’, starting from any initial configuration. Notice the similarity between this definition and that of the fractal dimension, D_F , given in equation 4.86. The analogs of the ϵ^d -sized boxes partitioning d -dimensional phase-space used in defining D_F are the k^N configurations in which the size- N lattice has a particular sequence of values. Although N remains strictly finite in this case, a *set dimension* for infinite lattices may be defined which is exactly analogous to the fractal dimension (see below).

Because $S_{\text{set}}^{(x)}(t)$ is determined by considering *all* possible evolutions on a finite lattice, it must obviously be related to certain properties of the global state-transition graph, G . For example, at large times, $S_{\text{set}}^{(x)}(t \rightarrow \infty)$ is given by the fraction of states that are on *cycles* in G .

Measure Entropy: In the same way as the information dimension, D_I , generalizes the fractal dimension, D_F , of an attractor $\mathcal{A}$, by taking into account the relative frequency with which the individual ϵ -boxes of a partition are visited by points on the attractor, so too the finite set entropy generalizes to a finite *measure entropy*,

[†]See Ya.B.Pesin, “Characteristic Lyapunov exponents and smooth ergodic theory”, *Russ. Math. Surveys* **32** (1977) 55.

by taking into account the probabilities for different configurations:

$$S_{\text{meas}}^{(x)}(t) = -\frac{1}{N} \sum_{i=1}^{k^N} p_i(t) \log_k p_i(t), \quad (4.104)$$

where $p_i(t)$ is the probability of the i^{th} configuration at time ' t '. $S_{\text{meas}}^{(x)}(t)$ can be interpreted as being the average number of k -ary bits necessary to completely specify a state in a statistical ensemble of all possible states.

We make three simple observations: (i) since entropy is maximum when the system is maximally disordered, $S_{\text{meas}}^{(x)}(t)$ takes its maximal value of *one k -ary bit per site* for an equiprobable ensemble – i.e., if all k^N possible configurations occur with equal probability, then $S_{\text{meas}}^{(x)}(t) = S_{\text{set}}^{(x)}(t) = 1$; (ii) If the system settles down into a unique cyclic state (which must be the null state if the rule is legal), then $S_{\text{meas}}^{(x)}(t \rightarrow \infty) = 0$; (iii) $S_{\text{meas}}^{(x)}(t) = S_{\text{set}}^{(x)}(t)$ if and only if all nonzero state probabilities, $p_i(t)$, are equal at time ' t '.

While the entropy for reversible systems almost always increase in time (see section 4.6), the evolution of irreversible rules typically leads to a decrease in entropy.[†]

4.5.2.1 Spatial Measures for Infinite Lattices

Although it is obviously impossible to enumerate all possible configurations for infinite lattices, so long as the values of far separated sites are statistically independent, the average entropy per site can nonetheless be estimated by a limiting procedure. To this end, we first generalize the definitions for the spatial *set* and spatial *measure* entropies given above to their respective *block-entropy* forms.

Block Entropies: The definitions are the same as for finite lattices except that whereas before we could sum over all possible configurations, we now perform the same calculations for all possible sequences of sites within *blocks* of finite size B :

$$\left\{ \begin{array}{ll} S_{\text{set}}^{(x)}(B, t) = \frac{1}{B} \log_k N^{(x)}(B, t) & \longleftrightarrow \text{spatial set block-entropy,} \\ S_{\text{meas}}^{(x)}(B, t) = -\frac{1}{B} \sum_{i=1}^{2^B} p_i^B(t) \log_k p_i^B(t) & \longleftrightarrow \text{spatial measure block-entropy,} \end{array} \right. \quad (4.105)$$

where $N^{(x)}(B, t)$ is the total number of length- B blocks generated at time ' t ', and $p_i^B(t)$ is the probability of the i^{th} sequence of site values within a block of size B at time ' t '.

While $S_{\text{set}}^{(x)}(B, t)$ is determined directly by the number of distinct sequences of length X generated at time ' t ', $S_{\text{meas}}^{(x)}(B, t)$ gives the average entropy per site by taking into account whatever correlations exist in blocks of length up to B .

[†]See figures 3.25 and 3.36 for the time evolution of both $S_{\text{set}}^{(x)}(t)$ and $S_{\text{meas}}^{(x)}(t)$ for elementary rules **R32** (class **c1**) and **R122** (class **c3**) for an ensemble of size $N = 10$ CA starting with an equiprobable ensemble.

From the above definition, we see immediately that

$$0 \leq S_{\text{meas}}^{(x)}(B, t) \leq S_{\text{set}}^{(x)}(B, t) \leq 1. \quad (4.106)$$

$S_{\text{set}}^{(x)}(B, t) = S_{\text{meas}}^{(x)}(B, t) = 0$ if and only if a single length- B block occurs (with nonzero probability); $S_{\text{set}}^{(x)}(B, t) = S_{\text{meas}}^{(x)}(B, t)$ only when all nonzero block probabilities, $p_i^B(t)$, are equal; $S_{\text{set}}^{(x)}(B, t) = 1$ if and only if all possible length- B blocks appear at time ' t ' (though possibly with unequal probabilities); $S_{\text{meas}}^{(x)}(B, t) = 1$ if and only if $p_i^B(t) = k^{-B}$ for all possible states ' i '.

It is also easy to see that

$$\begin{cases} (B_1 + B_2) S_{\text{set}}^{(x)}(B_1 + B_2, t) & \leq B_1 S_{\text{set}}^{(x)}(B_1, t) + B_2 S_{\text{set}}^{(x)}(B_2, t), \\ (B_1 + B_2) S_{\text{meas}}^{(x)}(B_1 + B_2, t) & \leq B_1 S_{\text{meas}}^{(x)}(B_1, t) + B_2 S_{\text{meas}}^{(x)}(B_2, t), \end{cases} \quad (4.107)$$

where B_1 and B_2 are two arbitrary block lengths and equality is achieved if and only if successive blocks are statistically uncorrelated. These relations imply that both the set and measure entropies decrease with block size. Indeed, for CA whose initial probability measures are translationally invariant, it is easy to deduce that

$$S^{(x)}(B, t) \leq S^{(x)}(B - 1, t), \quad (4.108)$$

where S stands for either S_{set} or S_{meas} [wolf84c].

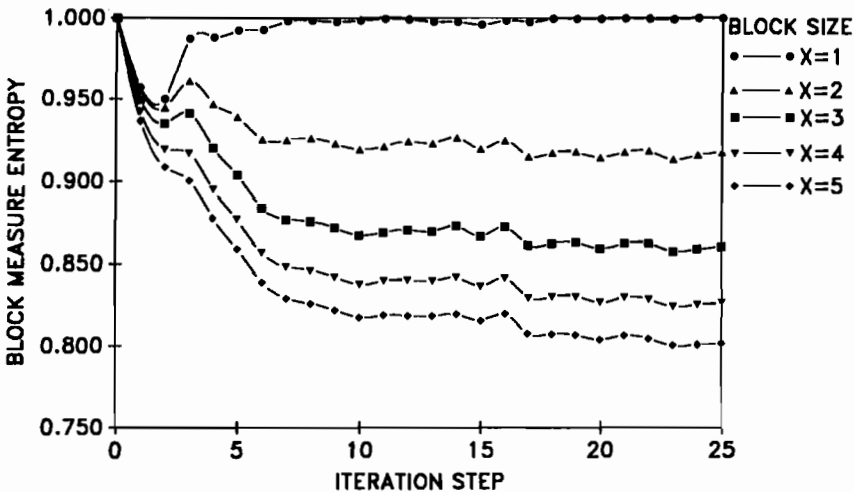


Fig. 4.14 Block measure entropy of rule **R122** versus iteration step for blocks with size $B \leq 5$; see text.

Figure 4.14 shows the first few iteration steps in the evolution of the spatial measure block-entropy of rule **R122** for blocks with size $B \leq 5$. Although the irreversibility of this rule predictably leads to a decrease of entropy with time, there nonetheless appears to be a 'relaxation' to equilibrium values. Observe also

that $S_{\text{meas}}^{(x)}(B, t) \leq S_{\text{meas}}^{(x)}(B - 1, t)$, consistent with the observation made above. In practice, reasonable estimates of the limit $\lim_{B \rightarrow \infty} S(B)$ may be obtained for relatively small B .

Dimensions: The limiting values of the block entropies as $B \rightarrow \infty$ gives the spatial set and spatial measure dimensions, of the set of configurations:

$$\begin{cases} d_{\text{set}}^{(x)} &= \lim_{B \rightarrow \infty} S_{\text{set}}^{(x)}(B, t \rightarrow \infty) \longleftrightarrow \text{spatial set dimension,} \\ d_{\text{meas}}^{(x)} &= \lim_{B \rightarrow \infty} S_{\text{meas}}^{(x)}(B, t \rightarrow \infty) \longleftrightarrow \text{spatial measure dimension.} \end{cases} \quad (4.109)$$

The relation given in equation 4.106 generalizes to

$$0 \leq d_{\text{meas}}^{(x)} \leq d_{\text{set}}^{(x)} \leq 1. \quad (4.110)$$

An ensemble of completely disordered configurations has set dimension $d_{\text{set}}^{(x)} = 1$. If the limit set consists only of a finite number of states, then $d_{\text{set}}^{(x)} = 0$. In general, the set of states for most irreversible class **c3** rules will occupy some fractal subspace of the space of all possible configurations, and thus be characterized by $0 < d_{\text{set}}^{(x)} < 1$.

Extensions to Higher Dimensional Lattices: Higher dimensional versions of each of the above measures may be obtained in a straightforward fashion. The two dimensional analogs of the set and measure dimensions, for example, are given by considering the sets of possible configurations on $x - y$ ‘patches’ of size $B_x \times B_y$:

$$\begin{cases} d_{\text{set}}^{(x)} &= \lim_{\substack{B_x \rightarrow \infty \\ B_y \rightarrow \infty}} \frac{1}{B_x B_y} \log_k N(B_x, B_y), \\ d_{\text{meas}}^{(x)} &= - \lim_{\substack{B_x \rightarrow \infty \\ B_y \rightarrow \infty}} \frac{1}{B_x B_y} \sum_{i=1}^{k^{B_x B_y}} p_i \log_k p_i, \end{cases} \quad (4.111)$$

where $N(B_x, B_y)$ is the total number of size $B_x \times B_y$ blocks generated in the course of the evolution, and p_i is the probability of the i^{th} $B_x \times B_y$ configuration.

Generalized Rényi Entropies and Dimensions: A hierarchy of generalized entropies and dimensions, $\{S_0^{(x)}(B, t), S_1^{(x)}(B, t), S_\nu^{(x)}(B, t), \dots\}$ – analogous to the hierarchy of fractal dimensions, $\{D_0, D_1, D_\nu, \dots\}$, introduced earlier in equation 4.94 for continuous systems – may also be defined:

$$\begin{cases} S_\nu(B, t) &= \frac{1}{1 - \nu} \log_k \left\{ \sum_{|\mathbf{B}|=B} p_{\mathbf{B}}^\nu(t) \right\}, \quad \nu \geq 0, \\ d_\nu^{(x)}(t) &= \lim_{B \rightarrow \infty} \frac{1}{B} S_\nu(B, t), \end{cases} \quad (4.112)$$

where $\sum_{|\mathbf{B}|=B}$ represents a sum over all blocks $\mathbf{B}$ of length- B and $p_{\mathbf{B}}(t)$ is the probability of the $\mathbf{B}^{\text{th}}$ block at time ‘ t ’.

It is easy to show that all of the above generalized spatial measure dimensions are *non-increasing in time* ([erik87a], [erik87b]):

$$\Delta d_\nu^{(x)}(t) \equiv d_\nu^{(x)}(t+1) - d_\nu^{(x)}(t) \leq 0 \quad \text{for all } t. \quad (4.113)$$

Proof: Using the fact that

$$\begin{aligned} S_\nu(B, t+1) &= \frac{1}{1-\nu} \log_k \left\{ \sum_{|\mathbf{B}|=B} p_{\mathbf{B}}^\nu(t+1) \right\}, \\ &= \frac{1}{1-\nu} \log_k \left\{ \sum_{|\mathbf{B}|=B} \left(\sum_{\substack{|\mathbf{B}'|=B+2r \\ \phi(\mathbf{B}')=\mathbf{B}}} p_{\mathbf{B}'}^\nu(t) \right) \right\}, \\ &\leq \frac{1}{1-\nu} \log_k \left\{ \sum_{|\mathbf{B}|=B+2r} p_{\mathbf{B}}^\nu(t) \right\}, \end{aligned} \quad (4.114)$$

we have that

$$\begin{aligned} \Delta d_\nu^{(x)}(t) &= \lim_{B \rightarrow \infty} \left\{ \frac{1}{B} S_\nu(B, t+1) - \frac{1}{B} S_\nu(B, t) \right\}, \\ &= \lim_{B \rightarrow \infty} \left\{ \frac{1}{B+2r} (S_\nu(B, t+1) - S_\nu(B+2r, t+1)) + \right. \\ &\quad \left. \frac{2r}{B(B+2r)} S_\nu(B, t+1) \right\}, \end{aligned} \quad (4.115)$$

Using the result in equation 4.114, the first term in the last expression is ≤ 0 , while the second term goes to zero as $B \rightarrow \infty$. Thus $\Delta d_\nu^{(x)}(t) \leq 0$ for all times ' t '. ■

Effective Measure Complexity: A convenient measure of the 'complexity' of a given site-value sequence (as opposed to simple measures of information content)[†], is provided by the so-called *effective measure complexity*, Υ , first used by Grassberger [grass86c] for isolating certain very long range correlations appearing in the spatial pattern of elementary rule **R22** (see section 3.1.4.1).

A heuristic 'derivation' of Υ is as follows ([grass86a], [grass86c]): Since the Shannon information stored in a block of length- B is given by

$$S_{\text{meas}}^{(x)}(B) = -\frac{1}{B} \sum_{i=1}^{2^B} p_i^B \log_k p_i^B, \quad (4.116)$$

where $B = |\mathbf{B}| \equiv \{\beta_1, \beta_2, \dots, \beta_B\}$ and p_i is the probability of the i^{th} block, the additional information that is needed to predict the value of β_{B+1} given $\mathbf{B}$ is $\delta_B S = S_{\text{meas}}^{(x)}(B+1) - S_{\text{meas}}^{(x)}(B)$. The average amount by which the uncertainty of the value of β_{B+1} decreases due to the knowledge of β_1 is then

$$\delta_B^2 S = \delta_{B-1} S - \delta_B S. \quad (4.117)$$

[†]A formal discussion of general measures of, and various relations between, the intrinsic *randomness* and *complexity* of sequences requires language-theoretic tools that are developed in chapter 6; see section 6.4.

$\delta_B^2 S$ represents the minimal information about β_1 necessary for making an optimal prediction of β_{B+1} , and thus the minimal amount of information – at any time ‘ t ’ and for every B – that must be stored for B iterations steps for optimal predictions. Υ itself is now defined as the minimal *total information* that must be stored at any time to make optimal predictions:

$$\begin{aligned}\Upsilon &\equiv \sum_{B=0}^{\infty} B \delta_B^2 S = \sum_{B=0}^{\infty} B \{ \delta_{B-1} S - \delta_B S \}, \\ &= \sum_{B=0}^{\infty} \{ \delta_B S - s \},\end{aligned}\tag{4.118}$$

where $s \equiv \lim_{B \rightarrow \infty} \delta_B S = S_{\text{meas}}^{(x)}(B)$ (compare to the *Kolmogorov-Sinai entropy*, defined in equation 4.101).

If sequences contain only short range spatial correlations, $\delta_B S$ converges to s exponentially fast, keeping Υ finite. On the other hand, if strong long-range correlations are present then increasingly large site-value sequences are able to store an increasing amount of information about their continuation, in which case, Υ diverges; in particular, Υ diverges whenever the block entropies converge to ‘ s ’ *slower than* $1/B$. Although Υ is finite for almost all elementary CA rules, Grassberger ([grass86a], [grass86c], and [grass88]) found that the block-length dependence of the decay of the spatial block entropy, $\delta_B S$, for the $k = 2, r = 1$ rule **R22**, is best fit by the power-law

$$\delta_B S \propto \frac{1}{B^{0.06}},\tag{4.119}$$

indicating the presence of very-long correlations in this rule (see earlier discussion in section 3.1.4).

4.5.2.2 Temporal Measures for Infinite Lattices

The entropies and dimensions introduced above were defined for purely *spatial* sequences of site values at given times; as such, they can be used to characterize sets of CA configurations. An alternative behavioral characterization is of the purely *temporal sequence of site-values at a given lattice site*.

Entropies: We rewrite the definitions for $S_{\text{set}}^{(x)}(B, t)$ and $S_{\text{meas}}^{(x)}(B, t)$ in terms of length- T blocks of site-values at ‘ T ’ successive time-steps:

$$\left\{ \begin{array}{lll} S_{\text{set}}^{(t)}(T, j) &= \frac{1}{T} \log_k N^{(t)}(T, j) & \longleftrightarrow \text{temporal set block-entropy,} \\ S_{\text{meas}}^{(t)}(T, j) &= -\frac{1}{T} \sum_{i=1}^{2^T} \tilde{p}_i^T(j) \log_k \tilde{p}_i^T(j) & \longleftrightarrow \text{temporal measure block-entropy,} \end{array} \right.\tag{4.120}$$

where $N^{(t)}(T, j)$ is the total number of length- T temporal-blocks generated at site ‘ j ’, and $\tilde{p}_i^T(j)$ is the probability of the i^{th} sequence of site values within a temporal-

block of size T at site ' j '. We hasten to point out that because spatial sequences of site-values generally have little in common with temporal site-value sequences at a given site, $S_{\text{set}}^{(t)}$ and $S_{\text{meas}}^{(t)}$ are typically very different. In the special case of a pure shift-map, however, it is true that the spatial entropy of a given configuration is the same as the temporal entropy of the shift-map rule applied to that configuration. The relation $S^{(t)}(T, j) \leq S^{(t)}(T - 1, j)$ holds only when the evolution has attained an 'equilibrium' in which the statistical properties are independent of time.

Dimensions: The analogous temporal *set* and *measure* dimensions, may likewise be defined:

$$\begin{cases} d_{\text{set}}^{(t)} &= \lim_{T \rightarrow \infty} S_{\text{set}}^{(t)}(T, j) & \longleftrightarrow & \text{temporal set dimension,} \\ d_{\text{meas}}^{(t)} &= \lim_{T \rightarrow \infty} S_{\text{meas}}^{(x)}(T, j) & \longleftrightarrow & \text{temporal measure dimension.} \end{cases} \quad (4.121)$$

with the analogue of equation 4.110 being given by

$$0 \leq d_{\text{meas}}^{(t)} \leq d_{\text{set}}^{(t)} \leq 1. \quad (4.122)$$

The spatial and temporal dimensions provide a convenient quantitative characterization of the various classes of large time behavior. The homogeneous final states of class **c1** CA, for example, are characterized by $d_{\text{set}}^{(x)} = d_{\text{set}}^{(t)} = d_{\text{meas}}^{(x)} = d_{\text{meas}}^{(t)} = 0$; such states are obviously analogous to *limit point* attractors in continuous systems. Similarly, the periodic final states of class **c2** CA are analogous to *limit cycles*; although there does not typically exist a unique invariant probability measure on the set of all possible configurations (*i.e.* , neither $d_{\text{set}}^{(x)}$ nor $d_{\text{meas}}^{(x)}$ can be assigned a unique value), finite periods imply that $d_{\text{set}}^{(t)} = d_{\text{meas}}^{(t)} = 0$. Finally, the aperiodic chaotic patterns produced by class **c3** CA are analogous to *strange attractors*; such patterns are characterized by nonzero spatial and temporal dimensions. These comments are summarized in the table below:

class	$d_{\text{meas}}^{(x)}$	$d_{\text{meas}}^{(t)}$
c1	0	0
c2	> 0	0
c3	> 0	> 0

Because of the generally unpredictable behavior of class **c4** rules, dimensions cannot meaningfully be defined for rules in this class.

4.5.2.3 Spatio-Temporal Measures for Infinite Lattices

Entropies: The individual space and time measures introduced above may also be generalized to *space-time blocks* of size $B \times T$:

$$\begin{cases} S_{\text{set}}^{(x,t)}(B, T; t) &= \frac{1}{T} \log_k N(B, T; t), \\ S_{\text{meas}}^{(x,t)}(B, T; t) &= -\frac{1}{T} \sum_{i=1}^{k^{BT}} p_i(t) \log_k p_i(t), \end{cases} \quad (4.123)$$

where $N(B, T; t)$ is the total number of size $B \times T$ space-time blocks generated at time ' t ', and $p_i(t)$ is the probability of the i^{th} size- $B \times T$ configuration at time ' t '. Comparing these two definitions with those for $S^{(x)}(B, t)$ (equations 4.105) and $S^{(t)}(T, t)$ (equations 4.120), we have the obvious relations

$$\begin{cases} S^{(t)}(T, t) &= S^{(x,t)}(1, T; t), \\ S^{(x)}(B, t) &= \frac{1}{B} S^{(x,t)}(B, 1; t), \end{cases} \quad (4.124)$$

where S stands for either S_{set} or S_{meas} . In order to obtain bounds on the possible values of these entropies, consider the schematic representation of a space-time block given in figure 4.15.

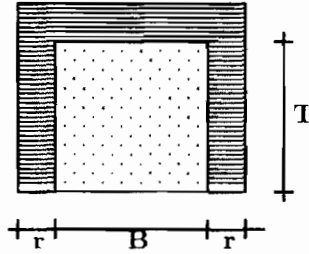


Fig. 4.15 Schematic view of a small space-time region of a one-dimensional CA. The site-values in the *dotted* region are completely determined by values in the surrounding *lined* area. See text for discussion.

The values of all of the sites contained within the $(B \times T)$ dotted inner region of this figure are completely determined by the values in the outer lined region. Since this surrounding area contains $(B + 2r(T - 1))$ sites (where ' r ' is, as usual, the range of the given CA rule), we have that

$$\begin{aligned} S_{\text{set}}^{(x,t)}(B, T; t) &\leq S_{\text{meas}}^{(x,t)}(B, T; t) \leq \frac{B + 2r(T - 1)}{T}, \\ \implies_{\text{fixed } B, \text{ large } T} S_{\text{set}}^{(x,t)}(B, T; t) &\leq S_{\text{meas}}^{(x,t)}(B, T; t) \leq 2r \end{aligned} \quad (4.125)$$

In particular, the last relation implies that if $B, T \rightarrow \infty$ with T/B fixed, then the *information per site* in a $B \times T$ space-time region, $\mathcal{I}_0 \equiv S_{\text{meas}}(B, T)/B \rightarrow 0$. In other words, completely random space-time patterns for one-dimensional CA *can never really be generated*.

If $T \rightarrow \infty$ with B fixed, the contribution by the length- B horizontal segment of the outer lined area in figure 4.15 can be effectively ignored. Noting that the entropy is largest when the $2r$ vertical columns are statistically independent, we find that

$$\begin{cases} S_{\text{set}}^{(x,t)}(B, T \rightarrow \infty) & \leq 2r S_{\text{set}}^{(t)}(T \rightarrow \infty) & = 2rd_{\text{set}}^{(t)}, \\ S_{\text{meas}}^{(x,t)}(B, T \rightarrow \infty) & \leq 2r S_{\text{meas}}^{(t)}(T \rightarrow \infty) & = 2rd_{\text{meas}}^{(t)} \end{cases} \quad (4.126)$$

Moreover,

$$\begin{cases} S_{\text{set}}^{(x,t)}(B, T \rightarrow \infty) & \leq S_{\text{set}}^{(x,t)}(B+1, T \rightarrow \infty), \\ S_{\text{meas}}^{(x,t)}(B, T \rightarrow \infty) & \leq S_{\text{meas}}^{(x,t)}(B+1, T \rightarrow \infty) \end{cases} \quad (4.127)$$

Dimensions: The limits of the set and measure entropies as $T, B \rightarrow \infty$ yield the *spatio-temporal set* and *measure dimensions*, respectively:

$$\begin{cases} \mathbf{h}_{\text{set}} & = \lim_{\substack{T \rightarrow \infty \\ B \rightarrow \infty}} S_{\text{set}}^{(x,t)}(B, T), \\ \mathbf{h}_{\text{meas}} & = \lim_{\substack{T \rightarrow \infty \\ B \rightarrow \infty}} S_{\text{meas}}^{(x,t)}(B, T). \end{cases} \quad (4.128)$$

$\mathbf{h}_{\text{set}}$ may be interpreted as yielding the asymptotic rate of increase of the number of possible ‘histories’, while $\mathbf{h}_{\text{meas}}$ is the entropy content of arbitrarily wide spacetime regions. Equations 4.126 and 4.127 lead to the relation

$$d^{(t)} \leq \mathbf{h} \leq 2rd^{(t)}, \quad (4.129)$$

where d stands for either d_{set} or d_{meas} and $\mathbf{h}$ stands for either $\mathbf{h}_{\text{set}}$ or $\mathbf{h}_{\text{meas}}$.

rule	$d_{\text{meas}}^{(x)}$	$d_{\text{set}}^{(x)}$
R18	1/2	1/2
R22	$< .795 \pm .001$	$< .744 \pm .003$
R30	1	1
R50	$.601 \pm .001$	0
R90	1	1
R110	0	0
R122	1/2	1/2

Table 4.2 Spatial and temporal measure dimensions for a few selected elementary one-dimensional rules (from table 6 of the appendix in [wolf86b]).

Chapter 5

Analytic Approach

One should not be surprised to learn that it is precisely that which makes CA so appealing as “toy” models of physical phenomena—namely, their propensity to exhibit a remarkably wide range of possible behaviors—that lies at the heart of what makes CA so difficult to study *analytically*. In fact, except for a relatively small class of so-called additive CA rules (that obey linear superposition laws), and other similarly small classes that can be organized according to some simplifying dynamical characteristics, it is generally very difficult to say anything meaningful about a particular CA rules’ time evolution. This chapter provides a brief survey of some analytical tools useful for describing CA. It discusses methods of inferring cycle-state structure from global eigenvalue spectra, the enumeration of limit cycles, the use of shift transformations, local structure theory, and Lyapunov functions. Some preliminary research on linking CA behavior with the topological characteristics of the underlying lattice is also described.

5.1 Deduction of Properties of General Rules

5.1.1 Cycle-State Structure from Global Eigenvalue Spectrum

Given any arbitrary *local* range- r one-dimensional CA rule, $\phi : \{0, 1, \dots, k-1\}^{2r+1} \rightarrow \{0, 1, \dots, k-1\}$, we can always explicitly construct the *global* rule, $\Phi : \Gamma \rightarrow \Gamma$:

$$\Sigma(t+1) = \Phi \Sigma(t), \quad (5.1)$$

where $\Sigma(t) = (\sigma_0(t), \sigma_1(t), \dots, \sigma_N(t)) \in \Gamma$ is the global state of the system at time ‘ t ’. The topological loop structure of the global state transition graph, $\mathcal{G}_\Sigma$, may then be partially inferred directly from the eigenvalue spectrum of Φ . The discussion given here closely follows that given in [gibb85].

To see this, we first rewrite equation 5.1 in matrix form as

$$\tilde{\Sigma}(t+1) = \Phi \tilde{\Sigma}(t), \quad (5.2)$$

where $\tilde{\Sigma}(t)$ is an k^N -dimensional column vector all of whose entries are equal to zero except for a single '1' in the i^{th} place (corresponding to the system being in the i^{th} global state at time ' t '), and Φ is an $k^N \times k^N$ $(0, 1)$ -matrix with entries $\Phi_{ij} = 1$ if and only if $\Phi \Sigma_j = \Sigma_i$.

Although any arbitrary labeling scheme for the global states may be used to define these matrices, the most convenient one for our purposes here is one that exploits our knowledge of the possible types of global states. In particular, we label Φ according to the following scheme:

1. assign the lowest global-state numbers $1, 2, \dots, n_g$ to all *garden-of-eden* states; that is, all states that can arise only as initial states of the system and can never be dynamically generated during the course of the subsequent evolution.
2. assign the numbers $n_g + 1, n_g + 2, \dots, n_g + n_t$ to all *transient* states; that is all states located on the (interior of) trees in $\mathcal{G}_L$.
3. assign the remaining numbers, $n_g + n_t + 1, n_g + n_t + 2, \dots, n_g + n_t + n_c = k^N$, to all global *cyclic* states; n_c is the total number of cycles in the system.

With this labeling, the matrix Φ effectively consists of nine submatrices, Φ_i , $i = 1, 2, \dots, 9$:

$$\Phi = \begin{array}{c} \text{eden} \\ \text{transient} \\ \text{cycle} \end{array} \begin{pmatrix} \text{eden} & \text{transient} & \text{cycle} \\ \Phi_1 & \Phi_2 & \Phi_3 \\ \Phi_4 & \Phi_5 & \Phi_6 \\ \Phi_7 & \Phi_8 & \Phi_9 \end{pmatrix} \quad (5.3)$$

Note that since for each state Σ_i , Φ assigns a unique successor state Σ_j , each *column* of the matrix Φ consists of all zeroes except for a single '1'; each *row*, on the other hand, is under no such constraint and can therefore have any number of 1's.

We can simplify this matrix by making the following two simple observations. First, since there cannot be predecessor states for garden-of-eden states, submatrices Φ_1 , Φ_2 and Φ_3 must all be equal to zero; second, since all cyclic states are predecessors only of other cyclic states, submatrices $\Phi_3 = \Phi_6 = 0$. Φ thus really looks like

$$\Phi = \begin{pmatrix} 0 & 0 & 0 \\ \Phi_4 & \Phi_5 & 0 \\ \Phi_7 & \Phi_8 & \Phi_9 \end{pmatrix}, \quad (5.4)$$

with eigenvalues, λ_i , given by the solution to the secular equation

$$|\Phi - \lambda| = (-\lambda)^{n_g} \cdot |\Phi_5 - \lambda| \cdot |\Phi_9 - \lambda|. \quad (5.5)$$

From the first part of this equation, we see that each of the n_g garden-of-eden states gives rise to a zero eigenvalue.

Consider now the contribution from submatrix Φ_5 . We know (i) that there is a single '1' in every column of either Φ_5 or Φ_8 , and (ii) that since at least one transient state must lead to a cycle, Φ_8 must contain at least one '1'. By relabeling the transient states making up Φ_5 so that the column containing the '1' in Φ_8 becomes column #1, we may rewrite the factor $|\Phi_5 - \lambda|$ as $-\lambda |(\Phi_5 - \lambda)'$, where $(\Phi_5 - \lambda)'$ is a $(k^N - 1) \times (k^N - 1)$ matrix obtained from Φ_5 by deleting its first row and column. There are three possibilities: (1) *the first (deleted) row contained a '1'*. If this was the case, the deletion left a zero column in the reduced submatrix, which, by another relabeling, may be put into the extreme leftmost position. The relabeled matrix is then again reduced in the same fashion as above, yielding another zero eigenvalue. (2) *the first (deleted) row did not contain a '1'*. In this case, the '1' leading to the transient state must be in submatrix Φ_4 . Assuming that the reduced submatrix is not null (see (3) below), there must therefore be another transient leading to a cycle; i.e., Φ_5 must have a zero column (and Φ_8 must contain another '1'). We again relabel this column so that it sits in the leftmost position. (3) *all entries of the reduced submatrix, $(\Phi_5 - \lambda)'$, are equal to zero*. In this case, the process is terminated. Putting this reasoning together with the contribution from the first part of the secular equation, we thus see that *each garden-of-eden and transient state contributes a zero eigenvalue*.

Finally, we consider the contribution from the last term, $|\Phi_9 - \lambda|$. To find the eigenvalues in this case, we note that we can relabel the submatrix Φ_9 so that it appears in block diagonal form, with each block corresponding to a particular cycle, C_i , $i = 1, 2, \dots, l$:

$$\Phi_9 = \begin{pmatrix} C_1 & 0 & \cdots & 0 \\ 0 & C_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & C_l \end{pmatrix}. \quad (5.6)$$

The secular equation takes the form

$$|\Phi_9 - \lambda| = \prod_{i=1}^l |C_i - \lambda|. \quad (5.7)$$

By relabeling each of the cyclic blocks, C_i , in such a way that the transition diagram proceeds systematically from state #1 to # $|C_i|$, C_i may be rewritten as a *circulant matrix* with first row = $(0, 0, \dots, 1)$:

$$C_i = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}. \quad (5.8)$$

It is well known (see section 2.1.4) that the eigenvalues of C_i are the $n = |C_i|$ roots

of unity:

$$1, e^{2\pi i(n-1)/n}, e^{2\pi i(n-2)/n}, \dots, e^{2\pi i/n}. \quad (5.9)$$

As suggested at the beginning of this subsection, we can – by reversing the above reasoning process – partially infer the topological structure of the global state transition graph, $\mathcal{G}_{\mathcal{L}}$:

1. Since each cycle yields a single eigenvalue $\lambda = 1$, *the number of eigenvalues equal to one gives the number of distinct cycles.*
2. *The degeneracy of the eigenvalue of the form $e^{2\pi i/m}$ with the largest value of ‘m’ (i.e., the one with the smallest nonzero phase-angle) gives the number of cycles of length ‘m’.*
3. Remove all eigenvalues corresponding to the cycles found in step (2) – i.e., remove $e^{2\pi i/m}, e^{2\pi i2/m}, \dots, 1$ – and repeat step (2).

In this way, the total number of loops of various sizes may be systematically found. We should hasten to point out, however, that such an analysis is in practice very difficult to carry out because of the potentially enormous size ($= k^N \times k^N$) of the matrix Φ . In the remaining sections of this chapter we consider a variety of alternative analytical tools.

5.1.2 Mathematical Characterization of Elementary CA

Despite being notoriously difficult to analyze formally, the behavior of general CA rules is nonetheless often amenable to an almost complete mathematical characterization. In this section we look at a simple method that exploits the properties of certain *implicit deterministic structures* of elementary one-dimensional rules to help determine the existence of periodic temporal sequences, rule inverses and homogeneous states. Additional details appear in [jen86a] and [jen86b].

5.1.2.1 Implicit Deterministic Structures

We recall that *elementary CA* are defined by nearest-neighbor rules of the form

$$\sigma_i(t+1) = \phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)), \quad \sigma_i(t) \in \{0, 1\}, \quad (5.10)$$

with rule-code $R[\phi] \equiv \sum_{\{\sigma_{i-1}, \sigma_i, \sigma_{i+1}\}} \phi(\sigma_{i-1}, \sigma_i, \sigma_{i+1}) 2^i = \sum_{i=0}^7 \alpha_i 2^i$. We will assume (without loss of generality) that $\phi(0, 0, 0) = 0$.

While the explicit ‘deterministic structure’ of such rules – by which me mean the set of sites whose value is fixed by values of other sites – appears as $[\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)] \Rightarrow \sigma_i(t+1)$, there may also exist an *implicit* underlying deterministic structure not immediately obvious from the definition of the rule itself. It may be

true, for example, that for all values of $\sigma_{i-1}(t)$ and $\sigma_i(t)$,

$$\begin{cases} \sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1} = 0 & \implies \alpha, \text{ and} \\ \sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1} = 1 & \implies \bar{\alpha} \end{cases} \quad (5.11)$$

where $\bar{\alpha} \equiv \alpha \oplus 2 \cdot 1$. In this case, the value of $\sigma_{i+1}(t)$ is determined by the values of $\sigma_{i-1}(t)$ and $\sigma_i(t)$ and the underlying deterministic structure is given by $[\sigma_{i-1}(t), \sigma_i(t), \sigma_i(t+1)] \Rightarrow \sigma_{i+1}(t)$; it may be represented schematically as

It is also easy to see what rules are of type specified by conditions given in equation 5.11. Since we must have

$$\begin{cases} 000 \rightarrow \alpha_0 & 010 \rightarrow \alpha_2 & 100 \rightarrow \alpha_4 & 110 \rightarrow \alpha_6 \\ 001 \rightarrow \alpha_1 & 011 \rightarrow \alpha_3 & 101 \rightarrow \alpha_5 & 111 \rightarrow \alpha_7, \end{cases} \quad (5.12)$$

the pairs $\{\alpha_0, \alpha_1\}$, $\{\alpha_2, \alpha_3\}$, $\{\alpha_4, \alpha_5\}$, and $\{\alpha_6, \alpha_7\}$ must all take on differing values. Any rule such that $\alpha_j \neq \alpha_{j+1}$, $j = 0, 2, 4, 6$ will therefore have the same implicit deterministic structure as defined above. Table 5.1 shows all eight possible deterministic structures.

5.1.2.2 Periodicity of Temporal Sequences

Among the global behavioral implications of rules possessing particular deterministic structures, are those having to do with the periodicity of temporal sequences.

We define a *finite initial state*, $\Sigma_{\alpha, \beta}(t=0)$, on an infinite lattice as an initial configuration $\Sigma(0) = \{\dots, \sigma_{\alpha-1}, \sigma_{\alpha}, \dots, \sigma_{\beta-1}, \sigma_{\beta}, \dots\}$ such that for some $-\infty < \alpha \leq \beta < \infty$, $\sigma_i = 0$ for $i < \alpha$ and $i > \beta$ and $\sigma_{\alpha} = \sigma_{\beta} = 1$. The sequences of site values, $\{\sigma_i(t=0), \sigma_i(t=1), \dots, \sigma_i(t=\tau), \dots\}$ is *periodic* if there exists T_i and s_i such that $\sigma_i(t+s_i) = \sigma_i(t)$ for $t \geq T_i$. We can now prove the following theorem:

Theorem 1 *Let ϕ be an elementary CA rule belonging either to deterministic structure type (1) (see table 5.1) with '100' $\rightarrow \alpha_4 = 1$ or type (2) with '001' $\rightarrow \alpha_1 = 1$. Then, with arbitrary finite initial states, there can exist at most one periodic sequence.*

Proof: First, it is easy to show that if $\{\sigma_i(t)\}$ and $\{\sigma_j(t)\}$ are two periodic sequences with $i < j$, then the sequence $\{\sigma_k(t)\}$ must also be periodic for $i < k < j$. In particular, $\{\sigma_{j-1}(t)\}$ is periodic. Suppose now that ϕ is of class (1). Then since $\sigma_{j+1}(t)$ is determined by $\sigma_j(t)$, $\sigma_{j-1}(t)$, and $\sigma_j(t+1)$, the periodicity of $\{\sigma_j(t)\}$ and $\{\sigma_{j-1}(t)\}$ implies the periodicity of $\{\sigma_{j+1}(t)\}$. Moreover, by induction, all sequences to the 'right' of the j^{th} site, $\{\sigma_{j+n}(t)\}$, $n > 0$, must also be periodic with the same $T = \max(T_j, T_{j-1})$ and $s = \text{lcm}(s_j, s_{j-1})$. Given that we start with finite initial conditions and the fact that $\alpha_4 = 0$, however, implies that there exists some N such that (i) $\sigma_{j+N}(t) = 0$ for some $T \leq t \leq T+s$ and (ii) $\sigma_{j+N}(T+m) = 1$ for some $m \geq s$. By contradiction, we conclude that there cannot exist two periodic temporal sequences of any period. The same conclusion is reached for rules of type (2). ■

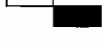
DETERMINISTIC STRUCTURE	COEFFICIENT CONSTRAINTS	RULES
(1) 	$\alpha_j \neq \alpha_{j+1}$ $j = 0, 2, 4, 6$	85, 86, 89, 90, 101, 102, 105, 106, 149, 150, 153, 154, 165 166, 169, 170
(2) 	$\alpha_j \neq \alpha_{j+4}$ $j = 0, 1, 2, 3$	15,30,45,60,75,90,105, 120,135,150,165,180,195, 210,225,240
(3) 	$\alpha_j = \alpha_{j+1}$ $j = 0, 2, 4, 6$	0,3,12,15,48,51,60,63,192, 195,204,207,240,243,252,255
(4) 	$\alpha_j = \alpha_{j+4}$ $j = 0, 1, 2, 3$	0,17,34,51,68,85,102, 119,136,153,170,187,204, 221,238,255
(5) 	$\alpha_0 = \alpha_1 = \alpha_4 = \alpha_5$ $\alpha_2 = \alpha_3 = \alpha_6 = \alpha_7$ $\alpha_0 \neq \alpha_2$	51,204
(6) 	$\alpha_0 = \alpha_1 = \alpha_2 = \alpha_3$ $\alpha_4 = \alpha_5 = \alpha_6 = \alpha_7$ $\alpha_0 \neq \alpha_4$	15,240
(7) 	$\alpha_0 = \alpha_2 = \alpha_4 = \alpha_6$ $\alpha_1 = \alpha_3 = \alpha_5 = \alpha_7$ $\alpha_0 \neq \alpha_1$	85,170
(8) 	$\alpha_j \neq \alpha_{j+2}$ $j = 0, 1, 4, 5$	51,54,57,60,99,102,105, 108,147,150,153,156,195, 198,201,204

Table 5.1 Deterministic structures for one-dimensional elementary CA [jen86b].

The rules satisfying the conditions of this theorem are given by $\phi = \mathbf{R30}, \mathbf{R86}, \mathbf{R90}, \mathbf{R150}, \mathbf{R154}, \mathbf{R210}$. Notice, in particular, that the theorem supports the conjecture (made earlier in section 3.1.4) that the center time sequence, $\{\sigma_0(t)\}$, of rule **R30** is in fact completely random (*i.e.*, aperiodic). The theorem may also be generalized to nearest-neighbor *non*-elementary CA rules: Allowing the sites to assume the values $\sigma \in S \equiv \{0, 1, \dots, k-1\}$, deterministic structure types (1) and (2) are defined by

$$\begin{cases} \alpha_{lk^2+mk+n_i} \neq \alpha_{lk^2+mk+n_j} & \text{for all } l, m, n_i, n_j \in S; \quad n_i \neq n_j \quad \longleftrightarrow \quad \text{type (1)} \\ \alpha_{l_i, k^2+mk+n} \neq \alpha_{l_j, k^2+mk+n} & \text{for all } l_i, l_j, m, n \in S; \quad l_i \neq l_j \quad \longleftrightarrow \quad \text{type (1)} \end{cases} \quad (5.13)$$

For rules satisfying these conditions, the theorem holds true provided that if ϕ is of type (1), $\{0, \dots, k-1\}00' \not\rightarrow 0$ and if ϕ is of type (2) that $00\{0, \dots, k-1\}' \not\rightarrow 0$.

5.1.2.3 Rule Inverses

A CA rule ϕ^{-1} is the *inverse* of rule ϕ if and only if $(\phi^{-1} \circ \phi) \{\sigma_i(t)\} = \{\sigma_i(t)\}$, where $\phi\{\sigma_i(t)\}$ is the sequence of sites obtained from $\{\sigma_i(t)\}$ by applying rule ϕ and $(\phi^{-1} \circ \phi) = \phi^{-1}\{\phi\{\sigma_i(t)\}\}$ is the *composition* of rules ϕ^{-1} and ϕ .

Theorem 2 *An elementary CA rule, ϕ , has an inverse, ϕ^{-1} , if and only if ($\Leftarrow$) ϕ has deterministic structure type (5), (6) or (7) (see table 5.1).*

Proof: (i) ($\Rightarrow$) Suppose ϕ is of type (5). Then $'*0*' \rightarrow \alpha$ and $'*1*' \rightarrow \bar{\alpha}$, where $\alpha \neq \bar{\alpha}$ and $'*' is a wildcard denoting both '0' and '1'. Assume that $'*0*' = 0$. Then ϕ^{-1} must be such that $'*1*' \rightarrow 1$ and $'*0*' \rightarrow 0$ and therefore $\phi^{-1} = \phi$. If ϕ is of type (6) then $'**0' \rightarrow \alpha$ and $'**1' \rightarrow \bar{\alpha}$, where $\alpha \neq \bar{\alpha}$. Assume that $'**0' = 0$. Then ϕ^{-1} must be such that $'1**' \rightarrow 1$ and $'0**' \rightarrow 0$ and therefore is of type (7). Similar analyses may be carried out for the cases $'*0*' \rightarrow 1$, $'**0' \rightarrow 1$, and $'0**' \rightarrow 1$.$

(ii) ($\Leftarrow$) First, define the set $\{\alpha_i, \beta_i, \gamma_i\}$ to be such that $\tilde{\phi}\{\alpha_i, \beta_i, \gamma_i\} = 0$, for some rule $\tilde{\phi}$. Then it is easy to show that if there exist x, y such that $\phi(x1y) = \beta_i$ for some $'i'$, then $\phi^{-1} = \tilde{\phi}$ implies that either there exists no $'w'$ such that $'wx1' \rightarrow \alpha_i$ or there exists no $'z'$ such that $'1yz' \rightarrow \delta_i$. Assume now that ϕ has inverse ϕ^{-1} and that $\phi(000) = 0$. Then ϕ can only have one of two possible forms: either (a) $'*0*' \rightarrow 0$ or (b) $'*0*' \rightarrow \{0, 1\}$. For case (a), we see that if either $'**0' \rightarrow 0$ or $'0**' \rightarrow 0$ then $(\phi^{-1} \circ \phi) \{ *010* \} = \phi^{-1}(000)$, inconsistent with our observation at the top of this paragraph. Thus, both $'**0'$ and $'0**'$ must be able to assume either value '0' or '1'. The only rule with an inverse is therefore such that $'*0*' \rightarrow 0$ and $'*1*' \rightarrow 1$; *i.e.*, ϕ must be of type (5). For case (b), on the other hand, no inverse exists if both $'**0' \rightarrow \{0, 1\}$ and $'0**' \rightarrow \{0, 1\}$. Thus, we must have either that $'**0' \rightarrow 0$ and $'**1' \rightarrow 1$ (type 6) or $'0**' \rightarrow 0$ and $'1**' \rightarrow 1$ (type 7). ■

5.1.2.4 Homogeneous States

A CA evolves to a *homogeneous state* if there exists a $T < \infty$ such that for all $'i'$ and $t \geq T$, $\sigma_i(t) = \alpha$, where α is a constant independent of both $'i'$ and $'t'$.

The following theorem defines the class of CA rules under which finite initial states evolve to homogeneous states, and thus describes all class **c1** rules:

Theorem 3 *All finite initial states, $\Sigma_{\alpha,\beta}(t=0)$, evolve under rule elementary CA ϕ to the homogeneous state $\{\dots, 0, 0, \dots, \sigma_{-1}(t) = 0, \sigma_0(t) = 0, \sigma_{i+1}(t) = 0, \dots, 0, 0, \dots\}$, $t < \infty$ if and only if the coefficients defining ϕ are such that $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_4 = 0$ and either (i) $\alpha_3 = 0$ or (ii) $\alpha_6 = 0$. The rules for which these conditions hold are given by $\phi = \mathbf{R0}, \mathbf{R8}, \mathbf{R32}, \mathbf{R40}, \mathbf{R64}, \mathbf{R96}, \mathbf{R128}, \mathbf{R136}, \mathbf{R160}, \mathbf{R168}, \mathbf{R192}, \mathbf{R224}$.*

Proof: We first show that the conditions are necessary. Observe that in order to prevent the leftmost and rightmost site values - $\sigma_{\alpha}(t=0)$ and $\sigma_{\beta}(t=0)$, respectively - from propagating outward indefinitely, we must have that '100' $\rightarrow \alpha_1 = 0$ and '001' $\rightarrow \alpha_4 = 0$. α_2 must equal zero since if $\alpha_2 = 1$ then any block of sites of the form ' $\dots 00100 \dots$ ' would remain invariant under ϕ . Similarly, if '011' $\rightarrow \alpha_3 = 1$ and '110' $\rightarrow \alpha_6 = 1$ then a block of the form ' $\dots 001100 \dots$ ' would remain invariant. We conclude that $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_4 = 0$ and either α_3 or α_6 must equal zero in order for ϕ to be able to evolve $\Sigma_{\alpha,\beta}(t=0)$ to a homogeneous state. We now turn to showing that the conditions are also sufficient. Assume that the first complete set is satisfied (i.e., that $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0$) and that $\sigma_i(t) = 0$ for all $i < \alpha$. The site value $\sigma_{\alpha}(t+1)$ will then equal zero, independently of the value of $\sigma_{\alpha+1}(t)$. Since a rightward propagation is prevented by '100' $\rightarrow \alpha_4 = 0$, $\Sigma_{\alpha,\beta}(t=0) \rightarrow \bar{0}$ in a finite number of iterations. A similar analysis may be carried out for the set $\alpha_0 = \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = 0$. ■

Define a *constant state* to be a sequence of site values $\{\dots, \sigma_{-1}(t), \sigma_0(t), \sigma_1(t), \dots\}$ such that there exists $T < \infty$ such that for all 'i' and $t \geq T$, $\sigma_i(t) = \alpha$, where α is a constant.

The following theorem - stated without proof (see [jen86a]) - gives necessary and sufficient conditions for CA rules to generate constant temporal sequences:

Theorem 4 *An arbitrary finite initial state, $\Sigma_{\alpha,\beta}(t=0)$, will evolve under an elementary CA rule, ϕ - defined by coefficients $\alpha_0, \dots, \alpha_7$ - to at least one constant nonzero temporal sequence if and only if one of the following conditions holds:*

(1) $\alpha_0 = 0, \alpha_1 = \alpha_4 = 1$ and any one of the following - (1a) $\alpha_3 = \alpha_6 = \alpha_7 = 1$ and '11' either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ ; (1b) $\alpha_2 = \alpha_3 = \alpha_6 = 1, \alpha_5 = 0$ and '101' either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ ; (1c) $\alpha_2 = \alpha_5 = \alpha_7 = 1, \alpha_3 = \alpha_6 = 0$ and $\beta - \alpha + 1$ (i.e., the length of the initial state) is odd and generates, for some $t \geq 0$, a symmetric state with respect to some i^* .

(2) $\alpha_0 = \alpha_1 = 0, \alpha_4 = 1$ and either of the following - (1a) $\alpha_3 = \alpha_6 = \alpha_7 = 1$ and '11' either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ ; (1b) $\alpha_2 = \alpha_3 = 1$.

(3) $\alpha_0 = \alpha_4 = 0, \alpha_1 = 1$ and either of the following - (1a) $\alpha_3 = \alpha_6 = \alpha_7 = 1$ and '11' either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ ; (1b) $\alpha_2 = \alpha_6 = 1$.

*By a symmetric state with respect to site 'i' we mean one in which $\sigma_{i-j}(t) = \sigma_{i+j}(t)$ for all $j \geq 0$.

(4) $\alpha_0 = \alpha_1 = \alpha_4 = 0$ and either of the following – (1a) $\alpha_3 = \alpha_6 = \alpha_7 = 1$ and ‘11’ either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ ; (1b) $\alpha_2 = 1$ and ‘00100’ either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ ; (1c) $\alpha_3 = \alpha_6 = 1$ and ‘001100’ either appears in $\Sigma_{\alpha,\beta}(t=0)$ or is generated under ϕ .

5.1.3 Enumeration of Limit Cycles

Consider once again a size- N , radius- r one-dimensional CA with periodic boundary conditions:

$$\begin{cases} \sigma_i(t+1) &= \phi(\sigma_{i-r}(t), \dots, \sigma_i(t), \dots, \sigma_{i+r}(t)), & \phi : S^{2r+1} \longrightarrow S, \\ \sigma_i(t) &= \sigma_j(t), & i \equiv j \pmod N, \end{cases} \quad (5.14)$$

where $S = \{0, 1, \dots, k-1\}$. We recall that a CA is *periodic* with period ‘ p ’ if there exists a $T \geq 0$ such that $\sigma_i(t) = \sigma_i(t+p)$ for all $0 \leq i < N$ and $t \geq T$; since there are a finite number of possible states, we know that $p \leq k^N$.

We will say that a state $\Sigma(t) \equiv (\sigma_0(t), \dots, \sigma_{N-1}(t))$ (and the limit cycle it generates) is *primitive* if there is no $M < N$ such that $\sigma_i(t) = \sigma_{(i+M) \bmod N}(t)$. We also define the following three quantities:

$$\begin{cases} C_{N,p} &\longleftrightarrow \text{ \# of limit cycles of period ‘} p \text{’} \\ \mathcal{P}_{N,p} &\longleftrightarrow \text{ \# of primitive limit cycles of \textit{least} period ‘} p \text{’} \\ \mathcal{T}_{N,p} &\longleftrightarrow \text{ total \# of (not necessarily primitive) states appearing} \\ &\quad \text{ in a limit cycle of (not necessarily least) period ‘} p \text{’} \end{cases} \quad (5.15)$$

It is easy to see that these quantities are related by

$$\begin{cases} C_{N,p} &= \sum_{M|N} \sum_{q|p} \mathcal{P}_{M,q}, \\ \mathcal{T}_{N,p} &= \sum_{M|N} \sum_{q|p} q \mathcal{P}_{M,q}, \end{cases} \quad (5.16)$$

where $\alpha \mid \beta$ means that *alpha* divides *beta*.

The key result in this section will be the derivation of linear recurrence relations for $\mathcal{T}_{N,p}$ in terms of $\mathcal{T}_{j,p}$, for $j < n$ [jen 88a]. We begin by introducing an *invariance matrix*, whose powers correspond to the lattice sizes on which ϕ is defined.

5.1.3.1 Invariance Matrix, $\mathcal{A}$

The technique for enumerating limit cycles for general rules consists essentially of two parts:

1. *identification of all invariant strings ‘ $\sigma_{-r}, \dots, \sigma_r$ ’ such that*

$$\phi(\sigma_{-r}, \dots, \sigma_r) = \sigma_0, \quad (5.17)$$

and

2. specification of a size $2^{2r} \times 2^{2r}$ $(0,1)$ invariance matrix, $\mathcal{A}$, whose entries are equal to one whenever they represent strings satisfying equation 5.17. To be more precise, if ' $i_{-r}i_{-r+1} \dots i_{r-1}$ ' and ' $j_{-r+1}j_{-r+2} \dots j_r$ ' represent the right-justified binary forms of ' i ' and ' j ', then the entries of $\mathcal{A} = a_{ij}$ are given by

$$a_{ij} = \begin{cases} 1 & \text{if } i_k = j_k, \quad -r+1 < k \leq r-1, \text{ and } \phi(i_{-r}, j_{-r+1}, j_{-r+2}, \dots, j_r) = j_0, \\ 0 & \text{otherwise.} \end{cases} \quad (5.18)$$

From this definition, it is easy to prove the following fundamental theorem relating the trace of powers of $\mathcal{A}$ to the number of fixed points of ϕ :

Theorem 5 *Let $\mathcal{A}$ be the invariance matrix of a range- r one-dimensional CA rule ϕ . Then, for $n \geq 2r+1$, the number of fixed points of ϕ ($= C_{N,1} = \mathcal{T}_{N,1}$) is given by $\text{Tr}(\mathcal{A}^{N-2r})$.*

Proof: The proof proceeds from the simple observation that the invariance matrix is analogous to the adjacency matrix of a graph. [†] In particular, we recall from section 2.1.2, that the entries of the n^{th} power of an adjacency matrix $\mathcal{A} = a_{ij}^{[n]}$ give the number of different paths of length ' n ' between the vertices ' i ' and ' j '. In the present case, the vertices represent tuples of site values and paths can be taken as spatial sequences of these tuples; an element of the invariance matrix is equal to one if a given value may be appended to a spatial sequence while preserving invariance under ϕ . Thus, an element $a_{ij}^{[2]}$ in $\mathcal{A}^2$ gives the number of length- $(2r+2)$ paths starting from the tuple $\mathbf{i} = (i_{-r}, \dots, i_r)$ and ending at the tuple $\mathbf{k} = (k_{-r}, \dots, k_r)$ such that each $(2r+1)$ -tuple in the string of site values satisfies equation 5.17. The generalization to arbitrary powers of $\mathcal{A}$ follows naturally. Since fixed points must begin and end at the same tuple, the total number is given by the sum of diagonal entries of $\mathcal{A}^{N-2r}$. Thus, $C_{N,1} = \mathcal{T}_{N,1} = \text{Tr}(\mathcal{A}^{N-2r})$. ■

We make three additional observations: (1) Denoting the set of eigenvalues of $\mathcal{A}$ by $\Lambda_{\mathcal{A}} = \{\lambda_1, \dots, \lambda_N\}$, we can relate the number of fixed points to $\Lambda_{\mathcal{A}}$: for $n \geq 2r+1$, $C_{N,1} = \mathcal{T}_{N,1} = \sum_{i=1}^N \lambda_i^{N-2r}$.

(2) Since these powers of eigenvalues correspond to terms in the characteristic equation of $\mathcal{A}$, we should not be surprised to learn that the number of strings on a given lattice belonging to limit cycles of a given period may be obtained as solutions to linear recurrence relations involving the number of strings on smaller lattices. Letting

$$\lambda^N + \alpha_{N-1}\lambda^{N-1} + \dots + \alpha_0 = 0 \quad (5.19)$$

represent the characteristic equation of $\mathcal{A}$, $C_{N,1} = \mathcal{T}_{N,1}$ in fact satisfies the linear recurrence relation

$$\mathcal{T}_{n,1} + \alpha_{N-1}\mathcal{T}_{n-1,1} + \dots + \alpha_0\mathcal{T}_{n-N,1} = 0, \quad (5.20)$$

[†]We recall, from section 2.1.2, that the adjacency matrix of a graph G , $A(G)$, is an $N \times N$ $(0,1)$ -matrix with entries $a_{ij} = 1$ if and only if there exists an edge between vertices ' i ' and ' j '.

for $n \geq N + 1$.

(3) Generalizing the second observation to cycles of arbitrary length, we note that since each primitive string in a limit cycle with least period equal to q must be a fixed point of the q^{th} order rule, $[\phi]^q$ (and thus also a fixed point of $[\phi]^p$, for any period p with $q \mid p$), each primitive limit cycle may be expressed by a term equal to its period:

$$\sum_i \lambda_i^{n-2rp} = \sum_{m \mid n} \sum_{q \mid p} q \mathcal{P}_{m,q} = \mathcal{T}_{n,p}. \quad (5.21)$$

Thus, if the characteristic equation of the invariance matrix of the p^{th} order composition of ϕ is

$$\lambda^N + \alpha_{N-1}^{(p)} \lambda^{N-1} + \cdots + \alpha_0^{(p)} = 0, \quad (5.22)$$

$\mathcal{T}_{n,p} = \sum_i \lambda_i^{n-2rp}$ satisfies the recurrence relation

$$\mathcal{T}_{n,p} + \alpha_{N-1}^{(p)} \mathcal{T}_{n-1,p} + \cdots + \alpha_0^{(p)} \mathcal{T}_{n-N,p} = 0. \quad (5.23)$$

5.1.3.2 Limit Cycle Enumeration

The above observations suffice for us to write down an algorithm for finding the total number of distinct cycles. Specifically, we can use the following procedure to compute $\mathcal{P}_{n,p}$ for all ‘ n ’ and some fixed ‘ p ’ [jen88a]:

1. Calculate $\mathcal{T}_{n,1}$, for all n , from equation 5.20; for all primes q , $\mathcal{P}_{q,1} = \mathcal{T}_{q,1}$.
2. Using equations 5.16, compute $\mathcal{P}_{n,1} = \mathcal{T}_{n,1} - \sum_{m \mid n; m \neq n} \mathcal{P}_{m,1}$.
3. Find $\mathcal{P}_{n,s}$ for all periods s with $s \mid p$ and $s \neq p$ by repeating steps one and two.
4. Using equation 5.23 to find $\mathcal{T}_{n,p}$, find $\mathcal{P}_{n,p} = \mathcal{T}_{n,p} - \sum_{m \mid n; m \neq n} \sum_{q \mid p; q \neq p} q \mathcal{P}_{m,q}$ from equations 5.16.

EXAMPLE: Consider the elementary rule **R18**, defined explicitly by $\{000, 010, 011, 101, 110, 111\} \rightarrow 0$, $\{001, 100\} \rightarrow 1$. Invariance under this rule is equivalent to a given 3-tuple being mapped to the value of the center component. Thus, any sequences constructed out of the 3-tuples 000 and 101 will be fixed points of the rule. Indexing the rows and columns

of $\mathcal{A}$ by $i, j = 00, 01, 10, 11$, we see that $\mathcal{A} = \begin{pmatrix} 1, 0, 0, 0 \\ 0, 0, 0, 0 \\ 0, 1, 0, 0 \\ 0, 0, 0, 0 \end{pmatrix}$. From the characteristic equation, $\lambda^3(1 - \lambda) = 0$, we conclude that $\sum_i \lambda^n = 1$ for all n , and thus that

$$\begin{aligned} \mathcal{T}_{n,1} &= 1, & n > 0, \\ \mathcal{L}_{n,1} &= 1, & n = 1, \\ &= 0, & \text{otherwise.} \end{aligned} \quad (5.24)$$

Omitting factors of λ , the characteristic equation for $p = 2$ is easily found to be $(\lambda - 1)(\lambda^6 - \lambda^2 - 2\lambda - 1) = 0$. Using equation 5.16 and observation #3 above, we find that

$$\sum_{m|n} \mathcal{L}_{m,2} = \frac{\mathcal{T}_{n,2} - 1}{2}, \quad \text{for all } n, \quad (5.25)$$

and the recurrence relation

$$\mathcal{T}_{n,2} = \mathcal{T}_{n-6,2} + \mathcal{T}_{n-4,2} + 2\mathcal{T}_{n-5,2} - 3, \quad n > 6, \quad (5.26)$$

where the following initial conditions may be found by computing traces of powers of the matrix $\mathcal{A}_2$: $\mathcal{T}_{1,2} = \mathcal{T}_{2,2} = \mathcal{T}_{3,2} = 1$, $\mathcal{T}_{4,2} = 5$, $\mathcal{T}_{5,2} = 11$ and $\mathcal{T}_{6,2} = 7$.

This same technique can be used to find the number of limit cycles of period p on lattice size n for any two-neighbor CA rule.

5.1.4 Shift Transformations

Feedback shift registers are essentially one-dimensional finite state machines consisting of a linear array of sites $i = 1, 2, \dots, n$, with each site i carrying value σ_i . At each time step, the system evolves according to the following two rules (see figure 5.1): (1) all of the sites are shifted one site to the right, $\sigma'_i = \sigma_{i-1}$, and (2) $\sigma'_0 = f(\sigma_{n-m+1}, \sigma_{n-m}, \dots, \sigma_n)$, where sites $i = n - m + 1, n - m, \dots, n$ label the positions of the “taps” on the shift-register. A feedback shift register is called *linear* if f is a linear function:

$$f(\sigma_{n-m+1}, \sigma_{n-m}, \dots, \sigma_n) = \alpha_0 \sigma_{n-m+1} \oplus_2 \alpha_1 \sigma_{n-m} \oplus_2 \dots \oplus_2 \alpha_m \sigma_n, \quad (5.27)$$

where $\alpha_i \in \{0, 1\}$ and *oplus₂* is addition modulo-two.

It is easy to see that an elementary size- n one-dimensional CA rule ϕ is equivalent to a size- n feedback shift register with $\sigma \in \{0, 1\}$, taps at positions $n - 2$, $n - 1$ and n , and $f = \phi$. The only difference is that it takes n “shift-register” time-steps to reproduce a single “CA” time step.

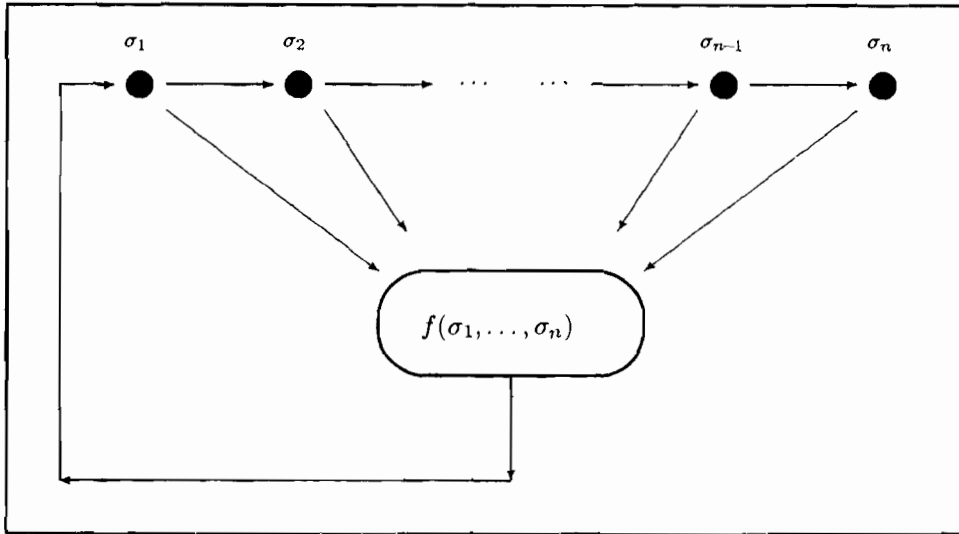


Fig. 5.1 Schematic diagram of a length- n feedback shift register.

There is a wealth of research that has been done on shift transformations. One of the best references is Golomb's classic *Shift Register Sequences* [golom67].

5.2 Algebraic Properties

A fairly complete analysis of the algebraic properties of cellular automata, including many of the most important global properties of finite CA evolving according to additive rules, was given by Martin, Odlyzko and Wolfram [martin84]. In particular, they derive the complete structure of state transition graphs of arbitrary additive rules in terms of various algebraic and number theoretic properties of polynomials over finite fields. This section summarizes the main points of their seminal paper.[†]

We begin by considering a one-dimensional CA consisting of N sites, and assume periodic boundary conditions. Letting, as always, $\sigma_0(t), \dots, \sigma_{N-1}(t)$ denote the values taken by each site at time ' t ', where $\sigma_i(t) \in \{0, 1\}$ [‡], we choose to represent

[†]An alternative approach, taken by Guan and He [guan86], is to first recast an additive rule in a "circulant matrix" form and then solve for the global behavior by exploiting the general properties of circulant matrices. In their paper, Guan and He talk apply their formalism to both non-Markovian rules (i.e. CAs that depend on s preceding time steps, $t-1, t-2, \dots, t-s$) and CAs existing in higher dimensions. An excellent additional background source for the properties of circulant matrices is *Circulant Matrices*, Philip J. Davis, John Wiley and Sons (1979).

[‡]We will generalize to letting $\sigma_i(t)$ take on values in a finite commutative ring $\mathcal{R}_k$ with k elements a bit later on in this section.

an arbitrary configuration at time ‘ t ’ by the generating function $A(x; t)$ defined by

$$A(x; t) \equiv \sum_{i=0}^{N-1} \sigma_i(t) x^i, \quad (5.28)$$

where the value of site ‘ i ’ is the coefficient of the term x^i , and all coefficients are equal to either ‘0’ or ‘1’.

It is convenient to consider generalized polynomials, called *dipolynomials*, containing both positive and negative powers of x . Dipolynomials possess the same divisibility and congruence properties as do conventional polynomials. A dipolynomial $P(x)$ is said to divide dipolynomial $Q(x)$, for example, if there exists a dipolynomial $R(x)$ such that $Q(x) = P(x)R(x)$. Similarly, $P(x) \equiv Q(x) \pmod{R(x)}$ if $R(x) \mid P(x) - Q(x)$. Observe that multiplying the generating function $A(x)$ by $\pm x^k$ yields another dipolynomial representing a configuration obtained from $A(x)$ by shifting each site k places to either the left (using $+x^k$) or right (using $-x^k$). The periodic boundary conditions are applied by reducing the generating function *modulo* the fixed polynomial ‘ $x^N - 1$ ’; i.e.,

$$\left(\sum_{i=0}^{N-1} \sigma_i x^i \right) \pmod{(x^N - 1)} = \sum_{i=0}^{N-1} \left(\sum_k \sigma_{i+kN} \right) x^i. \quad (5.29)$$

Notice that this reduction forces every dipolynomial to be congruent to a unique conventional polynomial with degree $d < N$.

An elementary additive rule

$$\sigma_i(t) = \alpha_{-1} \sigma_{i-1}(t-1) + \alpha_0 \sigma_i(t-1) + \alpha_{+1} \sigma_{i+1}(t-1), \quad (5.30)$$

may be represented by the polynomial

$$\mathcal{T}(x) = \alpha_{-1}x + \alpha_0 + \alpha_{+1}x^{-1}. \quad (5.31)$$

The state that emerges at time ‘ t ’, $A(x; t)$, is given as a function of the state at time ‘ $t-1$ ’ by

$$A(x; t) = \mathcal{T}(x)A(x; t-1) \pmod{(x^N - 1)}, \quad (5.32)$$

where it is understood that all arithmetic is performed *modulo* 2. We also recall that additive rules have the useful property that the configuration obtained from the initial configuration $A_1(x; 0) + A_2(x; 0)$ after t iterations is identical to the configuration $A_1(x; t) + A_2(x; t)$, where $A_1(x; t)$ and $A_2(x; t)$ are obtained separately after t iterations from states $A_1(x; 0)$ and $A_2(x; 0)$, respectively.

5.2.1 An Example: Elementary Rule R90

Let us first of all consider the simple additive rule **R90**, defined by

$$\sigma_i(t) = \sigma_{i-1}(t-1) + \sigma_{i+1}(t-1) \pmod{2}. \quad (5.33)$$

In our algebraic formalism, the time evolution of this system is represented by multiplying the generating function by the dipolynomial

$$\mathcal{T}(x) = x + x^{-1}. \quad (5.34)$$

An initial configuration consisting of single nonzero site therefore evolves after t iterations to a configuration given by

$$[\mathcal{T}(x)]^t \cdot 1 = (x + x^{-1})^t = \sum_{i=0}^t \binom{t}{i} x^{2*i-t}. \quad (5.35)$$

For $t < N/2$, the region of nonzero sites grows linearly with time with the position of the nonzero sites given by $\pm 2^{k_1} \pm 2^{k_2} \pm \dots$, where the k_i are the positions of the nonzero digits in the binary decomposition of the integer t . Patterns emerging from configurations containing more than one nonzero site may, according to the additive superposition property, be obtained by addition *modulo 2* of the patterns generated from states with a single nonzero site.

As we shall immediately, this algebraic formalism is deceptively deep; a great deal can be deduced from first principles alone. For example, we can easily prove the following characterization of *Garden-of-Eden*[†] configurations:

Lemma 1 *Configurations containing an odd number of sites with value 1 can never occur in the evolution of the CA evolving according to additive rule R90 (equation 5.34); they can occur only as initial states.*

Proof: Consider any initial configuration defined by the generating function $A(x; 0)$. Since the next state of the system is given by $A(x; 1) = (x + x^{-1})A(x; 0) \bmod (x^N - 1)$, we must have that

$$A(x; 1) = (x^2 + 1)P(x) + R(x)(x^N - 1) \quad (5.36)$$

for some dipolynomials $P(x)$ and $R(x)$. Since $x^2 + 1 = x^N - 1 = 0$ for $x = 1$, $A(1; 1) = 0$. We conclude that $A(x; 1)$ must contain an even number of terms, and therefore that only those configurations containing an even number of nonzero sites are reachable from an arbitrary initial configuration $A(x; 0)$. ■

Lemma 1 allows us to prove the following fundamental result concerning the density of reachable configurations for rule R90:

Theorem 1 *The fraction of the 2^N possible configurations of a size N CA evolving according to rule R90 that can occur only as initial states is equal to $1/2$ when N is odd, and is equal to $3/4$ when N is even.*

Proof: Consider first the case when N is even. We observe that, working *modulo 2*, (1) $(x^2 + 1) = (x + 1)^2 = (x - 1)^2$ and (2) $(x - 1)^2 | (x^{N/2} - 1)^2 = (x^N - 1)$, where

[†]Recall that *Garden-of-Eden* states are states that can appear only as initial states of an evolution; they can never be generated in the course of a CA's evolution.

the second result follows from a more general number theoretic property.[†] It follows that $(x-1)^2 \mid A(x;1)$ where $A(x;1) = (x^2+1)P(x) + (x^N-1)R(x)$, as in Lemma 1. But since $(x-1)^2$ contains a constant term, if $A(x;1)$ is a conventional polynomial, then $A(x;1)/(x-1)^2$ must also be a conventional polynomial. Thus, all reachable configurations represented by the generating function $A(x;1)$ have the form

$$A(x;1) = (x-1)^2 Q(x), \quad (5.37)$$

for some polynomial $Q(x)$. Since we know that the predecessor of this configuration is $xQ(x)$, any configuration of this form is therefore trivially reachable. Since $\deg(A(x)) < N$, $\deg(Q(x)) < N-2$. We conclude that there are exactly 2^{N-2} reachable configurations, or $1/4$ of all 2^N possible configurations.

Consider now the case when N is odd. Appealing to Lemma 1, the proof reduces to showing that all configurations containing an even number of nonzero sites have predecessors. Observing that any configuration with an even number of nonzero sites can always be written in the form $(x+1)S(x)$, we also have that

$$\begin{aligned} A(x;1) &= (x+1)S(x), \\ &\equiv (x+x^{-1})(x^2+x^4+\cdots+x^{N-1})S(x) \pmod{(x^N-1)}, \\ &\equiv \mathcal{T}(x)(x^2+x^4+\cdots+x^{N-1})S(x) \pmod{(x^N-1)}, \end{aligned} \quad (5.38)$$

which gives an explicit predecessor to $A(x;1)$. ■

In order to characterize some of the properties and density of cycles, we need two technical results:

Lemma 2 *The lengths of all cycles in a size N CA evolving according to rule **R90** must divide the length Π_N of the cycle obtained with an initial configuration containing a single nonzero site.*

Lemma 3 *For a size N CA evolving according to rule **R90**, $\Pi_N = 1$ if $N = 2^j$ (for some j) and $\Pi_N = 2\Pi_{N/2}$ if N is even but not of the form $N = 2^j$.*

Lemma 2 follows immediately from the additivity of rule **R90**, since any configuration is a superposition of configurations emerging from the initial states with a single nonzero site. The proof of Lemma 3 is left as an exercise for the reader. Note, however, that the first part of Lemma 3 shows that when $N = 2^j$ all configurations must eventually evolve to a fixed point consisting of all zero sites, since

$$(x+x^{-1})^{2^j} \cdot 1 \equiv (x^{2^j} + x^{-2^j}) \equiv (x^N + x^{-N}) \equiv 0 \pmod{(x^N-1)}. \quad (5.39)$$

Lemmas 1 and 2 allow us to characterize cycle lengths for all even-sized systems. The following result effectively determines the cyclic structure for the case when N is odd.

[†]It is generally true that over the finite field of size p , where p is some prime, $x^N-1 = (x^n-1)^{D_p(N)}$, where $n = N/D_p(N)$ and $D_p(N)$ is the maximum power of p that divides N .

Theorem 2 For a CA of size $N = 2m + 1$ and evolving according to rule **R90**,

$$\Pi_N | \Pi_N^* = 2^{\text{sord}_N(2)} - 1, \quad (5.40)$$

where $\text{sord}_N(2)$ is the multiplicative suborder function, defined as the least integer ' j ' such that $2^j = \pm 1 \pmod N$.

Proof: Lemma 1 shows that no initial configuration containing a single nonzero site can be reached at any time $t > 0$. Letting $A(x; 0)$ be such an initial state, we have that

$$A(x; 1) = (x + x^{-1})A(x; 0) \pmod{(x^N - 1)}, \quad (5.41)$$

which is a configuration that occurs again after exactly $2^{\text{sord}_N(2)} - 1$ time steps, since

$$\begin{aligned} \mathcal{T}(x)^{2^{\text{sord}_N(2)}} \cdot 1 &\equiv (x + x^{-1})^{2^{\text{sord}_N(2)}} \equiv (x^{2^{\text{sord}_N(2)}} + x^{-2^{\text{sord}_N(2)}}) \\ &\equiv (x^{\pm 1} + \mp 1) \equiv (x + x^{-1}) \pmod{(x^N - 1)}. \blacksquare \end{aligned} \quad (5.42)$$

Using Lemmas 1 and 2 and Theorem 2 we can easily compute Π_N for, say, $N = 3$ to 20: $\Pi_N = 1, 1, 3, 2, 7, 1, 7, 6, 31, 4, 63, 14, 15, 1, 15, 14, 511, 12$. The random-like behavior of Π_N as a function of N is a consequence of the dependence of Π_N on the number theoretic properties of N . Similar reasoning to that above allows us to determine the number and length of the distinct cycles of rule **R90**:

Lemma 4 If N is a multiple of 3, there are exactly four distinct fixed points (i.e. cycles of length one); otherwise, only the null configuration is a fixed point.

5.2.1.1 Topology of the State Transition Graph

The following lemma shows that the tree structure of the state transition graph $\mathcal{G}$ is very regular. Notice, in particular, that since the proof makes no assumption on the form of $\mathcal{T}$, the result is generally valid for all additive rules.

Lemma 5 The trees rooted on each node of all cycles of $\mathcal{G}$ are identical.

Proof: We prove this statement by showing that all trees rooted on cycles are equal to the tree rooted on the null configuration. Let $A(x)$ represent the configuration that evolves into the null state after exactly t iterations; i.e. $[\mathcal{T}(x)]^t A(x) \equiv 0 \pmod{(x^N - 1)}$. Let $R(x)$ and $R^{(-t)}(x)$ be two states on the same cycle so that $[\mathcal{T}(x)]^t R^{(-1)}(x) \equiv R(x) \pmod{(x^N - 1)}$. Now define

$$\Psi[A(x), R^{(-t)}(x)] = A(x) + R^{(-1)}(x), \quad (5.43)$$

and note that

$$\begin{aligned} [\mathcal{T}(x)]^t \Psi[A(x), R^{(-t)}(x)] &= [\mathcal{T}(x)]^t A(x) + [\mathcal{T}(x)]^t R^{(-1)}(x) \\ &\equiv R(x) \pmod{(x^N - 1)}. \end{aligned} \quad (5.44)$$

This says that all configurations $\Psi[A(x), R^{(-t)}(x)]$ evolve to the state $R(x)$ after t time steps. It is also easy to show that all of these configurations must lie on the tree rooted at $R(x)$ (assume that the evolution reaches another cycle at some time $s < t$ and arrive at a contradiction). Thus, as $A(x)$ ranges over all configurations in the tree rooted on the null configuration, $\Psi[A(x), R^{(-t)}(x)]$ ranges over all configurations on the tree rooted at $R(x)$. That Ψ also preserves the time evolution structure of the trees follows trivially from the definition of Ψ : i.e. if $\mathcal{T}(x)A(x; 0) = A(x; 1)$ then

$$\mathcal{T}(x)\Psi[A(x; 0), R^{(-t)}(x)] = \Psi[A(x; 1), R^{(-t)}(x)]. \quad (5.45)$$

Since Ψ is therefore an isomorphism, we have proven that any tree rooted on a cyclic state is identical to the tree rooted on the null configuration. ■

Suppose N is odd. Under rule **R90**, the predecessor state to the null state is the state consisting of all 1's: $\Sigma_0^{(-1)} = (1, 1, \dots, 1, 1) \rightarrow \Sigma_0 = \vec{0}$. Lemma 1 assures us that $\Sigma_0^{(-1)}$ can itself have no predecessors; i.e. we have shown that, under rule **R90**, each node of each cycle on $\mathcal{G}$ is the root of a tree consisting of a single arc.

Define a *balanced tree* as any tree such that all of its leaves are located at the same distance from its root. Let the *height* of a tree equal the maximum number of arcs that are traversed while descending from any leaf or terminal node to the root of the tree. Let $D_2(N)$ be the maximum 2^j dividing N . We state the following theorem for rule **R90** for the case when N is even without proof (see [martin84]):

Theorem 3 *Each node on each cycle of $\mathcal{G}$ is the root of a balanced tree of height $D_2(N)/2$; except for their roots (which have in-degree three), the non-terminal nodes of all trees have in-degree four.*

5.2.1.2 Cycle Length Distribution

The previous discussion has shown us how to calculate the total number of possible cyclic states. We also know, from Lemma 2, that all cycle lengths must divide the maximal cycle length $\prod_N$. To obtain the exact number of distinct cycles and their lengths takes a little bit more work. If $\prod_N$ is prime, we know that the only possible cyclic lengths are 1 and $\prod_N$. It can then be shown that only the null configuration is a fixed point unless N is some multiple of 3, in which case there are exactly four distinct cycles of length one. If $\prod_N$ is not prime, there can exist as many cycles as there are divisors of $\prod_N$. Although there is no currently known closed form expressions for either the lengths or multiplicities of these cycles, Martin, *et.al.* [martin84] do give a relatively straightforward algorithm for their determination. Before outlining their scheme, we pause briefly to digest a few necessary facts and theorems from basic number theory.

Some Number Theory Definitions: Let $\mathcal{F}$ be a field. We recall that any subset $\mathcal{K} \subset \mathcal{F}$ that is itself a field under the operations of $\mathcal{F}$ is a subfield of $\mathcal{F}$. Relative to this subfield, $\mathcal{F}$ is called an *extension field* of $\mathcal{K}$. Now let $f \in K[x]$ be some polynomial of positive

degree. Then f 'splits' in $\mathcal{F}$ if f can be written as a product of linear factors in $F[x]$ (the extension-field of $\mathcal{K}$): i.e. if $f(x) \sim \prod (1 - \alpha_i)$. $\mathcal{F}$ is called the *splitting field* of f over $\mathcal{K}$ if f splits in $\mathcal{F}$; the splitting field of f over $\mathcal{K}$ is thus effectively the smallest field that contains all of the roots of f .

The splitting field of $x^n - 1$ (n a positive integer) over $\mathcal{K}$ is the n^{th} Cyclotomic field over $\mathcal{K}$, denoted by $\mathcal{K}^{(n)}$. The roots of $x^n - 1$ in $\mathcal{K}^{(n)}$ are the n^{th} roots of unity over $\mathcal{K}$.

The n^{th} *Cyclotomic Polynomial* over a field $\mathcal{F}$ of characteristic p is defined by

$$\mathcal{Q}_n(x) = \prod_{\substack{d=1 \\ \gcd(d,n)=1}}^n (x - \zeta^d), \quad (5.46)$$

where n is a positive integer not divisible by p , ζ is the n^{th} primitive root of unity over $\mathcal{F}$, and the coefficients all belong to n^{th} Cyclotomic field over $\mathcal{K}$. $\mathcal{Q}(x)$ is independent of the choice of ζ . The degree of $\mathcal{Q}_n(x)$ is given by the *Moebius Function*, $\mu(n)$, defined by

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1, \\ (-1)^k & \text{if } n \text{ is the product of } k \text{ distinct primes,} \\ -1 & \text{if } n \text{ is divisible by the square of a prime.} \end{cases} \quad (5.47)$$

We state the following basic theorems without proof.[†]

(i) If $\mathcal{K}$ is a field of characteristic p and n a positive integer not divisible by p , then

$$x^n - 1 = \prod_{d|n} \mathcal{Q}_d(x) = (x - 1) \prod_{\substack{d|n \\ d \neq 1}} \prod_{i=1}^{\phi(d)} \mathcal{Q}_{d,i}(x), \quad (5.48)$$

where $\phi(d)$ is the *Euler Totient function*, defined as the number of integers less than d which are relatively prime to d , and $\text{ord}_d(p)$ is the *multiplicative order function*, and is defined as the minimum positive integer ' j ' such that $p^j \equiv 1 \pmod{d}$.

(ii) If d is a divisor of positive integer n with $1 \leq d \leq n$, then $\mathcal{Q}_n(x)$ divides $(x^n - 1)/(x^d - 1)$ wherever $\mathcal{Q}_n(x)$ is defined.

(iii) If $\mathcal{K}$ is a field of characteristic p and n a positive integer not divisible by p , the n^{th} Cyclotomic polynomial $\mathcal{Q}_n$ over $\mathcal{K}$ satisfies

$$\mathcal{Q}_n = \prod_{d|n} (x^d - 1)^{\mu(n/d)} = \prod_{d|n} (x^{n/d} - 1)^{\mu(d)}, \quad (5.49)$$

where $\mu(x)$ is the Moebius function defined above.

Cycle Lengths. Suppose we want to find the possible cycle lengths for a size N system. Theorem 2 shows that any configuration $A(x)$ on a cycle may be written in the form $A(x) = (1 + x)^{D_2(N)} B(x)$, where $B(x)$ is some polynomial and (we recall)

[†]The reader may wish to consult a standard text on finite fields. One of the best texts is the *Introduction to Finite Fields and Their Applications* by Lidl and Niederreiter [lid86].

$D_2(N)$ is defined as the largest value of 2^j that divides N . The cycle length must then be the minimum power π such that

$$(x + x^{-1})^\pi B(x) \equiv B(x) \pmod{\left(\frac{x^n - 1}{x + 1}\right)^{D_2(N)}}, \quad (5.50)$$

where $n = N/D_2(N)$ and $(x^n - 1)^{D_2(N)} = x^N - 1$. Using the factorization given in equation 5.48, we have that

$$x^n - 1 = (x - 1) \prod_{\substack{d|n \\ d \neq 1}} \prod_{i=1}^{\frac{\phi(d)}{\text{ord}_d(2)}} Q_{d,i}(x), \quad (5.51)$$

where $Q_{d,i}$ is the i^{th} irreducible cyclotomic polynomial over $\mathcal{F}_2$ of order $\text{ord}_d(2)$, we can rewrite equation 5.50 as

$$(x + x^{-1})^\pi B(x) \equiv B(x) \pmod{Q_{d,i}(x)^{D_2(N)}}, \quad (5.52)$$

for all $d | n$, $d \neq 1$ and for all i such that $1 \leq i \leq \phi(d)/\text{ord}_d(2)$. The length of the cycle on which $A(x)$ occurs, $L[\mathcal{C}_{A(x)}]$ is then given by the least common multiple of the smallest values of π for all possible d and i , $\text{lcm}(\{\pi_{d,i}[B(x)]\})$, where $\pi_{d,i}[B(x)]$ is the smallest value of π for which equation 5.52 is true for given ' d ' and ' i '.

Now, it is clear from equation 5.52, that (1) if $Q_{d,i}(x)^{D_2(N)}$ divides $B(x)$, then $\pi_{d,i}[B(x)] = 1$; (2) if $r_{d,i}[B(x)]$ is the largest power of $Q_{d,i}(x)$ that divides $B(x)$, where $0 \leq r_{d,i}[B(x)] \leq D_2(N)$, then equation 5.52 may be rewritten as

$$(x + x^{-1})^\pi \equiv 1 \pmod{Q_{d,i}(x)^{D_2(N) - r_{d,i}[B(x)]}}. \quad (5.53)$$

In this case we see that the value for $\pi_{d,i}$ will be the same for all configurations with $r_{d,i} = s$; let us call this value $\pi_{d,i,s}$, where $0 \leq s \leq D_2(N)$.

We have at least one other helpful hint. Notice that $Q_{d,i}(x)$ must divide $(x^d - 1)/(x + 1)$ ($d \neq 1$), it must be true that $\pi_{d,i,1}$ divides the minimum value of π for which $(x + x^{-1})^\pi \equiv 1 \pmod{(x^d - 1)/(x + 1)}$. Recognizing that this is exactly the same relation as the one we used to prove theorem 2, we conclude that $\pi_{d,i,1}$ must divide $2^{\text{sord}_d(2)} - 1$.

To summarize, we must perform the following two basic computations to find the lengths of all possible cycle lengths for a system of size N :

Step 1: Use equation 5.51 to factorize $x^N - 1 = x^N + 1 \pmod{2}$ into a product of irreducible cyclotomic polynomials over $\mathcal{F}_2$. For example, for $N = 30$, we would find that

$$x^{30} + 1 = Q_{1,1}(x)^2 Q_{3,1}(x)^2 Q_{5,1}(x)^2 Q_{15,1}(x)^2 Q_{15,2}(x)^2, \quad (5.54)$$

where

$$\begin{cases} Q_{1,1}(x) = x + 1, \\ Q_{3,1}(x) = x^2 + x + 1, \\ Q_{5,1}(x) = x^4 + x^3 + x^2 + x + 1, \\ Q_{15,1}(x) = x^4 + x + 1, \\ Q_{15,2}(x) = x^4 + x^3 + 1. \end{cases} \quad (5.55)$$

Step 2: Find the values of $\pi_{d,i,s}$ for all $0 \leq s \leq D_2(N)$. In the case that $N = 30$ we find that

$$\begin{cases} \pi_{3,1,0} = 2 & \pi_{3,1,1} = 1 & \pi_{3,1,2} = 1, \\ \pi_{5,1,0} = 6 & \pi_{5,1,1} = 3 & \pi_{5,1,2} = 1, \\ \pi_{15,1,0} = 30 & \pi_{15,1,1} = 15 & \pi_{15,1,2} = 1, \\ \pi_{15,2,0} = 30 & \pi_{15,2,1} = 15 & \pi_{15,2,2} = 1. \end{cases} \quad (5.56)$$

We thus find that the only cycles that can occur for $N = 30$ have lengths of 1, 2, 3, 6, 15 and 30.

Number of Distinct Cycles of Given Length. The number of distinct cycles of a given length, $\mathcal{N}[\mathcal{L}]$, is found by finding the number of polynomials $B(x)$ for each possible set of values of $r_{d,i}[B(x)]$. This number is given by [martin84]

$$\mathcal{N}[\mathcal{L}] = \prod_{\substack{d|N \\ d \neq 1}} \prod_i f(r_{d,i}, d, D_2(N)), \quad (5.57)$$

where

$$f(r, d, D_2(N)) = 2^{\text{ord}_d(2)(D_2(N)-r)} - 2^{\text{ord}_d(2)(D_2(N)-r-1)}, \quad 0 \leq r < D_2(N). \quad (5.58)$$

5.2.2 CA over $\mathcal{F}_p$, p Prime

Most of the theorems and lemmas of the previous section have an easily proven counterpart for the case of an arbitrary additive rule, represented by dipolynomial $\mathcal{T}(x)$, acting on states $\sigma \in \{0, 1, \dots, p-1\}$, where p is prime. Since the proof of Lemma 2 of the previous section, for example, depended only on the *additivity* property, it carries over exactly:

Lemma 2' *The lengths of all cycles in any size N additive CA over $\mathcal{F}_p$ must divide the length $\prod_N$ of the cycle obtained with an initial configuration containing a single nonzero site.*

Lemma 3 of the previous section, on the other hand, generalizes only slightly to read:

Lemma 3' For a size N additive CA, $\prod_N \mid p \prod_{N|p}$ if N is a multiple of p and $\prod_N = p \prod_{N|p}$ if N is a multiple of P but not a power of p (and $\mathcal{T}(x) = (x + x^{-1})$).

Let $\Lambda_1(x) \equiv \gcd(x^N - 1, \mathcal{T}(x))^\dagger$ and suppose that the dipolynomial $A(x)$ represents a reachable configuration. If $A(x)$ can be reached, then it must be that $A(x) \equiv \mathcal{T}(x)A^{(-1)}(x) \bmod (x^N - 1)$, for some $A^{(-1)}(x)$. Since $\Lambda_1(x) \mid (x^N - 1)$ and $\Lambda_1(x) \mid \mathcal{T}(x)$, Λ_1 must also divide $A^{(-1)}(x)$. On the other hand, we now show that all configurations $A^{(-1)}(x)$ divisible by $\Lambda_1(x)$ must have predecessors: by definition, $\Lambda_1(x)$ can be expressed as

$$\Lambda_1(x) = \alpha(x)\mathcal{T}(x) + \beta(x)(x^N - 1), \quad (5.59)$$

where $\alpha(x)$ and $\beta(x)$ are dipolynomials; i.e.

$$\Lambda_1(x) \equiv \alpha(x)\mathcal{T}(x) \bmod (x^N - 1). \quad (5.60)$$

We then see that the dipolynomial $A(x) = \Lambda_1(x)B(x)$ provides an explicit predecessor to $A(x)$, since

$$\mathcal{T}(x)\alpha(x)B(x) \equiv \Lambda_1(x)B(x) \equiv A(x) \bmod (x^N - 1). \quad (5.61)$$

We can go through similar arguments for states reachable in more than one step to obtain the general result that a configuration $A(x)$ is reachable in n steps if and only if $\gcd(x^N - 1, \mathcal{T}^n(x))$.

Let $D_p(N)$ be the maximum p^j dividing N . Let m_i be the multiplicity of the i^{th} irreducible factor of $\Lambda_1(x)$ in $\tilde{\mathcal{T}}(x)$, where $\tilde{\mathcal{T}}(x) = x^s \mathcal{T}(x)$ is a polynomial with a nonzero constant term. Finally, define $\chi = \min_i \{m_i\}$, so that $0 \leq \chi \leq D_p(N)$. Using these definitions, Martin, et.al. [martin84] prove the following basic theorem:

Theorem 4 The state transition diagram for an additive CA of size N over $\mathcal{F}_p$ has the following properties: (1) a set of identical $p^{\deg(\Lambda_1(x))}$ -ary trees are rooted at each node of each cycle; (2) a fraction $f_C = p^{-D_p(N) \deg(\Lambda_1(x))}$ of the possible configurations are cyclic states; (3) for $\chi > 0$, the height of the tree is given by $\lceil D_p(N)/\chi \rceil$; (4) the trees are all balanced if and only if (a) $m_i \geq D_p(N)$ for all i , or (b) $m_i = m_j$ for all i and j , and $m_i \mid D_p(N)$.

The proof for the first parts of this theorem is straightforward. Suppose that we have some configuration $A(x)$ with two predecessor states $B_1(x)$ and $B_2(x)$; i.e. $\mathcal{T}(x)A(x) \equiv B_i(x) \bmod (x^N - 1)$, $i = 1, 2$. Then, since $\Lambda_1(x)$ divides $x^N - 1$, it follows that $B_1(x) - B_2(x) \equiv 0 \bmod ((x^N - 1)/\Lambda_1(x))$. The number of solutions to this congruence – that is, the number of predecessor states $B_i(x)$ to $A(x)$ – is given by $p^{\deg(\Lambda_1(x))}$. Now, consider the state $C(x)$ that evolves to the null configuration in n steps. By definition, we must have that $\mathcal{T}^n C(x) \equiv 0 \bmod (x^N - 1)$, so that $(x^N - 1)/\Lambda_n(x)$ divides $C(x)$, where $\Lambda_n(x) \equiv \gcd(x^N - 1, \mathcal{T}^n(x))$. Therefore, defining

[†]The greatest common divisor of two dipolynomials $D_1(x)$ and $D_2(x)$ is defined as $\gcd(x^{s_1} D_1(x), x^{s_2} D_2(x))$, where s_1 and s_2 are chosen such that $x^{s_1} D_1(x)$ and $x^{s_2} D_2(x)$, respectively, become ordinary polynomials with a nonzero constant term.

$\Lambda_\infty \equiv \lim_{n \rightarrow \infty} \Lambda_n(x)$, all states on trees must be divisible by $(x^N - 1)/\Lambda_\infty(x)$. But the configuration $(x^N - 1)/\Lambda_\infty(x)$ evolves to the null state in exactly $\lceil D_p(N)/\chi \rceil$ steps; i.e. the height of all trees must be given by $\lceil D_p(N)/\chi \rceil$. We leave the remaining steps of the proof of the theorem as an exercise to the reader.

5.3 Local Structure Theory

We have already seen ample evidence for what is arguably the single most impressive general property of CA, namely their capacity for self-organization. Starting from completely random initial configurations, CA evolution typically builds up correlations between separated site values. Moreover, the characteristic statistical features describing the emerging correlated spatial patterns do not depend on the details of the initial state, but depend only on the particular rule and type of lattice. Although a variety of different correlation measures used to gauge the degree of self-organization in a given system have already been introduced, a tool that has heretofore been conspicuously lacking is a strictly analytical approach to predicting or estimating many of these same measures. A powerful and elegant analytical tool of this type is provided by the *local structure theory* (LST), developed by Gutowitz, et. al. ([guto87a],[guto87b],[guto89]) .

The LST is a finitely parameterized model of the action of a given CA rule, Φ , on probability measures on the space of configurations on an arbitrary lattice. In a very simple manner – which may be thought of as a generalization of the simple *mean field theory* (MFT) introduced in section 3.1.3. – the LST provides a sequence of approximations of the statistical features of evolving CA patterns.

We recall that the MFT assumes that Φ does not induce any correlation between separated sites: if all of the sites are mutually uncorrelated at $t = 0$, MFT assumes that they remain uncorrelated at all later times $t > 0$. A virtue of this approach is that it permits an easy derivation of the limiting value density, $\rho_{t \rightarrow \infty}$. Because the underlying assumption is generally not valid, however, we should hardly be surprised to learn that the limiting densities obtained for most of the interesting (i.e. nonlinear) rules differ significantly from those obtained by Monte Carlo simulations of those same rules.

The LST, on the other hand, explicitly takes into account all correlations (up to an arbitrary N^{th} order) that arise between different cells on a given lattice, by considering the probabilities of local blocks of N sites. For one dimensional lattices, for example, it is simply formulated as a set of recursive equations expressing the time evolution of the probabilities of blocks of length N (to be defined below). As the order of the LST increases, so does the accuracy with which the LST is able to predict the statistical behavior of a given rule.

There are two additional points of interest concerning the LST:

Behavioral Classification: We will shortly see that many rules may in fact give rise to the same set of recursive equations of a given order. This suggests that the LST provides an alternative behavioral classification scheme to the four (thus far

largely phenomenological) classes, **c1-c4**, introduced by Wolfram.

Complexity Engineering: Specific applications of CA to physical problems typically involve enormous efforts spent on obtaining just the right set of rules appropriate for a given problem. By succinctly summarizing the statistical behavior of a well-defined class of rules for a variety of lattice structures, the LST equations may be used to effectively *guide* searches for particular rules displaying the set of desired statistical behaviors.

We will have more to say about both of these two possibilities later. In the remaining paragraphs of this section, we introduce (and remind ourselves of) some basic terminology, outline the LST for one dimensional systems and provide a few simple examples of its use. The section concludes with a brief discussion of some subtleties needed to define a LST for systems with dimension $d > 1$.

5.3.1 Blocks, Measures and Bayesian Extensions

We restrict our attention for the moment to elementary one-dimensional systems, so that each cell of the lattice is indexed by an integer $i \in \mathcal{Z}$ and takes on one of two possible values, $\sigma_i \in \Sigma \equiv \{0, 1\}$. We recall from section 2.2.1 that the collection of all configurations, or the CA *phase space*, $\Gamma \equiv \Sigma^{\mathcal{Z}}$, is a compact metric space under the metric

$$\partial(\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}) = \sum_{i=-\infty}^{\infty} 2^{-|i|} |\vec{\sigma}^{(1)} - \vec{\sigma}^{(2)}|, \quad \vec{\sigma}^{(1)}, \vec{\sigma}^{(2)} \in \Gamma. \quad (5.62)$$

Open sets ‘ $\mathcal{O}$ ’ in the topology imposed by this metric, are defined as unions of *N-cylinders*: $\mathcal{O} \equiv \bigcup_i c_i^{(N)}$, where $c_i^{(N)} \equiv \{\vec{\sigma} \in \Gamma \mid \vec{\sigma}_i = c_i, \dots, \vec{\sigma}_{i+N-1} = c_{i+N-1}\}$. Cylinders thus specify configurations with prescribed values at a finite number of cells.

Each *N-cylinder* may be put into a one-to-one correspondence with an *N-block*, B_N : given B_N , the corresponding cylinder set is defined by $c_i(B_N) \equiv \{\vec{\sigma} \in \Gamma \mid \sigma_i = b_1, \sigma_{i+1} = b_2, \dots, \sigma_{i+N-1} = b_N\}$. B_N are thus simply explicit lists of a specified finite sequence of contiguous sites. The *size* of B_N will be written as $|B_N| = N$. Denoting the state of the i^{th} cell in B_N by $(B_N)_i$, we recall that the action of the *shift operator*, γ , is given by $(\gamma B_N)_i = (B_N)_{i+1}$. The symbol $\mathbf{B}_N$ will denote the collection of all blocks (or cylinders) of size N .

Left ($\mathcal{L}$) and right ($\mathcal{R}$) *truncation operators* map *N-blocks* to $(N-1)$ -blocks by truncation from the left and right, respectively: if $B_N = (b_1, b_2, \dots, b_N)$ then $\mathcal{L}B_N = (b_2, b_3, \dots, b_N)$ and $\mathcal{R}B_N = (b_1, b_2, \dots, b_{N-1})$. When applied to B_1 , both $\mathcal{L}$ and $\mathcal{R}$ yield the null block.

A CA rule ϕ of radius r maps $\mathbf{B}_{(2r+1)}$ into $\mathbf{B}_1$, and is extended to a map $\mathbf{B}_{(2r+n)} \rightarrow \mathbf{B}_n$, for arbitrary n , by the shift operator, γ . Thus, by infinite extension, the shift-commuting dynamical map $\Phi : \Gamma \rightarrow \Gamma$ is defined by

$$[\Phi(\vec{\sigma})]_i = \phi(\sigma_{i-r}, \sigma_{i-r+1}, \dots, \sigma_{i+r-1}, \sigma_{i+r}). \quad (5.63)$$

CA Action on Probability Measures: To facilitate the mathematical description of the general action of Φ on Γ , we introduce a *probability measure* μ on Γ . The action of Φ on block-subsets of Γ induces an action on measures on Γ of the following form [guto87a]:

$$(\Phi\mu)(c(B_N)) = \mu(\Phi^{-1}(c(B_N))), \quad (5.64)$$

where $c(B_N)$ is the cylinder corresponding to block B_N of size N . Expressed in words, this equation states that the probability of B_N under $(\Phi\mu)$ is the sum of the probabilities under μ of all of the pre-images of B_N under Φ . Because Φ is a local map, we know that the inverse image of B_N will typically consist of a finite collection of larger blocks B_M , where $M \geq N$.

We will, in particular, be interested in the *invariant* (or *limit*) *measure*, $\mu_\infty(\Phi)$, of Φ , defined as

$$\mu_\infty(\Phi) \equiv \lim_{t \rightarrow \infty} [\Phi]^t \mu. \quad (5.65)$$

Since CA are shift invariant, we need only consider probability measures that are themselves shift invariant: *i.e.* μ such that $\mu(\gamma E) = \mu(E)$, for all measurable subsets E of Γ . We can therefore use the probabilities of finite blocks to rewrite equation 5.64 for a range- r CA rule as the following infinite set of equations:

$$P^{(t+1)}(B) = \sum_{B' \mid |B'|=|B|+2r} \delta(\Phi(B'), B) P^{(t)}(B'), \quad (5.66)$$

where $P^{(t)}(B)$ is the probability of block B at time ' t ', and

$$\delta(\Phi(B'), B) = \begin{cases} 1 & \text{if } \Phi(B') = B, \\ 0 & \text{else.} \end{cases} \quad (5.67)$$

Equation 5.66 shows that if we are given the probabilities of all blocks of length $|B| + 2r$ at time ' t ', then we can directly obtain the probabilities of all blocks of length $|B|$ at time ' $t + 1$ '. Since the size of blocks for which probabilities must be initially known in order to determine the probability of a block of given length at time ' t ' grows with ' t ', the *exact* determination of the probabilities of blocks of a given length for large times can obviously pose a formidable challenge.

The LST alleviates this problem by systematically approximating the probabilities of B_M , with $M > N$, from the set of probabilities of smaller blocks, $B_1, B_2, \dots, B_N$. In this way, N^{th} order correlation information is used to predict the statistical properties of evolving patterns for arbitrarily large times. The outline of the approach begins with a formal definition of block probability functions.

Block Probability Functions: We define the *block probability function of order- N* , P_N , to be a map from $\{B_N, B_{N-1}, \dots, B_0\}$ into the reals that satisfies the

following four *Kolmogorov consistency conditions* [guto87a]:

$$\left\{ \begin{array}{ll} \text{I:} & P_N(B_j) \geq 0 \quad \text{for } j = 0, 1, \dots, N, \\ \text{II:} & \sum_{B \in B_j} P_N(B) = 1 \quad \text{for } j = 0, 1, \dots, N, \\ \text{III:} & P_N(B'_j) = \sum_{B_{j+1} | \mathcal{R}B_{j+1}=B'_j} P_N(B_{j+1}) \quad \text{for } j = 0, 1, \dots, N-1, \\ \text{IV:} & P_N(B'_j) = \sum_{B_{j+1} | \mathcal{L}B_{j+1}=B'_j} P_N(B_{j+1}) \quad \text{for } j = 0, 1, \dots, N-1, \end{array} \right. \quad (5.68)$$

where, in conditions III and IV, the sums are over all blocks B such that either $\mathcal{R}B = B'$ or $\mathcal{L}B = B'$, respectively. Together, these conditions assure that (a) P_N is non-negative for all blocks within its domain (condition I), (b) P_N is a probability function for each set of blocks of fixed size (condition II), and (c) that the probability of a given block within the domain of P_N is the sum of the probabilities of the blocks containing the given block at a particular position (*self-consistency* conditions III and IV).

The set of all block probability functions of order- N is denoted by $\mathbf{P}_N$. If two block probability functions, P_N and P_M , with $M > N$, are self-consistent and are equal on blocks of size $s \leq N$, they are said to be *mutually consistent*.

The Kolmogorov consistency theorem [guto88] asserts that *any set of self- and mutually-consistent probability functions* $\{P_j\}$, $j = 1, 2, \dots, N$ may be extended to a unique shift-invariant measure on Γ .

Below, we will define a canonical procedure for constructing probabilities of blocks of arbitrary lengths consistent with a given block probability function P_N . The Kolmogorov consistency theorem will then allow us to use this set of *finite* block probabilities to define a measure on the set of *infinite* configurations, Γ .

Bayesian Extension of Finite Block Probabilities: Given a block probability function P_N , the *Bayesian extension process* [guto87a] generates the set of block probabilities $\{P_j\}$, $j > N$ that are consistent with P_N . This is done recursively two steps: (1) the ‘best-possible’ $(N+1)$ -block probability is constructed from the given set of N -block probabilities by using a general operator mapping N -block to $(N+1)$ -block probabilities, and (2) the set $\{P_j\}$ for $j > N+1$ is generated by repeated application of this operator to successively defined sets of lower order block probabilities.

Consider the first step. We are looking for an operator $\pi_{N \rightarrow N+1}$ that will map P_N into P_{N+1} , and require that $(\pi_{N \rightarrow N+1} P_N)(B_j) = P_N(B_j)$ for $j \leq N$. A heuristic derivation of such an operator proceeds as follows [guto87b]: assume that the length s of some block B_s is much longer than the correlation length of the spatial CA pattern. Then the conditional probability of finding either $B_s^R = B_s \sigma = (b_1, b_2, \dots, b_s, \sigma)$ or $B_s^L = \sigma B_s = (\sigma, b_1, b_2, \dots, b_s)$ should be approximately independent of the state of either the left-hand-most or right-hand-most sites of B_s , respectively. The first case, for example, implies that the following

condition is satisfied:

$$\frac{P(B_s^R)}{P(B_s)} = \frac{P(\mathcal{L}B_s^R)}{P(\mathcal{L}B_s)}, \quad (5.69)$$

where P is a block probability function. Letting $B_s^R \equiv B$, and noting that $B_s = \mathcal{R}B_s^R$ we solve for $P(B) = P(B_s^R)$ to obtain:

$$P(B) = \frac{P(\mathcal{L}B) \cdot P(\mathcal{R}B)}{P(\mathcal{L}\mathcal{R}B)}. \quad (5.70)$$

Notice that the truncation operators $\mathcal{R}$ and $\mathcal{L}$ appear in a symmetric fashion. We could have anticipated this, of course, since it should not matter whether an additional site is appended to the *left* or the *right* of B_s . More importantly, however, notice that the block B is of size $(s+1)$, so that the relation is already of the form of a map from s -block probabilities to $(s+1)$ -block probabilities. In order to use this to define the operator $\pi_{N \rightarrow N+1}$ we make the additional assumption that the form of the relation is valid for *all* block sizes $j \leq s$. We make two further observations: (1) if $P(\mathcal{L}\mathcal{R}B) = 0$, then the probability of any block $B' \supset B$ should also equal zero, and (2) the $(N+1)$ -block probability function should be identical to the N -block probability function for all blocks of size $j \leq N$. These observations suffice to define the operator $\pi_{N \rightarrow N+1}$:

$$[\pi_{N \rightarrow N+1} P_N] B \equiv \begin{cases} \frac{P_N(\mathcal{R}B) P_N(\mathcal{L}B)}{P_N(\mathcal{L}\mathcal{R}B)} & \text{if } |B| = N+1 \text{ and } P_N(\mathcal{L}\mathcal{R}B) > 0, \\ 0 & \text{if } |B| = N+1 \text{ and } P_N(\mathcal{L}\mathcal{R}B) = 0, \\ P_N(B) & \text{if } |B| \leq N. \end{cases} \quad (5.71)$$

It is an easy exercise to show that if P_N satisfies the Kolmogorov consistency conditions (equations 5.68) for all blocks B_j of size $j \leq N$, then $(\pi_{N \rightarrow N+1} P_N)$ satisfies the Kolmogorov consistency conditions for blocks B_j of size $j \leq N+1$. Given a block probability function P_N , therefore, we can generate a set of block probability functions $\{P_j\}$ for arbitrary $j > N$ by successive applications of the operator $\pi_{N \rightarrow N+1}$; this set is called the *Bayesian extension* of P_N .

The Local Structure Operator: By the Kolmogorov consistency theorem, we can use the Bayesian extension of P_N to define a measure on Γ . This measure – called the *finite-block measure*, μ_N , where N denotes the order of the block probability function from which it is derived by Bayesian extension – is defined by assigning to each cylinder $c(B_j) \equiv \{\vec{\sigma} \in \Gamma \mid \sigma_1 = b_1, \sigma_2 = b_2, \dots, \sigma_j = b_j\}$ a value equal to the probability of its associated block:

$$\mu_N(\mathcal{C}(B_j)) \equiv P_j(B_j), \quad j = 1, 2, \dots \quad (5.72)$$

The CA action of rule Φ on measures – $(\Phi\mu)(c(B_N)) = \mu(\Phi^{-1}(c(B_N)))$ – is approximated formally by the *local structure operator* $\Lambda_N(\Phi)$, mapping measures

to finite-block measures:

$$[\Lambda_N(\Phi)]\mu \equiv [S_N\Phi S_N]\mu, \quad (5.73)$$

where S_N (called the *scramble operator*) maps the measure μ to the finite-block measure μ_N that agrees with μ on cylinders corresponding to all blocks whose size is N or less.

The first application of S_N in equation 5.73 generates an order- N finite block measure. This is followed by the CA rule Φ , which induces a general measure. Finally, the second application of S_N truncates the general measure back to an order- N finite-block measure. The net effect is that $\Lambda_N(\Phi)$ maps the set of N -block measures to itself. The fundamental assumption of LST is that $\Lambda_N(\Phi)$ approximates the action of Φ on the measure μ increasingly well as the order N of the underlying finite block measures is increased. Certainly, $\Lambda_N(\Phi) \rightarrow \Phi$ as $N \rightarrow \infty$, since as N increases the scramble operator gets increasingly closer to being the identity map.

Note that, since $S_N\mu_n = \mu_n$ for all finite block measures μ_n with $n \leq N$ and, in particular, $\Phi(\mu_\infty) = \mu_\infty$, we can show that if the invariant measure $\mu_\infty(\Phi)$ of Φ is a finite block measure of order $n \leq N$, then $\mu_\infty(\Phi)$ is also invariant under $\Lambda_N(\Phi)$.

Having thus outlined the formal theoretical structure of one-dimensional LST, we now turn to a more pragmatic discussion of its use and applications.

5.3.2 LST for One-dimensional Lattices

The N^{th} -order LST is defined by the same infinite system of equations appearing in equation 5.66, but with $P_{(n \rightarrow m)}^{(t)}(B) \equiv m^{\text{th}}$ -order Bayesian extended probability of block B at time ' t ', given the set of n -block probabilities at time ' t ' substituted for the general block probability $P^{(t)}(B)$:

$$P^{(t+1)}(B) = \sum_{B' \in \mathbf{B}_{|B|+2r}} \delta((\Phi(B'), B)) P_{(N \rightarrow |B|+2r)}^{(t)}(B'), \quad (5.74)$$

The LST approximation itself resides solely in the determination of $P_{N \rightarrow (|B|+2r)}^{(t)}(B')$; the general combinatorial structure of the CA rule Φ is retained (for blocks of size N or less) by the function $\delta(\Phi(B'), B)$ (defined in equation 5.67).

The general LST algorithm for approximating the temporal evolution of N -block measures using $\Lambda_N(\Phi)$ is therefore as follows:

1. Obtain the length $(N + 2r)$ inverse block images of each possible length N block under the range- r rule Φ .
2. Find the Bayesian extended set of probabilities of each of the inverse $(N + 2r)$ -block images of all possible N -blocks.
3. Calculate the N -block probabilities for the next time step by summing the inverse image block probabilities of the current time step found in step 2.

4. Repeat steps 2 and 3 to generate the LST approximation of the temporal evolution.

As a simple example, consider the N^{th} -order LST equations for range $k = 2$, $r = 1$ CA. Since the inverse image of an N -block is a block of size $(N + 2)$, we need to apply the operator $\pi_{N \rightarrow N+1}$ to P_N twice in succession to define the $(N + 2)$ -block probabilities:

$$\begin{aligned} P_{(N+2)}(B) &= [\pi_{N+1 \rightarrow N+2}(\pi_{N \rightarrow N+1} P_N)](B), \\ &= \frac{\pi_{N \rightarrow N+1} P_N(\mathcal{L}B) \cdot \pi_{N \rightarrow N+1} P_N(\mathcal{R}B)}{\pi_{N \rightarrow N+1} P_N(\mathcal{L}\mathcal{R}B)}, \\ &= \frac{P_N(\mathcal{R}^2 B) \cdot P_N(\mathcal{R}\mathcal{L}B) \cdot P_N(\mathcal{L}^2 B)}{P_N(\mathcal{R}^2 \mathcal{L}B) \cdot P_N(\mathcal{L}^2 \mathcal{R}B)}. \end{aligned} \quad (5.75)$$

The set of recursive N^{th} -order LST equations then appear as follows:

$$P_{(N)}^{(i+1)}(B) = \sum_{B' \in \mathbf{B}_{N+2}} \left\{ \delta(\Phi(B', B)) \cdot \frac{P_N^{(t)}(\mathcal{R}^2 B') \cdot P_N^{(t)}(\mathcal{R}\mathcal{L}B') \cdot P_N^{(t)}(\mathcal{L}^2 B')}{P_N^{(t)}(\mathcal{R}^2 \mathcal{L}B') \cdot P_N^{(t)}(\mathcal{L}^2 \mathcal{R}B')} \right\}. \quad (5.76)$$

Probabilities for blocks B_j with length $j < N$ may be calculated by appealing to the Kolmogorov consistency conditions (equation 5.68). We now examine some low order LST approximations in more detail.

0th-order LST: Although the lowest order LST is trivial in the sense that the approximation involves no dynamics, it is not entirely vacuous. 0th-order block probabilities are independent of time and are simply functions of block-length: $P^{(t)}(B) = 2^{-|B|}$ for all times ' t '. Thus the 0th-order LST equations define the trivial 'evolution' of the probability of 1-blocks, or individual sites, having value $\sigma = 1$: $P^{(t=1)}(B_1 = 1) = P^{(t=2)}(B_1 = 1) = \dots = P^{(t=n)}(B_1 = 1) = \rho_1$, where ρ_1 is just the density of 1's in the configuration. ρ_1 is then formally calculated from

$$\begin{aligned} \rho_1 &= \sum_{B' \in \mathbf{B}_{2r+1}} \frac{\delta(\Phi(B', 1))}{2^{2r+1}}, \\ &= \frac{1}{2^{2r+1}} \cdot \sum_{B' \in \mathbf{B}_{2r+1}} \delta(\Phi(B', 1)), \\ &= \frac{1}{2^{2r+1}} \cdot \lambda^{(0)}(\Phi), \end{aligned} \quad (5.77)$$

where we have introduced the 0th-order LST class coefficient for rule Φ , $\lambda^{(0)}(\Phi)$. It is defined by

$$\lambda^{(0)}(\Phi) \equiv \text{Number of neighborhoods that yield } \sigma = 1 \text{ under } \Phi. \quad (5.78)$$

Thus, despite the absence of any sort of dynamics, the preservation of the 0th-order combinatorial structure of Φ by $\delta(\Phi, B)$ nonetheless allows us to define $2^{2r+1} + 1$

0th-order LST behavioral classes, $C_0^{\text{LST}}(\lambda)$, one for each possible value of $\lambda^{(0)}(\Phi)$:

$$\Phi \in C_0^{\text{LST}}(\lambda) \longleftrightarrow \lambda^{(0)}(\Phi) = \lambda, \quad \lambda = 0, 1, 2, \dots, 2^{2r+1}. \quad (5.79)$$

Since each class, $C_0^{\text{LST}}(\lambda)$, therefore consists of range- r rules Φ such that exactly λ neighborhoods are mapped to '1', we see that the total number of rules in class $C_0^{\text{LST}}(\lambda)$ is $\binom{2^{2r+1}}{\lambda}$.

The 0th-order LST approximation of the invariant measure of Φ is given simply by the fraction of neighborhoods that yield 1 under Φ .

1st-order LST: The 1st-order LST – which is identical to the mean field theory – is a refinement of the 0th-order LST in that it uses the probabilities of states of sites within blocks to estimate the probabilities of those blocks. Consider, for example, the set of LST equations for $r = 1$ given in equation 5.76.

In the present case, we may set $B = 1$ and replace $P_N^{(t)}(B)$ by the density $\rho_1(t)$. Furthermore, with $B_3 \equiv (b_1, b_2, b_3)$, and P now a 1-block measure, the set of block probabilities that are used to calculate the Bayesian extended 3-block probability are reduced to the following:

$$\begin{aligned} P^{(t)}(\mathcal{R}^2 B_3) &= \rho_1(t)b_1 + (1 - \rho_1(t))(1 - b_1), \\ P^{(t)}(\mathcal{L}^2 B_3) &= \rho_1(t)b_3 + (1 - \rho_1(t))(1 - b_3), \\ P^{(t)}(\mathcal{R}\mathcal{L} B_3) &= \rho_1(t)b_2 + (1 - \rho_1(t))(1 - b_2), \end{aligned} \quad (5.80)$$

and, since the probability of the null block is one, $P^{(t)}(\mathcal{R}^2 \mathcal{L} B_3) = P^{(t)}(\mathcal{L}^2 \mathcal{R} B_3) = 1$. Making these substitutions, we find that equation 5.76 simplifies to

$$\rho_1(t+1) = \sum_{B \in \mathbf{B}_3} \delta(\Phi(B), 1) \rho_1(t)^{\#1_B} (1 - \rho_1(t))^{\#0_B} \quad (5.81)$$

where $\#1_B$ and $\#0_B$ are, respectively, the number of 1's and 0's in the block B .

Note that any two blocks with the same number of sites in the state $\sigma = 1$ contribute the same factor to the summation; such blocks are said to be of the same 1st-order block type. We can then put equation 5.81 into a more suggestive form by summing over 1st-order block types:

$$\sum_{i=0}^{2r+1} \lambda_i^{(1)}(\Phi) \rho_1(t)^i (1 - \rho_1(t))^{2r+1-i}, \quad (5.82)$$

where, analogously to the 0th-order case, we have introduced the 1st-order LST class coefficients for rule Φ , $\lambda_i^{(1)}(\Phi)$:

$$\begin{aligned} \lambda_i^{(1)}(\Phi) &= \text{Number of neighborhood blocks} \\ &\quad \text{containing } i \text{ 1's that yield 1 under } \Phi, \quad i = 0, 1, 2, \dots, 2r+1. \end{aligned} \quad (5.83)$$

Since $0 \leq \lambda_i^{(1)}(\Phi) \leq \binom{2r+1}{i}$, these coefficients define a total of $\prod_{i=0}^{2r+1} (\binom{2r+1}{i} + 1)$ possible 1st-order LST behavioral classes, $C_1^{\text{LST}}(\vec{\lambda})$ – one for each possible set of

values of $\lambda_i^{(1)}(\Phi)$'s, where $\vec{\lambda} \equiv (\lambda_0, \dots, \lambda_{2r+1})$:

$$\Phi \in C_1^{\text{LST}}(\vec{\lambda}) \longleftrightarrow \begin{cases} \lambda_0^{(1)}(\Phi) = \lambda_0, \\ \lambda_1^{(1)}(\Phi) = \lambda_1, \\ \vdots \\ \lambda_{2r+1}^{(1)}(\Phi) = \lambda_{2r+1} \end{cases} ; \quad \lambda_i = 0, 1, \dots, \binom{2r+1}{i}. \quad (5.84)$$

Since the total number of ways of obtaining a given value of the i^{th} coefficient, λ_i , is $\binom{2r+1}{\lambda_i}$, we find that the number of rules in each class, $C_1^{\text{LST}}(\vec{\lambda})$, is equal to $\prod_{i=0}^{2r+1} \binom{2r+1}{\lambda_i}$.

Note that $\lambda^{(0)} = \sum_{i=0}^{2r+1} \lambda_i^{(1)}$, so that the 1st-order LST, or mean field theory, behavioral classification is a strict *refinement* of the 0th-order LST classification. All rules belonging to 1st-order LST classes such that the sum of the $2r+2$ 1st-order coefficients defining that class are the same, also belong to the same 0th-order LST class.

The 1st-order LST approximation of the invariant measure of any rule Φ in the class $C_1^{\text{LST}}(\vec{\lambda})$ is given by the fixed point ρ_1^* of the equation 5.82.

2nd-order LST: 2nd-order LST improves upon the predictions of mean field theory by explicitly taking into account the correlations between separated site values. Specifically, probabilities of blocks of an arbitrary length N are estimated by probabilities of the various 2-blocks that they contain.

The 3-block probability, $P_3(B_3 = (b_1, b_2, b_3))$, for example, is determined from P_2 by a single application of the operator $\pi_{2 \rightarrow 3}$ (equation 5.71): $P_3(b_1, b_2, b_3) = P_2(b_2, b_3)P_2(b_1, b_2)/P_2(b_2)$. More generally, if the 2-block probabilities $P_2(b_1, b_2)$ are known for all b_1, b_2 , then the N -block probability, for arbitrary N is estimated by

$$P_N(b_1, b_2, \dots, b_N) = \prod_{i=2}^{N-1} \pi_{i \rightarrow i+1} P_i = \frac{\prod_{i=1}^{N-1} P_2(b_i, b_{i+1})}{\prod_{i=2}^{N-1} P(b_i)}, \quad (5.85)$$

where the $P(b_i) = P_2(b_i, 1) + P_2(b_i, 0)$.

Two blocks, B and B' , are of the same 2nd-order block type if $P_N(B) = P_N(B')$. Thus, B and B' must share three characteristics: (1) the same number of sites (excluding the right-most and left-most sites) with value '1' ($= n_1$), (2) the same number of '11' sub-blocks ($= n_{11}$), and (3) the same total number of '01' and '10' sub-blocks ($= n_{10+01}$). Accordingly, 2nd-order blocks of length N types are characterized by the 3-tuple $\vec{\xi}_N \equiv (n_1, n_{11}, n_{10+01})_N$.

In the same way as we found the 1st-order equations, we obtain the 2nd-order LST equations by first substituting equation 5.85 into the general form for the temporal evolution of block probabilities given by equation 5.76, and then simplifying the resulting expression by summing over sets of blocks of the same 2nd-order type.

The 1 and 2 block probabilities can be parameterized by any pair of linearly independent 1 and/or 2 block probabilities. For example, choosing the density ρ_1

and probability of '11' 2-blocks, ρ_{11} ,[†] we have

$$\begin{aligned}\rho_1^{(t+1)} &= \sum_{\vec{\xi}_{2r+1}} \lambda_a^{(2)}(\xi_{2r+1}; \Phi) P^{(t)}(\vec{\xi}_{2r+1}), \\ \rho_{11}^{(t+1)} &= \sum_{\vec{\xi}_{2r+2}} \lambda_b^{(2)}(\xi_{2r+2}; \Phi) P^{(t)}(\vec{\xi}_{2r+2}),\end{aligned}\tag{5.86}$$

where the sums are over all 2nd-order block types of size $(2r+1)$ and $(2r+2)$, respectively, $P^{(t)}(\vec{\xi})$ is the probability at time 't' of a 2nd-order type defined by $\vec{x}i$, and we have introduced two 2nd-order LST class coefficients, $\lambda_a^{(2)}(\xi_{2r+1}; \Phi)$ and $\lambda_b^{(2)}(\xi_{2r+2}; \Phi)$, one for each of the two block types:

$$\begin{aligned}\lambda_a^{(2)}(\xi_{2r+1}; \Phi) &= \text{Number of } (2r+1)\text{-blocks of type specified by } \xi_{2r+1} \text{ that,} \\ &\quad \text{yield '1' under } \Phi \\ \lambda_b^{(2)}(\xi_{2r+2}; \Phi) &= \text{Number of } (2r+2)\text{-blocks of type specified by } \xi_{2r+2} \text{ that} \\ &\quad \text{yield the 2-block '11' under } \Phi\end{aligned}\tag{5.87}$$

Analogously to the 0th- and 1st-order cases, each set of 2nd-order coefficients $\vec{\lambda}_a^{(2)}$ and $\vec{\lambda}_b^{(2)}$,

$$\begin{aligned}\vec{\lambda}_a^{(2)} &\equiv (\lambda_a^{(2)}(\xi_{2r+1,1}; \Phi), \lambda_a^{(2)}(\xi_{2r+1,2}; \Phi), \dots, \lambda_a^{(2)}(\xi_{2r+1,s}; \Phi), \\ \vec{\lambda}_b^{(2)} &\equiv (\lambda_b^{(2)}(\xi_{2r+2,1}; \Phi), \lambda_b^{(2)}(\xi_{2r+2,2}; \Phi), \dots, \lambda_b^{(2)}(\xi_{2r+2,s'}; \Phi)\end{aligned}\tag{5.88}$$

where s and s' are the total number of $(2r+1)$ and $(2r+2)$ blocks of 2nd-order type, respectively, defines a 2nd-order LST behavioral class, $C_2^{\text{LST}}(\vec{\lambda}_a, \vec{\lambda}_b)$:

$$\Phi \in C_2^{\text{LST}}(\vec{\lambda}_a, \vec{\lambda}_b) \longleftrightarrow \begin{cases} \lambda_a^{(2)}(\xi_{2r+1,1}; \Phi) = \vec{\lambda}_{a,1}, & \lambda_b^{(2)}(\xi_{2r+2,1}; \Phi) = \vec{\lambda}_{b,1} \\ \lambda_a^{(2)}(\xi_{2r+1,2}; \Phi) = \vec{\lambda}_{a,2}, & \lambda_b^{(2)}(\xi_{2r+2,2}; \Phi) = \vec{\lambda}_{b,2} \\ \vdots & \vdots \\ \lambda_a^{(2)}(\xi_{2r+1,s}; \Phi) = \vec{\lambda}_{a,s}, & \lambda_b^{(2)}(\xi_{2r+2,s'}; \Phi) = \vec{\lambda}_{b,s'} \end{cases}\tag{5.89}$$

Each 2nd-order LST class is a strict refinement of some mean field class. There are no simple closed forms for either the total number of 2nd-order class or the the number of rules within a given 2nd-order class.

N^{th} -order LST: The determination of the N^{th} -order LST equations proceeds in five steps as a generalization of the 0th, 1st and 2nd order systems of equations described above:

[†]the other 2-block probabilities are obtained by appealing to the Kolmogorov consistency conditions, defined in equation 5.68: $P_{10} = P_{01} = \rho_1 - \rho_{11}$.

1. Equation 5.85, giving the Bayesian extension of 2-block probabilities, is first generalized to give the Bayesian extension of N -block probabilities to probabilities of arbitrarily large M -blocks, P_M , $M \geq N$:

$$P(B_M) = \frac{\prod_{B \in \mathbf{B}_N} P(B)^{\#B_{B_M}}}{\prod_{B \in \mathbf{B}_{N-1}} P(B)^{\#B_{\mathcal{L}\mathcal{R}B_M}}}, \quad (5.90)$$

where $\#B_{B_M}$ is the number of blocks B in the M -block B_M (counting overlaps) and $\#B_{\mathcal{L}\mathcal{R}B_M}$ is the number of blocks B in the central $(M-2)$ portion of the block B_M (again, counting overlaps).

2. All $(2r+1)$ -, $(2r+2)$ -, $\dots$, and $(2r+N-1)$ - blocks of the same N^{th} -order type are identified; two blocks, B and B' , are of the same N^{th} -order type if they are assigned the same probability by equation 5.90.
3. A basis set of probabilities, $\mathcal{B} \equiv \{p_{(1)}, p_{(2)}, \dots, p_{(s)}\}$ is selected for parameterizing arbitrary N -block probabilities. It is a simple exercise to show that, because of the constraints imposed by the the Kolmogorov consistency conditions (equation 5.68, $s = 2^{N-1}$ basis elements are necessary.
4. A set of N^{th} -order LST class coefficients, $\vec{\xi}(\mathcal{T}_B)$, is assigned to each block type, $\mathcal{T}_B$; each coefficient is equal to the number of blocks of a given type that yield a block in the basis set $\mathcal{B}$.
5. Finally, the N^{th} -order LST equations for the temporal evolution of the i^{th} basis probability, $p_{(i)}$, are given by

$$p_{(i)}^{(t+1)} = \sum_{\mathcal{T}_B} \vec{\xi}(\mathcal{T}_B) P^{(t)}(\mathcal{T}_B), \quad (5.91)$$

where the summation is over all blocks of type $\mathcal{T}_B$ whose size is appropriate for being mapped by Φ to the block size corresponding to the i^{th} basis probability, and $P^{(t)}(\mathcal{T}_B)$ is the probability at time ' t ' of a block of N^{th} -order type $\mathcal{T}_B$.

Figure 5.2, for example, shows all N^{th} -order ($N \leq 10$) LST approximations of the invariant (*i.e.*, fixed point) density, $\rho_1^{(N)}$, for elementary rule **R22**. As N increases, $\rho_1^{(N)}$ approximates the density derived by Monte Carlo simulation [guto87a] (indicated by the dotted line) increasingly well.

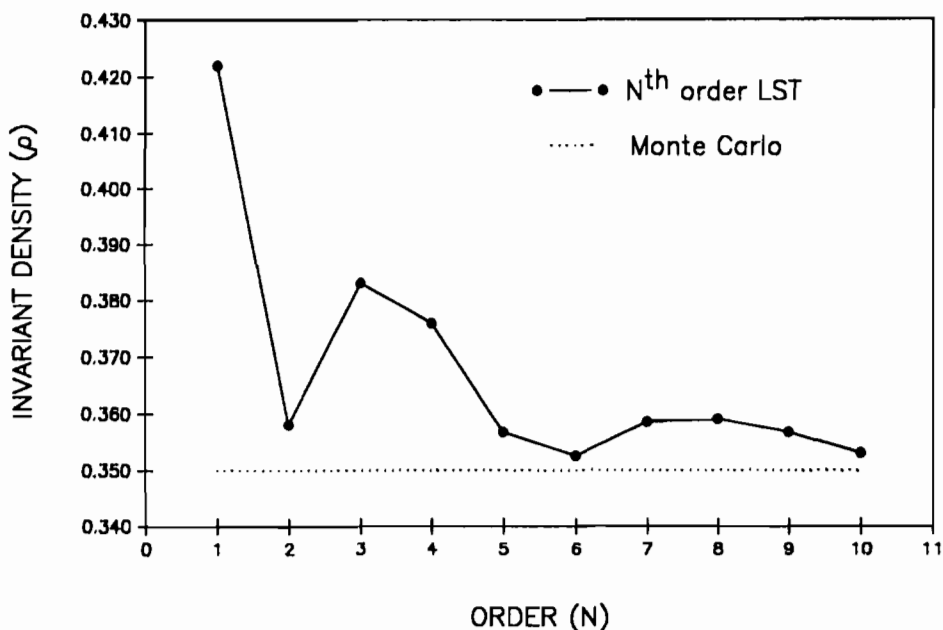


Fig. 5.2 Plots of 11 N^{th} -order ($N \leq 10$) LST' approximations of the invariant (*i.e.*, fixed point) density, $\rho_1^{(N)}$, for elementary rule **R22**; see text.

As alluded to earlier, there are no closed form expressions either for the total number of classes or rules within a given class. It is generally true, however, that for a given radius- r rule, classes both increase in number and decrease in size as the order N of the LST increases; for fixed order, on the other hand, the number and size of classes increases with radius.

5.3.3 LST for d -Dimensional Lattices, $d > 1$

The essence of the LST for one-dimensional lattices resides in the fact that an operator $\pi_{N \rightarrow N+1}$ could be constructed (equation 5.71), mapping N -block probability functions to $(N + 1)$ -block probabilities in a manner which satisfies the Kolmogorov consistency conditions (equation 5.68). A sequence of repeated applications of this operator allows us to define a set of Bayesian extended probability functions $\{P_M\}$, $M \geq N$, and thus a shift-invariant measure on the set of all one-dimensional configurations, Γ . Unfortunately, a simple generalization of this procedure to lattices with more than one dimension, does not, in general, produce a set of consistent block probability functions. Extensions must instead be made by using some other, approximate, method. We briefly sketch a heuristic outline of one approach below (details are worked out in [guto87b]).

We first generalize the nomenclature. Consider a Euclidean d -dimensional lattice L , with translation group G_L . A *frame*, F , of L is defined to be a finite subset of (not necessarily contiguous) sites of L that is closed under (i) intersection, (ii) union, (iii) difference and (iv) operations $g \in G_L$. A *block*, B_F , is a specific assignment

of values to the sites in frame F . $\mathbf{B}_F$ denotes the set of all blocks on frame F . A *block probability function* $P_F : \mathbf{B}'_F \rightarrow \mathcal{R}$, is a map from all blocks $B_{F'}$, $F' \subseteq F$ to the reals that satisfies the generalized Kolmogorov consistency equations:

$$\left\{ \begin{array}{ll} \text{I:} & P_F(B) \geq 0, \\ \text{II:} & \sum_{B \in \mathbf{B}_{F'}} P_{F'} = 1, \\ \text{III:} & P_{F'}(B') = \sum_{B| B \downarrow F' = B'} P_F(B), \end{array} \right. \quad (5.92)$$

where, in condition III, $B' \subseteq B$) and the sum is over blocks B such that B restricted to frame F' is equal to block B' .

The d -dimensional analogue of the operator π , mapping N -block probabilities to $(N+1)$ -block probabilities, is an operator, π_j , defining the *Bayesian extension* of P_F to $P_{F'}$ along dimension j . Here, $P_{F'} \equiv F^{e,j}$, where $F^{e,j}$ is an extension of frame $F \equiv (i_1 \times i_2 \times \cdots \times i_d)$ by one unit along dimension ' j '. π_j is defined by

$$[\pi_j P_F]B \equiv \begin{cases} \frac{P_F(\mathcal{R}_j B) P_F(\mathcal{L}_j B)}{P_F(\mathcal{R}_j \mathcal{L}_j B)} & \text{if } B \in \mathbf{B}_{F^{e,j}}, \\ 0 & \text{if } P_F(\mathcal{R}_j \mathcal{L}_j B) = 0, \\ P_F(B) & \text{if } B \in \mathbf{B}_F. \end{cases} \quad (5.93)$$

The problem is that for $d > 1$, it is no longer guaranteed that π_j induces a set of block probabilities obeying all of the generalized consistency conditions in equation 5.92. If correlations exist *only in one dimension*, then it is possible to define what essentially amounts to being a one-dimensional LST for a higher dimensional state space. In the presence of bona-fide multi-dimensional correlations, however, appropriate modifications must be made to compensate for whatever consistency violation appears. For example, if the local shift invariance condition is violated, then we could instead consider *average block probabilities* by averaging P_F on all frames F related by a local shift [guto87a]. Modified Bayesian extensions of this sort have been conducted for simple two-dimensional Euclidean and hexagonal lattices.

The construction of LST's for higher dimensional lattices is particularly significant for studying questions concerning the role the underlying lattice L plays in shaping the dynamical behavior of a given system. Since, as we have seen, order N LST, for $N \geq 2$, takes an explicit account of the local lattice structure, an analysis of such theories may reveal heretofore hidden lattice-generated dynamical mechanisms responsible for some part of the emerging statistical behaviors.

5.4 Dependence on Lattice Topology

In this section we investigate the relationship between global dynamical properties, as characterized, for example, by certain features of the state transition graph $G_{\mathcal{L}}$, and the topology of the underlying lattice $\mathcal{L}$. To do so, we first introduce the notion of a *natural topology*, which effectively transforms the dynamical content of the problem into more useful structural information. We next provide explicit solutions for general systems whose site values are taken from finite fields of arbitrary size, directly linking behavioral characteristics with topological properties of the lattice $\mathcal{L}$. The more typical binary valued CA are discussed in some detail; we make predictions about specific kinds of system behaviors from basic knowledge of the topological features of $\mathcal{L}$.

5.4.1 Natural Topology

Consider a finite but structurally arbitrary lattice $\mathcal{L}$, with geometry completely specified by the $(N \times N)$ *adjacency matrix* $\mathbf{L}$:

$$(\mathbf{L})_{ij} = \begin{cases} 1 \longleftrightarrow & \text{'i' is linked to 'j'} \\ 0 \longleftrightarrow & \text{otherwise} \end{cases} \quad (5.94)$$

At each of N sites is a variable σ_i belonging to a finite field $\mathcal{F}[q = p^n]$ (p is a prime, n is any integer), so that a particular configuration is specified by the vector $\Sigma(t) \equiv (\sigma_1(t), \dots, \sigma_N(t))^T$.

Defining a distance function $d(i, j) \equiv \min_{\text{paths}} \{ \# \text{ of links } (i, j; \text{ path}) \}$ and a ' d '-size neighborhood of ' i ' as $\mathcal{N}_d(i) \equiv \{ 'k' \text{ such that } d(i, k) \leq d \}$, we wish to study the discrete time-evolution of $\Sigma(t)$ in which the site variables undergo transitions of the general form

$$\sigma_i(t+1) = \phi_{\mathcal{L}} \left[\sum_{j \in \mathcal{N}_d(i)} \sigma_j(t) \right], \quad (5.95)$$

where the subscript on ' ϕ ' is to emphasize that $\phi_{\mathcal{L}}$ acts on a particular lattice. Since there is no universally applicable *local* labeling procedure for sites in a random lattice $\mathcal{L}$, this is in fact the most general form possible. As always, $\phi_{\mathcal{L}} : \mathcal{Z} \rightarrow \mathcal{F}[q]$ is the same for all ' i ' and is defined explicitly by enumerating, for all $y \in \mathcal{F}[q]$, all possible values $x \in \mathcal{Z}$ for which $\phi_{\mathcal{L}}(x) = y$.

Given any lattice $\mathcal{L}$ and arbitrary transition rule ' $\phi_{\mathcal{L}}$ ' we define a *natural topology* $\mathcal{L}_{\phi}$:

$$(\mathbf{L}_{\phi})_{ij} = \begin{cases} 1 \longleftrightarrow & \sigma_i(t+1) \text{ depends on } \sigma_j(t) \text{ through } \phi_{\mathcal{L}} \\ 0 \longleftrightarrow & \text{otherwise,} \end{cases} \quad (5.96)$$

upon which the site transitions become strictly *local*:

$$\phi_{\mathcal{L}} \left[\sum_{j \in \mathcal{N}_d(i)} \sigma_j(t) \right] = \phi_{\mathcal{L}_{\phi}} \left[\sum_{j \in \mathcal{N}_{d=1}(i)} \sigma_j(t) \right]. \quad (5.97)$$

We are effectively transforming functional identity into topological information: *i.e.* different choices of rules correspond to different topologies and all rules are taken to be simple functions of local sums.

The general form of the global transition function may then be written

$$\Sigma(t+1) = \Phi[\mathbf{L}^* \cdot \Sigma(t)], \quad (5.98)$$

where $[\Phi(\mathbf{x})]_i = \phi(x_i)$, $x_i \equiv \mathbf{L}_{ij}^* \Sigma_j$ and the matrix product is taken over $\mathcal{Z}$. *Additive* rules are defined by $\phi(x) = x \pmod{q}$, so that our goal is to explore the dependence of the global dynamics of the system

$$\Sigma(t+1) = \mathbf{L} \cdot \Sigma(t) \quad (5.99)$$

on the topological features of the lattice represented by $(\mathbf{L})_{ij}$. Throughout this section, *outer-totalistic OT* rules will refer to loopless graphs ($\mathbf{L}_{ii} = 0$); *totalistic T* rules to graphs with loops ($\mathbf{L}_{ii} = 1$).

Figure 5.3 shows $\mathcal{L}^*$ for three different additive rules in 1-dim (*i.e.* $\mathcal{L} \equiv 1$ -dim topology). The dynamics may be equally well represented either as taking place entirely on a one-dimensional lattice but under three different rules, or obeying the same rule ($\equiv \oplus_q (\sigma_{\text{neighbors}})$) but defined on three different lattices. Having subsumed, in this way, the dynamical content of a given rule into the underlying natural topology, the fundamental question becomes: *What are the topological characteristics of $\mathcal{L}_\phi$ which determine the system's global dynamical behavior?*

5.4.2 General Solution in $\mathcal{F}[q]$

Exact calculations have already been carried out for simple *one* and *two* dimensional Euclidean geometries by exploiting properties of *polynomials* (chapter 5.2.1) and *circulant matrices* (chapter 5.2.2) over the finite field $\mathcal{F}[q]$, $q = p^n$ where p is prime. We will here rely instead on the theory of *input-free modular systems*, which is more suitable for dealing with the dynamics of completely arbitrary lattices.

The goal, as before, is to find the *state graph* ($\equiv G_L$) description of the system, where G_L is a directed graph with q^N vertices and is defined by $G_{Lij} = 1 \Leftrightarrow \Sigma^{(j)} = \mathbf{L} \cdot \Sigma^{(i)}$.[†] Familiar quantities of interest include *cycle lengths*, *number of distinct cycles* and *transients*. G_L has been successfully characterized when its (formal) *cycle sum* $\mathcal{C}[L] \equiv \sum_i [n_i, \ell_i]$, where $n_i = \#$ of cycles of length ℓ_i , has been computed.

We define the *order* of some state Σ to be the least positive integer such that $\mathbf{L}^t \Sigma = \Sigma$. Suppose $\mathbf{L}$ is a direct sum of two matrices, $\mathbf{L}_1 \oplus \mathbf{L}_2$, and $\begin{pmatrix} \sigma_1 \\ 0 \end{pmatrix}$, $\begin{pmatrix} 0 \\ \sigma_2 \end{pmatrix}$ are two states partitioned according to the labeling of $\mathbf{L}$, with orders t_1 and t_2 , respectively. Since $\mathbf{L}^t \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} \Leftrightarrow \mathbf{L}^t \sigma_i = \sigma_i$, we have $\text{order} \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \text{lcm}(t_1, t_2)$. If, in particular, G_{L_i} has n_i cycles of length ℓ_i , so that there are $n_1 \ell_1$ states of order ℓ_1 of the form $\begin{pmatrix} \sigma_1 \\ 0 \end{pmatrix}$ and $n_2 \ell_2$ states of order ℓ_2 of the form $\begin{pmatrix} 0 \\ \sigma_2 \end{pmatrix}$, then G_L has $n_1 n_2$

[†]Subscripts indicate individual state components; superscripts label distinct configurations.

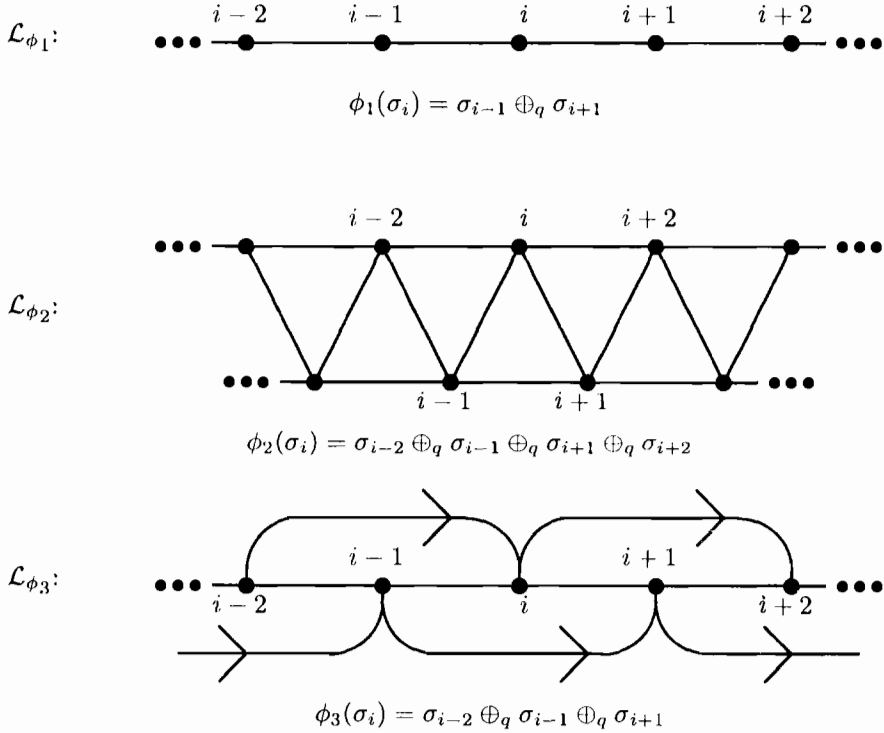


Fig. 5.3 Natural topologies $\mathcal{L}_\phi$ for three one-dimensional additive rules ($\oplus_q \equiv \text{sum modulo } q$). For an arbitrary $\phi^{(\mathcal{L})}$ acting on a given lattice $\mathcal{L}$, $\phi^{(\mathcal{L}_\phi)}$ is always ' $\oplus_q(\sigma_{\text{neighbors}})$ ' on $\mathcal{L}^*$. In this way we may effectively study one generic rule: the study of the *different rules* on $\mathcal{L}$ becomes a study of a *fixed rule on a variety of topologies*. Solid edges represent symmetric dependence; arrows imply one-way communication.

$\gcd(t_1, t_2)$ cycles of length $\text{lcm}(t_1, t_2)$. That is, we may define the *formal product* of two cycle terms by

$$[n_1, t_1][n_2, t_2] = [n_1 n_2 \gcd(t_1, t_2), \text{lcm}(t_1, t_2)]. \quad (5.100)$$

If $\mathcal{C}_{L_1}$ and $\mathcal{C}_{L_2}$ are the cycle sums for $\mathbf{L}_1$ and $\mathbf{L}_2$, then the cycle sum for $\mathbf{L}$ consists of all pairwise products of all possible combinations of cycle terms from $\mathbf{L}_1$ and $\mathbf{L}_2$: $\mathcal{C}_L = \mathcal{C}_{L_1} \mathcal{C}_{L_2}$.[†] It is straightforward to obtain, inductively, the general result that if $\mathbf{L} = \oplus_{i=1}^r \mathbf{L}_i$ and $\mathbf{L}_i$ have cycle sums $\mathcal{C}_i$, then $\mathcal{C}_L = \prod_{i=1}^r \mathcal{C}_i$.

[†]Sums of cycle terms of equal length are handled in the obvious manner: $[n_1, t] + [n_2, t] = [n_1 + n_2, t]$.

Now, suppose the entries of an $(N \times N)$ matrix $\mathbf{M}$ are polynomials over the field $\mathcal{F}[q]$. Then $\mathbf{M}$ is similar to a matrix $\tilde{\mathbf{M}}$ ($\equiv$ *Smith Canonical Form* (SCF) of $\mathbf{M}$): $\mathbf{M} \sim \tilde{\mathbf{M}} \equiv \oplus_{i=1}^N f_i(x)$, where $f_i(x) \mid f_{i+1}(x)$ for $i=1, 2, \dots, N-1$ and each $f_i(x)$ is monic (leading coefficient is '1'). The $f_i(x)$ are the *similarity invariants* of $\mathbf{M}$ [174].

If, in particular, we convert a matrix ' $\mathbf{L} - x\mathbf{1}$ ' into its SCF, where now the $(0, 1)$ -entries of $\mathbf{L}$ are elements of $\mathcal{F}[q]$, and factor the similarity invariants into products of powers of monic irreducible polynomials $p_j(x)$, so that $f_i(x) = \prod_{j=1}^r [p_j(x)]^{\nu_{ij}}$, we obtain the *elementary divisors* $\{\varepsilon_i^{(L)}(x)\}$ of $\mathbf{L}$:

$$\{\varepsilon_i^{(L)}(x)\} \equiv \text{set of all nonconstant factors } [p_i(x)]^{\nu_{ij}}. \quad (5.101)$$

It is this set of polynomials, uniquely defined for all similar matrices, which effectively determines the complete dynamics.

Recalling that the *companion matrix* of any monic polynomial, $\varepsilon(x) = x^N + a_1x^{N-1} + \dots + a_N$, is defined by

$$C[\varepsilon(x)] \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 & -a_n \\ 1 & 0 & 0 & \cdots & \cdots & 0 & -a_{N-1} \\ 0 & 1 & 0 & \cdots & \cdots & 0 & -a_{N-2} \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -a_1 \end{pmatrix}, \quad (5.102)$$

we make use of the extremely useful fact that every matrix $\mathbf{L}$ over a finite field $\mathcal{F}[q]$ is similar to (its *Rational Canonical Form* (RCF)) $\tilde{\mathbf{L}} \equiv \oplus_{i=1}^r C[\varepsilon_i^{(L)}(x)]$.

In general, $\varepsilon(x)$ can be one of two types:

$$\begin{cases} \varepsilon_I(x) &= x^r + a_1x^{r-1} + \dots + a_r = [p(x)]^\nu, \quad a_r \neq 0 \\ \varepsilon_{II}(x) &= x^r, \end{cases} \quad (5.103)$$

where $C[\varepsilon_I]$ is *nonsingular* and $C[\varepsilon_{II}]$ is *nilpotent* (i.e. $C^t[\varepsilon_{II}] = 0$ for some 't'). Thus, the RCF of $\mathbf{L}$ will be of the general form

$$\mathbf{L} \sim \mathbf{L}_{\text{nilpotent}} \oplus \mathbf{L}_{\text{nonsingular}}. \quad (5.104)$$

$\mathbf{L}_{\text{nonsingular}}$ contributes only *cycles*[†], while from $C[\varepsilon_{II}] \equiv \delta_{i,i-1}$, we see that all states must reach $\Sigma = \mathbf{0}$ in $t \leq r$; i.e. $\mathbf{L}_{\text{nilpotent}}$ contributes the *transient* (or *tree*) structure of G_L .

Although we will not worry about the precise tree structure, we note that *for all graphs*, and therefore *all additive rules*, every cyclic state is a root of a tree which is isomorphic to the null tree (the one terminating on $\Sigma = \mathbf{0}$):

Proof: define $\Sigma \equiv \begin{pmatrix} \sigma_1 \\ \mathbf{0} \end{pmatrix}$ to be a state reaching '0' in r -steps. If $\mathbf{L} \sim \mathbf{L}_1 \oplus \mathbf{L}_2$, with $\mathbf{L}_1$ 'nilpotent' and $\mathbf{L}_2$ 'nonsingular' then $\mathbf{L}_1^r \sigma_1 = \mathbf{0}$. Consider the state $\Sigma' \equiv$

[†]Each state Σ has a unique *successor* $\mathbf{L}\Sigma$ and unique *predecessor* $\mathbf{L}^{-1}\Sigma$.

$\begin{pmatrix} \sigma_1 \\ (\mathbf{L}_2^{-r})\sigma_2 \end{pmatrix}$. It is clear that the null tree, consisting of all states of the form Σ , is isomorphic to the subgraph consisting of all states of form Σ' for any σ_2 such that $\begin{pmatrix} \mathbf{0} \\ \sigma_2 \end{pmatrix}$ is a cyclic state: simply use the isomorphism $\psi(\Sigma) = \Sigma'$. Then, for $\sigma_1 \neq \mathbf{0}$, Σ' cannot be cyclic. Since $\mathbf{L}'\Sigma' = \begin{pmatrix} \mathbf{0} \\ \sigma_2 \end{pmatrix}$, it must be a tree isomorphic to the null tree with root $= \begin{pmatrix} \mathbf{0} \\ \sigma_2 \end{pmatrix}$. ■

Since the topology of G_L is invariant under similarity transformations of $\mathbf{L}$,[†] its complete structure can be computed using $\tilde{\mathbf{L}}$. It remains only to find the cycle sum of a general block $C[(\varepsilon_I)_i]$. We quote the result ([biggs74], [cvet79]):

Let $p(x)$ be a monic irreducible polynomial over $\mathcal{F}[q]$ of degree $= d$ and $t_m \equiv \text{ord}([p(x)]^m)$ [‡], then

$$C_C[(p(x))^\nu] = [1, 1] + \sum_{i=1}^{\nu} \left[\frac{q^{id} - q^{(i-1)d}}{t_i}, t_i \right]. \quad (5.105)$$

EXAMPLE: Consider a one-dimensional lattice of size $N = 5$. The adjacency matrix, $\mathbf{L}$, and *Smith Canonical Form* of $\mathbf{L} - x\mathbf{1}$, are, respectively,

$$\mathbf{L} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{L} - x\mathbf{1} \sim \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & x(1+x^4) \end{pmatrix},$$

from which we obtain the *similarity invariants*: $f_1(x) = \cdots = f_4(x) = 1$, $f_5(x) = x(1+x)^4$, and *elementary divisors*: $\epsilon_1(x) = x$, $\epsilon_2(x) = (1+x)^4$. Now, the companion matrix of $\epsilon_1(x)$,

$C_1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ is *nilpotent*, giving rise to the transient states; since $t_1 = \text{ord}(1+x) = 1$, $t_2 = 2$, $t_3 = t_4 = 4$, the cyclic states are characterized by

$$C[(1+x)^4] = [1, 1] + \sum_{i=1}^4 \left[\frac{2^i - 2^{i-1}}{t_i}, t_i \right] = [2, 1] + [1, 2] + [3, 4]$$

5.4.3 Connection with Lattice Topology

We can relate the dynamics, which, as is clear from the discussion of the previous section, depends solely on the set of elementary divisors $\{\varepsilon_i(x)\}$, to the topology $\mathcal{L}$

[†]With $\mathbf{L}$ and $\mathbf{L}' = \mathbf{PLP}^{-1}$, let $\Sigma \rightarrow \Sigma' = \mathbf{P}\Sigma$. Then $\mathbf{L}'\Sigma' = (\mathbf{PLP}^{-1})(\mathbf{P}\Sigma) = \mathbf{P}(\mathbf{L}\Sigma)$.

[‡]If $p(0) \neq 0$ then $\text{ord}(p)$ is the least positive integer 't' such that $p(x)|x^t - 1 \pmod{q}$. If $p(0) = 0$ then $p(x) = x^a g(x)$ with $g(0) \neq 0$ and $\text{ord}(p) \equiv \text{ord}(g)$.

by noting that $\prod_{i=1}^r \varepsilon_i(x) = P_L(x) \equiv \det(\mathbf{L} - x\mathbf{1})$ (the characteristic polynomial of $\mathbf{L}$). Writing $P_L(x)$ in the form ' $x^N + a_1x^{N-1} + a_2x^{N-2} + \dots + a_N$ ', we have that $a_i = (-1)^i \text{tr}_i(\mathbf{L})$, where ' $\text{tr}_i(\mathbf{L})$ ' is the sum of determinants of all principal minors of $\mathbf{L}$: $\text{tr}_1(\mathbf{L})$, for example, ' $= 0$ ' for OT rules, while $\text{tr}_2(\mathbf{L}) = \sum_{i < j} \begin{vmatrix} 0 & \ell_{ij} \\ \ell_{ij} & 0 \end{vmatrix} = \sum_{i < j} \ell_{ij} = \text{'# of links in } \mathcal{L}\text{'}$. A convenient representation for all of these coefficients is provided by the following fundamental result.

A graph is called a *primitive graph* if its components are either *single edges* (E) or *circuits* ($\hat{C}_i$, $i \geq 1$). The coefficients of $P_L(x)$ for an undirected graph may then be related to the topological content of $\mathcal{L}$ by a decomposition into all primitive subgraphs [harary73]:

$$a_i = \sum_{G \in G[i]} (-1)^{r(G)} 2^{s(G)}; \quad 0 \leq i \leq N, \quad (5.106)$$

where $G[i]$ is the set of all primitive graphs in $\mathcal{L}$ with ' i ' vertices, $r(G)$ is the # of components of a graph G and $s(G) \equiv \text{'# of circuits contained in } G\text{'}$.

Proof: consider the last coefficient, a_N . Using the *Leibnitz* expansion for the determinant, we have $a_N = (-1)^N \det(\mathcal{L}) = (-1)^N \sum_p \pi(p) \prod [\mathbf{L}_{i, \pi(i)}]$, where ' $\pi(p)$ ' is the *parity* of the permutation ' p '. Now, we have a non-zero contribution *if and only if* $\mathbf{L}_{i, p(i)} \neq 0$, $\forall i \implies p(i) \neq i$. Thus, $p = \prod_{\text{cycle of length } l \geq 2} (i_1, i_2, \dots, i_n)$. Since length-2 cycles contribute *edges* in ' $\mathcal{L}$ ' and length- $n > 2$ contribute factors corresponding to *circuits* in ' $\mathcal{L}$ ', we see that each non-zero factor contributes a *primitive graph* ' G '. Now, the parity $\pi(p) = (-1)^{n_{\text{even}}}$, where n_{even} is the number of even cycles. Since $N = \sum_i (n_{2i+1} \hat{C}_{2i+1} + n_{2i} \hat{C}_{2i})$, we see that *number of odd cycles* $= N \pmod{2}$. Thus $(-1)^N \pi(p) = (-1)^{N+n_{\text{even}}} = (-1)^{n_{\text{odd}}+n_{\text{even}}} = (-1)^{\text{'# components'}} = (-1)^{r(G)}$. Since we can choose two *cycles* for each *circuit*, there are ' $2^{s(G)}$ ' permutations for which a particular term in the determinant expansion remains nonvanishing. Each ' G ' thus contributes a factor ' $(-1)^{r(G)} 2^{s(G)}$ ' to $\det(\mathcal{L})$. We arrive at equation (5.106) by applying this result to all principal minors (each of which is the determinant of a subgraph of $\mathcal{L}$ of size ' i '). ■

Using the notation $N(i) \equiv \text{'# of subgraphs of type } i\text{'}$, and $N(i_1, \dots, i_n) \equiv \text{'# of } n\text{-disjoint subgraphs } i_1, \dots, i_n\text{'}$, the first few coefficients for OT rules are given explicitly by

$$\left\{ \begin{array}{ll} a_1^{\text{OT}} & = 0 \\ a_2^{\text{OT}} & = -N(E) \\ a_3^{\text{OT}} & = -2N(\hat{C}_3) \\ a_4^{\text{OT}} & = N(E, E) - 2N(\hat{C}_4) \\ a_5^{\text{OT}} & = 2N(E, \hat{C}_3) - 2N(\hat{C}_5) \\ a_6^{\text{OT}} & = -N(E, E, E) + 2N(E, \hat{C}_4) + 4N(\hat{C}_3, \hat{C}_3) - 2N(\hat{C}_6) \\ a_7^{\text{OT}} & = -2N(E, E, \hat{C}_3) + 2N(E, \hat{C}_5) - 2N(\hat{C}_7) \\ \vdots & \quad \quad \quad \vdots \end{array} \right. \quad (5.107)$$

Since $\mathbf{L}^{\mathbf{T}} = \mathbf{L}^{\mathbf{OT}} + 1$, we obtain the *totalistic* $\mathbf{T}$ coefficients by computing $P_L^{\mathbf{T}}(x) = P_L^{\mathbf{OT}}(x+1)$:

$$a_i^{\mathbf{T}} = \sum_{j=0}^i \binom{N-j}{N-i} a_j^{\mathbf{OT}}. \quad (5.108)$$

In the more general case of a directed graph, we have that

$$a_i^{\mathbf{OT}} = \sum_{G \in L[i]} (-1)^{r(G)}, \quad (5.109)$$

where $L[i]$ is the set of all linear directed subgraphs in $\mathcal{L}$ with ' i ' vertices (*i.e.* all subgraphs consisting of pure cycles), and $r(G)$ is as above.

Although the actual cycle decomposition (as well as the tree structure) of a particular graph is determined exactly by the set of elementary divisors $\{\varepsilon_i(x)\}$, much of the general form of the possible dynamics may be extracted from $P_L(x)$ itself. All graphs $\mathbf{L}_i$ whose characteristic polynomials $P_{L_i} = P^* = x^\alpha \prod_{i=1}^r [p_i(x)]^{\nu_i} \pmod{q}$, for some fixed $P^*(x)$, for example, must share the following properties:

- 1: $\text{vol}(\mathcal{C}_i) \equiv \text{number of cyclic states in } \mathbf{L}_i = q^{N-\alpha}$ for all $\mathbf{L}_i$.
- 2: $f_0 \equiv \text{fraction of initial states} \rightarrow 0 = [\text{vol}(\mathcal{C})]^{-1}.$ [†]
- 3: $T_M \equiv \text{maximal transient time} \leq \alpha$.
- 4: the cyclic sum decomposition $\mathcal{C}_i = [n_1^{(i)}, t_1^{(i)}] + \dots + [n_{m_i}^{(i)}, t_{m_i}^{(i)}]$ can only have cycle lengths $n_j^{(i)} \in \{\text{lcm}(t_{a_1}^{(1)}, t_{a_2}^{(2)}, \dots, t_{a_r}^{(r)}); 0 \leq a_k \leq \nu_k, 1 \leq k \leq r\}$ determined from $\mathcal{C}[P^*]$, where $t_{a_k}^{(k)} \equiv \text{ord}([p_k(x)]^{a_k})$. In this way we can easily determine both the *maximal* possible cycle length and the set of cycle lengths *shared* by all $\mathbf{L}_i$: $\{\text{lcm}(t_{a_1}^{(1)}, \dots, t_{a_r}^{(r)}); a_i = 0, 1, 0 \leq i \leq r\}$.

The set of all topologically distinct graphs (of which there are $\sim 2^{N(N-1)/2}/N!$ for large N) may thus be broken up into a much smaller set of *cyclic equivalence classes* $\mathcal{Q}$: each $\mathcal{Q}$ corresponds to a particular choice for a set of values of the coefficients $\{a_i\}$ yielding a unique set of possible dynamics. From equation (5.12) we see that sets of different $\{p_i(x)\}$ for which $\{d_i = \deg(p_i(x))\}$ and $\{t_i^{(j)} = \text{ord}(p_i(x))^j\}$ are the *same for all 'i'*, must give topological characteristics of graphs belonging to the same $\mathcal{Q}$.

To find the number of distinct G_L 's for each $\mathcal{Q}$, we must count, for each term $[p_i(x)]^{\nu_i}$ appearing in the factorization, the number of equivalent sets of $\{\varepsilon_i(x)\}$ which can be formed. That is, for each ' i ', count the number of ways of forming the products

$$p_i(x)]^{\nu_{i1}} [p_i(x)]^{\nu_{i2}} \dots [p_i(x)]^{\nu_{in_i}} = [p_i(x)]^{\nu_i}, \text{ with}$$

[†]This follows from the fact that all *trees* are *isomorphic*: each of the $q^{N-\alpha}$ cyclic states has an isomorphic copy of the null tree; all ' $q^N - q^{N-\alpha}$ ' states available for the tree structures must then be equally distributed. Thus, $f_0 = q^{-N} \{1 + (q^N - q^{N-\alpha})/q^{N-\alpha}\} = q^{\alpha-N} = [\text{vol}(\mathcal{C})]^{-1}$.

$$\begin{cases} \sum_{j=1}^{n_i} \nu_{ij} = \nu_i \\ \nu_{i1} \geq \nu_{i2} \geq \cdots \geq \nu_{in_i} \geq 1. \end{cases} \quad (5.110)$$

Defining $p(\nu_i, n_i) \equiv \#$ of partitions of an integer ν_i into n_i parts', we thus have that the maximum number of distinct topologies of G_L ($\equiv \mathcal{N}(G_L)$) is

$$\mathcal{N}(G_L) = \prod_{i=1}^r \sum_{n_i=1}^{\nu_i} p(\nu_i, n_i). \quad (5.111)$$

The much more difficult task of finding how often a given state transition graph G_L appears when one samples all possible topologies $\mathcal{L}$ (or how the $\mathcal{Q}$ sets are individually *weighted*), remains an open question.

In table 5.2, we list the maximal numbers of possible cycle states $|\mathcal{C}_{\mathbf{OT}}|$ and $|\mathcal{C}_{\mathbf{T}}|$ for $\mathbf{OT}$ and $\mathbf{T}$ rules, respectively, the total number of possible distinct state transition topologies (including trees), $\mathcal{N}(G_L)$, and the number of equivalence classes $\mathcal{Q}$, for small N in $\mathcal{F}[2]$. The number of possible state transition topologies is evidently much smaller than the number of distinct connected topologies ($= \mathcal{L}$, [cvt79]). Note that the sets $\mathcal{C}_{\mathbf{OT}}$ and $\mathcal{C}_{\mathbf{T}}$ are the same for *even*- N , while for *odd*- N , $\mathcal{C}_{\mathbf{OT}}$ is the same as $\mathcal{C}_{\mathbf{OT}}$ for $(N-1)$ (since $\{P_L^{(N=2j+1)}\} = \{xP_L^{(N=2j)}\}$).

N	$ \mathcal{L} $	$\mathcal{Q}$	$ \mathcal{C}_{\mathbf{OT}} $	$ \mathcal{C}_{\mathbf{T}} $	$\mathcal{N}(G_L^N)$
5	21	4	10	13	20
6	112	7	27	27	54
7	853	7	27	38	69
8	11,117	13	72	72	168
9	261,080	13	72	105	217
10	11,716,571	22	200	200	502
11	$\sim 10^9$	22	200	272	641
12	$\sim 1.6 \cdot 10^{11}$	36	491	491	1354

Table 5.2 Number of topologically distinct connected graphs $|\mathcal{L}|$, number of *cyclic equivalence classes* $\mathcal{Q}$, maximal numbers of possible cycle sets $|\mathcal{C}_{\mathbf{OT}}|$ and $|\mathcal{C}_{\mathbf{T}}|$ for $\mathbf{OT}$ and $\mathbf{T}$ rules, respectively, and the maximal number of possible distinct topologies of the state transition graph, $\mathcal{N}(G_L)$, calculated for graphs with size $N=5, 6, \dots, 12$ in $\mathcal{F}[2]$.

Apart from knowing whether particular topologies *do or do not* support cycles with prescribed length (i.e *period*), which, as seen above is *exactly* answerable from the graph's edge topology, we may also be interested in knowing the *minimal size* of arbitrary topologies necessary to support desired cycles. Table 5.3 gives the *minimal sizes* of *symmetric* and *directed* graphs necessary to support cycles of a given period $p \leq 36$ in $\mathcal{F}[2]$.

We make the following observations:

period	N_{min}^{sym}	N_{min}^{gen}	period	N_{min}^{sym}	N_{min}^{gen}	period	N_{min}^{sym}	N_{min}^{gen}
1	1	1	13	24	12	25	40	20
2	2	2	14	6	5	26	24	14
3	4	2	15	8	4	27	36	18
4	4	3	16	10	9	28	10	7
5	8	4	17	16	8	29	56	28
6	4	4	18	12	8	30	8	6
7	6	3	19	36	18	31	10	5
8	6	5	20	12	7	32	18	17
9	12	6	21	10	5	33	20	10
10	8	6	22	20	12	34	16	10
11	20	10	23	22	11	35	12	7
12	8	5	24	10	8	36	14	9

Table 5.3 Minimal sizes of *symmetric OT* and *general* (i.e. directed) graphs necessary to support cycles of given *period* for the first 36 periods in $\mathcal{F}[2]$.

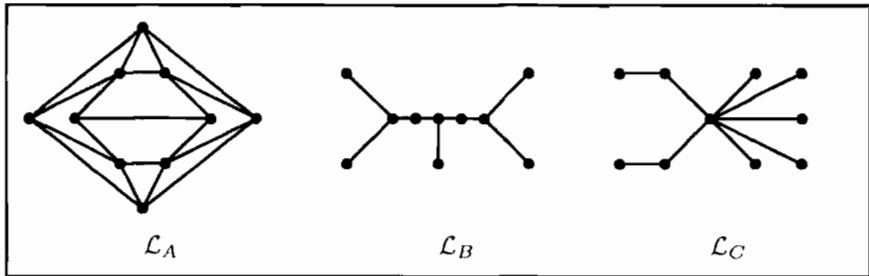


Fig. 5.4 Three distinct topologies on 10 vertices belonging to the same cyclic equivalence class $\mathcal{Q}$, with $P_{L_A}(x)=P_{L_B}(x)=P_{L_C}(x)=x^4(1+x)^6 \pmod{2}$. All three graphs therefore have $\text{vol}(\mathcal{C}) = 2^6$ and can support only those cycles taken from the set $\{1, 2, 4, 8\}$: $\mathcal{C}_A = [4, 1] + [6, 2] + [12, 4]$, $\mathcal{C}_B = \mathcal{C}_C = [2, 1] + [1, 2] + [3, 4] + [6, 8]$.

Observation 1: Since primitive graph decompositions are not particularly representative of global topologies, it can hardly be surprising to find a large number of nonisomorphic topologies supporting virtually the same dynamics.

Observation 2: There are well established theorems and techniques for almost all cases of interest in which one is interested either in finding $P_L(x)$ for some arbitrarily complicated topology or in constructing complex graphs out of simpler

topologies whose $P_i(x)$ are already known. The problem is thus effectively reduced to polynomial factorization over $\mathcal{F}[q]$. Reference [harary73] provides an excellent summary of the most important results concerning evaluation of $P(x)$.

Observation 3: Whenever $P(x) = \sum_{i=1}^r [p_i(x)]^{\nu_i}$ is such that $\sum_{i=1}^r \nu_i$ is *small*, it becomes possible to determine the exact dynamics with relatively little direct calculation. *Ex:* of the $2^7 = 128$ possible distinct $P(x) \pmod{2}$ in $\mathcal{F}[2]$ for graphs of order ‘ $N = 14$ ’, ‘ 18 ’ are in the same class $\mathcal{Q}$ for which $P(x) = [p(x)]^2$, with $\deg[P(x)] = 7$ and $\text{ord}[p(x)] = 127$. Any $\mathcal{L} \in \mathcal{Q}$ is able to support only one of two possible cycle sums ($\mathcal{C}_a = [1, 1] + [129, 127]$ or $\mathcal{C}_b = [1, 1] + [1, 127] + [64, 254]$) so that the actual system must be studied exactly for a *maximum* of ‘256’ steps to be certain of its overall behavior. A majority of systems can be analyzed very rapidly in this manner; particularly easy to study are those defined over $\mathcal{F}[2]$.

5.4.4 Simplifications in $\mathcal{F}[2]$

The general problem simplifies considerably in the finite field $\mathcal{F}[2]$. Because circuits are always counted at least twice, their number contributes a factor ‘ $\equiv 0 \pmod{2}$ ’: we see from equation (5.14), therefore, that the *only* structural information necessary to obtain $P_L(x)$ is that of the *parity of disjoint edge distributions*. Moreover, since there is no way to distribute disjoint edges among an *odd* number of vertices, equation (5.13) gives

$$a_i = \begin{cases} 0 & \text{if ‘} i \text{’ is odd} \\ 1 & \text{if the \# of } (\frac{i}{2})\text{-disjoint edges} \\ & \text{in } \mathcal{L} \text{ is odd for ‘} i \text{’ even} \end{cases} \quad (5.112)$$

Figure 5.3 shows three distinct *size* $N = 10$ topologies belonging to the same $\mathcal{Q}$ in $\mathcal{F}[2]$: notice that superficial topological dissimilarities such as *average degree* and *diameter* are clearly irrelevant in predicting a similarity in dynamic behavior. Also, since all $\mathcal{Q}$ contain at least one representative *tree*, a significant range of possible dynamical evolutions for a given N can actually be studied by observing trees alone (for which topological decompositions are especially easy [boll79]). In appendices A and B we calculate essentially all possible dynamical behaviors under additive rules for any (undirected) graph of order $5 \leq N \leq 10$.

Below, we give a sampling of the sorts of dynamical behaviors that can immediately be deduced from basic topological features of $\mathcal{L}$.

Reversible Behavior: *all states Σ are on cycles if and only if x does not divide $P_L(x)$* , a fact requiring only that the last coefficient $a_N \equiv 1 \pmod{2}$. We conclude that

1. there are *no* $\mathcal{L}$ with reversible dynamics under **OT** rules for *odd* N .
2. for $N = 2j$ we can have reversible behavior if and only if the number of ‘ j -disjoint edges’ in $\mathcal{L}$ is *odd*.[†] The topological content of reversible dynamics is

[†]This tells us, for example, that *no size- N 1-dim CA with periodic boundary conditions* obeying

thus effectively defined by solutions of the *dimer* problem on arbitrary lattices

EXAMPLE: Consider an $m \times n$ lattice, where ‘ m ’ is even. From the explicit solution to the dimer problem [boll79], given by

$$\text{Number of dimer coverings} = 2^{mn} \prod_{j=1}^{m/2} \prod_{i=1}^n \left\{ \cos^2 \frac{\pi}{m+1} j + \cos^2 \frac{\pi}{n+1} i \right\},$$

we find that $a_N \equiv 1 \pmod{2}$ if and only if the $\gcd(m+1, n+1)=1$.

3. structural stability: Given a graph G supporting reversible behavior we want to know whether the reversibility is retained upon either an *addition* or *deletion* of a single link. We ‘*perturb*’ a lattice by $\mathbf{L}_{ij} \rightarrow \mathbf{L}_{ij} + \ell_{ab}$, where ℓ_{ab} is an $(N \times N)$ matrix all of whose entries are *zero* except for $\ell_{ab} = 1$. Since

$$a_N = \det(\mathbf{L}) = \sum_{\text{permutations } \pi} \ell_{1\pi(1)} \ell_{2\pi(2)} \cdots \ell_{N\pi(N)} \pmod{2}, \quad (5.113)$$

we have $\tilde{a}_N = \det(\mathbf{L}) \oplus_2 \det(\tilde{\mathbf{L}})$, where $\tilde{\mathbf{L}}$ is the ‘ $(N-2) \times (N-2)$ ’ adjacency matrix for a graph $\tilde{G} \equiv G - \{a, b\} - \{\ell_{ia}, \ell_{jb} | i, j \in G \text{ and } \ell_{ia} = 1, \ell_{jb} = 1\}$. We see that reversible dynamics on a graph G is stable with respect to single link addition or deletion if and only if the number of $(\frac{N-2}{2})$ -disjoint edges in $\tilde{G}$ is *even*.

4. to get an idea of how frequently an **OT** additive rule yields reversible behavior in the most general case of a (not necessarily symmetric) lattice $\mathbf{L}$ with *weighted* links (weights $\in \mathcal{F}[p]$, ‘ p ’ prime), we calculate the fraction of $(N \times N)$ matrices which are nonsingular:

$$f_{\text{nonsingular}}(p, N) = \frac{1}{p^{N^2}} \prod_{i=1}^N (p^N - p^{i-1}) \quad (5.114)$$

The first few values are given by $f(2, N > 9) \sim 0.29$, $f(3, N > 7) \sim 0.56$, $f(5, N > 4) \sim 0.76$. The (approximate) fraction of *symmetric* $(0, 1)$ matrices which are nonsingular (*i.e.* defining **OT** additive rules) is given for $7 \leq N \leq 15$ for small ‘ p ’ in table 5.4. [†]

Trivial Behavior: by *trivial* we mean that all states $\Sigma \rightarrow \mathbf{0}$ in finite time. This occurs if $\mathbf{L}$ is nilpotent $\implies P_L(x) = x^N \implies$ the number of decompositions into r -disjoint edges is *even* for all r . We see immediately that

the rule $\phi(\sigma_i) = \sigma_{i-1} \oplus_2 \sigma_{i+1}$ can support a reversible dynamics. On the other hand, *all even size* 1-dim lattices with *free ends* (*i.e.* *even length paths*) have reversible dynamics.

[†]The dimer problem effectively consists of exactly enumerating the number of ways an arbitrary lattice can be decomposed into non-intersecting edges, without any leftover links: covering an $n \times n$ chessboard with $n^2/2$ dominoes, for example, so that the entire board is covered without overlap or gaps.

[‡]Results were obtained by averaging over computer generated ensembles of random matrices.

N	p:	2	3	5	7	11
7		0	0.39	0.42	0.42	0.42
8		0.42	0.50	0.57	0.58	0.59
9		0	0.51	0.57	0.58	0.59
10		0.42	0.55	0.67	0.68	0.70
11		0	0.58	0.68	0.72	0.74
12		0.42	0.60	0.74	0.77	0.80
13		0	0.62	0.75	0.80	0.84
14		0.42	0.63	0.77	0.82	0.87
15		0	0.63	0.78	0.84	0.88

Table 5.4 Fraction of symmetric $(0, 1)$ -matrices which are nonsingular in finite fields $\mathcal{F}[p]$ (p -prime) – gives the probability that a random (undirected) lattice evolving according to an **OT** $\oplus_p$ rule yields *reversible behavior*.

1. No lattices with an *odd* number of edges can support a trivial dynamics. *Ex:* all *even- N trees*.

2. *Paths:* using the explicit form $P = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{N-k}{k} x^{N-2k} \pmod{2}$ for paths [harary73], it is easy to see that $P_{\text{path}}(x) = x^N \Leftrightarrow N = 2^n - 1, n \geq 1$.

3. *Circuits:* from $P = x^N + \sum_{i=1}^{\lfloor n/2 \rfloor} \frac{N}{i} \binom{N-i-1}{i-1} x^{N-2i} \pmod{2}$ [cvet79], we similarly find that $P_{\text{circuit}} = x^N \Leftrightarrow N = 2^n, n \geq 1$.

4. *r -regular graphs* ($r \geq 2$): the first two coefficients of $P_{r\text{-reg}}(x)$ can be calculated exactly:[†]

$$\begin{cases} a_2 = Nr/2 \pmod{2} \\ a_4 = Nr \{ r(\frac{N}{2} - 2) + 1 \} / 4 \pmod{2}. \end{cases} \quad (5.115)$$

From this we can deduce that

$$a_2 \equiv a_4 \equiv 0 \iff \begin{cases} N \equiv 0 \pmod{8}, & 2 \leq r < N, \text{ or} \\ r \equiv 0 \pmod{8}, & N \geq r + 1, \text{ or} \\ N \equiv 4 \pmod{8}, & r \text{ even, or} \\ r \equiv 4 \pmod{8}, & N \text{ even,} \end{cases} \quad (5.116)$$

and that trivial dynamics *cannot* occur for any r -regular graphs either when N is *odd* and $r \not\equiv 0 \pmod{8}$, or r is *odd* and $N \not\equiv 0 \pmod{8}$.

5. From equation 5.108 we see that $a_N^T = 1 + \sum_{i=2}^N a_i^{\text{OT}}$. Thus, if an **OT** additive rule yields *trivial* dynamics on $\mathcal{L}$, the corresponding **T** rule supports *reversible*

[†]To get a_4 , we observe that each edge has ' $a_2 - 2(r-1) - 1$ ' disjoint edges to pair with. Summing over a_2 edges and dividing by '2' for the double counting we get the result.

behavior on the same lattice.

Complexity: Let C_i be the ' i^{th} ' cycle in the cycle set $\mathcal{C}$ in G_L , corresponding to the $[n_i, t_i]$ term in the cycle sum expansion. Using ' $v(T_\sigma) \equiv \#$ of states on the tree rooted at the state σ ', so that $p[C_i] \equiv$ 'fraction of the number of initial configurations which are attracted into each cycle C_i ' $= n_i(1 + v(T_\sigma))/2^N$, we introduce the *global complexity*[‡]

$$S_g \equiv - \sum_{C_i \in \mathcal{C}} p[C_i] \ln p[C_i]. \quad (5.117)$$

S_g gives the amount of information of the initial state necessary to predict the final state of the system. In the present notation, with ' $\alpha \equiv$ largest integer such that $x^\alpha | P_L(x)$ ', we can calculate this quantity exactly:

$$S_g = (N - \alpha) \ln 2 - 2^{\alpha-N} \sum_{C_i \in \mathcal{C}} n_i \ln n_i. \quad (5.118)$$

For trivial dynamics $S_g = 0$; in general, $S_g \leq 2^N$, with equality holding when $\alpha = 0$ and $n_i = 1$ for all ' i '. Since $\varepsilon = (1+x)$ is the only irreducible polynomial with $\text{ord}(\varepsilon) = 1$, this is possible only if $\{\varepsilon_i\}$ consists of $\{\varepsilon_1 = \varepsilon_2 = \dots = \varepsilon_N = (1+x)\} \implies S_g = 2^N$ only if $P_L(x) = (1+x)^N$, which therefore defines the appropriate equivalence class $\mathcal{Q}$ for *maximal complexity*. Note that $\mathcal{L} \in \mathcal{Q}_{\text{OT}}^{S_{\text{max}}} \Rightarrow \mathcal{L} \in \mathcal{Q}_T^{S=0}$.

To gain useful information as to the structure of the transient and cycle sets, we define the *external* (S_E) and *internal* (S_I) complexities:

$$\begin{cases} S_E \equiv - \sum_{T_i \in \mathcal{C}} p[T_i] \ln p[T_i]; & p[T_i] \equiv \frac{\sum_{\sigma \in \mathcal{C}} v(T_\sigma)}{2^{N-v(\mathcal{C})}} \\ S_I \equiv - \sum_{C_i \in \mathcal{C}} \tilde{p}[C_i] \ln \tilde{p}[C_i]; & \tilde{p}[C_i] \equiv \frac{n_i}{v(\mathcal{C})}, \end{cases} \quad (5.119)$$

which give the information content of the *tree* and *cycle* structure, respectively, taken as independent sets, and where $v(\mathcal{C})$ is the volume of the cycle set ($= \sum_i n_i t_i$).

The three complexities are typically related by $S_E \leq S_g \leq S_I$, with equality occurring for additive rules. For the more general rules dealt with in the next sections the magnitudes of the deviation from equality give some indication of the organization of various parts of the topology of G_L as compared with the additive case.

Similarity: Arbitrarily large families of distinct (directed) topologies can be generated graphically by observing that there is only a single non-trivial elementary row(r)/column(c) operation on matrices over $\mathcal{F}[2]$: $r_i(c_i) \rightarrow r_i(c_i) \oplus 2^j(c_j)$. Defining the three vertex neighborhoods $C_1(i)$, A_{ij} and $B_j(i)$,

[‡]Called the *basin complexity* by Kaneko in [kaneko86a].

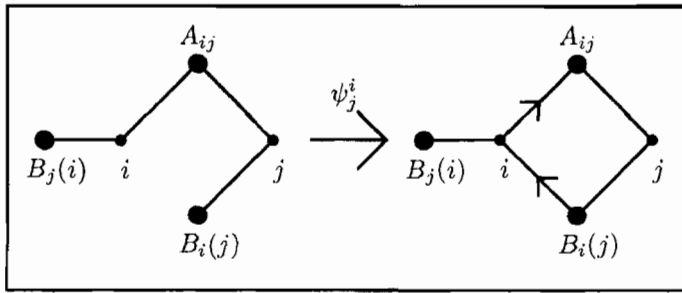


Fig. 5.5 Local action of the topological operator ' ψ ' with which any number of distinct structures supporting exactly the same global dynamics can be constructed. The various quantities are defined in equation (5.27). Solid lines represent 2-cycles.

$$\begin{cases} C_1(i) \equiv \{\text{vertices } 'k' \mid d(i, k) = 1\}, \\ A_{ij} \equiv \{k \mid d(i, k) = d(j, k) = 1\}, \\ B_j(i) \equiv C_1(i) - A_{ij}, \end{cases} \quad (5.120)$$

we introduce a *topological operator* ψ_j^i , acting on vertex ' i ' with respect to ' j ', which has the following action: $\psi_j^i : C_1(i) \rightarrow C_1(i) - A_{ij} + B_i(j)$ (see figure 3.3). That is, for any two vertices ' i, j ' such that all incoming arrows from A_{ij} are deleted and incoming arrows from all vertices in $B_j(i)$ are added to ' i ', we get a new topology $\mathcal{L}'$ supporting exactly the same global dynamics.

5.4.5 Discussion

In this section we have presented some preliminary results of a study of the lattice topology influence on the global dynamics of deterministic cellular automata. For the general class of additive rules, whose behavior is well known to be amenable to an exact analysis, it is found that an elementary topological specification of a given lattice (such as that provided by finding the number of disjoint-circuit subgraphs present), often suffices in giving an effective description of the sorts of dynamical behaviors possible on that lattice. In the simplest case, when the site variables $\sigma \in \mathcal{F}[2]$, it is only the *parity of n -disjoint edge subgraphs* present in a lattice which determines the scope of behavior: since this kind of topological decomposition depends only minimally on the exact global structure, there are typically very large numbers of nonisomorphic graphs supporting essentially the same kind of dynamical behavior. In the appendix 5-B, for example, we list most of the ~ 200 possible cycle-sum sets for systems of size $N = 10$ – a negligible fraction of the $\sim 10^6$ possible distinct connected topologies of that same size.

We have treated the problem from one point of view only, of course (for a phenomenological analysis of CA behavior as a function of lattice structure, see section 3.3). Many of the questions concerning the exact relationship between lattice topology and dynamics remain unanswered, awaiting a deeper study. We mention

only a few of the outstanding fundamental problems deserving attention:

1. *What is the complete behavioral specification of a given transition rule on arbitrary lattices?* Which topologies yield trivial or complex dynamics? What fraction of topologies of given size induce a particular variety of dynamical behavior?
2. *What are the generic effects of minimal topological deformations to a given lattice?* How well organized does the cycle set structure remain when the lattice is slightly altered? What fraction of the complete cycle-set typically survives such an alteration? Concerning *class-4* automata, which are really defined only for infinitely large lattices, a most important question is how the capacity for supporting universal computation is compromised by particular structural deficiencies?
3. *What can be said of local topology dependence in larger (and infinite) systems (for which direct calculation of global measures becomes clearly impractical)?* How does the average information transmission speed depend on local peculiarities of structure?

Studies of these kinds are of particular importance to all theoretical information storage and retrieval systems incorporating some form of geometry modification, such as those modeled by certain neural networks.

5.5 Lyapunov Functions and Threshold CA Rules

Classical *Lyapunov functions* are an important tool for determining the stability of solutions to continuous dynamical systems [sanch68]. An analogous discrete construct, which is the subject of this section, has also proven to be enormously useful in characterizing the behavior of certain kinds of CA rules; most notably the class of *threshold* (or *voting*; see section 3.4.3) rules. In particular, Lyapunov functions help to both characterize the long-term behavior of a finite system by specifying the possible cycle lengths, and provide bounds on the length of transients.

A discrete version of classical Lyapunov functions was first introduced by Hopfield in his analysis of the fixed point behavior of random sequential updates of associative neural networks [hopf82]. Cohen and Grossberg [cohenm83] constructed global Lyapunov functions for a large class of continuous neural nets. The Lyapunov functions to be described below were originally introduced by Fogelman-Soulie and Goles for studying both sequential of threshold CA rules ([fogel83], [fogel85]) and parallel updating ([goles82], [goles85], [goles87b]). A similar class of functions was also applied by Pomeau to reversible automata [pomeau84].[†] An extensive formal mathematical treatment of the material presented appears in the excellent book by Goles and Martinez [goles90].

[†]Section 8.1 contains a discussion of additive invariants, including Pomeau's, within the context of reversible CA systems.

5.5.1 Generalized Threshold Automata

Threshold automata date back to McCulloch and Pitts' [mccul43] interconnected networks of binary valued neurons. In their networks, a given neuron becomes *active* if and only if the number of active neighboring neurons exceeds some threshold. In order to emphasize the broad applicability of Lyapunov functions, we will actually deduce both the long-term and transient behavior for slightly more generalized (but still binary valued) versions of threshold rules than those originally introduced by McCulloch and Pitts. In particular, we will prove results for rules for which different sites may have different thresholds, and the underlying lattice structure (or, more correctly, the neuronal interconnectivity pattern) is essentially arbitrary. Properties of simpler one and two dimensional systems, such as the class of voting rules, will then be seen as immediate consequences of much more general theorems.

Using site variables $\sigma \in \{0, 1\}$, the generalized threshold transition function ϕ_{gtf} is defined by:

$$\sigma_i(t+1) = \phi_{\text{gtf}}[\vec{\sigma}(t); A, \vec{b}] = \begin{cases} 1 & \text{if } \sum_{j=1}^N a_{ij}\sigma_j(t) \geq b_i, \\ 0 & \text{else,} \end{cases} \quad (5.121)$$

where $A = a_{ij}$ is a symmetric (i.e. $a_{ij} = a_{ji}$ for all i, j) real-valued but otherwise arbitrary *synaptic-weight matrix*, b_i is the i^{th} element of an arbitrary *threshold vector* $\vec{b} = (b_1, \dots, b_N)$ and N is the total number of sites. In what follows, the dynamics itself proceeds in the usual parallel fashion; that is to say, all sites i are simultaneously updated throughout the lattice on each iteration step. Sequential updates, such as used by Hopfield [hopf82], are intriguing in their own right, of course – the Lyapunov Functions defined for sequentially updated threshold rules take on the form of *spin-glass* energies, for example – and are discussed briefly in the last section.

Notice that the lattice structure is implicit in the synaptic-weight matrix A ; indeed, the astute reader no doubt wants to jump ahead a few lines, set $a_{ij} \in \{0, 1\}$ for all i, j , and interpret A as the adjacency matrix for the underlying lattice. The more general interpretation for the elements of A is an outgrowth of ϕ_{gtf} 's neural-net origins: $a_{ij} > 0$ is interpreted as being an *excitatory* synaptic weight and $a_{ij} < 0$ as an *inhibitory* weight – the i^{th} neuron is excited if and only if the weighted sum $\sum_j a_{ij}\sigma_j$ is greater than its threshold b_i . We invite the reader to show that there is no loss in generality in assuming that the threshold vector always satisfies the condition

$$b_i \neq \sum_j a_{ij}\sigma_j \quad \text{for all } i, \vec{\sigma}. \quad (5.122)$$

As we shall see immediately, this condition, together with the linearity of the neuronal excitations in the threshold condition, allows us to determine a finite system's fate (*almost* entirely) analytically.

5.5.2 Lyapunov Functions

A classical *Lyapunov Function* of a continuous dynamical system $\dot{\vec{x}} = \vec{f}(\vec{x}, t)$, is any non-increasing function g on the orbits of $\vec{f}$: i.e. for all $t \geq 0$, $g[\vec{x}(t+1)] \leq g[\vec{x}(t)]$ [sanch68]. Now let $\mathcal{X}_{\vec{\phi}}(t) = \{\vec{\sigma}(0), \vec{\sigma}(1), \dots, \vec{\sigma}(t)\}$ be the orbit set of a discrete system $\vec{\sigma}(t+1) = \vec{\phi}[\vec{\sigma}(t)]$. The analogous discrete Lyapunov function is a function $\tilde{g}$ on the orbits of $\mathcal{X}_{\vec{\phi}}(t)$ such that, for all $t \geq 0$, $\tilde{g}[\vec{\sigma}(t+1)] \leq \tilde{g}[\vec{\sigma}(t)]$.

Consider the following function L for all $t \geq 1$:

$$L[\vec{\sigma}(t), \vec{\sigma}(t+1)] = -\sum_i \sigma_i(t+1) \sum_j a_{ij} \sigma_j(t) + \sum_i b_i \{\sigma_i(t+1) + \sigma_i(t)\}. \quad (5.123)$$

We first note that since A is symmetric,

$$\begin{aligned} \Delta_t L &= L[\vec{\sigma}(t), \vec{\sigma}(t+1)] - L[\vec{\sigma}(t-1), \vec{\sigma}(t)], \\ &= -\sum_{i=1}^N [\sigma_i(t+1) - \sigma_i(t-1)] \left(\sum_{j=1}^N a_{ij} \sigma_j(t) - b_i \right). \end{aligned} \quad (5.124)$$

Now consider each of the possible terms in the summation at right. If in the i^{th} sum, $\sigma_i(t+1) = \sigma_i(t-1)$, that term vanishes identically; if the terms are unequal, say, $\sigma_i(t+1) = 1$ and $\sigma_i(t-1) = 0$, then, using equation 5.122, we have that $\sum_j a_{ij} \sigma_j(t) - b_i > 0$ and thus that $[\sigma_i(t+1) - \sigma_i(t-1)] \left(\sum_j a_{ij} \sigma_j(t) - b_i \right) > 0$. We therefore find that

$$\Delta_t L \leq 0, \quad (5.125)$$

and $\Delta_t L < 0$ if and only if $\sigma_i(t+1) \neq \sigma_i(t-1)$. In other words, we have shown that the function $L = L[\vec{\sigma}(t), \vec{\sigma}(t+1)]$ is a *Lyapunov function of the generalized threshold rule defined by equation 5.121*. As the next two subsections show, variants of this function allow us to both characterize the nature of the system's orbits and place bounds on the possible transient lengths; we follow mainly [goles85b], [goles87b], and [goles90].

5.5.3 Characterization of Orbits

If the number of sites $N < \infty$, we know that the system will eventually reach some cyclic state. Suppose we obtain a cycle of period T : $\vec{\sigma}(0) \rightarrow \vec{\sigma}(1) \rightarrow \dots \rightarrow \vec{\sigma}(T-1) \rightarrow \vec{\sigma}(0)$. Then, since we have just concluded that L must be strictly decreasing for cyclic states,

$$\begin{cases} \Delta_1 L &= L[\vec{\sigma}(1), \vec{\sigma}(2)] - L[\vec{\sigma}(0), \vec{\sigma}(1)] &< 0 \\ \Delta_2 L &= L[\vec{\sigma}(2), \vec{\sigma}(3)] - L[\vec{\sigma}(1), \vec{\sigma}(2)] &< 0 \\ \vdots &\vdots & \\ \Delta_{T-1} L &= L[\vec{\sigma}(T-1), \vec{\sigma}(0)] - L[\vec{\sigma}(T-2), \vec{\sigma}(T-1)] &< 0 \\ \Delta_0 L &= L[\vec{\sigma}(0), \vec{\sigma}(1)] - L[\vec{\sigma}(T-1), \vec{\sigma}(0)] &< 0, \end{cases} \quad (5.126)$$

and thus that

$$L[\vec{\sigma}(0), \vec{\sigma}(1)] > L[\vec{\sigma}(1), \vec{\sigma}(2)] > \cdots L[\vec{\sigma}(T-1), \vec{\sigma}(0)] > L[\vec{\sigma}(0), \vec{\sigma}(1)], \quad (5.127)$$

which is an obvious contradiction. It must therefore be true that either $\vec{\sigma}(t+1) = \vec{\sigma}(t)$ or $\vec{\sigma}(t+1) = \vec{\sigma}(t-1)$. In other words, we have just proven the following theorem.

Theorem 5 [goles87a] *If the synaptic-weight matrix A is symmetric, and the number of sites in the lattice is finite, then the orbits of the generalized threshold rule (equation 5.121) are either fixed points or cycles of period two.*

5.5.4 Bound on Possible Transient Lengths

A slightly different Lyapunov function from the one defined above can be used to put bounds on the transient length. Let

$$\begin{aligned} L'[\vec{\sigma}(t), \vec{\sigma}(t+1)] &= -\sum_i [2\sigma_i(t+1) - 1] \sum_j a_{ij} [2\sigma_j(t) - 1] \\ &\quad + \sum_i [2b_i - \sum_j a_{ij}] [2\sigma_i(t+1) - 1 + \sigma_i(t) - 1]. \end{aligned} \quad (5.128)$$

A simple calculation shows that $\Delta_t L' = L'[\vec{\sigma}(t), \vec{\sigma}(t+1)] - L'[\vec{\sigma}(t-1), \vec{\sigma}(t)] = 4\Delta_t L$, so that if L is a decreasing Lyapunov function, L' must also be a decreasing Lyapunov function.[‡]

Let $\mathcal{X}_\tau = \{\vec{\sigma}(0), \vec{\sigma}(1), \dots, \vec{\sigma}(\tau-1)\}$ be the transient set, and $\vec{\sigma}(\tau)$ the first global state belonging to the stationary (i.e. cyclic) state associated with initial state $\vec{\sigma}(0)$.

We introduce two useful quantities: (1) From the definition of L (equation 5.123), we know that L is strictly decreasing for all $\vec{\sigma} \in \mathcal{X}_\tau$. We can therefore define the positive quantity

$$e = \min_{1 \leq t \leq \tau-1} |\Delta_t L'| = \min_{1 \leq t \leq \tau-1} |L'[\vec{\sigma}(t), \vec{\sigma}(t+1)] - L'[\vec{\sigma}(t-1), \vec{\sigma}(t)]| > 0. \quad (5.129)$$

(2) From equation 5.122, we know that $\sum_j a_{ij} \sigma_j - b_i \neq 0$ for any vector $\vec{\sigma}$, so that we can also define the positive quantities

$$e_i = \min_{\vec{\sigma}} \left| \sum_j a_{ij} \sigma_j - b_i \right|, \quad i = 1, 2, \dots, N. \quad (5.130)$$

[‡]The minor difference in form between L and L' is due to our choice of $\sigma \in \{0, 1\}$ variables as opposed to $S \in \{+1, -1\}$ variables. This particular form for L' just happens to be more convenient to work with when using σ variables. The reader is encouraged to retrace our steps using S instead of σ variables and the same L as used in proving Theorem 5. How our variables are labeled obviously cannot affect the dynamics.

Now consider the i^{th} term in the expression for L' (equation 5.128):

$$\begin{aligned} L'_i[\vec{\sigma}(t), \vec{\sigma}(t+1)] &= -[2\sigma_i(t+1) - 1] \sum_j a_{ij} [2\sigma_j(t) - 1] \\ &\quad + [2b_i - \sum_j a_{ij}] [2\sigma_i(t+1) - 1 + \sigma_i(t) - 1]. \end{aligned} \quad (5.131)$$

We see that L' is bounded below by

$$L' \geq L'_{\text{lower}} = -\sum_j |a_{ij}| - 2|2b_i - \sum_j a_{ij}|. \quad (5.132)$$

Rewriting L' as

$$\begin{aligned} L'_i[\vec{\sigma}(t), \vec{\sigma}(t+1)] &= -2[2\sigma_i(t+1) - 1] \sum_j a_{ij} [2\sigma_j(t) - b_i] \\ &\quad + [2b_i - \sum_j a_{ij}] [2\sigma_i(t) - 1], \end{aligned} \quad (5.133)$$

and using the definition of e_i in equation 5.130, we also see that L' is bounded above by

$$L' \leq L'_{\text{upper}} = -2e_i + |2b_i - \sum_j a_{ij}|. \quad (5.134)$$

Thus,

$$-\|A\| - 2\|2\vec{b} - A\vec{1}\| \leq L'_i[\vec{\sigma}(t), \vec{\sigma}(t+1)] \leq -2\sum_i e_i + \|2\vec{b} - A\vec{1}\|, \quad (5.135)$$

where $\|A\| = \sum_{ij} |a_{ij}|$, $\vec{1} = (1, 1, \dots, 1)$ is the constant 1-vector and $\|\vec{v}\| = \sum_i |v_i|$ for any vector $\vec{v}$.

To see how to use this result to bound the transient length, we first note that since L' is strictly decreasing in the transient phase, equation 5.129 yields

$$L'[\vec{\sigma}(t), \vec{\sigma}(t+1)] \leq L'[\vec{\sigma}(t-1), \vec{\sigma}(t)] - e \leq L'[\vec{\sigma}(0), \vec{\sigma}(1)] - te. \quad (5.136)$$

Therefore, using equation 5.135 and setting $t = \tau$, we have that

$$-\|A\| - 2\|2\vec{b} - A\vec{1}\| \leq L'[\vec{\sigma}(\tau), \vec{\sigma}(\tau+1)] \leq L'[\vec{\sigma}(0), \vec{\sigma}(1)] - \tau e. \quad (5.137)$$

Now, since $L'[\vec{\sigma}(0), \vec{\sigma}(1)] \geq -\|A\| - 2\|2\vec{b} - A\vec{1}\|$, we conclude that $\tau e \leq L'[\vec{\sigma}(0), \vec{\sigma}(1)] + \|A\| + 2\|2\vec{b} - A\vec{1}\|$. Finally, adding the fact that $L'[\vec{\sigma}(0), \vec{\sigma}(1)] \leq -2\sum_i e_i + \|2\vec{b} - A\vec{1}\|$,

we have proven the following theorem.

Theorem 6 [goles87b] *If A is symmetric, then the transient length of the generalized threshold rule defined in equation 5.121 is bounded by*

$$\tau(A, \vec{b}) \leq \frac{1}{e} \left(-2\sum_i e_i + 3\|2\vec{b} - A\vec{1}\| + \|A\| \right). \quad (5.138)$$

We now consider two special cases of the symmetric matrix A ; namely, (1) the entries of A are allowed to take on only integer values, and (2) the entries of A are all binary valued.

5.5.4.1 A Is an Integer Valued Symmetric Matrix

In the special case where A is an integer matrix – i.e. where $a_{ij} \in \mathbb{Z}$, for all i, j – we can obtain bounds on the quantities e (equation 5.129) and e_i (equation 5.130) and thereby get an explicit form for τ as a function of A and $\vec{b}$.

We first observe that if $\alpha_i \in \mathbb{Z}$, $i = 1, 2, \dots, n$, then, for all $v_i \in \mathbb{Z}$, $\sum_i \alpha_i v_i \geq \lceil x \rceil$ if and only if $\sum_i \alpha_i v_i \geq \lceil x \rceil - \frac{1}{2}$, where $\lceil x \rceil$ is the least integer greater than or equal to x . This means that if A is an integer matrix, we can always assume that the individual components of the threshold vector $\vec{b}$ are of the form $b_i = z_i + \frac{1}{2}$, $z_i \in \mathbb{Z}$. Using this form for $\vec{b}$, we see from equation 5.129 that

$$e_i = \min_{\vec{\sigma}} \left| \sum_j a_{ij} \sigma_j - b_i \right| \geq \frac{1}{2}, \quad i = 1, 2, \dots, N. \quad (5.139)$$

From the fact that $\Delta_t L' = 4\Delta L = -4 \sum_{i=1}^N [\sigma_i(t+1) - \sigma_i(t-1)] (\sum_{j=1}^N a_{ij} \sigma_j(t) - b_i)$ (equation 5.124 and comment following equation 5.128), and $e > 0$ (equation 5.129), we see that $e \geq 4 \cdot 1 \cdot \frac{1}{2} = 2$. By substituting these two bounds on e and e_i in equation 5.138, we obtain the following corollary to theorem 6:

Corollary 1 [goles87a] *If A is an $n \times n$ integer-valued symmetric matrix, then the transient length of the generalized threshold rule defined in equation 5.121 is bounded by*

$$\tau(A, \vec{b}) \leq \frac{1}{2} \left(-n + 3\|2\vec{b} - A\vec{1}\| + \|A\| \right). \quad (5.140)$$

5.5.4.2 A is a Binary Valued Symmetric Matrix

Another special case of theorem 6 occurs for matrices A that actually reflect the local neighborhood structure around each site. Suppose that $a_{ij} = a_{ji} = 0$ unless $\sigma_j \in \mathcal{N}_i$, where $\mathcal{N}_i$ is the neighborhood of site i , in which case $a_{ij} \in \{-1 \text{ (inhibitory)}, +1 \text{ (excitatory)}\}$. Suppose also that the size of the neighborhood $|\mathcal{N}_i| = \mathcal{N}$ for all i . It is then easy to show from corollary 1 that [goles85b]

$$\tau(A, \vec{b}) \leq 5n\mathcal{N}. \quad (5.141)$$

While this bound is not a particularly strong one and convergence is generally faster in practice [goles90], it does clearly point out the important fact that transient times are *linearly bounded by the lattice size n* . Notice that this is not true of more general classes of matrices, even those of the preceding section that are both symmetric and integer-valued. Equation 5.140 shows that the transient time depends on both $\|A\|$ and $\|2\vec{b} - A\vec{1}\|$; if both A and $\vec{b}$ are arbitrary (save, perhaps, for A 's symmetry), there is of course no particular reason to expect τ to be linearly

bounded by the size of the system. Goles, *et.al.* in fact show that for any n , there exists a symmetric $n \times n$ matrix A and size n threshold vector $\vec{b}$ such that the transient length $\tau(A, \vec{b}) \geq 2^{n/3}$ ([goles81], [goles89]); [goles90] provides an explicit construction.

5.5.5 One-dimensional Majority Rules

Consider the one-dimensional majority rule defined on a radius- r neighborhood:

$$\sigma_i(t+1) = \phi_{1d \text{ majority}}[\sigma_{i-r}, \dots, \sigma_{i+r}] = \begin{cases} 1 & \text{if } \sum_{j=i-r}^{i+r} \sigma_j(t) \geq r+1, \\ 0 & \text{else.} \end{cases} \quad (5.142)$$

We recognize that $\phi_{1d \text{ majority}}$ is merely a special case of the generalized threshold rule defined in equation 5.121. In particular, $\phi_{1d \text{ majority}}$ may be defined using that more general definition by setting

$$\begin{cases} a_{ij} = \begin{cases} 1 & \text{if } |i-j| \leq r, \\ 0 & \text{else,} \end{cases} & \text{for all } i, j \\ b_i = r + \frac{1}{2} & \text{for all } i. \end{cases} \quad (5.143)$$

5.5.5.1 Cyclic States

Since theorem 5 applies to this system, we immediately conclude that $\phi_{1d \text{ majority}}$ can yield only either fixed points or cycles of period two. It turns out that one can actually prove a stronger result for this particular rule. Let a *finite state* be any state consisting of a finite number of nonzero sites. Then we have the following theorem.

Theorem 7 ([tch82], [goles84], [goles90]) *All finite initial states evolve, under the map $\vec{\phi}_{1d \text{ majority}}$, to a fixed point in a finite number of steps.*

Proof: The proof consists of two parts. The first part, which we leave to the reader to show, is to observe that if a state $\vec{\sigma}$ is a fixed point of $\phi_{1d \text{ majority}}$ then it *must* be of the following form:

$$\vec{\sigma} = (\vec{0}^\infty, \vec{1}^{n_1}, \vec{0}^{n_2}, \vec{1}^{n_3}, \dots, \vec{0}^{n_{m-1}}, \vec{1}^{n_m}, \vec{0}^\infty), \quad n_j \geq r+1, \quad j = 1, 2, \dots, m, \quad (5.144)$$

where $\vec{\alpha}^p$ represents a block of p consecutive α 's.

The second part is to show that if we assume a finite state $\vec{\sigma}$ is *not* a fixed point – which, according to theorem 5, necessarily makes it period two, or that

$\vec{\phi}_{1d \text{ majority}}^2[\vec{\sigma}] = \vec{\sigma}$ – then a contradiction ensues; we thus conclude that only fixed points are allowed.

To show this second part, we first write the finite state $\vec{\sigma} = (\vec{0}^\infty, \vec{1}^{n_1}, \vec{0}^{n_2}, \vec{1}^{n_3}, \dots, \vec{0}^{n_{m-1}}, \vec{1}^{n_m}, \vec{0}^\infty)$, and note that, since it is of period two, it cannot be true that $n_j \geq r+1$ for any $j = 1, 2, \dots, m$. Let i_0 be the first coordinate such that $\sigma_{i_0-1} \neq \sigma_{i_0} = \sigma_{i_0+1} = \dots = \sigma_{i_0+m-1} \neq \sigma_{i_0+m}$ with $m < r$. Since, by construction, all sites $i < i_0$ belong to equal-valued blocks of length $l \geq r+1$, $\sigma'_i = (\vec{\phi}_{1d \text{ majority}}[\vec{\sigma}])_i = \sigma_i$. On the other hand, since the number of elements σ_j in the radius- r neighborhood of i_0 that are *unequal* to σ_{i_0} exceeds $r+1$, $(\vec{\phi}_{1d \text{ majority}}[\vec{\sigma}])_{i_0} = 1 - \sigma_{i_0}$. Moreover, since the same holds true for all sites $i < i_0$, $(\vec{\phi}_{1d \text{ majority}}[\vec{\sigma}])_{i_0} = (\vec{\phi}_{1d \text{ majority}}[\vec{\sigma}])_{i_0-1} = \dots = (\vec{\phi}_{1d \text{ majority}}[\vec{\sigma}])_{i_0-(m+1)} = 1 - \sigma_{i_0}$. We therefore have that $(\vec{\phi}_{1d \text{ majority}}^2[\vec{\sigma}])_{i_0} = (\vec{\phi}_{1d \text{ majority}}[\vec{\sigma}])_{i_0} = 1 - \sigma_{i_0} \neq \sigma_{i_0}$, which contradicts our original assumption that $\vec{\sigma}$ was a cyclic state of period two. ■

5.5.5.2 Transient Length

A bound on the transient length of the one-dimensional majority rule (equation 5.142) follows in straightforward fashion from our more general results of the previous section.

Suppose we have a finite initial state $\vec{\sigma} = (\vec{0}^\infty, \sigma_{i_{\min}}, \dots, \sigma_{i_{\max}}, \vec{0}^\infty)$, where $i_{\min}$ and $i_{\max}$ are, respectively, the minimum and maximum coordinate values of the finite block of non-zero sites. Since A is a symmetric integer valued matrix, the conditions for corollary 1 are met. The transient length τ is thus bounded by $\tau \leq \frac{1}{2} \left(-n(\vec{\sigma}) + 3\|2\vec{b} - A\vec{1}\| + \|A\| \right)$, where A and $\vec{b}$ are given by equation 5.143 and $n(\vec{\sigma}) = i_{\max} - i_{\min} + 1$. Substituting the explicit forms for A and $\vec{b}$ leads to the bound [goles90]

$$\tau_{1d \text{ majority}} \leq r(r + n(\vec{\sigma}) + 1). \quad (5.145)$$

A sharper bound is given by Tchuente [tch82], who showed that $\tau_{1d \text{ majority}} \leq r(x)$, where $r(x)$ is the cardinality of the set of blocks of consecutive 1-valued sites making up the finite initial state (see also [goles90]).

5.5.6 Two-dimensional Majority Rules

Consider the two-dimensional majority rule defined on the 4-neighbor von Neumann neighborhood:

$$\sigma_{i,j}(t+1) = \phi_{2d \text{ majority}}[\sigma_{k,l} \in \mathcal{N}_{ij}] = \begin{cases} 1 & \text{if } \sum_{\sigma_{k,l} \in \mathcal{N}_{ij}} \sigma_{k,l}(t) \geq b, \\ 0 & \text{else,} \end{cases} \quad (5.146)$$

where $\mathcal{N}_{ij} = \{\sigma_{i,j}, \sigma_{i-1,j}, \sigma_{i+1,j}, \sigma_{i,j-1}, \sigma_{i,j+1}\}$ and $1 \leq b \leq 4$. Recall that the qualitative behavior of such rules was discussed in sections 5.5.5 and 5.5.6.

5.5.6.1 Cyclic States

Just as was the case for one-dimensional majority rules considered in the previous section, we again recognize that the two-dimensional majority rule is but a special case of the generalized threshold rule defined in equation 5.121. Intuitively, the idea is simply to let a_{ij} represent a two-dimensional lattice that is built out of our a-priori structureless set of sites, $i = 1, 2, \dots, N$. Suppose we arrange these N sites into n rows with m sites per row, so that $N = n \times m$. Then the site (i, i') , positioned on the i^{th} row and i'^{th} column, can be identified with the original site number $I = (i - 1) * m + i'$. Making a similar identification between the site (j, j') and $J = (j - 1) * m + j'$, we see that a symmetric adjacency matrix a_{IJ} can be defined as follows:

$$a_{IJ} = \begin{cases} 1 & \text{if } \begin{cases} |i - j| = 0 & \text{and } |i' - j'| = 0 & \text{or} \\ |i - j| = 0 & \text{and } |i' - j'| = 1 & \text{or} \\ |i - j| = 1 & \text{and } |i' - j'| = 0 \end{cases} \\ 0 & \text{else,} \end{cases} \quad \text{for all } I, J \quad (5.147)$$

Equation 5.121 is then reproduced in full by setting $b_i = b - 1/2$ for all i . Since a_{IJ} is symmetric, the condition of theorem 5 is met. We conclude that ϕ_{2d} majority can only yield either fixed points or cycles of period two.

Notice that if the threshold is either $b = 1$ or $b = 4$, the resulting behavior is essentially trivial. If $b = 1$, for example, all initial states that have at least one nonzero site $\sigma_{i,j} \neq 0$ must converge to the state consisting of all 1's. This is because the threshold is low enough so that all neighboring sites of a non-zero site become 1 on the next time step. The opposite is true for a threshold of $b = 4$: all states with at least one site $\sigma_{i,j} \neq 1$ converge to $\vec{\sigma} = \vec{0}$. Figure 5.6 shows a few snapshot views of ϕ_{2d} majority for $b = 2$ and a random initial state with density $\rho_0 = 0.075$.

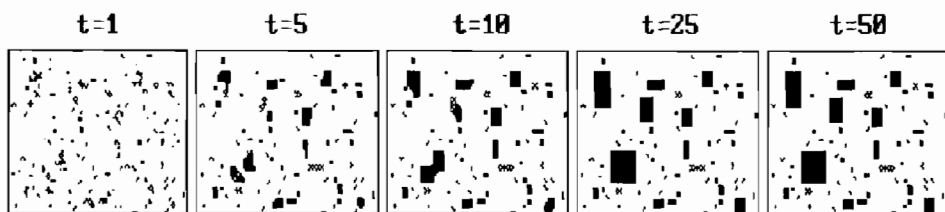


Fig. 5.6. Some snapshots of the evolution of the 5-neighbor (von Neumann neighborhood) majority rule ϕ_{2d} majority with threshold $b = 2$. The initial state is random with density $\rho_0 = 0.075$.

We now consider the transient behavior of the two non-trivial cases, $b = 2$ and $b = 3$.

5.5.6.2 Transient Length

Suppose that the initial state is confined to a rectangle $R = (i_{\min}, i_{\max}) \times (j_{\min}, j_{\max})$, where $i_{\min}$ and $i_{\max}$ are the minimal and maximal i coordinates of the region containing nonzero sites and $j_{\min}$ and $j_{\max}$ are the minimal and maximal j coordinates of that same region. Then according to corollary 1, the transient length $\tau_{2d \text{ majority}}$ is bounded by

$$\tau_{2d \text{ majority}}(A, \vec{b}) \leq \frac{1}{2} \left(-\text{Area}(R) + 3\|2\vec{b} - A\vec{1}\| + \|A\| \right), \quad (5.148)$$

where $\text{Area}(R) = (i_{\max} - i_{\min}) \times (j_{\max} - j_{\min})$.

Threshold $b = 2$: Using the form of A in equation 5.147, we see that $\|A\| = 5 \cdot \text{Area}(R) - 2(i_{\max} - i_{\min} + 1) - 2(j_{\max} - j_{\min} + 1)$ and that $\|2\vec{b} - A\vec{1}\| = 2 \cdot \text{Area}(R) - 3[(i_{\max} - i_{\min} + 1) + (j_{\max} - j_{\min} + 1)] + 8$. Thus, $\frac{1}{2} \left(-\text{Area}(R) + 3\|2\vec{b} - A\vec{1}\| + \|A\| \right) = 5 \cdot \text{Area}(R) - \frac{11}{2}[(i_{\max} - i_{\min} + 1) + (j_{\max} - j_{\min} + 1)] + 36$, or

$$\tau_{2d \text{ majority}}(A, b = 2) \leq 5 \cdot \text{Area}(R) - \frac{11}{4} P(R) + 37, \quad (5.149)$$

where $P(R) = 2[(i_{\max} - i_{\min}) + (j_{\max} - j_{\min})]$ is the *perimeter* of rectangle R [goles90].

Threshold $b = 3$: Using the form of A in equation 5.147, we see that $\|A\| = 5 \cdot \text{Area}(R) - 2(i_{\max} - i_{\min} + 1) - 2(j_{\max} - j_{\min} + 1)$ and that $\|2\vec{b} - A\vec{1}\| = (i_{\max} - i_{\min}) + (j_{\max} - j_{\min}) + 6$. Thus $\frac{1}{2} \left(-\text{Area}(R) + 3\|2\vec{b} - A\vec{1}\| + \|A\| \right) = 2 \cdot \text{Area}(R) + \frac{1}{2}[(i_{\max} - i_{\min} + 1) + (j_{\max} - j_{\min} + 1)] + 6$. Using the above expression for the perimeter $P(R)$, we have [goles90]

$$\tau_{2d \text{ majority}}(A, b = 3) \leq 2 \cdot \text{Area}(R) + \frac{P(R)}{4} + 7 \quad (5.150)$$

5.5.7 Additional Remarks

The purpose behind this section was not to provide an exhaustive account of the entire set of known properties of generalized threshold rules, but merely to acquaint the reader with Lyapunov Functions as a tool in ascertaining some of those properties. We conclude by briefly discussing (1) What happens when the matrix A is *anti-symmetric*?; (2) What happens when the updating is sequential rather than parallel?; (3) Multi-threshold rules, and (4) The relationship between generalized threshold rules and spin-glasses. In addition to the many fine papers by Fogelman-Soulie ([fogel82]–[fogel87]), Goles ([goles81a]–[goles89]), Tchuente ([tch82]–[tch87]) and Vichniac ([vich84]–[vich90]) that are listed in the reference section at the end of this book, the interested reader will find a wealth of useful information in the book by Goles and Martinez [goles90].

5.5.7.1 *A is Anti-Symmetric*

Consider the following rule

$$\sigma_i(t+1) = \begin{cases} 1 & \text{if } \sum_{j=1}^N a_{ij}(2\sigma_j(t) - 1) \geq 0, \\ 0 & \text{else,} \end{cases} \quad (5.151)$$

and where $a_{ij} = -a_{ji}$ for all i, j ; in particular, all of A 's diagonal entries are equal to zero. We also assume that $\sum_j [a_{ij}(\sigma_j - \frac{1}{2})] \neq 0$ for any $\vec{\sigma}$.

Using the Lyapunov function $L_{\text{anti-symmetric}}$, given by

$$L_{\text{anti-symmetric}}[\vec{\sigma}(t)] = -\sum_{i=1}^n [(2\sigma_i(t) - 1) \sum_{j=1}^n a_{ij}(2\sigma_j(t-1) - 1)], \quad (5.152)$$

Goles [goles86c] shows that (1) only period $T = 4$ orbits are allowed, and (2) the transient length $\tau_{\text{anti-symmetric}} \leq \|A\|$.

5.5.7.2 *Multithreshold Rules*

Multithreshold rules are natural extensions of the (binary-valued) generalized threshold rule defined in equation 5.121. Using k -state variables $\sigma \in \{0, 1, \dots, k-1\}$ and using the j^{th} entry of the i^{th} threshold vector to define the j^{th} threshold at that site ($= b_{i,j}$), the generalized multithreshold rule is defined as follows:

$$\sigma_i(t+1) = \phi_{\text{multi-thresh}}[\vec{\sigma}(t); A, b] = \begin{cases} 0 & \text{if } \sum_{j=1}^N a_{ij}\sigma_j(t) < b_{i,0}, \\ 1 & \text{if } b_{i,0} \leq \sum_{j=1}^N a_{ij}\sigma_j(t) < b_{i,1}, \\ \vdots & \vdots \\ k-1 & \text{if } b_{i,k-2} \leq \sum_{j=1}^N a_{ij}\sigma_j(t) < b_{i,k-1}, \\ k & \text{else,} \end{cases} \quad (5.153)$$

Although it is certainly not immediately obvious from the rule itself, it turns out that, just as is the case for generalized threshold rules, the only possible asymptotic states of finite symmetric *multi*-threshold rules are either fixed points or cycles of period two [goles90]. Unlike their binary brethren, however, multi-threshold rules possess some intriguing additional properties.

For example, consider a radius- r one-dimensional neighborhood, set $k = 4$, and let $b_{i,j} = b_j$ for all j (i.e. assign the same set of thresholds b_0, b_1 and b_2 to each site i). The asymptotic behavior of this rule – in particular, the question whether

an initial state converges to a final state consisting of all zeroes or to fixed state or period-two cycle containing some nonzero sites – depends on the sum $B = \sum_i b_i$. If the final state $\bar{\sigma}(\infty) = \bar{0}$, the rule is said to be *erasing* [goles90]. Goles [goles85a] shows that if $b_0 \in [r+2, 2r+1)$, $b_1 \in [2r+3, 4r+2)$, $b_2 \in [4r+3, 5r+3)$ and $b_0 + b_1 \in [4r+5, +\infty)$ (where ‘ $[x$ ’ denotes a closed left-boundary and ‘ $x]$ ’ denotes an open right-boundary, then (1) $B \leq 9r+8 \implies$ *Erasing*, (2) $B \geq 9r+10 \implies$ *Not-Erasing*, and (3) if $B = 9r+9$ then both types of behaviors can occur. This erasing problem is actually very difficult to solve in general. Toom [toom76b] has in fact shown that for the restricted class of monotone local rules, the problem is formally undecidable. Some additional details may be found in [gal78].

5.5.7.3 Sequential Updating

Consider the same generalized threshold rule ϕ_{gtf} as defined in equation 5.121, but apply now a *sequential updating* to the sites $i = 1$ through $i = n$. More precisely, for any initial state $\vec{S} = (S_1, S_2, \dots, S_n)$ (with $S_i \in \{-1, +1\}$), begin by updating only the first coordinate of $\vec{S}$ by $S_1 \rightarrow S'_1 = \phi_{\text{gtf}}[\vec{S}; A, \vec{b}]$, followed by $\vec{S} \rightarrow \vec{S}' = (S'_1, S_2, \dots, S_n)$. Next, update the second coordinate of $\vec{S}$ by $S_2 \rightarrow S'_2 = \phi_{\text{gtf}}[\vec{S}'; A, \vec{b}]$, followed by $\vec{S}' \rightarrow \vec{S}'' = (S'_1, S'_2, \dots, S_n)$. And so on. More formally, apply the following rule

$$S_i(t+1) = \phi_{\text{gtf, seq}}[\vec{S}(t+1), \vec{S}(t); A, \vec{b}] = \begin{cases} 1 & \text{if } \sum_{j=1}^{i-1} a_{ij} S_j(t+1) + \sum_{j=i}^n a_{ij} S_j(t) \geq b_i, \\ 0 & \text{else.} \end{cases} \quad (5.154)$$

The sequential update at time t is actually composed of n successive iterates at times $t_i = t + i/n$, where only the i^{th} coordinate changes state at time t_i ; i.e. $\vec{S}(t) = (S_1(t), \dots, S_n(t))$ and $\vec{S}(t + i/n) = (S_1(t+1), \dots, S_i(t+1), S_{i+1}(t), \dots, S_n(t))$, for $1 < i \leq n$.[†]

Now, consider the following function E :

$$E[\vec{S}(t)] = -\frac{1}{2} \sum_i S_i(t) \sum_j a_{ij} S_j(t) + \sum_i b_i S_i(t). \quad (5.155)$$

[†]We may, of course, generalize this sequential updating to entire blocks of m sites at a time. See [goles90] for discussion.

We find that

$$\begin{aligned}
 \Delta_t E &= E[\vec{S}(t+1)] - E[\vec{S}(t)], \\
 &= \sum_{k=1}^n \left(E[\vec{S}(t+k/n)] - E[\vec{S}(t+(k-1)/n)] \right), \\
 &= \sum_{k=1}^n \left(-[S_k(t+1) - S_k(t)] \left[\sum_{j=1}^{k-1} a_{kj} S_j(t+1) + \sum_{j=k}^n a_{kj} S_j(t) + b_k \right] \right. \\
 &\quad \left. - \frac{1}{2} a_{kk} [S_k(t+1) - S_k(t)]^2 \right),
 \end{aligned} \tag{5.156}$$

Equation 5.154 assures us that the first term on the right-hand-side of this last expression is strictly negative. If we also assume that all of the diagonal entries of A are positive - that is, that $a_{ii} \geq 0$ for all $i = 1, 2, \dots, n$ - then the second term on the right-hand-side is negative as well. We conclude that, provided $\vec{S}(t+1) \neq \vec{S}(t)$, $\Delta_t E < 0$; i.e. E is a *Lyapunov Function* for the sequentially updated generalized threshold rule defined in equation 5.154. Moreover, since any cycle of period $T > 2$ would necessarily imply the contradiction that $E[\vec{S}(0)] > E[\vec{S}(1)] > \dots > E[\vec{S}(T-1)] > E[\vec{S}(0)]$, equation 5.156 also demonstrates that this system can only have *fixed points* [goles87b].

Goles, *et.al.* [goles90] prove that for symmetric A and $a_{ii} \geq 0$, $i = 1, \dots, n$, the transient time for sequential updates is bounded by

$$\tau_{\text{seq}} \leq \frac{1}{4 \left(e + \frac{1}{2} \min_i a_{ii} \right)} (\|A\| + 2\|2\vec{b} - A\vec{1}\|), \tag{5.157}$$

where e is defined by equation 5.129.

Other details may be found in [fogel83], [goles85b], [goles87b], [goles89], and [goles90].

5.5.7.4 Spin Glasses

Spin glasses are magnetic materials in which the interaction among the constituent magnetic moments, or spins, is random.[‡] Much of what is currently known about spin glasses can be traced back to the pioneering work of Edwards and Anderson [edw75]. Their idea was to try to capture the essential properties of real spin glasses with a simple *Ising*-like Hamiltonian of the form:

$$\mathcal{H}_{\text{spin-glass}} = - \sum_{ij} J_{ij} S_i S_j, \tag{5.158}$$

where the sites i and j are on some regular two or three dimensional lattice, the spins S_i take on the values ± 1 , the sum is taken over nearest neighbors, and the

[‡]An expanded discussion of spin glasses appears in section 7.1.7

couplings J_{ij} 's are assumed to be independent random variables. The problem is to find the minimal energy configurations of this system.

Because of the randomness of the spin-spin couplings (if not simply the complexity of the space itself – particularly if the dimension $d > 2$, for which the combinatorial minimization problem has been shown to be NP-complete ([bara80], [goles85b])),[§] one typically must resort either to an approximation scheme, such as a mean-field theory [sherr75], or a direct Monte-Carlo simulation. In the latter case, the ground states are approximated by choosing spins at random throughout the lattice and changing their states with a probability that depends on a local majority, or threshold, rule. It should therefore not be surprising to learn that spin glasses and threshold rules are related. The connection between spin glasses and neural nets (which, we may recall, are themselves related to threshold rules via McColluch and Pitt's original neuronal activation rules [mccul43]), was first made by Little ([lit74], [lit78]).

In the case of the threshold rules defined in this section, we must consider sequential iterations of deterministic rules. Also, the choice of spins that may change state is not random but is fixed by some random permutation of the sites on the lattice. Such rules may be shown to correspond to spin glasses in the zero-temperature limit.

Consider a two-dimensional lattice $\mathcal{L}$ with periodic boundary conditions, and suppose each site belongs to a 5-neighbor von Neumann neighborhood. Furthermore, suppose that the N sites of the lattice are randomly partitioned into two sets, $\mathcal{L}_1$ and $\mathcal{L}_2$ ($\mathcal{L} = \mathcal{L}_1 \cup \mathcal{L}_2$). On this set, Goles, et.al. ([goles85b], [goles87b]) define a *generalized spin glass* as a threshold network evolving according to

$$S_i(t+1) = \begin{cases} \begin{cases} -1 & \text{if } \sum_{j<i} a_{ij}S_j(t+1) + \sum_{i<j\leq N} a_{ij}S_j(t) - b_i < 0, \\ S_i(t) & \text{if } \sum_{j<i} a_{ij}S_j(t+1) + \sum_{i<j\leq N} a_{ij}S_j(t) - b_i = 0, \\ +1 & \text{if } \sum_{j<i} a_{ij}S_j(t+1) + \sum_{i<j\leq N} a_{ij}S_j(t) - b_i > 0 \end{cases} & \text{if } i \in \mathcal{L}_1, \\ \begin{cases} -1 & \text{if } \sum_{j<i} a_{ij}S_j(t+1) + \sum_{i<j\leq N} a_{ij}S_j(t) - b_i < 0, \\ -S_i(t) & \text{if } \sum_{j<i} a_{ij}S_j(t+1) + \sum_{i<j\leq N} a_{ij}S_j(t) - b_i = 0, \\ +1 & \text{if } \sum_{j<i} a_{ij}S_j(t+1) + \sum_{i<j\leq N} a_{ij}S_j(t) - b_i > 0 \end{cases} & \text{if } i \in \mathcal{L}_2, \end{cases} \quad (5.159)$$

where $a_{ij} \in \{-1, 0, +1\}$ is a symmetric matrix and $a_{ii} = 0$. We see that the i^{th} spin can change its state only if it belongs to the set $\mathcal{L}_2$, and it is only these sites that can “disturb” the system; that is, induce local oscillation. In case of tie votes, sites belonging to the set $\mathcal{L}_2$ remain fixed and thus act as “freezing elements”, tending to induce fixed states. The cycle-length and transient-time bound theorems of the main section thus provide some insight into the expected properties of spin glasses.

[§]Just as there are universal computers that, given a particular input, can simulate any other computer, there are NP-complete problems that, with the appropriate input, are effectively equivalent to any NP-hard problem of a given size. For example, Boolean “satisfiability” -i.e. the problem of determining truth values of the variable's of a Boolean expression so that the expression is true -is known to be an NP-complete problem. See section 12.3.5.2

5.6 Appendix 5-A

Although the exact cycle decomposition of a finite-size CA depends on the set of elementary divisors of $\mathbf{L}_{ij}$ (see section 5.4), it is convenient to classify topologies according to their cyclic equivalence classes ‘ $\mathcal{Q}$ ’. Any $P_1(x) = \prod [p_{1i}(x)]^{\nu_{1i}}$ and $P_2(x) = \prod [p_{2i}]^{\nu_{2i}}$, where $\{deg(p_{1i}) = deg(p_{2i})\}$ and $\{ord(p_{1i}) = ord(p_{2i})\}$ for all ‘ i ’, must share the same cycle sums and so belong to the same class $\mathcal{Q}$.

Table 5.5 gives all possible cycle lengths supported by (symmetric) $\mathcal{L} \in \mathcal{Q}$ (for systems in $\mathcal{F}[2]$), along with the volume of cycle state $vol(\mathcal{C}) = \sum_i n_i t_i$. Bracketed cycle lengths are those which appear for all $\mathcal{L} \in \mathcal{Q}$. The coefficients ‘ a_i ’ are defined by $P_L(x) = 1 + \sum_{i=1}^N a_i x^{N-i}$.

N	a_2	a_4	a_6	a_8	OT	vol (C)	T	vol (C)
5	0	0			[1]	1	[1,2,4,8]	32
	0	1			[1,2,4]	16	[1]	2
	1	0			[1,2]	4	[1,2,4]	8
	1	1			[1,3],6	16	[1,3],6	32
6	0	0	0		[1]	1	[1,2,4,8]	64
	0	0	1		[1,3],2,6	64	[1,3],6	16
	0	1	0		[1,2,4]	16	[1,2]	4
	0	1	1		[1,7],14	64	[1,7],14	64
	1	0	1					
	1	0	0		[1,2]	4	[1,2,4]	16
	1	1	0		[1,3],6	16	[1,3],2,6	64
	1	1	1	1	[1,2,4,8]	64	[1]	1
7	0	0	0		[1]	1	[1,2,4,8]	128
	0	0	1		[1,3],2,6	64	[1,3],6	32
	0	1	0		[1,2,4]	16	[1,2,4]	8
	0	1	1		[1,7],14	64	[1,7],14	128
	1	0	1					
	1	0	0		[1,2]	4	[1,2,4,8]	32
	1	1	0		[1,3],6	16	[1,3],2,6,12	128
	1	1	1	1	[1,2,4,8]	64	[1]	2
8	0	0	0	0	[1]	1	[1,2,4,8]	256
	0	0	0	1	[1,2,4,8]	256	[1]	1
	0	0	1	0	[1,3],2,6	64	[1,3],2,6	64
	0	0	1	1	[1,15],30	256	[1,15],30	256
	0	1	0	0	[1,2,4]	16	[1,2,4]	16
	0	1	0	1	[1,3],6,12	256	[1,3],6,12	256
	0	1	1	0	[1,7],14	64	[1,7],14	256
	0	1	1	1				
	1	0	1	0	[1,7],14	256	[1,7],14	64
	1	1	0	1				
	1	0	0	0	[1,2]	4	[1,2,4,8]	64
	1	0	0	1	[1,15],30	256	[1,5],10	256
	1	0	1	1	[1,3],2,6,12	256	[1,3],6	16
	1	1	0	0	[1,3],6	16	[1,3],2,6,12	256
	1	1	1	0	[1,2,4,8]	64	[1,2]	4
	1	1	1	1	[1,5],10	256	[1,15],30	256
9	0	0	0	0	[1]	1	[1,2,4,8,16]	512
	0	0	0	1	[1,2,4,8]	256	[1]	2
	0	0	1	0	[1,3],2,6	64	[1,3],2,6,12	128
	0	0	1	1	[1,15],30	256	[1,15],30	512
	0	1	0	0	[1,2,4]	16	[1,2,4,8]	32
	0	1	0	1	[1,3],6,12	256	[1,3],6,12	512
	0	1	1	0	[1,7],14	64	[1,7],14,28	512
	1	0	1	0				
	1	0	1	1	[1,7],14	256	[1,7],14	128
	1	1	0	1				
	1	0	0	0	[1,2]	4	[1,2,4,8]	128
	1	0	0	1	[1,15],30	256	[1,5],10	512
	1	0	1	1	[1,3],2,6,12	256	[1,3],6	32
	1	1	0	0	[1,3],6	16	[1,3],2,4,6,8,12,24	512
	1	1	1	0	[1,2,4,8]	64	[1,2,4]	8
	1	1	1	1	[1,5],10	256	[1,15],30	512

Table 5.5. All possible cycle lengths supported by (symmetric) $\mathcal{L} \in \mathcal{Q}$ (for systems in $\mathcal{F}[2]$), along with the volume of cycle state $vol(\mathcal{C}) = \sum_i n_i t_i$.

5.7 Appendix 5-B

Table 5.6 lists the distinct classes $\mathcal{Q}$ for **T** and **OT** rules, and gives all possible cycle sets supported by $\mathcal{L} \in \mathcal{Q}$ for topologies of size $N=10$. $\mathcal{Q}_T$ gives the corresponding class for **T** rule behavior on the same lattice. *Ex:* the **T** behavior on a lattice which has a single *odd* decomposition into ' n -disjoint edges' for $n=5$ (i.e. $P(x) = 1+x^{10}$), belongs to the same cyclic class as **OT** behavior on a lattice whose $P(x) = x^2+x^8+x^{10}$ (or $[a_2, a_4, a_6, a_8, a_{10}] = [1, 0, 0, 1, 0]$). $\mathcal{Q} = 22 : [1, 0, 0, 1, 1]$, which has 50 *distinct cycle sets* with periods $\in \{1, 2, 4, 8, 16\}$, is not listed.

$\mathcal{Q}_{OT}$	a_2	a_4	a_6	a_8	a_{10}	$\mathcal{Q}_T$	$ \mathcal{C} $	$\mathcal{C} = \sum_i [n_i, t_i]$
1	0	0	0	0	0	22	1	[1,1]
2	0	0	0	0	1	6	84 112 156 208	[2,1]+[1,2]+[30,5]+[51,10] [4,1]+[12,5]+[96,10] [2,1]+[1,2]+[102,5]+[51,10] [4,1]+[204,5]
3	0 1	0 0	0 0	1 0	1 1	3 2	32 36 40 60	[1,1]+[1,3]+[2,6]+[1,7]+[4,14]+[1,21]+[22,42] [1,1]+[5,3]+[1,7]+[4,14]+[5,21]+[20,42] [1,1]+[1,3]+[2,6]+[9,7]+[9,21]+[20,42] [1,1]+[5,3]+[9,7]+[45,21]
4	0	0	1	0	0	14	14 16 18 24	[2,1]+[1,2]+[2,3]+[9,6] [4,1]+[4,3]+[8,6] [2,1]+[1,2]+[10,3]+[5,6] [4,1]+[20,3]
5	0 0 0 1 1 1	0 1 1 0 1 1	1 0 1 1 0 1	0 0 1 1 1 0	1 1 1 1 1 1	5 5 5 5 5 5	18 34	[1,1]+[1,31]+[16,62] [1,1]+[33,31]
6	0 1	0 0	1 0	1 0	0 1	10 2	10 18	[1,1]+[1,15]+[8,30] [1,1]+[17,15]
7	0 1	0 1	1 0	1 0	1 1	11 11	40 52 64 80 84 88 96 100 120 160	[2,1]+[1,2]+[3,4]+[18,7]+[9,14]+[27,28] [2,1]+1,2+3,4+2,7+17,14+27,28 [4,1]+[2,2]+[2,4]+[4,7]+[34,14]+[18,28] [4,1]+[2,2]+[2,4]+[36,7]+[18,14]+[18,28] [4,1]+[6,2]+[4,7]+[70,14] [8,1]+[4,2]+[8,7]+[68,14] [16,1]+[16,7]+[64,14] [4,1]+[6,2]+[36,7]+[54,14] [8,1]+[4,2]+[72,7]+[36,14] [16,1]+[144,7]
8	0	1	0	0	0	17	6 8 10 12 16	[2,1]+[1,2]+[3,4] [4,1]+[2,2]+[2,4] [4,1]+[6,2] [8,1]+[4,2] [16,1]
9	0	1	0	1	0	19	24 28 44 54 86	[1,1]+[1,3]+[2,6]+[20,12] [1,1]+[2,3]+[8,6]+[1,9]+[16,12] [1,1]+[2,3]+[16,6]+[1,9]+[24,6] [1,1]+[21,3]+[32,6] [1,1]+[85,3]
10	0 1	1 0	0 1	1 0	1 1	18 6	38 40 54 72	[2,1]+[1,2]+[2,15]+[33,30] [4,1]+[4,15]+[32,30] [2,1]+[1,2]+[34,15]+[17,30] [4,1]+[68,15]
11	0 1	1 0	1 1	0 0	0 0	7 7	6 10	[1,1]+[1,7]+[4,14] [1,1]+[9,7]
12	0	1	1	1	0	16	22 24 30 40	[2,1]+[1,2]+[2,7]+[17,14] [4,1]+[4,7]+[16,14] [1,2]+[2,1]+[18,7]+[9,14] [4,1]+[36,7]
13	1	0	0	0	0	20	3 4	[2,1]+[1,2] [4,1]

Table 5.6. All possible cycle sets supported by $\mathcal{L} \in \mathcal{Q}$ for topologies of size $N=10$.

$\mathcal{Q}_{OT}$	a_2	a_4	a_6	a_8	a_{10}	$\mathcal{Q}_T$	$ C $	$C \equiv \sum_i [n_i, \epsilon_i]$
14	1	0	1	1	0	4	32 36 40 48 52 56	$[2,1]+[1,2]+[2,3]+[3,4]+[9,6]+[15,12]$ $[2,1]+[1,2]+[10,3]+[3,4]+[5,6]+[15,12]$ $[4,1]+[2,2]+[4,3]+[2,4]+[18,6]+[10,12]$ $[4,1]+[2,2]+[20,3]+[2,4]+[10,6]+[10,12]$ $[4,1]+[6,2]+[4,3]+[38,6]$ $[8,1]+[4,2]+[8,3]+[36,6]$
							60 64 72 96	$[4,1]+[6,2]+[20,3]+[30,6]$ $[16,1]+[16,3]+[32,6]$ $[8,1]+[4,2]+[40,3]+[20,6]$ $[16,1]+[80,3]$
15	1	1	0	0	0	21	4 6	$[1,1]+[1,3]+[2,6]$ $[1,1]+[5,3]$
16	1	1	0	1	0	12	18 24 30 40	$[4,1]+[1,2]+[2,7]+[13,14]$ $[4,1]+[4,7]+[16,14]$ $[2,1]+[1,2]+[18,7]+[9,14]$ $[4,1]+[36,7]$
17	1	1	1	0	0	8	12 16 22 24 28 32 36 40 48 64	$[2,1]+[1,2]+[3,4]+[6,8]$ $[4,1]+[2,2]+[6,4]+[4,8]$ $[4,1]+[6,2]+[12,4]$ $[8,1]+[4,2]+[12,4]$ $[8,1]+[12,2]+[8,4]$ $[16,1]+[8,2]+[8,4]$ $[8,1]+[28,2]$ $[16,1]+[24,2]$ $[32,1]+[16,2]$ $[64,1]$
18	1	1	1	1	0	10	27 52	$[1,1]+[3,5]+[24,10]$ $[1,1]+[51,5]$
19	1	1	1	1	1	9	94 96 114 120 178 184 194 216 258 344	$[2,1]+[1,2]+[2,3]+[9,6]+[80,12]$ $[4,1]+[4,3]+[8,6]+[80,12]$ $[2,1]+[1,2]+[10,3]+[37,6]+[64,12]$ $[4,1]+[20,3]+[32,6]+[64,12]$ $[2,1]+[1,2]+[10,3]+[165,6]$ $[4,1]+[20,3]+[160,6]$ $[2,1]+[1,2]+[42,3]+[149,6]$ $[4,1]+[84,3]+[128,6]$ $[2,1]+[1,2]+[170,3]+[85,6]$ $[4,1]+[340,3]$
20	0	0	0	1	0	13	36 40 44 46 48	$[2,1]+[1,2]+[3,4]+[30,8]$ $[4,1]+[2,2]+[6,4]+[28,8]$ $[4,1]+[6,2]+[22,4]+[12,8]$ $[4,1]+[6,2]+[12,4]+[24,8]$ $[8,1]+[4,2]+[12,4]+[24,8]$
20							60 64 70 76 84 88 96 103 112	$[8,1]+[12,2]+[24,4]+[16,8]$ $[16,1]+[8,2]+[24,4]+[16,8]$ $[4,1]+[6,2]+[60,4]$ $[8,1]+[12,2]+[56,4]$ $[8,1]+[28,2]+[48,4]$ $[16,1]+[24,2]+[48,4]$ $[32,1]+[16,2]+[48,4]$ $[16,1]+[56,2]+[32,4]$ $[32,1]+[48,2]+[32,4]$
							128 136 144 160 192 256	$[64,1]+[32,3]+[32,4]$ $[16,1]+[120,2]$ $[32,1]+[112,2]$ $[64,1]+[96,2]$ $[128,1]+[64,2]$ $[256,1]$
21	0	1	1	0	1	15	68 72 88 96 124 128	$[2,1]+[1,2]+[2,3]+[3,4]+[9,6]+[6,8]+[15,12]+[36,24]$ $[2,1]+[1,2]+[10,3]+[3,4]+[5,6]+[6,8]+[15,12]+[30,24]$ $[4,1]+[2,2]+[4,3]+[6,4]+[18,6]+[4,8]+[30,12]+[30,24]$ $[4,1]+[2,2]+[20,3]+[6,4]+[10,6]+[4,8]+[30,12]+[20,24]$ $[4,1]+[6,2]+[4,3]+[12,4]+[38,6]+[60,12]$ $[8,1]+[4,2]+[8,3]+[12,4]+[36,6]+[40,12]$
							132 144 152 152 160 192 200 208 216 224 240 256 288 384	$[4,1]+[6,2]+[20,3]+[12,4]+[30,6]+[60,12]$ $[8,1]+[4,2]+[40,3]+[12,4]+[20,6]+[60,12]$ $[8,1]+[12,2]+[40,3]+[8,4]+[60,6]+[24,12]$ $[8,1]+[12,2]+[8,3]+[8,4]+[76,6]+[40,12]$ $[16,1]+[8,2]+[16,3]+[8,4]+[72,6]+[40,12]$ $[16,1]+[8,2]+[80,3]+[8,4]+[40,6]+[40,12]$ $[8,1]+[28,2]+[8,3]+[156,5]$ $[16,1]+[24,2]+[16,3]+[152,6]$ $[8,1]+[28,2]+[40,3]+[140,6]$ $[32,1]+[16,2]+[32,3]+[144,6]$ $[16,1]+[24,2]+[80,3]+[120,6]$ $[64,1]+[64,3]+[128,6]$ $[32,1]+[16,2]+[160,3]+[80,6]$ $[64,1]+[320,3]$

Table 5.6 (continued) All possible cycle sets supported by $\mathcal{L} \in \mathcal{Q}$ for topologies of size $N=10$.

Chapter 6

Cellular Automata and Language Theory

An elegant and powerful description of the self-organizing processes of CA is provided by *formal computation theory*, or the mathematical theory of *formal languages*.^{*} The idea is to exploit perhaps the simplest interpretation of CA systems as being nothing more than *basic information processors*. That is to say, we can think of the action of a generic CA system as a “computation”, processing the information encoded within a given initial state. The outcome of this computation, at an arbitrary time step ‘ t ’, is a string—or, to use a slightly more suggestive term, a *word*—of symbols (such as ‘0’ and ‘1’ in the case when $k = 2$), that are arranged in some definite (rule-defined) ‘order’. Now, we recall that formal languages themselves consist essentially of abstract *words* formed from strings of symbols from a finite alphabet A according to some definite set of grammatical rules. Accordingly, sets of CA configurations may be considered to be formal languages, in which different words in a given language represent different CA states. This chapter consists of a short primer on CA and language theory. It discusses formal language theory, the relationship between CA and formal language theory, power spectra of regular languages and reversible computation.

Using the notation

$$\Phi : \Gamma \longrightarrow \Gamma \tag{6.1}$$

to represent the global form of the local (one-dimensional) mapping $\phi : \Sigma^{2r+1} \rightarrow \Sigma$, where $\Gamma = \Sigma^N$, the ensemble of configurations generated after ‘ t ’ iterations (which we will refer to as the *finite-time limit set* of the rule ϕ), $\Omega_t = \Omega_t[\phi]$, is given by

$$\Omega_t[\phi] = \Phi^t \Gamma. \tag{6.2}$$

While Wolfram [wolf84a] showed (and, as we will summarize below, made quite a few *interesting* deductions from the fact) that $\Omega_t[\phi]$ is a *regular language* for all

^{*}Recall that the basic notions of abstract automata and formal language theory were very briefly touched upon in our introductory survey in section 2.1.5.

finite ‘ t ’, Hurd [hurd87] gives a few explicit examples proving that $\lim_{t \rightarrow \infty} \Omega_t[\phi]$ need not be a regular language.

In the remaining paragraphs of this section, we follow mostly [wolf84a], [hurd87], [li87] and [li89]. There are many excellent texts on formal language theory. We recommend the ones by Brookshear [brooksh89], Hopcroft and Ullman [hopc79], Davis and Weyuker [davis83] and the classic by Minsky [minsky67].

6.1 Formal Language Theory: A Primer

Just as *points* and *lines* are formally undefined geometrical objects, a *symbol* represents an abstract undefined object. Typical representations include *letters* and *digits*. An *alphabet* is then simply a finite nonempty set A of symbols. An n -tuple of symbols of A is defined to be a *string* on A (also called a *word* on A). If $A = \{a_1, a_2, \dots, a_n\}$, for example, then we would write the string $s(A) = a_1 a_2 \cdots a_n$; the *length* of the string is the number of symbols of which it is composed, and is written $|s(A)| = n$. The *null* string, s_0 , is a unique string consisting of zero symbols (so that $|s_0| = 0$). Letting S^* denote the set of all strings, we introduce a binary *concatenation* operator: if $s_1, s_2 \in S^*$, then the concatenation $\overline{s_1 s_2}$ is obtained by placing the string ‘ s_2 ’ after the string ‘ s_1 ’. For example, if $s_1 = a_1 a_2 a_3$ and $s_2 = b_1 b_2$ then

$$\overline{s_1 s_2} = a_1 a_2 a_3 b_1 b_2 \neq \overline{s_2 s_1} = b_1 b_2 a_1 a_2 a_3. \quad (6.3)$$

It is clear that $\overline{s\{\}} = \{\}s = s$. If ‘ s ’ is a string and $n \in \mathcal{N}$, $n > 0$ then we write $s^{[n]} = \underbrace{ss \cdots s}_n$. By convention, $s^{[0]} = \{\}$.

Define the set $S(A)$ to be the set of all subsets on A . Then a *language on A* (or a *language with alphabet A*) is any subset of $S(A)$. The set of all strings over a fixed finite alphabet A , for example, is a language; it is denoted by $\mathcal{L}(A)$. If $A = \{0, 1\}$, then $\mathcal{L}(A) = \{\{\}, 0, 1, 00, 01, 10, 000, \dots\}$.

Formal languages are subsets of $S(A)$ formed according to definite grammatical rules. Different formal languages are defined by using sets of different constraints on allowable words. A computer – or an *abstract automaton*, $\mathcal{M}$ – can then be used to implement the grammatical rules to generate (or recognize) the strings in the formal language; different *types* of languages being distinguished by different requirements for the computer’s memory size.

Abstract automata are machines with internal states, an input tape, and sometimes an auxiliary information storage stack. Automata read symbols from the tape, making transitions from one state to another, while performing other operations on the tape and stack. The simplest example of such an idealized machine is the *finite automaton*:

DEFINITION: A finite automaton (FA) $\mathcal{M}$ is specified by three sets A , Σ and Σ^* and a state-transition function $\phi: \Sigma \times A \rightarrow \Sigma$, where

$$\left\{ \begin{array}{ll} A &= \{a_1, \dots, a_n\} \text{ is a finite input alphabet,} \\ \Sigma &= \{\sigma_1, \dots, \sigma_m\} \text{ is a finite set of states,} \\ \Sigma^* \subset \Sigma &\text{ is the set of output (or accepting) states.} \end{array} \right. \quad (6.4)$$

Given an automaton $\mathcal{M}$ that starts in state σ_1 , and any finite string $s \in A^*$, $\phi^*(\sigma, s)$ will represent the final output state that $\mathcal{M}$ will enter after having processed s , one symbol at a time, from left to right. $\mathcal{M}$ is said to *accept* the word s if $\phi^*(\sigma_1, s) \in \Sigma^*$; the word s is *rejected* if and only if it is not accepted. Finally, we may define the *language* $\mathcal{L}(\mathcal{M})$ accepted by $\mathcal{M}$ as the set of all words $s \in A^*$ that are accepted by $\mathcal{M}$.

Notice that there are two kinds of symbols that appear: *non-terminal* symbols, appearing only in the generating stages of a word, and *terminal* symbols, which are the constituents of the final word. In order to generate a given word, one starts at some non-terminal *start* symbol and uses the grammatical “production” rules to obtain output strings of terminal symbols. According to the classification scheme developed by Noam Chomsky [chom56], there are essentially four types of formal languages, each defined by a particular kind of grammatical production rule and recognized by a particular kind of abstract automaton (see also table 6.1):

Regular Languages: allow only those productions that are of the form $a \rightarrow \sigma a'$ or $a \rightarrow \sigma$. Recognized by *Finite Automata*.

Context-Free Languages: allow only productions of the form $a \rightarrow \tilde{\sigma}$, where $\tilde{\sigma}$ is an arbitrary string of terminal and non-terminal symbols; there is also a fixed bound on the length of $\tilde{\sigma}$ ($=|\tilde{\sigma}|$). Recognized by *Push-Down Automata*.

Context-Sensitive Languages: the only constraint is that the length of successive words cannot be decreased; i.e. any productions of the form $\tilde{\sigma}_1 \rightarrow \tilde{\sigma}_2$ are allowed provided that $|\tilde{\sigma}_2| \geq |\tilde{\sigma}_1|$. Recognized by *Linear-Bounded Automata*.

Unrestricted Languages: no restrictions; all arbitrary productions of the form $\tilde{\sigma}_1 \rightarrow \tilde{\sigma}_2$ are allowed. Recognized by *Turing Machines*.

Notice that only the last class of unrestricted languages requires a full universal computer (i.e. *Turing Machine*); the other classes require progressively simpler kinds of computers. Each one of these four automata act as a kind of black-box into which is fed a tape of symbols, sequentially, one cell at a time. During each cycle, the black-box reads the symbol at the appropriate cell, responds to that

Level	Language Class	Class of Accepting Automata	Memory
0	Unrestricted	Universal computer	arbitrarily large
1	Context-Sensitive	linear-bounded	$\sim s_{\text{input}} $
2	Context-Free	pushdown	fixed length
3	regular	finite	none

Table 6.1 Chomsky Language Hierarchy.

symbol according to a set of model-specific rules, and then moves the tape forward by one cell. The type of computational model a particular black-box represents depends on the form of its response.

Below we present evidence that (1) the infinite-time limit sets of class **c1** and **c2** CA form regular languages, (2) the infinite-time limit set of class **c3** CA (appear to) form context-sensitive languages and (3) the infinite-time limit set of class **c4** CA (appear to) to form unrestricted languages. While the evidence is very strong that the assertions about the infinite time limit sets of class **c3** and **c4** CA are in fact correct, a formal proof has yet to be provided.

6.1.1 Regular Languages/ Finite Automata

Finite Automata: A language $\mathcal{L}$ is called *regular* if there is a finite automaton $\mathcal{M}$ that accepts it. The *grammars* for regular languages can be conveniently specified by *finite state transition graphs* (or finite STGs) for the finite automata that recognize them. The vertices of these graphs represent the system states $\sigma_i \in \Sigma$ and the arcs represent the possible input states $a_i \in A$. The arrows point to the next state that will result from the initial state when the input on the arc is applied. Consider the following simple example:

EXAMPLE: Consider an automaton $\mathcal{M}$ with alphabet $A = \{0, 1\}$, state space $\Sigma = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4\}$ and transition rule ϕ given by

$$\left\{ \begin{array}{llll} \phi(\sigma_1, 0) = \sigma_2, & \phi(\sigma_1, 1) = \sigma_4, & \phi(\sigma_2, 0) = \sigma_2, & \phi(\sigma_2, 1) = \sigma_3, \\ \phi(\sigma_3, 0) = \sigma_4, & \phi(\sigma_3, 1) = \sigma_3, & \phi(\sigma_4, 0) = \sigma_4, & \phi(\sigma_4, 1) = \sigma_4. \end{array} \right\}$$

Assume that the initial state is σ_1 and that the accepting set is $\Sigma^* = \{\sigma_3\}$. It is easy to see that $\mathcal{M}$ will reject the strings $s_1 = 00110$ and $s_2 = 10011$ (since $\phi^*(\sigma_1, s_1) = \phi^*(\sigma_1, s_2) = \sigma_4$), and accept $s_3 = 00111$ (since $\phi^*(\sigma_1, s_3) = \sigma_3 \in \Sigma^*$). In fact, $\mathcal{M}$ accepts the regular language

$$\mathcal{L} = \{0^{[n]}1^{[m]}, n, m \geq 0\}.$$

The finite STG for this example is given in figure 6.1.

The computational capabilities of finite automata are actually very limited. Consider, for example, the problem of constructing an “arithmetic expression parser”,

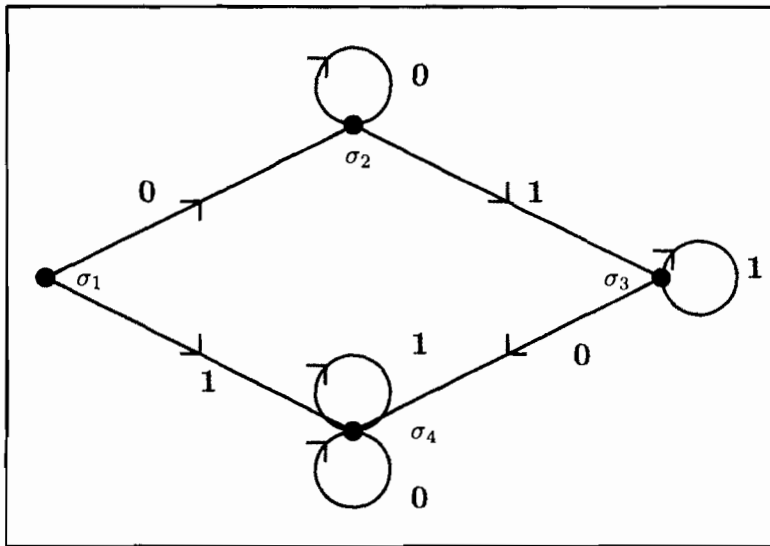


Fig. 6.1 Finite State Transition graph (STG) for the regular language $\mathcal{L} = \{0^n 1^m\}$.

one of whose functions must clearly be to make sure that all of the *parentheses* are correctly nested. Intuitively, we expect that in order to be able to do this, the automaton must be able to remember how many *left* parentheses that have not yet been matched with a *right* parenthesis have been encountered at any given time. Since a finite automaton has no built-in ability to save such information for later reference, it is not difficult to show that the parsing of arithmetic expressions is beyond the computational powers of finite automata. Similarly, as the reader may be interested in showing, no finite automaton can accept the set of all *palindromes* over some specified alphabet. Nonetheless, as alluded to in the preamble (and shown below) the finite-time limit set of a given CA rule can always be expressed as a regular language.

Deterministic vs Non-deterministic STGs: There are two possible kinds of finite STGs: *deterministic* and *non-deterministic*. Deterministic state transition graphs (DSTGs), such as the one appearing in figure 6.2, are such that they are (1) *fully defined* (i.e. there exists, from each state, at least one directed arc for each symbol in the alphabet) and (2) *unambiguous* (i.e. each state has only one directed arc leaving it for each symbol in the alphabet). In contrast to DSTGs, the transitions appearing in NDSTGs can be ambiguous. This can be a result of there being either more than one possible applicable transition or perhaps none at all (in the case where the automaton is not fully defined). Despite the “looser” definition, however, NDSTGs do not actually provide any additional processing power. Indeed, it can easily be shown that for each non-deterministic finite automaton there exists a deterministic finite automaton that accepts exactly the same language. In

fact, a stronger theorem asserts that the set of languages accepted by deterministic and non-deterministic finite automata are identical [hopc79]. This equivalence is actually quite useful: since, in practice, it is usually easier to construct a nondeterministic automaton to accept a given language, it guarantees that the design can be later physically implemented by a deterministic machine.

6.1.2 Context-Free Languages/ Push-Down Automata

Push-down Automata: push-down automata generalize finite automata by introducing an internal *memory*. Just as for finite automata, push-down automata have a finite input alphabet and a finite set of intermediate states, a subset of which constitutes the set of its output (or accepting) states. The difference is that push-down automata have an additional *stack-space*, consisting of some or all of the symbols of the machine's alphabet (along with perhaps some additional symbols to be used as internal markers) which they can use to store information for later use. We can therefore generalize our definition for finite automata (equation 6.4) to:

DEFINITION: A push-down automaton $\mathcal{M}$ is specified by four sets A , Σ , Δ and Σ^* and a finite set of state-transition functions $\Phi \ni \phi : \Sigma \times A \rightarrow \Sigma$, where

$$\left\{ \begin{array}{ll} A & = \{a_1, \dots, a_n\} \text{ is a finite input alphabet,} \\ \Sigma & = \{\sigma_1, \dots, \sigma_m\} \text{ is a finite set of states,} \\ \Delta & = A^* \subset A \cup \{\delta_1, \dots, \delta_d\} \text{ is a finite set of stack-symbols,} \\ \Sigma^* \subset \Sigma & \text{ is the set of output (or accepting) states.} \end{array} \right. \quad (6.5)$$

The general sequence of state-transitions executed by push-down automata proceeds as follows: (1) a symbol is read from the input, (2) a symbol is 'popped' from the stack, (3) a symbol is 'pushed' into the stack, (4) the automaton enters a new state. Symbol-strings are analyzed by push-down automata in much the same way as by finite automata. The automaton is first initialized with an empty stack. The string to be analyzed is placed on an input tape and is fed into the machine, and is "accepted" if the automaton reaches an accept-state after it has read the entire string. (Note that we do not require the automaton to be in an accept-state *immediately* after reading the last symbol of the input string – numerous internal stack-transitions can still occur after the last symbol is read and before the input string is finally declared as "accepted."). As for finite automata, the set of all strings accepted by the push-down automaton $\mathcal{M}$ is called the language accepted by $\mathcal{M}$, and is denoted by $L(\mathcal{M})$. Observe that we are perfectly free to consider the restricted class of push-down automata that effectively ignore the presence of a stack (i.e. no symbols are either popped from, or pushed into, the stack). Thus, the set of languages accepted by push-down automata includes all regular languages.

Context-Free Grammars: context-free grammatical rules $\{\alpha_i \rightarrow \beta_j\}$ are such that (1) α_i consist only of a single nonterminal symbol and (2) β_j are arbitrary strings of terminal and nonterminal symbols. It is easy to see why such a grammar is called context-free: consider a transition rule whose left-hand side contains a nonterminal portion, say $\alpha\alpha^{(\text{non})} \rightarrow \alpha\beta$, where $\alpha^{(\text{non})}$ is the nonterminal substring. The transition rule states that $\alpha^{(\text{non})}$ can be replaced by β only when it is preceded by the terminal α . Whether or not a replacement is made therefore depends on the "context" within which the nonterminal symbol finds itself.

Although it might also appear at first sight as though context-free grammars have an inherent ambiguity as to which nonterminal symbol to replace when a given grammatical rule involves more than one nonterminal symbol, no real ambiguity exists. For example, we may wonder what happens when we have the string $\alpha_1\beta_1^{(\text{non})}\beta_2^{(\text{non})}\alpha_2$ and the two rules $\beta_1^{(\text{non})} \rightarrow \alpha_3\beta_1^{(\text{non})}\alpha_3$ and $\beta_1^{(\text{non})} \rightarrow \alpha_4\beta_1^{(\text{non})}\alpha_4$. We could choose to be consistent and always work our way either from right to left replacing the *rightmost* nonterminal $\beta_1^{(\text{non})}$ or from left to right replacing the *leftmost* nonterminal $\beta_2^{(\text{non})}$ first. In the end, it turns out that such consistency 'ordering' does not really matter: if a string can be generated by any derivation, it can be generated by, say, a leftmost derivation [brooksh89].

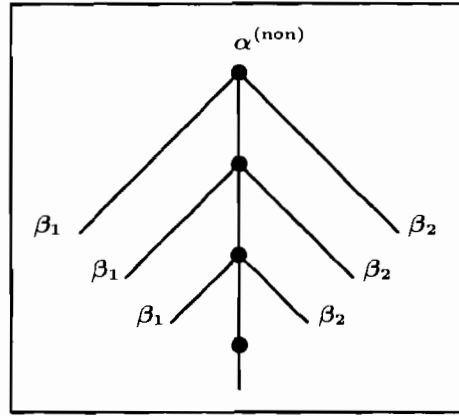
It can be shown that *the set of languages generated by context-free grammars is exactly equal to the set of languages accepted by pushdown automata* [hopc79].

Parse Trees: The words of a context-free language form sequences of terminal nodes in 'parse trees,' constructed according to the context-free grammar. A *parse tree* (or *derivation tree*) is a tree whose nodes are equal to terminal and nonterminal symbols of the grammar. The root node is equal to the start symbol while all descendent nodes of each nonterminal node are the symbols that replace given nonterminals according to the grammatical production rules. (No terminal can be an interior node, of course, and no nonterminal symbol can be a leaf.) Regular languages are context-free languages whose parse trees consist only of a "trunk" and a sequence of leaves that emerge one at a time out of the trunk.

EXAMPLE: Consider the following context-free grammar:

$$\begin{cases} \alpha^{(\text{non})} \longrightarrow \beta_1 \alpha^{(\text{non})} \beta_2, \\ \alpha^{(\text{non})} \longrightarrow \{\}, \end{cases} \quad (6.6)$$

where $\alpha^{(\text{non})}$ is a nonterminal symbol and β_1 and β_2 are terminal symbols. The parse-tree for this language is given by



so that this context-free language consists of all strings of the form $\beta_1^n \beta_2^n$, $n \in \mathcal{N}$.

6.2 Relationship Between CA and Formal Languages

We begin this section by showing that the finite-time limit set of an arbitrary CA rule ϕ , $\Omega_t = \Omega_t[\phi] = \Phi^t \Gamma$ (equation 6.2), is a regular language for all 't'. To this end, consider an explicit construction for the elementary rule **R178**, defined by

$$\begin{cases} 000 \rightarrow 0, & 001 \rightarrow 1, & 010 \rightarrow 0, & 011 \rightarrow 0, \\ 100 \rightarrow 1, & 101 \rightarrow 1, & 110 \rightarrow 0, & 111 \rightarrow 0. \end{cases} \quad (6.7)$$

We first show how to construct a STG for this rule. In the course of the construction it will become obvious how to generalize to other rules.

6.2.1 CA Rule $\rightarrow$ Finite State Transition Graph

The value $\sigma_i(1) \in \Gamma^{(1)}$ of site 'i' at time $t = 1$ in a configuration $\Gamma^{(1)} = \Phi \Gamma^{(0)} \in \Omega_1$ is, of course, a function of the values of the sites in its neighborhood at time $t = 0$: $\sigma_i(1) = \phi(\sigma_{i-1}(0), \sigma_i(0), \sigma_{i+1}(0))$, where $\sigma_{i-1}(0), \sigma_i(0), \sigma_{i+1}(0) \in \Gamma^{(0)}$. The value of the site 'i + 1', on the other hand, depends on the overlapping neighborhood, $\{\sigma_i(0), \sigma_{i+1}(0), \sigma_{i+2}(0)\}$. The dependence of $\sigma_{i+1}(1)$ on $\sigma_i(0)$ associated with this two site overlap may be represented by the graph g in figure 6.2.

The nodes of g represent all possible values of the overlap $\{\sigma_i(0), \sigma_{i+1}(0)\}$. These nodes are joined by arcs representing all possible values of the full three-site neighborhood. The symbol ($= 0$ or 1) associated with each arc is the value assigned to the center site of the neighborhood by the CA rule ϕ . In this way, (1) each possible path through the graph g corresponds to a particular initial configuration $\Gamma^{(0)}$, and (2) the configuration at time $t = 1$, $\Gamma^{(1)}$, is given by the sequence of symbols assigned to arcs on the path. By following all possible paths through g , one thus

obtains the set of all possible configurations Ω_1 obtained through a single step in the evolution of the CA defined by rule ϕ . It is in this sense that the set Ω_1 is completely represented by the graph g .

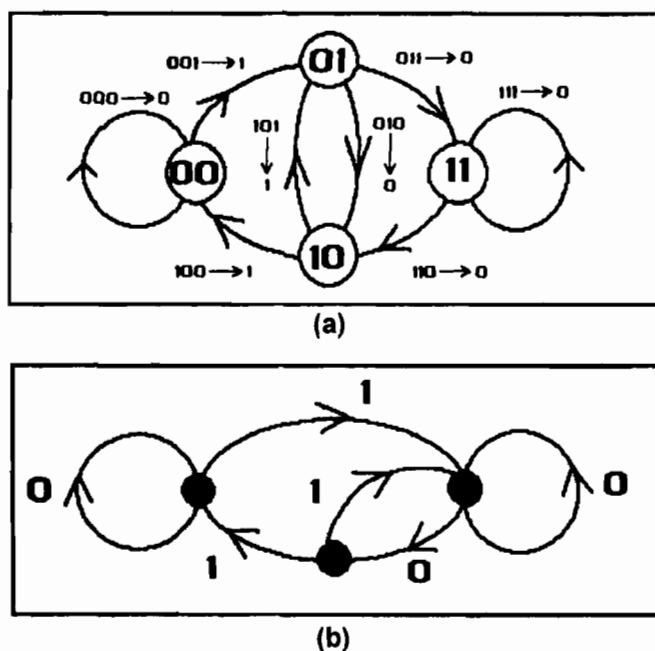


Fig. 6.2 Finite state transition graph for the CA rule defined in equation 6.8; see text.

The graph g in figure 6.2 may be considered as the finite STG for a finite automaton generating the formal language Ω_1 . To make the correspondence transparent, we associate each node of g with a state in the finite automaton, and each arc to a transition (or production rule according to the grammar prescribed by the finite automaton). Labeling the states in g as $\alpha_0 \equiv 00$, $\alpha_1 \equiv 01$, $\alpha_2 \equiv 10$, and $\alpha_3 \equiv 11$, we see that the grammar for this language consists of the following production rules:

$$\begin{cases} \alpha_0 \rightarrow 0\alpha_0, & \alpha_0 \rightarrow 1\alpha_1, & \alpha_1 \rightarrow 0\alpha_3, & \alpha_1 \rightarrow 0\alpha_2, \\ \alpha_2 \rightarrow 1\alpha_0, & \alpha_2 \rightarrow 1\alpha_1, & \alpha_3 \rightarrow 0\alpha_3, & \alpha_3 \rightarrow 0\alpha_2. \end{cases} \quad (6.8)$$

This finite set of production rules completely specifies the infinite set Ω_1 , which thus forms a regular language.

We make four additional comments about figure 6.2-a:

1. Not all possible sequences of 0's and 1's appear in Ω_1 . Since no path can include the sequence '111', for example, all configurations $\Gamma^{(1)} \in \Omega_1$ must exclude this particular block of sites.

2. The graph g is not unique. An alternative, and “simpler”, finite STG (call it $\tilde{g}$) is shown in figure 6.2-b. It is obtained from g by deleting all of the equivalent nodes in g , where two nodes are defined to be *equivalent* if all paths passing through them carry exactly the same symbols. In our example, nodes α_1 and α_2 are equivalent and can thus be combined into a single node.

3. Both g and $\tilde{g}$ are *non-deterministic*, in the sense that multiple arcs originating from the same node carry the same symbol. A given word in the resulting formal language therefore need not originate from a unique path.

4. There is nothing special about the particular rule we have chosen as an example. Indeed, if we would have chosen a different rule, the *template* for the state transition graph (figure 6.2-a) would have remain exactly the same, with only the symbols carried by the arcs changing. The construction outlined above therefore holds true for arbitrary rules. Moreover, it generalizes easily to rules with both larger neighborhood and/or greater number of local states. Figure 6.3, for example, shows the *template* analogous to that appearing in figure 6.2-a but for $k = 3$, $r = 1$ rules.

6.2.2 The Myhill-Nerode Theorem and the Minimization Algorithm

The Myhill-Nerode Theorem asserts that for every regular language there exists an *essentially unique deterministic finite automaton (DFA) containing a minimum number of nodes*.[†] We can arrive at this minimal DFA, or, equivalently, its minimal DSTG, in two steps: (1) use a simple canonical *subset construction* to form a DSTG $\mathcal{G}$, equivalent to the NDSTGs g and $\tilde{g}$ (we follow [hopc79] and [wolf84a]), and (2) reduce $\mathcal{G}$ by combining sets of all equivalent nodes, just as we had done previously in obtaining $\tilde{g}$ from g . It can be shown that the resulting graph $\tilde{\mathcal{G}}$ is the *minimal graph that recognizes the language Ω_1* .[‡]

We begin step one of the construction by forming the power set of the set of nodes in g . That is, we form the set Ψ , consisting of all $2^4 = 16$ subsets of the set $\{\alpha_0, \alpha_1, \alpha_2, \alpha_3\}$: $\Psi = \{\{\}, \{\alpha_0\}, \dots, \{\alpha_0, \alpha_1, \alpha_2, \alpha_3\}\}$.

Now, beginning with the *start node* $\Psi_0 = \{\alpha_0, \alpha_1, \alpha_2, \alpha_3\}$, we must find the set of NDSTG nodes reached by ‘0’ and ‘1’ arcs, in turn, according to the grammar defined by equation 6.8. These sets simply consist of the NDSTG nodes in g that are reached by ‘0’ and ‘1’ arcs from any of the $\alpha_i \in \Psi_0$. We repeat the construction for each such set – or *node* – in $\mathcal{G}$:

[†]The content of the actual theorem is somewhat more technical. The assertion given in italics in the main text above is one of the more important *consequences* of the Myhill-Nerode Theorem. Details may be found in [hopc79] and [davis83].

[‡]Note that the analogous procedure carried out for NDSTGs does not, in general, yield the *minimal graph*.

$$\begin{array}{ll}
 \Psi_0 = \{\alpha_0, \alpha_1, \alpha_2, \alpha_3\} & \rightarrow 0\{\alpha_0, \alpha_2, \alpha_3\}, & \Psi_0 = \{\alpha_0, \alpha_1, \alpha_2, \alpha_3\} & \rightarrow 1\{\alpha_0, \alpha_1\}, \\
 \{\alpha_0, \alpha_2, \alpha_3\} & \rightarrow 0\{\alpha_0, \alpha_2, \alpha_3\}, & \{\alpha_0, \alpha_2, \alpha_3\} & \rightarrow 1\{\alpha_1\}, \\
 \{\alpha_1\} & \rightarrow 0\{\alpha_2, \alpha_3\}, & \{\alpha_1\} & \rightarrow 1\{\}, \\
 \{\alpha_2, \alpha_3\} & \rightarrow 0\{\alpha_2, \alpha_3\}, & \{\alpha_2, \alpha_3\} & \rightarrow 1\{\alpha_0, \alpha_1\}.
 \end{array}
 \quad (6.9)$$

Note that only 5 of the 16 possible nodes are actually reached by transitions in $\mathcal{G}$. The notation $\{\alpha_1\} \rightarrow 1\{\}$ is meant to imply that there is no '1' arc originating at the $\{\alpha_1\}$ node. Figure 6.3 shows the DSTG for the deterministic finite automaton defined by the grammar in equation 6.9. By convention the starting node Ψ_0 is circled. Words in the regular language Ω_1 correspond to paths through $\mathcal{G}$ starting at Ψ_0 . Unlike the nondeterministic graph g in figure 6.2-a, each path in $\mathcal{G}$ is uniquely defined.

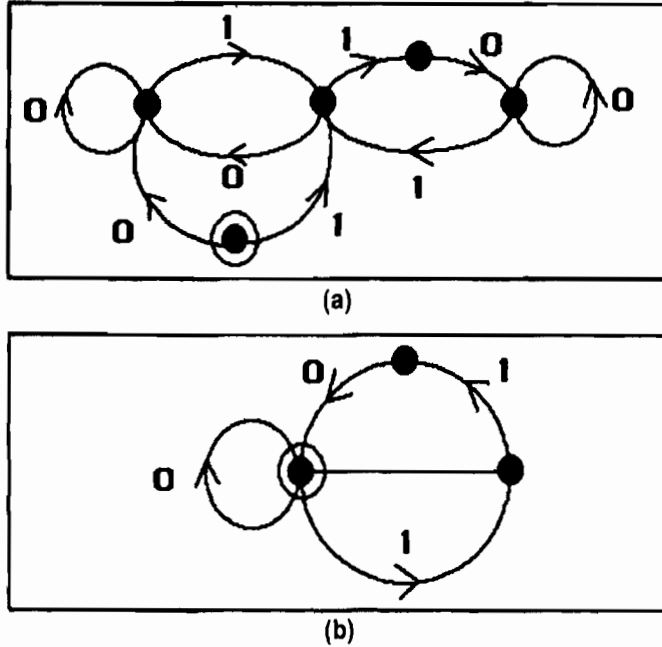


Fig. 6.3 Minimum DSTG defined by the grammar defined by equation Finite state transition graph for the CA rule defined in equation 6.9.

Proceeding to step two of our construction, we now *combine all equivalent nodes* in $\mathcal{G}$, in exactly the same way as we had done earlier in obtaining graph $\tilde{g}$ from g . The resulting graph $\tilde{\mathcal{G}}$ is shown in figure 6.3-b. It can be shown that this minimized DSTG is in fact the minimal one that recognizes the regular language Ω_1 [wolf84a]; it is unique *modulo* node relabelings.

Given that a unique minimal DFA exists and can always be found, it behooves

Rule	Class	Ξ_0	Ξ_1	Ξ_2	Ξ_3	Ξ_4	$\lambda_{\max}$
4	c2	1	2	2	2	2	1.618
22	c3	1	15	280	4506	$\sim 20,000$	1.917
32	c1	1	2	5	7	9	1.618
36	c2	1	3	3	3	3	1.755
90	c3	1	1	1	1	1	2.000
122	c3	1	15	179	5088	$\sim 20,000$	1.883
126	c3	1	3	13	107	2867	1.755
232	c2	1	11	15	19	23	1.785

Table 6.2 Number of nodes Ξ_t , $t = 0, \dots, 4$ in the minimal deterministic state transition graph (DSTG) representing the regular language $\Omega_t[\phi]$, where ϕ is an elementary $k = 2$, $r = 1$ CA rule; $\lambda_{\max}$ is the maximal eigenvalue of the adjacency matrix for the minimal DSTG and determines the entropy of the limit set in the infinite time limit (see text). Values are taken from Table 1 in [wolf84a].

us to exploit this fact in characterizing the set of CA rules, In particular, measures of complexity of minimal DFA provide insights into (if not outright estimates for) measures of complexity for CA limit sets.

6.2.3 Regular Language Complexity

Recall, from our discussion of complexity and entropy in chapter 4, that there is an entire hierarchy of complexity measures (or dimensions) describing the CA evolution in increasingly finer detail. The coarsest measure is one that merely counts the number of attainable states at a given time step ‘ t ’. The analogous *state complexity* (or *regular language complexity*) of a regular language, or of the set Ω_t , is given simply by the *number of states in the minimal DFA that accepts (or generates) the language (or limit set)*. Call this number Ξ_t . Ξ_t is equal to the minimal number of states required to define the set Ω_t in terms of a regular language, and is clearly bounded at all finite times ‘ t ’ by

$$1 \leq \Xi_t \leq 2^{k^{2rt}} - 1,$$

(6.10)

where r is the radius of the neighborhood. It has been experimentally confirmed that Ξ_t is nondecreasing in time, and that class **c1** and **c2** rules yield complexities that tend to constants after a very few time steps (or increase at most quadratically in time). The complexity of class **c3** and **c4** rules, on the other hand, typically increases exponentially with time. There are exceptions, of course. Some rules, such as the two additive rules such as **R90** and **R150**, for which $\Phi\Gamma = \Gamma$, so that all configuration can be reached at all times. Such surjective rules can be easily identified from their (deterministic) STG, since surjectivity requires that to each node must be attached all k possible outgoing arcs. Table 6.2 gives values for Ξ_t , $t = 0, \dots, 4$ for a few sample elementary rules.

6.2.4 Entropy

Let us recall some basic facts from our earlier discussion of elementary graph theory in chapter 2. Denote the *adjacency matrix* of a graph G by $A(G)$. Then the entries of the n^{th} power of $A(G)$, $[a_{ij}^{[n]}]$, $n \geq 1$, are equal to the number of different paths from vertex ' i ' to vertex ' j ' of length ' n ' in G ($= N_n(i, j)$). If $V = (\vec{v}_1, \dots, \vec{v}_n)$ is the set of mutually orthogonal normalized eigenvectors of $A(G)$, and $\Lambda = \delta_{ij} \lambda_i$, where $\{\lambda_i\}$ is the set of eigenvalues, then $a_{ij}^{[n]} = \sum_{l=1}^n v_{il} v_{jl} \lambda_l^n$, and the total number of length- n paths in G is given by

$$N_n = \sum_{ij} N_n(i, j) = \sum_{ij} a_{ij}^{[n]} = \sum_{l=1}^n C_l \lambda_l^n, \quad (6.11)$$

where $C_l = (\sum_{i=1}^n v_{il})^2$. For large n , we can use the approximation

$$N_n \sim \text{Tr}(A^n) = \sum_i \lambda_i^n \sim \lambda_{\max}^n, \quad (6.12)$$

where ' $\text{Tr}(A)$ ' denotes the *trace* of matrix A , and $\lambda_{\max}$ is the magnitude of the largest eigenvalue.

The (finite time) limit set Ω_t may be considered to be a *Cantor Set*, with dimension S given by (see section 4.5.2):

$$S = \lim_{n \rightarrow \infty} \frac{1}{n} \log_k N_n = \log_k \lambda_{\max}. \quad (6.13)$$

6.2.5 What Happens as $t \rightarrow \infty$?

The above discussion lends at least some heuristic validity to the assertion that the set of configurations generated after a *finite* number of iteration steps Ω_t forms a regular language. The problem obviously becomes more difficult, however, when we consider the large time limit. While some CA rules yield regular languages even as $t \rightarrow \infty$, other rules appear to yield more complicated formal languages. It has been suggested, for example, that class **c3** and **c4** rules give rise to regular languages whose complexity increases exponentially in time. This suggests that no finite description will suffice in the *infinite time limit*, and that Ω_∞ *must* therefore be specified in terms of a more complex formal language. Our attempts at describing this more complex formal language must unfortunately face at least two formidable obstacles: (1) given any arbitrary generative grammar, such as the one we could presumably write down for a suspected "complex" rule, it is, in general, *undecidable* to which level of the Chomsky hierarchy that grammar actually belongs, and (2) given this grammar, there does not, in general, exist any finite algorithm for constructing its minimal form (i.e. there are no analogs of the regular-language minimization algorithm outlined in section 6.2.2 above for higher level formal languages). An important fundamental consequence of these "obstacles" is that the (analogue of a regular) language complexity is *formally uncomputable*; i.e. if class **c3** and **c4** rules do indeed yield limit sets corresponding to either context-free or unrestricted

formal languages, their entropies are generally not computable. (Note that this fact does not in any way preclude us from using numerical data to estimate these same entropies). While it may be undecidable to what level of the Chomsky hierarchy a given generative grammar belongs, there is a well-known set of properties that can be used to very easily verify that a given language is *not* in a given class. These properties are collectively called the *pumping lemmas*.

Pumping Lemmas: The pumping lemma for regular languages states that for every regular language L_R there exists a symbol-sequence length l such that every string with length greater or equal to l can be written in the form $\alpha_1\alpha_2\alpha_3$, such that for any n the symbol-sequence $\alpha_1\alpha_2^n\alpha_3$ is also in the language. The lemma is merely a restatement of the obvious fact that any sufficiently long “walk” through a finite graph must contain a cycle. Since cycles can be traversed an arbitrary number of times, symbol-sequences can be repeated an arbitrary number of times.

Now, if one can show that a given language has a set of strings for which this lemma is not satisfied, that language cannot be regular. This immediately shows that the language $\alpha_1^n\alpha_2^n$, for example, is not regular. More importantly, it is possible to construct CA rules for which the regular language pumping lemma fails as $t \rightarrow \infty$. Hurd [hurd87] shows an explicit construction.

The regular language pumping lemma can be generalized to context-free languages. It states that given a context-free language L_F , there exists a length l such that every symbol-sequence of length greater than or equal to l can be written in the form $\alpha_1\alpha_2\alpha_3\alpha_4\alpha_5$ such that $\alpha_1\alpha_2^n\alpha_3\alpha_4^n\alpha_5$ is also in L_F for all n . Thus, for example, the language $\alpha_1^n\alpha_2^n\alpha_3^n$ cannot be a context-free language.

6.3 Power Spectra of Regular Languages

Fourier transforms and power spectra are frequently used in physics to reveal otherwise hidden regularities in apparently irregular behavior. Li ([li87], [li89b]) has exploited a connection between regular languages and Markov chains to derive closed form expressions for the spatial power spectra for some periodic CA. The key insight is the generalization of STGs to graphs with *weighted* arcs, where the value of the weight of a given arc corresponds to the probability of the transition defined by that arc. The resulting “weighted” regular grammars generate sequences in the same way as do Markov chains, which specify the probability that a given value will appear on the next time step. Since the correlation function (and, hence, the power spectrum; see below) is related to the probabilities for two values to appear separated by some distance τ , it is also related to the τ^{th} power of the one-step transition probability specified by the regular language grammar. By using the definition of a regular language, we can deduce some of the properties of its spectrum. This section summarizes Li’s methodology, and follows [li87] and [li89b].

Given a real-valued sequence $\sigma_0, \sigma_1, \dots, \sigma_{N-1}$, the *correlation function* $R(\tau)$ and *Fourier Transformation* $\mathcal{F}(f)$ may be defined in both a continuous and discrete form:

$$\begin{aligned}
\text{Discrete} & \longleftrightarrow \begin{cases} R(\tau) = \left[\frac{1}{N} \sum_{i=0}^{N-1} \sigma_i \sigma_{i+\tau} \right] - \left[\frac{1}{N} \sum_{i=0}^{N-1} \sigma_i \right]^2, \\ \mathcal{F}(f) = \frac{1}{N} \sum_{j=0}^{N-1} e^{-i2\pi(f/N)j} \sigma_j, \quad f = 0, 1, \dots, N-1. \end{cases} \\
\text{Continuous} & \longleftrightarrow \begin{cases} R(\tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sigma(t) \sigma(t+\tau) dt - \left(\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sigma(t) dt \right)^2, \\ \mathcal{F}(f) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_{-\infty}^{\infty} e^{-i2\pi ft} \sigma(t) dt, \quad f = 0, 1, \dots, N-1. \end{cases}
\end{aligned} \tag{6.14}$$

We give both forms here because, depending on the problem, either of the two forms may yield a “simpler” answer. Although the discrete form may appear *a-priori* to be the natural choice, for example, its discrete nature actually introduces some spurious periodicity into the resulting power spectra, thus washing away some of its characteristic features. We therefore follow Li [li87] in working mainly with the continuous forms of $R(\tau)$ and $\mathcal{F}(f)$.

The energy spectral density function (or *power spectrum*) $P(f)$ is given by the absolute square of $\mathcal{F}(f)$:

$$P(f) = \begin{cases} N |\mathcal{F}(f)|^2 & \leftrightarrow \text{Discrete,} \\ \lim_{T \rightarrow \infty} \left| \frac{1}{T} \int_{-\infty}^{\infty} e^{-i2\pi ft} \sigma(t) dt \right|^2 \cdot T & \leftrightarrow \text{Continuous.} \end{cases} \tag{6.15}$$

It is a well known fact, called the *Wiener-Khintchine Theorem* [gardi85], that the correlation function and power spectrum are Fourier Transforms of one another:

$$P(f) = \int_{-\infty}^{\infty} e^{-i2\pi f\tau} R(\tau) d\tau = 2 \int_0^{\infty} \cos(2\pi f\tau) R(\tau) d\tau. \tag{6.16}$$

6.3.1 Numerical Estimates

Figures 6.4 shows some of the variety of possible shapes of $P(f)$ for elementary rules; shown in the figures are the power spectra for rules **R11**, **R56**, **R150** and **R200**. The plots were generated for lattice size $N = 2048$, ignoring the first 15 transient steps and averaging a total of 20 runs. Also, since there are only N data points but $2N$ real Fourier components, half of the components are redundant. Thus, only the first half of the components are shown (see [li89b] or [li87] for a complete set of power spectra).

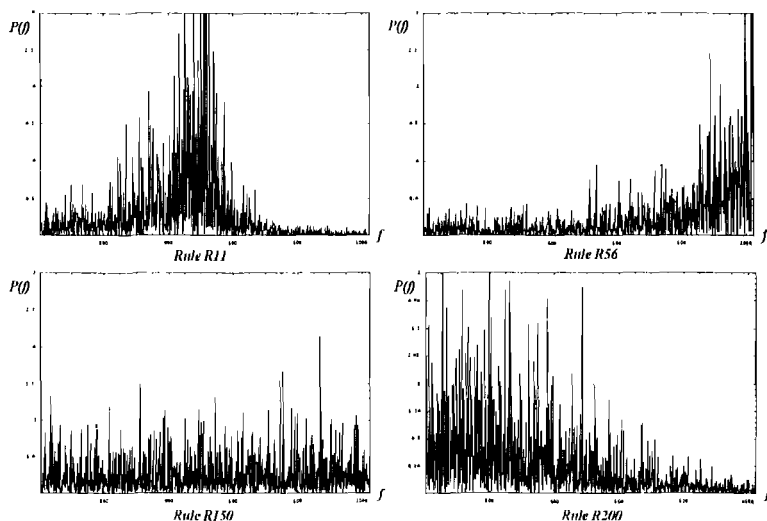


Fig. 6.4 Numerical estimates of $P(f)$ versus frequency f for four elementary CA rules; see text.

The power spectrum of some rules (whose evolution of random initial states typically yields complex class **c3** behavior, corresponding to the ‘trivial’ regular language in which all possible words can occur) is essentially ‘white’ (i.e. $P(f) \sim \text{constant}$); some rules, such as rule **R200**, have $P(f)$ with $1/f^2$ tails (i.e. Brownian noise); other rules have $P(f)$ that do not appear to be fit by any $1/f^n$ -like distribution. The power spectra of rules leading to periodic behavior typically show discrete peaks. In the next section we outline Li’s algorithm for generating closed form expressions for the power spectra of *periodic* rules, or those for which a regular language description can (at least in principle) always be found. Nonperiodic rules may or may not be described by regular languages, and are for this reason considerably more difficult to deal with.

6.3.2 Li’s Algorithm for Generating Power Spectra

Li’s algorithm for generating closed form solutions for the power spectra of CA attractors consists essentially of five main parts ([li87], [li89b]):

Step 1 – Construct the STG: The first step consists of constructing the STG for the CA attractor. We do this in exactly the same manner as discussed earlier in section 6.2.2, deleting all arcs that do not satisfy a prescribed invariance condition defining the simple attractor state. Were we to do this for rule **R42**, for example, for which the evolution leads into an essentially time invariant state in which the state at time ‘ t ’ is equal to the state at ‘ $t - 1$ ’ shifted to the left by one site, the invariance condition would simply be $\sigma_{i-1}(t+1) = \sigma_i(t)$. Only those arcs satisfying this condition would be kept.

Step 2 – Specify the Arc-to-Arc Transition Matrix $\mathcal{P}$: Each element $[\mathcal{P}_{ij}]$ of this matrix is equal to the probability that arc ‘ i ’ will be followed by arc ‘ j ’.[‡] Although it will taken for granted in the following examples that the values of $\mathcal{P}$ can be specified, we should be quick to point out that there is actually no well-defined scheme to find these values. The best one can do in practice is to either use a mean-field-theory estimate (see section 7.4) or perhaps use a more refined approach like that given by higher-order local-structure-theory (see section 5.3).

Step 3 – Calculate $\mathcal{P}^\tau$: If $\mathcal{P}$ is diagonalizable, we can proceed as follows [horn85]. Let $\vec{p}_1, \vec{p}_2, \dots, \vec{p}_n$ denote the eigenvectors of $\mathcal{P}$, corresponding to eigenvalues $\lambda_1, \dots, \lambda_n$. Define a matrix V by placing in the j^{th} column of V the components of $\vec{p}_j$; i.e. set $[V_{ij}] = [\vec{p}_j]_i$. Then, defining $[\Lambda_{ij}] \equiv \delta_{ij}\lambda_i$, we have that $P = V\Lambda V^{-1}$, $P^2 = (V\Lambda V^{-1})(V\Lambda V^{-1}) = V\Lambda(V^{-1}V)\Lambda V^{-1} = V\Lambda^2 V^{-1}$, and, in general, for any positive integer τ ,

$$P^\tau = V\Lambda^\tau V^{-1}. \quad (6.17)$$

Step 4 – Calculate the Autocorrelation Function $R(\tau)$: Assuming that $\sigma \in \{0, 1\}$, $R(\tau)$ simplifies to

$$\begin{aligned} R(\tau) &= \left(\sum_{i=1}^n \sum_{j=1}^n \beta_i \mathcal{P}_{ij}^\tau \sigma_i \sigma_j \right) - \left(\sum_{i=1}^n \beta_i \sigma_i \right)^2, \\ &= \sum_{i'j'(\sigma_{i'}=1, \sigma_{j'}=1)} \beta_{i'} \mathcal{P}_{i'j'}^\tau - \left(\sum_{i'(\sigma_{i'}=1)} \beta_{i'} \right)^2, \end{aligned} \quad (6.18)$$

where β_i and σ_i are, respectively, the equilibrium probability distribution and value for the i^{th} arc.

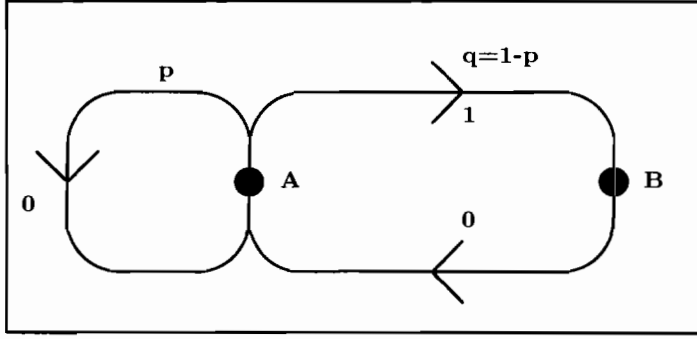
Step 5 – Calculate the Power Spectrum $P(f)$: Having calculated $R(\tau)$, we can use either equation 6.15 or 6.16. In the case where all of the eigenvalues λ_i are real, the (continuous) spectrum is given by

$$P(f) = \sum_{i=1}^n \left[a_i \frac{2/t_{pi}}{(2\pi f)^2 + (1/t_{pi})^2} + b_i \left(\frac{1/t_{ni}}{(2f+1)^2\pi^2 + (1/t_{ni})^2} + (f \rightarrow -f) \right) \right], \quad (6.19)$$

where $t_{pi} \equiv \log(1/\lambda_{pi})$, $t_{ni} \equiv \log(1/|\lambda_{ni}|)$ and λ_{pi} and λ_{ni} are the positive and negative eigenvalues, respectively; the coefficients a_i and b_i are simply related to the eigenvectors of $\mathcal{P}$ [li89b]. We see that (in this simplest case) positive eigenvalues lead to spectral peaks at $f = 0$ while negative eigenvalues lead to peaks at $f = 1/2$. When the eigenvalues are complex, the positions of the peaks are generally functions of the phase angles of the eigenvalues.

[‡]Note that $\mathcal{P}$ is not equal to the more conventional node-to-node (weighted) adjacency-matrix.

EXAMPLE:[†] Consider a simple but non-trivial STG consisting of two nodes and three arcs (the reader can check that this regular language actually characterizes the attractors of many one dimensional CA – rules **R12**, **R56** and **162**, among others):



Let $i = 1$ represent arc $\bar{A}\bar{B} = 1$, $i = 2$ represent arc $\bar{B}\bar{A} = 0$ and $i = 3$ represent arc $\bar{A}\bar{A} = 0$. The arc-to-arc transition matrix $\mathcal{P}$ is then equal to

$$\mathcal{P} = \begin{pmatrix} 0 & 1 & 0 \\ q & 0 & p \\ q & 0 & p \end{pmatrix}.$$

The eigenvalues are the zeros of the characteristic equation $\det(\mathcal{P} - \lambda \cdot I) = -\lambda(\lambda - 1)(\lambda + q)$: $\lambda_1 = 0$, $\lambda_2 = 1$ and $\lambda_3 = -q$. The corresponding eigenvectors are given by $\vec{v}_1 = (-p/(1-p), 0, 1)$, $\vec{v}_2 = (1, 1, 1)$ and $\vec{v}_3 = (-p/(((1-p)/(p-1) + 1 - p)(p-1)), -p/((1-p)/(p-1) + 1 - p), 1)$. The τ^{th} power of the arc-to-arc transition matrix $\mathcal{P}^\tau$ is given by

$$\mathcal{P}^\tau = \begin{pmatrix} \bar{\sigma} + (-q)^\tau/(1+q) & \bar{\sigma} - (-q)^\tau/q(1+q) & p/q(\bar{\sigma} + (-q)^\tau/(1+q)) \\ \bar{\sigma} + (-q)^{\tau+1}/(1+q) & \bar{\sigma} - (-q)^{\tau+1}/q(1+q) & p/q(\bar{\sigma} + (-q)^\tau/(1+q)) \\ \bar{\sigma} + (-q)^{\tau+1}/(1+q) & \bar{\sigma} - (-q)^{\tau+1}/q(1+q) & p/q(\bar{\sigma} + (-q)^\tau/(1+q)) \end{pmatrix}$$

where the average value $\bar{\sigma} = q/(1+q)$. Now, it is easy to show that the equilibrium value for arc $\bar{A}\bar{B}$, $b_1 = \bar{\sigma}$ (since it is the only arc with value '1'), so that the correlation function

$$R(\tau) = b_1[\mathcal{P}_{11}^\tau] - \bar{\sigma}^2 = \frac{q}{(1+q)^2}(-q)^\tau.$$

Using equation 6.16 we obtain the (continuous form of the) power spectrum:

$$\begin{aligned} P(f) &= 2 \int_0^\infty \cos(2\pi f\tau) \frac{q}{(1+q)^2} q^\tau \cos(\pi\tau) d\tau \\ &= \log\left(\frac{1}{q}\right) \frac{q}{(1+q)^2} \left[\frac{1}{(f - \frac{1}{2})^2 4\pi^2 + \log^2(q)} + (f \rightarrow -f) \right]. \end{aligned}$$

[†]This example appears as example-2 in chapter 2 of Li's thesis [li89b].

Notice that $P(f)$ has a maximum at $f = 1/2$. The presence of this maximum can be directly traced back to the length-2 loop of the STG shown above, which yields a period-2 component in the spatial configurations. The half-width of the peak ($=\log(1/q)$) is seen to decrease as q decreases, a natural consequence of the period-2 part of the STG being visited more often as q increases. Figure 6.4 shows an empirical estimate of the power spectrum for rule **R56** obtained for a size $N = 2^{11} = 2048$ system.

We conclude this section with a few general comments: We note first that the methodology outlined above is applicable only to those rules having relatively simple attractor states (exceptions may include rules **R30** and **R90** whose long-time states may be characterized by a simple “white-noise” random process). Moreover, only regular-language structures were considered. Higher-level languages, such as context-free languages, could be used to explain the spectra of some CA rules whose attractors are not amenable to the description discussed above (for an application of context-free languages to $1/f$ -noise see [li89b]).

Second, observe that the methodology need not be constrained to CA systems alone. With a suitable coarse-graining, the same methodology can easily be extended to provide the spectra of continuous dynamical systems, such as one-dimensional mappings of the unit interval to itself.

Finally, notice that the general methodology exploits a connection between “topology” (of the STG) and the resulting “dynamics” (in the form of the power spectrum). This connection has been explored in slightly different guises by both local structure theory (section 5.3) and more direct efforts to isolate the effect that the underlying lattice structure has on the overall dynamics for systems evolving according to additive rules (section 5.4). Though immensely important, this connection is also an immensely difficult one to isolate. Indeed, it is arguable that most fundamental results probably remain to be discovered. The difficulty stems largely from our general inability to obtain exact closed form results for any systems other than a few isolated classes of rules (additive rules forming the prototypical class of rules that are amenable to such an analysis). One suspects, however, that in the general case, the situation ought not really be too different from say, that in chemistry, where the energy levels of a molecule are related in a very fundamental way to the topological configurations of its constituent atoms.[‡]

6.4 Reversible Computation

Any computation, whether performed by a slide rule, computer workstation or brain, is inherently a *physical* process, and as such is subject to whatever laws and limitations apply to physical systems in general. It is a natural question to ask, then, whether there exists a fundamental thermodynamic limit to computation; i.e.

[‡]For an interesting discussion of the connection between the spectra of graphs (i.e. the set of eigenvalues of adjacency matrices of given graphs) and some properties of various chemical and physical systems, the reader should consult chapter eight of [cvet79].

whether there is a minimum amount of energy that is required to perform a given logical operation? This section provides a concise history of the development of an answer to this most-important basic question and discusses how it relates to formal CA studies. The interested reader can find additional details in papers by Bennett ([benn73], [benn82], [benn84], [benn85], [benn87], [benn88]), Fredkin [fredkin82], Keyes [keyes75], Landauer ([land61], [land67], [land82], [land84a], [land84b], [land86], [land87a], [land87a]), Margolus ([marg84], [marg88]), Toffoli ([toff77a], [toff77b], [toff80]) and an excellent collection of reprints edited by Leff and Rex [leff90].

Although the basic question arguably dates back to Maxwell and the paradox of *Maxwell's Demon*[†], the formal connection between thermodynamics and computation seems to have been made first by von Neumann in a 1949 lecture [vonN66].[‡] Von Neumann asserted that any computer operating at temperature T must dissipate at least $kT \ln 2$ units of energy ($\sim 3 \cdot 10^{-21}$ joules at room temperature) "per elementary act of information, that is per elementary decision of a two-way alternative and per elementary transmittal of one unit of information." Brillouin, in his well-known information theory text *Science and Information Theory* [brill56], came to a very similar conclusion. He argued that, within the context of physical measurement, the minimal energy dissipation must increase with certainty of the measurement as $kT \ln(1/\epsilon)$, where ϵ represents the probability of error within the measurement.

Von Neumann's and Brillouin's assertions are both certainly very plausible ones, in view of the fact that each mechanical degree of freedom used to store one bit of information (such as a capacitor, for example) involves at least an amount of kT of thermal noise which must then "apparently" be overcome to reliably read or manipulate the given bit of information [benn82]. We have inserted the word "apparently" in quotes, however, because this supposition is now known to be false:

[†]*Maxwell's Demon* was conceived by James Clerk Maxwell in his 1871 book, *Theory of Heat*. Towards the end of the book, in a section entitled, "Limitations of the Second Law of Thermodynamics", Maxwell writes: "...conceive a being whose faculties are so sharpened that he can follow every molecule in its course, such a being, whose attributes are still as essentially finite as our own, would be able to do what is at present impossible to us. For we have seen that the molecules in a vessel full of air at uniform temperature are moving with velocities by no means uniform, though the mean velocity of any great number of them, arbitrarily selected, is almost exactly uniform. Now let us suppose that such a vessel is divided into two portions, A and B, by a division in which there is a small hole, and that a being, who can see the individual molecules, opens and closes this hole, so as to allow only the swifter molecules to pass from A to B, and only the slower ones to pass from B to A. He will thus, without expenditure of work, raise the temperature of B and lower that of A, in contradiction to the second law of thermodynamics." (The actual term *Demon* was first introduced by W. Thomson in his 1879 paper, "The Sorting Demon of Maxwell").

[‡]The 'intellectual climate' was ripened for such abstract considerations by a number of important earlier contributions, including those by Szilard [szil29], who provided a detailed analysis of the thermodynamics of Maxwell's Demon, Turing [turing36], who laid the groundwork for formal computation theory (see section 12.8), and Shannon [shan48], who developed the mathematical formalism appropriate for discussing the fundamental limitations to information transmission through noisy channels.

computers can, in principle, provide an *arbitrary* amount of *reliable* computation per kT of dissipated energy (see discussion below).

Although von Neumann's original assertion articulated the prevailing sentiment of the time, a deeper understanding of the relationship between energy dissipation and computation was not really reached until the issue was critically re-examined by Rolf Landauer in a landmark 1961 paper [land61]. Landauer observed that the existence of logically irreversible operations (i.e. those involving the erasure of some information in the course of a computation) necessarily implies a strictly *physical* irreversibility in the mechanism responsible for the actual computation.

Consider the logical **AND** and **OR** operators or *gates*, schematic representations and truth tables for which are shown in figure 6.5. Notice that both gates destroy information. Whenever the output of the **OR** gate equals '1', for example, it is unclear as to what two input values were responsible. Indeed, just as elementary CA are typically irreversible because the size of their output state-space is smaller than that of their input state-space, so too all logic gates possessing fewer output lines than input lines must inevitably discard some information.

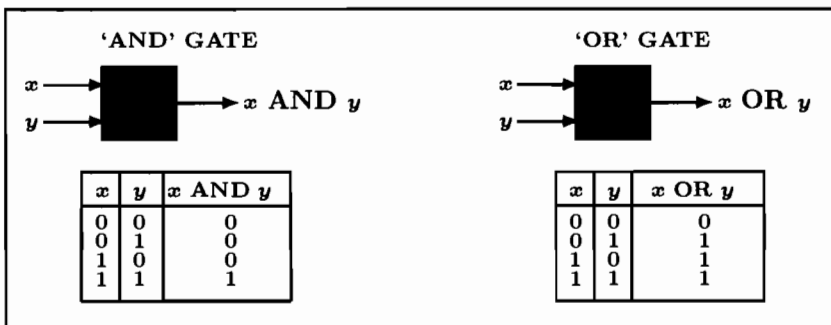


Fig. 6.5 Schematic representations and truth tables for conventional **AND** and **OR** gates. Observe that both gates dissipate energy: if the output of the **AND** gate equals '0' (or the output of the **OR** gate equals '1'), there is no way of deducing the values of the respective inputs.

Assuming that the underlying dynamics of any computing device is reversible – so that the global information content of the system remains constant – the thermodynamic cost of losing a single bit of information must be paid for by an accompanying transfer of at least $kT \ln 2$ of work into various *non-computational* degrees-of-freedom. Similarly, whenever a 'bit' is simply erased from memory (i.e. whenever any two-state subsystem is reset to its cleared, or zero, state), the information loss to the system must be compensated for by a simultaneous transfer of information into the surrounding (non-computational) 'heat bath'. Landauer concluded that whenever computations depend on irreversible logical operations (which, it is important to point out, were the *only* ones known at that time), the computation must inevitably induce a minimum energy dissipation on the order of kT per elementary logical operation. What Landauer did not ask was whether ir-

reversible gates are themselves essential to computation. It was not until 1973 that Charles Bennett showed that computation need not, in fact, depend on irreversible logical primitives [benn73]. Before we discuss the implications of Bennett's brilliant insight, however, we must first briefly review the concept of a *universal logic gate*.

6.4.1 Universal Logic Gates

A set G of logic gates is *universal* if an arbitrary n -variable Boolean function $\mathcal{F}$ can be written as a composition of the logic gates in G ; a universal set of gates $g_1, \dots, g_m$ is sometimes also said to form a *basis set* for $\mathcal{F}$. It is easy to show that the set consisting of the Boolean operators **AND**, **OR** and **NOT**, for example, is universal.[†]

Consider an arbitrary set of Boolean input values, $x_1, \dots, x_n$. Using only the Boolean operators **AND** and **NOT**, we can write down an expression which takes the value '1' *if and only if* a particular configuration of 0's and 1's appears in the input. Suppose that $n = 6$ and we want to construct an expression that equals one if and only if $x_1 = x_3 = x_4 = x_5 = 1$ and $x_2 = x_6 = 0$. A little thought will show that the required expression is given by joining the string of six Boolean variables with the **AND** operator, substituting **NOT**(x_i) for all values x_i that are required to equal zero:

$$x_1 \text{ AND } (\text{NOT } x_2) \text{ AND } x_3 \text{ AND } x_4 \text{ AND } x_5 \text{ AND } (\text{NOT } x_6). \quad (6.20)$$

In order to construct an expression representing an arbitrary Boolean function $\mathcal{F}$, we must therefore perform two simple steps: (1) construct expressions of the above form for each occurrence of a '1' in $\mathcal{F}$'s truth table, and (2) join each such expression by the **OR** operator. Since each term is explicitly constructed so as to pick out a particular input configuration yielding the value '1' under $\mathcal{F}$, no more than one such term in the resulting **OR** expansion can yield the value '1' for a given input. All other configurations are identically zero.

EXAMPLE: Consider the two-input function $\mathcal{F}: \{0, 1\}^2 \rightarrow \{0, 1\}$, defined by the truth table:

x_1	x_2	$\mathcal{F}(x_1, x_2)$
0	0	0
0	1	1
1	0	1
1	1	0

We see that $\mathcal{F}(x_1, x_2) = 1$ if and only if either $x_1 = 0$ and $x_2 = 1$, or $x_1 = 1$ and $x_2 = 0$ (i.e. $\mathcal{F}$ is the **EXCLUSIVE-OR** operator). An equivalent Boolean expression,

[†]Truth tables for the **AND** and **OR** gates are shown in figure 6.5. The one-input/one-output **NOT** operator simply negates the input value: **NOT**(0)=1 and **NOT**(1)=0.

constructed using only **AND**, **OR** and **NOT** gates, is therefore given by

$$((\text{NOT } x_1) \text{ AND } x_2) \text{ OR } (x_1 \text{ AND } (\text{NOT } x_2)).$$

Note that while the set $\{\text{AND}, \text{OR}, \text{NOT}\}$ forms a complete basis, it is not a *minimal* basis; i.e. a basis set such that no subset of the set is itself a complete basis. It is easy to show, however, that the subset consisting of the **AND** and **NOT** operators is a minimal basis. Similarly, there also exist *individual* gates, such as the **NAND** and **NOR** gates (see figure 6.6), that are universal by themselves.

x_1	x_2	$x_1 \text{ NAND } x_2$	x_1	x_2	$x_1 \text{ NOR } x_2$
0	0	1	0	0	1
0	1	1	0	1	0
1	0	1	1	0	0
1	1	0	1	1	0

Fig. 6.6 Truth tables for the universal Boolean operators **NAND** and **NOR**.

Consider the **NAND** gate. The **NAND** gate yields a '1' unless both input values equal '1'. If the value of either one of input lines is fixed at '1', the gate is equivalent to the **NOT** operator; i.e. the gate yields an output of '1' if the free input-line equals '0' and a '0' if the free input-line equals '1'. If we now use the **NOT** operator to complement the **NAND** operator input line, we obtain the **AND** operator. Since we have already observed that the set $\{\text{AND}, \text{NOT}\}$ is universal, we have thus also shown that the **NAND** operator is, by itself, universal.[‡]

The question which Landauer failed to ask in 1961 [land61] and which was answered first by Bennett in 1973 [benn73] and later, independently, by Fredkin [fredkin82], is whether *irreversible* logic gates are essential to computation. Might it be possible to construct a universal set out of *reversible* gates?

6.4.2 Universal Reversible Logic Gates

As commented earlier, the reason that conventional logic gates are generally irreversible is that an information loss is inevitable whenever a gate has fewer output lines than input lines. To find reversible primitives, therefore, we must start by looking at gates that have an equal number of input and output lines.

A simple exercise should convince the reader that the set of 24 possible 2-input/2-output reversible gates fails to be universal.[†] To find a universal set we must there-

[‡]We could also just as easily construct the **OR** operator by complementing each of the two input-lines to a **NAND** gate with a **NAND** constructed **NOT** gate.

[†]An examination of the $(4^4) = 256$ possible truth tables for 2-input/2-output functions reveals that only 24 are invertible. These 24 functions are, in fact, identical to the set of functions that can be constructed using compositions of only the Boolean **XOR** function. Since there is no way

fore either enlarge the state space to $k > 2$ or increase the number of input/output lines.

Consider a logic gate with 3-input and 3-output lines. Edward Fredkin, motivated by a deep conviction in a fundamental connection between a discrete, finite physics and reversible computation [wright88],[†] discovered a simple universal 3-input/ 3-output logic function that now bears his name [fredkin82].

6.4.2.1 The Fredkin Gate

In reversible systems, it is generally true that all signal processing must effectively reduce to *conditional routing* of signals. The Fredkin gate, shown in figure 6.7, consists of three inputs and three outputs. One of the input lines, labeled ‘c’ in the figure, is the *control* line and carries the input value through the gate unchanged. If the value of the control line $c = 0$, the values of the other two input lines than pass through unchanged as well. If $c = 1$, the outputs of the other two lines are *switched*; i.e. the output of line x becomes the output for y and vice versa. Notice that, in this way, the gate does not discard any information. Given an output state, the exact input state responsible for that output can be immediately deduced.

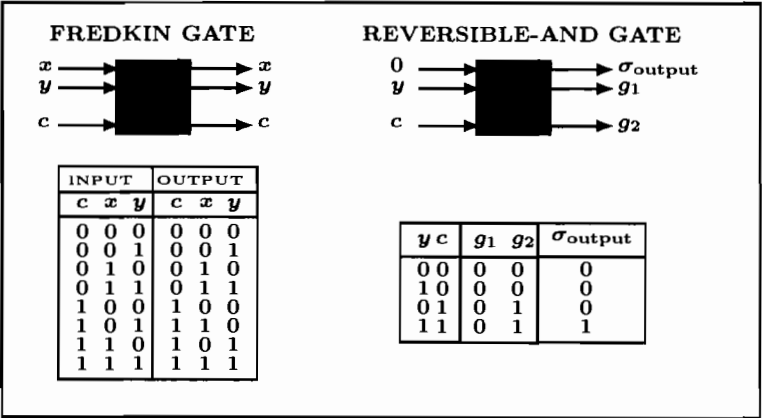


Fig. 6.7 Schematic representations and truth tables for the *Fredkin gate* and *Reversible-AND gate*. In the Fredkin gate, the c -line is the control line; in the reversible-AND gate, lines g_1 and g_2 are the “garbage” lines (see text).

Fredkin was able to show that an *arbitrary logic gate, reversible or not, can be reproduced by a suitable arrangement of Fredkin gates* [fredkin82]. To reproduce the **AND** gate, for example, we must fix one input, say line x , to have the value ‘0’ (see figure 6.5). Ignoring, for the moment, the output to lines y and c – which,

to reproduce the **NAND** function out of **XOR** alone, this set cannot be universal [marg88].

[†]We discuss Fredkin’s philosophy and ideas on a finite, fundamentally discrete physics in section 12.6.4.

because they play no direct role in interpreting this particular configuration of the Fredkin gate as an **AND** gate, are called *garbage bits* – the output to line x is easily verified to be equivalent to the **AND** operator. Figure 6.8 shows the Fredkin-gate realizations of conventional **OR**, **NOT** and **FAN-OUT** operators.[†]

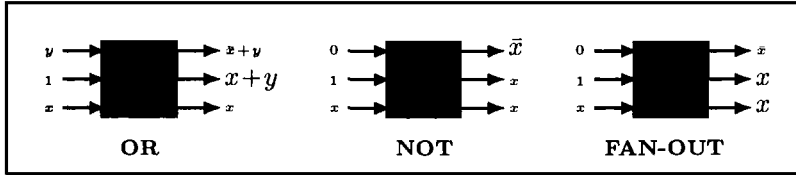


Fig. 6.8 Fredkin-gate realizations of conventional **OR**, **NOT** and **FAN-OUT** operations. The desired outputs of each gate are shown in large type; the other output lines are the garbage lines.

The garbage bits g_1 and g_1 appearing in both figures 6.7 and 6.8 appear, at first sight, to serve no useful purpose. They are generated in the course of the computation, but play no role in the effective functionality of the gate. Moreover, if the gate (or circuit, or even the computer built out of these gates) is to be used again, an information loss is sure to arise since these garbage bits must first be cleared out of memory. It was Bennett's and Fredkin's insights that first paved the way out of this dilemma. They both showed that the garbage bits in fact play a very important role in assuring that no energy dissipation results. The trick is to first copy down the result of the desired computation, such as the output of our reversible **AND** gate, and then *run the gate backwards with the garbage bits and desired output as our new inputs*. Since the gate is reversible, no energy needs be dissipated, and we are assured of returning to exactly the same state that the system had originally started in. In other words, provided we copy down our desired answer at the end of each computation, it is possible to complete an entire *computing cycle* – starting from and returning to a given starting state – without dissipating any energy.

The Fredkin gate satisfies two obvious, but nonetheless, important properties: (1) it is reversible, with the inverse gate equal to itself (i.e. if the values of the output lines x , y and c are fed back in and the gate is run backwards, the result is the set of original input values), and (2) the number of 1's in the output always equals the number of 1's in the input. Whenever a logic gate satisfies the second property it is said to be a *conservative logic gate*. Fredkin had, in fact, intentionally searched for a conservative gate in order to make it easier to find an actual physical realization of it. Anticipating our discussion in the next section, it is tempting to think of the values '0' and '1' as somehow representing the 'absence' or 'presence' of binary signals, respectively. As we shall shortly see, it in fact takes relatively little work to jump from such modest temptations to finding an actual physical realization of a reversible computing device.

[†]The **FAN-OUT** operator is discussed in the following section.

6.4.2.2 Conservative Logic Circuits

We have thus far discussed the processing of only individual logic gates. In order to perform useful computations, however, we need to construct entire circuits. Luckily, building circuits does not involve any great jump in complexity, as we need only two additional abstract primitives to begin talking of real computation.

Fundamentally, computation consists of the *storage*, *transmission* and *processing* of information, which in the present context we will assume takes the form of *discrete signals*. We have already tacitly assumed the existence of a transmission medium, or wire, along which our signals travel both to and out of various logic gates. The processing itself is handled, at least at the local level, by each individual logic gate. In order to link gates, it is, in general, necessary to route output signals of some gates to the input lines of others; i.e. an arbitrary signal *fan-out* may be required. In our case of reversible systems, however, we have to be a bit careful. If we were to allow signals to split in the forward direction, we would then also have to allow two signals to 'join' in the reverse direction. We therefore require that all *fan-outs* occur only *within individual signal processing elements*; i.e. we will use the Fredkin-gate itself to handle fan-outs rather than arbitrarily splitting signals along their routes on a wire [fredkin82].

The last element necessary for the construction of a universal computer is a simple *time delay*; i.e. a circuit primitive whose output at time ' $t+1$ ' equals the input at time ' t ' and which allows us to feed outputs back into gates as inputs.

The functionality of any conventional circuit can now be exactly reproduced by a conservative-logic circuit in which conventional gates are replaced by Fredkin gates. Figure 6.9 (taken from [marg88] and [fredkin82]), for example, shows a conservative-logic realization of a conventional *serial-adder* circuit. That is to say, a circuit whose output equals the sum *modulo 2* of the bits appearing at the input. In the figure, all outputs labeled *g* are *garbage bits* and locations along wires marked with a dot are unit time delays. Note that the output of this circuit, equal to $y^t = x^{t-5} \oplus y^{t-5}$, represents a sum of the bits appearing at the input and output of the circuit *five* time steps prior to a given output; i.e. our straightforward transcription of the serial adder into conservative logic has slowed down the conventional processing speed by a factor of five. Had we designed a serial-adder circuit directly in conservative logic instead of transcribing it from a conventional circuit without regard for optimizing the overall computational cost, we could have constructed a circuit that significantly improves on the computational cost of our transcribed circuit.

Recalling Bennett's and Fredkin's trick to erase the garbage bits, the way in which the reversible logic circuit in figure 6.9 can be made to act as a real reversible serial-adder circuit is to first operate the circuit as shown, store the desired output, and then operate it backwards using the output and all intermediary garbage bits as new input. After all operations are completed in the reverse direction, we will be left with our desired answer stored on the side and with the serial-adder circuit back in its original state ready for another run.

In summary then, any computation that can be carried out by a conventional circuit can be reproduced by a conservative logic circuit (assuming only that some

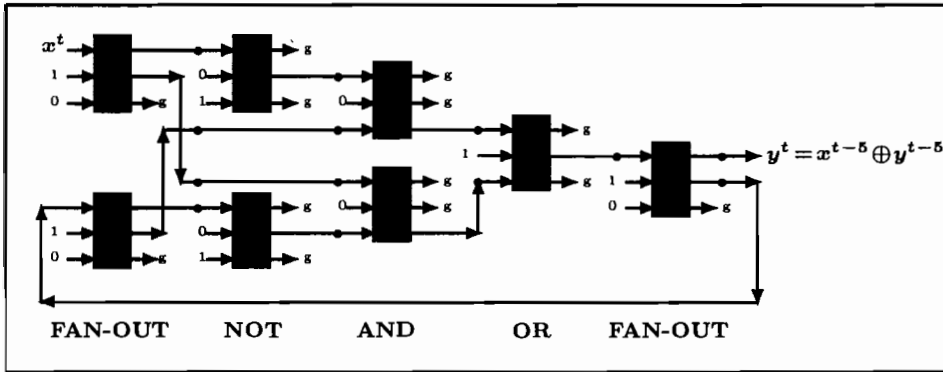


Fig. 6.9 A conservative-logic realization of a conventional *serial adder* circuit; it is built entirely of Fredkin gates. Places along the wires marked with a dot represent unit time delays at those locations. Illustration patterns after [marg88] and [fredkin82]

source of suitable constant-valued inputs is available and, if the system is not going to be run backwards, provision is made to *drain* off the unwanted garbage bits of the system). We now turn to a discussion of a well-known *physical realization* of a conservative-logic system.

6.4.3 The Billiard Ball Model

The *Billiard-Ball Model* (BBM), first introduced by Fredkin and Toffoli in 1982 [fredkin82], is a classical mechanical model of digital computation based on an idealization of a gas.[†] Although all of the variables of the model (masses, positions, velocities, etc.) are real-valued, the model may be induced to perform digital computations by treating integers as real numbers. In particular, by starting with precisely defined initial conditions and observing the system only at discrete intervals in time, the resulting behavior can be appropriately ‘discretized’. As we shall see, it is also a relatively simple matter to transcribe this discrete classical mechanical system into a CA. We begin by reviewing Fredkin’s original construction.

6.4.3.1 Classical Mechanical Incarnation

The BBM ‘gas’ consists of an arbitrary number of hard spheres (or balls) of finite diameter that collide elastically both among themselves and with any solid ‘walls’ (or mirrors) that they may encounter during their motion.[‡] Starting out on some site of a two-dimensional Euclidean lattice, each ball is allowed to move only in one of four directions (see figure 6.10). The lattice spacing, $d = 1/\sqrt{2}$ (in arbitrary units), is chosen so that balls collide while occupying adjacent sites. Unit ‘time’ is

[†] Additional details may be found in papers by Margolus ([marg84], [marg88]) and Toffoli ([toff87], [toff90a]).

[‡] Thus, physically, kinetic energy is conserved in this system, but, due to the presence of fixed (i.e. infinitely massive) mirrors, momentum is not.

defined as the time it takes for one ball to move from one site to another. Collisions between any two balls or a ball and a mirror always proceed at right-angles (see figure 6.11).

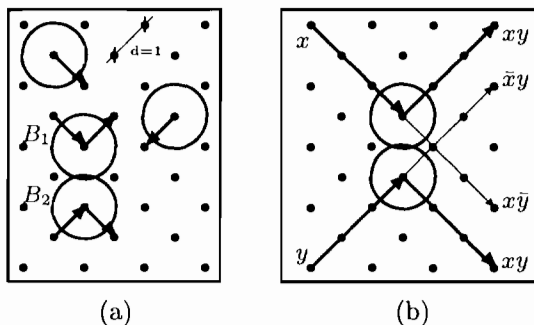


Fig. 6.10 (a) Billiard balls of radius $r = 1/\sqrt{2}$ traveling on a unit-spaced lattice; balls B_1 and B_2 are shown undergoing a right-angle elastic collision; (b) An example of an interaction gate (see text for discussion).

Fredkin was able to show that this system is capable of universal computation ([fredkin82], [marg84], [marg88]). Intuitively, it certainly makes sense that any configuration of gas molecules evolving according to well-defined classical laws (or rules) performs some sort of computation. At the very least, it computes its own future states. To see that such a system can in fact carry out *arbitrary* computations, with its initial shape defining the ‘hardware’ and the initial configuration of balls corresponding to the ‘software’, requires a bit more thought. There are two critical observations that need to be made in order to appreciate why this might be so: (1) *the presence or absence of a ball at a site ‘ (i, j) ’ can be interpreted as a binary variable σ_{ij} taking on either the value 1 or 0*, and (2) *all lattice neighborhoods in which collisions might occur can be interpreted as Boolean logic gates*.

The first observation consists merely of an alternative but natural interpretation of the presence or absence of balls: the ‘movement’ of balls is equated with the communication of *binary signals*. Once this interpretation is made, the second observation also becomes a natural one: wherever balls collide, either among themselves or with some collection of rigid mirrors, the effect of the collision may be viewed as a Boolean logic gate.

Consider the simple collision shown in figure 6.10-b. Labeling the incoming balls from the left by x and y , respectively, the figure shows that the result of the collision, or ‘output signal’, is effectively given by a Boolean function of the ‘input signal’. Reading from top to bottom, we see that the four possible output signals are given by, respectively, xy , $\bar{x}y$, $x\bar{y}$ and $\bar{x}\bar{y}$, where $\bar{\sigma}$ indicates the absence of ball σ in the input signal. In other words, if both balls are initially present, they collide and scatter at right angles to their original trajectory; on the other hand, if either one of the balls is missing from the input, the output consists of the continuation of the trajectory of the only ball initially present. (Obviously, if both balls are initially missing, there is no output.)

We make three observations about the *interaction gate* shown in figure 6.10-b: (1) since the number of balls ‘out’ always equals the number of balls ‘in’, it is trivially ball-conserving, (2) because each input is mapped into a unique output, it is also reversible, and (3) since it realizes both the Boolean AND function and (if we keep one of its inputs, say y , fixed by continually feeding in a stream of balls) the Boolean NOT function, it is a *universal logic gate* (see section 6.4.1). Indeed, if we (formally) add to it two additional inputs that are constrained to always have the value zero (i.e. null input), we obtain a four-input/ four-output conservative-logic gate.

Entire *logic circuits* can be built out of these interaction gates by a judicious routing of balls (or signals) from one interaction region to another, the outputs of one interaction being used as inputs to another. Basic routing effects induced by appropriate arrangements of fixed ‘mirrors’ include signal-path deflections (figure 6.11-a), sideways shifts (figure 6.11-b), time-delays (figure 6.11-c) and nontrivial crossovers (figure 6.11-d). Building actual ‘working’ circuits out of these, and similar, primitives, of course, requires that careful attention be paid to all collision ‘timings’, ‘angles’, the relative ‘speeds’ among balls, etc.

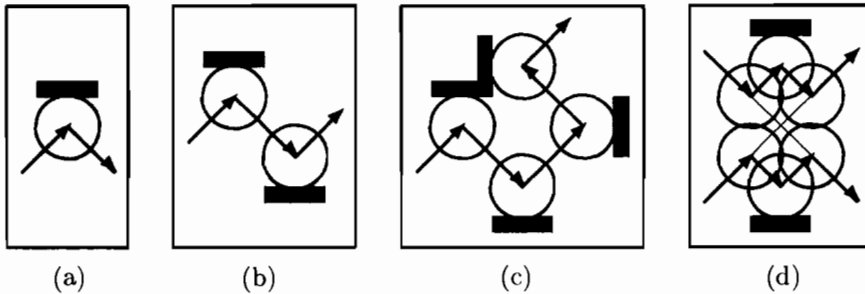


Fig. 6.11 Four examples of the use of *mirrors* (solid bars) in the BBM: (a) deflection, (b) sideways-shift, (c) time-delay and (d) crossover. (After [fredkin82]).

The **BBM** construction shows that an infinite two-dimensional hard-sphere gas in a periodic potential (i.e. a periodic array of mirrors) is *computationally universal*. The system may, at least in principle, be induced to perform arbitrary digital computations by a suitable programming of the its initial state. It should be mentioned, however, that there are at least two major drawbacks to using such a system for performing real computations [benn82]: (1) the sensitivity of the ball's trajectories to small perturbations and (2) the difficulty in making all of the collisions be truly elastic. Because errors in positions and velocities are magnified by a factor of roughly 2 at each collision, the smallest initial misalignment of mirrors and balls would result in trajectories that would become effectively unpredictable after only a relatively few collisions. The problem is that there is no practical method to completely isolate the the system's kinetic energy from the BBM's other degrees of freedom; all initial configurations must eventually degenerate into a gas, with velocities distributed according to the Maxwell distribution. Although there are

ways of partially circumventing this problem, they can only be implemented at the cost of eliminating the system's reversibility [benn86].

6.4.3.2 The BBM CA

If we choose to look at the state of the BBM only at integer valued times, corresponding to when all balls are located at the vertices of the lattice, the resulting system certainly appears amenable to a CA-like description. Margolus ([marg84], [marg88]) showed that the classical realization of the BBM can in fact easily be transcribed into a CA, although not necessarily in what might at first sight be the most straightforward manner.[†] The rules for his transcription, shown in figure 6.12, are defined on the 4-square *Margolus* neighborhood of a partitioning CA (see section 8.1.3.3).

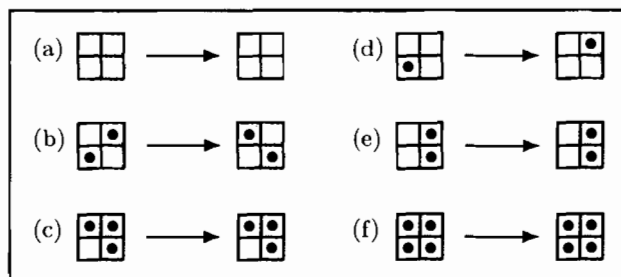


Fig. 6.12 The BBMCA rules, defined by using the *Margolus* neighborhood (see section 8.1.3.3). The complete set of rules may be obtained by writing down all rotations of the rules defined explicitly above.

Note that if we label the 4-squares of the *Margolus* neighborhood by a , b , c and d (i.e. let the neighborhood be given by $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$) and equate the presence (or absence) of a particle with the value '1' (or '0'), then rules (a), (b) and (d) in figure 6.12 are in fact identical with the (completion of) the conservative-logic *interaction gate* defined in the previous section.

Balls: the *balls* in this CA model are not to be identified with individual particles (i.e. solid dots at given sites) but are actually composite objects, and consist of two particles moving in the same direction but located in different partitions. Partitioning CA evolve in time by successively applying a rule to alternating partitions of the lattice. In this way, applying rule (d) in figure 6.12 to two overlapping sublattices induces a single particle to move along a diagonal (see figure 6.13); in

[†]Margolus ([marg84], [marg88]) points out that the most straightforward transcription of the classical BBM to a conventional (non-partitioning) CA, in which a ball is identified with a single particle, requires 6-state sites and neighborhoods of size 17. The exact definition of the appropriate rules also becomes a more subtle matter in this case. One must be careful, for example, to encode both the *presence* and *direction of motion* of a given ball at each site.

the figure, rule (d) is first applied to the even lattice (consisting of Margolus neighborhoods outlined by *thick*-lines), then to the *odd* lattice (consisting of Margolus neighborhoods outlined by *thin*-lines), and so on.

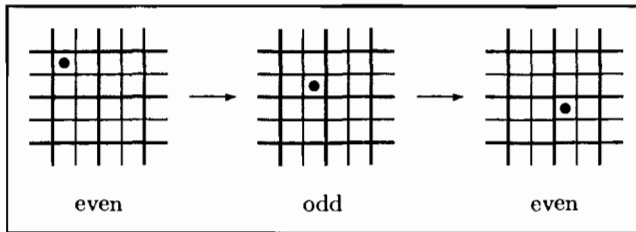


Fig. 6.13 Diagonal motion of a single particle (represented by solid dot) as induced by successively applying BBMCA rule (b) (see figure 6.12) to *even* (i.e. *thick*-lined) and *odd* (i.e. *thin*-lined) partitions of the lattice.

Figure 6.14 shows a right-angle collision between two *balls*, each of which consists of two particles. Notice that this collision process, which makes use of BBMCA rules (a)-(d) in figure 6.12, involves a slight *time-delay* that was not present in the classical incarnation. Specifically, each ball winds up one block-column *behind* where it would have been had the collision not taken place. This delay actually proves to be only a minor nuisance, however, as some additional work must be done to properly synchronize signals when constructing functioning circuits (see below).

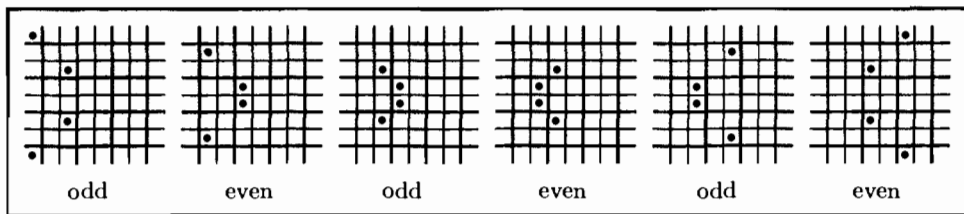


Fig. 6.14 Collision between two BBMCA Balls.

Mirrors: BBMCA rule (e), and its rotated equivalents, allows groups of particles to be built up to form stable configurations. Such configurations can then be used as *mirrors* to reflect balls, and thereby to act as signal routers. Figure 6.15, for example, shows the smallest possible fixed configuration consisting of four particles. Since adjacent ‘squares’ remain uncoupled from one another, mirrors of arbitrary size can be built up from this basic four-particle mirror.

BBMCA rule (c) in figure 6.12 allows for ball-mirror collisions to mimic their classical incarnations. Figure 6.16, for example, shows a collision between a (two-particle) *ball* and an 8-particle mirror. Notice that, just as for the ball-ball collision shown earlier in figure 6.14, a slight time-delay is again introduced.

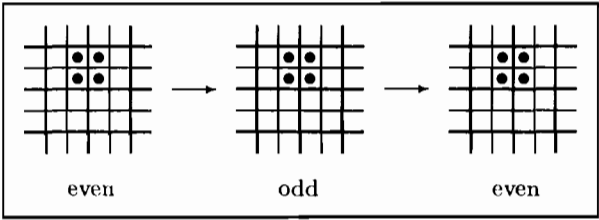


Fig. 6.15 Smallest possible fixed *mirror*, formed by a stable arrangement of four particles. BBMCA rule (e) (see figure 6.12) is successively applied to *even* (i.e. *thick-lined*) and *odd* (i.e. *thin-lined*) partitions of the lattice.

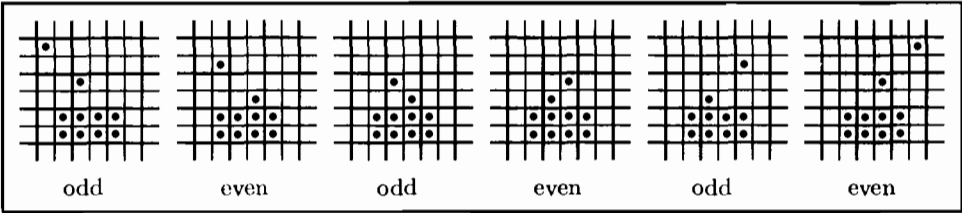


Fig. 6.16 Collision between a *Ball* and a *Mirror*.

Margolus [marg88] suggests that whenever ‘timing’ is a critical issue, such as when coordinating the arrival of signals in time-sensitive circuits, additional mirrors can be used to offset the effects of any time-delays. Two 8-particle mirrors positioned as shown in figure 6.17, for example, may be used to provide a 2-block delay in the diagonal motion of incoming balls. Circuits with any desired timing-features can then be constructed out of a set of similar delay-circuits. Proper signal timing also allows for the creation of signal path cross-overs without having the signals interact with one another.

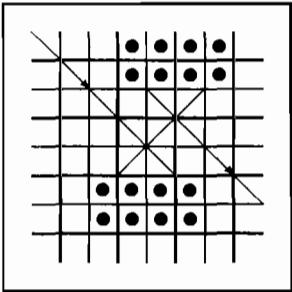


Fig. 6.17 Two-mirror configuration that acts as a 2-block delay to an incoming ball; ball’s motion follows sequence of arrows.

The most important observation about the BBMCA is that since any BBM circuit can be translated into a BBMCA circuit (albeit with whatever number of time and/or cross-over delays might be required), the BBMCA is, like the BBM itself, a *universal computer*.

Energy: since there is such a close analogy between the BBM and its CA incarnation, we may well ask whether there is, within the BBMCA, some conserved quantity analogous to physical *energy* in the BBM? Well, we know that the total number of balls, or total number of 1's, is conserved. Let $\sigma_{x,y}(t)$ equal the value of site (x,y) , and define $p_{x,y}(t) \equiv \sigma_{x,y}(t) - \sigma_{x,y}(t-1)$. We see that $p_{x,y}^2 = 1$ if and only if the value of site (x,y) changes from time $t-1$ to t . Since a 'moving' 1 must leave one site and enter another, the sum over all sites $\frac{1}{2} \sum_{x,y} p_{x,y}^2(t)$ counts the total number of moving 1's (the factor of $1/2$ accounts for the double counting). Similarly, since stationary 1's are precisely those sites with fixed value 1 at times t and $t-1$, the sum $\sum_{x,y} \sigma_{x,y}(t)\sigma_{x,y}(t-1)$ counts the total number of stationary ones. Putting these two expressions together, we get the following expression for the BBMCA *energy*:

$$E = \frac{1}{2} \sum_{x,y} p_{x,y}^2(t) + \sum_{x,y} \sigma_{x,y}(t)\sigma_{x,y}(t-1), \quad (6.21)$$

which, as we have just seen from our derivation, is really just a complicated way of writing down the total number of 1's on our lattice ([marg84], [marg88]).

Chapter 7

Probabilistic CA

This chapter covers a variety of topics related to the class of probabilistic CA (PCA); i.e. CA that involve some elements of probability in their state-space definition and/or time-evolution. We begin with a physicist's overview of critical phenomena, then move on to discuss the equivalence between PCA and spin models, critical behavior of PCA, mean-field theory, and CA simulation of conventional spin models. The chapter concludes with a discussion of a stochastic version of Conway's *Life* rule.

7.1 Critical Phenomena: A Heuristic Discussion

We are all familiar with the gas-liquid phase transition undergone by water. In such a transition, a plot of density versus temperature shows a distinct discontinuity at the critical temperature marking the transition point. There are many other common examples of similar phase transitions.

For example, consider an iron bar sitting in a magnetic field H parallel to its axis. The bar will be almost completely “magnetized”; using appropriate units, we can write $M = 1$. If we decrease the magnetic field to zero, however, we will find that the iron bar still possesses some residual nonzero *spontaneous magnetization* $M_0(T)$, whose value depends on the temperature T . On the other hand, if we start with a reversed field $-H$, then, assuming that the microscopic interactive forces within the iron bar are time reversal invariant, we would expect to find a spontaneous magnetization $-M_0(T)$. A plot of $M_0(H)$ versus H would therefore reveal a *discontinuous* function with $M \rightarrow -M_0(T)$ for $H \rightarrow 0^-$ and $M \rightarrow +M_0(T)$ for $H \rightarrow 0^+$. What happens if we increase the temperature? At first, for T' just a bit larger than T , we see no qualitative change; the only different is that $M_0(T') < M_0(T)$. There is a critical temperature, T_c – called the *Curie Temperature* – such that if $T > T_c$, $M_0(T) \rightarrow 0$ and $M_0(H)$ becomes a continuous function of H . A plot of $M_0(T)$ versus T thus shows a singularity at $T = T_c$; see figure 7.1.

These are but two examples of a whole class of critical phenomena and are the subject of statistical mechanics, in many ways the prototypical field of study of “complex systems,” trying as it does to predict the emergent macroscopic properties of systems from a knowledge only of the microscopic interactions among its constituent parts. In this section we provide a brief heuristic sketch of critical phenomena as understood by statistical mechanics. The aim is to provide some basic terminology and a few analytical tools before embarking on a discussion of the relationship between some statistical mechanical models and the behavior of particular CA models. The reader is encouraged to explore the ideas touched upon in this section further by making use of the references. Some of the better texts include those by Baxter [bax82], Huang [huang87] and Ma [ma85].

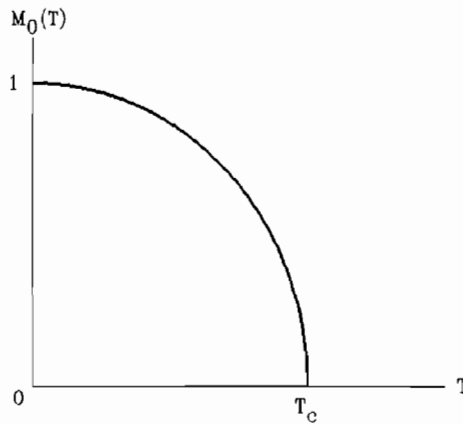


Fig. 7.1 Spontaneous magnetization $M_0(T)$ as a function of temperature T .

7.1.1 Boltzman Distribution

Consider a physical system with a set of states $\{\sigma\}$, each of which has an energy $\mathcal{H}(\sigma)$. If the system is at some finite temperature T , random thermal fluctuations will cause σ – and therefore $\mathcal{H}(\sigma)$ – to vary. While a system might initially be driven towards one direction (decreasing $\mathcal{H}$, for example) during some transient period immediately following its preparation, as time increases, it eventually fluctuates around a constant average value. When a system has reached this state, it is said to be in *thermal equilibrium*. A fundamental principle from thermodynamics states that when a system is in thermal equilibrium, each of its states σ occurs with a probability equal to the *Boltzman distribution* $P(\sigma)$:

$$P(\sigma) = \frac{1}{Z} e^{-\mathcal{H}(\sigma)/k_B T}, \quad (7.1)$$

where the normalization factor, called the *partition function*, is defined by

$$Z = \sum_{\sigma} e^{-\mathcal{H}(\sigma)/k_B T}, \quad (7.2)$$

where T is the temperature, $k_B = 1.38 \times 10^{-16}$ erg/K is Boltzman's constant and the sum is taken over all possible states of the system. For continuum systems, the sum becomes an integral; for quantum systems it is a trace.

7.1.2 Free Energy

For small T , we see from equations 7.1 and 7.2 that the probability of low-energy states is larger than for high-energy states. As the temperature increases, higher energy configurations become more and more likely. At $T = 0$, the system evolves towards the minimal energy state. For finite T , it evolves in such a way as to minimize the free energy F of the system, where F is defined by

$$F = -k_B T \ln Z, \quad (7.3)$$

and can also be written as

$$F = U - TS, \quad (7.4)$$

where $S = -\sum_{\sigma} P(\sigma) \log P(\sigma)$ is the entropy. As we have seen from previous discussions of entropy (see chapter 3), we know that the greater the number of accessible states there are, the greater the entropy. For small T we can therefore expect there to be a relatively few accessible states and the contribution of S to F to be small – the minima for U and F will be about the same. For large T , the system will typically occupy a large number of states, and S will be large.

Knowing the energy function $\mathcal{H}(\sigma)$ allows us, at least in principle, to calculate the average (or expected) value of any observable $\mathcal{O}$ of the system:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{\sigma} \mathcal{O}(\sigma) e^{-\mathcal{H}(\sigma)/k_B T}. \quad (7.5)$$

In particular, the internal energy U is equal to

$$U = \langle \mathcal{H} \rangle =; \frac{1}{Z} \sum_{\sigma} \mathcal{H}(\sigma) e^{-\mathcal{H}(\sigma)/k_B T}. \quad (7.6)$$

Using equation 7.3, U can also be expressed in terms of the free energy F :

$$U = k_B T^2 \frac{\partial}{\partial T} \ln Z = -T^2 \frac{\partial}{\partial T} \left(\frac{F}{T} \right). \quad (7.7)$$

The basic problem of statistical mechanics is to evaluate the sum-over-states in equation 7.2 and obtain Z and F as functions of T and any other variables (such as external magnetic fields) that might appear in $\mathcal{H}$. Any thermodynamic observable of interest can then be obtained in a straightforward manner from equation 7.5. In practice, however, the sum-over-states often turns out to be prohibitively difficult to evaluate. Instead, the physical system is usually replaced with a simpler model system and/or some simplifying approximations are made so that the sum-over-states can be evaluated directly.

7.1.3 Stochastic Dynamics

So far we have discussed mainly *stable* configurations that have reached an equilibrium. What about the evolution of a system from an arbitrary initial state? In particular, what do we need to know in order to be assured of reaching an equilibrium state that is described by the Boltzman distribution (equation 7.1) from an arbitrary initial state? It turns out that it is not enough to know just the energies $\mathcal{H}(\sigma)$ of the different states σ . We also need to know the *set of transition probabilities between all pairs of states of the system*.

Let $P(\sigma \rightarrow \sigma')$ be the probability of transition from state σ to state σ' . In general, the set of transition probabilities will define a system that is not describable by an equilibrium statistical mechanics. Instead, it might give rise to limit cycles or even chaotic behavior. Fortunately, there exists a simple condition called *detailed balance* such that, if satisfied, guarantees that the evolution will lead to the desired thermal equilibrium. Detailed balance requires that *the average number of transitions from σ to σ' equal the number of transitions from σ' to σ* :

$$P(\sigma)P(\sigma \rightarrow \sigma') = P(\sigma')P(\sigma' \rightarrow \sigma), \quad (7.8)$$

or

$$\frac{P(\sigma \rightarrow \sigma')}{P(\sigma' \rightarrow \sigma)} = \frac{P(\sigma')}{P(\sigma)} = e^{-\Delta\mathcal{H}(\sigma, \sigma')/k_B T}, \quad (7.9)$$

where $\Delta\mathcal{H}(\sigma, \sigma') = \mathcal{H}(\sigma') - \mathcal{H}(\sigma)$.

It is important to realize that detailed balance does not uniquely prescribe the set of transition probabilities; many different choices are possible. One common choice, due to Glauber [glaub63], is to let

$$P(\sigma \rightarrow \sigma') = \frac{1}{1 + \exp(\Delta\mathcal{H}(\sigma, \sigma')/k_B T)}. \quad (7.10)$$

Another widely used choice is the *Metropolis Algorithm* [metrop53], given by

$$P(\sigma \rightarrow \sigma') = \begin{cases} 1 & \text{if } \Delta\mathcal{H}(\sigma, \sigma') < 0, \\ e^{-\Delta\mathcal{H}(\sigma, \sigma')/k_B T} & \text{otherwise} \end{cases} \quad (7.11)$$

It is easy to show that both of these choices satisfy equation 7.9.

7.1.3.1 Monte Carlo Dynamics

Given that we have found a set of transition probabilities satisfying detailed balance, we can use a simple *Monte Carlo* method to “find” the low energy states of the model system. We begin by preparing the system in a random state. Then, choosing an arbitrary element i that may potentially undergo a change, we calculate the energy difference $\Delta\mathcal{H}$ between the original state of the system with the element unchanged and the potential new state with the given element changed. The given element is then actually changed, and the system is put into a new state, with a

probability $P(\Delta\mathcal{H})$. We repeat this procedure, iteratively, until the fluctuations in the observables that we are interested in die down; i.e. until the system reaches equilibrium. Of the two sets of probabilities defined above, the Metropolis algorithm is used more frequently in practice because it makes more transitions and therefore reaches thermal equilibrium faster.

7.1.4 Critical Exponents

Figure 7.1 shows a plot of the spontaneous magnetization $M_0(T) = \lim_{H \rightarrow 0^+} M(H, T)$ as a function of temperature T . In particular, we see that there is a singularity at the critical temperature T_c . It is expected that around this singularity, $M_0(T)$ behaves as a simple non-integer power; i.e. that

$$M_0(T) \sim (1 - \frac{T}{T_c})^\beta, \quad \text{as } T \rightarrow T_c^-. \quad (7.12)$$

The particular power β is an example of a *critical exponent*. There are many more such examples of critical exponents, of course, as a variety of thermodynamic functions have singularities at $H = 0$ and $T = T_c$ and are all similarly expected to be non-integer powers; for example, it is expected that

$$\left\{ \begin{array}{lll} M(H, T_c) & \sim H^{1/\delta} & \text{as } H \rightarrow 0, \\ C(H = 0) & \sim (1 - \frac{T}{T_c})^{-\alpha'} & \text{as } T \rightarrow T_c^-, \\ C(H = 0) & \sim (\frac{T}{T_c} - 1)^{-\alpha} & \text{as } T \rightarrow T_c^+, \\ \chi(H = 0, T) & \sim (1 - \frac{T}{T_c})^{-\gamma'} & \text{as } T \rightarrow T_c^-, \\ \chi(H = 0, T) & \sim (\frac{T}{T_c} - 1)^{-\gamma} & \text{as } T \rightarrow T_c^+, \end{array} \right. \quad (7.13)$$

where $C(H = 0) = \frac{\partial}{\partial T} U(H = 0, T)$ is the zero-field specific heat, and $\chi(H, T) = \partial M(H, T) / \partial H$ is the susceptibility.

7.1.4.1 Universality

Critical exponents are widely believed to be *universal*, in the sense of their being independent of the details of an underlying energy function $\mathcal{H}$. There is strong experimental evidence, for example, to suggest that critical exponents do not particularly care whether the system is a fluid system or a magnetic system [stan71]. In theory, there are only a few parameters, such as the dimensionality of the lattice and any underlying “symmetries” of $\mathcal{H}$, that are relevant near the critical point; what those relevant parameters are remains an open problem. If true, universality lends credence to the practice of studying very simplified versions of a “real” system; though the energy functions may be idealized facsimiles, if the underlying symmetries have been preserved so will be its critical exponents. For example, it has been shown that (within experimental error), CO_2 , Xe and the three-dimensional Ising

model all have the same critical exponents. On the other hand, a long-held conjecture that all one-dimensional two-state probabilistic CA with a single absorbing state formed a universality class has recently been shown to be false (see section 7.4.5).

7.1.4.2 Scaling Hypothesis

The critical exponents are not all independent of one another. For example, it can be shown on purely thermodynamic grounds that the inequality $\alpha' + 2\beta + \gamma' \geq 2$ must be satisfied [Rush63]. A number of such relations can be easily derived from the *scaling hypothesis*. First suggested by Widom [widom65] and Domb and Hunter [domb65], the scaling hypothesis asserts that, near the critical point, certain thermodynamic functions are *homogeneous* (see below). The general scaling hypothesis near the critical point has been verified experimentally both for fluid and magnetic systems [binn92].

Homogeneous Functions: A function $f(x)$ is called *homogeneous* if

$$f(\lambda x) = g(\lambda)f(x)$$

for all values of λ . An obvious example of a homogeneous function is $f(x) = x^2$, since $f(\lambda x) = \lambda^2 x^2$ and the above equation is satisfied using $g(\lambda) = \lambda^2$. More generally, it is easy to show that $g(\lambda)$ is actually not at all arbitrary. We first note that

$$f(\lambda \mu x) = g(\lambda \mu)f(x) = g(\lambda)f(\mu x) = g(\lambda)g(\mu)f(x),$$

so that

$$g(\lambda \mu) = g(\lambda)g(\mu).$$

Differentiating with respect to μ , we get

$$\frac{\partial}{\partial \mu} g(\lambda \mu) = \lambda g'(\lambda \mu) = g(\lambda)g'(\mu).$$

If we now substitute $\mu = 1$, let $g'(1) = p$ and integrate the resulting expression from 1 to λ , we find that

$$g(\lambda) = \lambda^p.$$

Thus, a homogeneous function must be of the form $f(\lambda x) = \lambda^p f(x)$, and, in particular (if we let $\lambda = 1/x$), $f(x) = f(1)x^p$; i.e. a homogeneous function has a simple power-law dependence on its argument.

The concept of homogeneity naturally extends to functions of more than one variable. For example, a generalized homogeneous function of two variables, $f(x, y)$, can be written in the form

$$f(\lambda^a x, \lambda^b y) = \lambda f(x, y),$$

or, using $\lambda = y^{-1/b}$, in the alternate form

$$f(x, y) = y^{1/b} f\left(\frac{x}{y^{a/b}}, 1\right).$$

We can now turn to a brief discussion of how these ideas relate to critical exponents.

As an example of how the scaling hypothesis leads to certain relationships among the critical exponents, let us once again consider an iron bar sitting in a magnetic field H . We will assume that its free energy per lattice site f (equation 7.3, say, can be written as a sum of a *regular part* $f_r(T, H)$, which does not change appreciably as $T \rightarrow T_c$ and a *singular part* $f_s(T, H)$, which shows critical behavior for $T \sim T_c$. Since we are probing for the behavior near T_c , it is convenient at this point to introduce the variable $t \equiv (T - T_c)/T$, so that $t \rightarrow 0$ is equivalent to $T \rightarrow T_c$. Focusing our attention on the singular part of f , we now assume that f_s is a generalized homogeneous function of t and H :

$$f_s(\lambda^a H \lambda^b t) = \lambda f_s(H, t). \quad (7.14)$$

We will now show how some of the critical exponents defined in equation 7.13 can be deduced in terms of the generalized exponents a and b above.

$\boxed{\beta}$ – The critical exponent β is defined in equation 7.12: $M_0(H = 0, t) \sim (-t)^\beta$. Recalling that $M = -\partial f / \partial H$, we first differentiate equation 7.14 with respect to H :

$$\lambda^a M(\lambda^a H, \lambda^b t) = \lambda M(t, H). \quad (7.15)$$

Setting $\lambda = (-t)^{-1/b}$ and $H = 0$, we obtain

$$M(t, 0) = (-t)^{(1-a)/b} M(-1, 0). \quad (7.16)$$

Comparing to equation 7.12, we see that

$$\beta = \frac{1-a}{b}. \quad (7.17)$$

$\boxed{\delta}$ – Differentiating equation 7.14 with respect to H , and setting $t = 0$ and $\lambda = H^{-1/a}$, we find

$$M(H, 0) = H^{(1-a)/a} M(1, 0). \quad (7.18)$$

Comparing this to the first expression in equation 7.13, we see that

$$\delta = \frac{a}{1-a}. \quad (7.19)$$

$\boxed{\alpha}$ – Since the specific heat at constant H is defined by $C_H = (\partial U / \partial T) |_{H = -(\partial^2 f / \partial T^2) |_{H}}$, we differentiate equation 7.14 to get:

$$\lambda^{2b} C(\lambda^a H, \lambda^b t) = \lambda C_H(H, t). \quad (7.20)$$

Setting $H = 0$ and $\lambda = t^{-1/b}$, we get

$$C_H(0, t) = t^{(1-2b)/b} C(0, 1). \quad (7.21)$$

Comparing to the expression for $C(H = 0)$ as $T \rightarrow T_c^+$ in equation 7.13, we see that

$$\alpha = 2 - \frac{1}{b}. \quad (7.22)$$

It can similarly be shown that $\alpha' = \alpha$.

$\boxed{\gamma}$ – Recalling that $\chi(H, T) = \partial M(H, T) / \partial H$, we differentiate equation 7.15 to obtain

$$\lambda^{2a} \chi(\lambda^a H, \lambda^b t) = \lambda \chi(H, t). \quad (7.23)$$

Setting $H = 0$ and $\lambda = t^{-1/b}$, we get

$$\chi(0, t) = t^{(1-2a)/b} \chi(0, 1). \quad (7.24)$$

Comparing to the last expression in equation 7.13, we see that

$$\gamma = \frac{2a - 1}{b}. \quad (7.25)$$

It can similarly be shown that $\gamma' = \gamma$.

Having now expressed α , α' , β , γ , γ' and δ in terms of the generalized exponents a and b appearing in expression 7.14, we can immediately deduce the following two relations: (1) Combining equations 7.17, 7.19 and 7.25, we see that

$$\gamma = \gamma' = \beta(\delta - 1). \quad (7.26)$$

(2) Combining equations 7.17, 7.19 and 7.22, we see that

$$\alpha + \beta(\delta + 1) = 2. \quad (7.27)$$

Many more such relationships can be derived in a similar manner (see [ma85] or [stan71]). For our purposes here, it will suffice to merely take note of the fact that certain relationships among the critical exponents do exist and are in fact commonly exploited. Indeed, we shall soon see that certain estimates of critical behavior in probabilistic CA system are predicated on the assumptions that (1) certain rules fall into in the same universality class as *directed percolation*, and (2) the same relationships known to exist among critical exponents in directed percolation must also hold true for PCA (see section 7.2).

7.1.5 Ising Model

The *Ising* model is arguably the simplest “system” that undergoes a nontrivial phase transition. The one-dimensional version was originally introduced as a model for ferromagnetism and solved by Ising in 1925 [ising25]. Ising was disappointed to find no evidence for a phase transition in one-dimension and had in fact argued that neither the two nor three dimensional versions of the model could exhibit a phase transition as well, an assertion that we now know to be false. Onsager was the first to solve (i.e. find the partition function for) and rigorously prove the existence of

a phase transition for the two-dimensional Ising model (in zero external magnetic field) in 1944 [onsag44]. Although it is beyond the scope of this book to go into detail about this one particular model and its many interesting variants, a discussion of its basic properties is a natural way to introduce the reader to some of the concepts and methodology that we will be using later on in this chapter.

7.1.5.1 General

The Ising model is the prototype for all models of physical magnets. The Ising model idealizes a magnet by describing it as consisting of N microscopic magnets (or *spins*), S_i , constrained to lie on sites of a lattice, $i = 1, 2, \dots, N$. These spins “point” either along, or exactly opposite to, some preferred axis; we will say that a particular spin S is *up* if $S = +1$ and that S is *down* if $S = -1$.

The energy $\mathcal{H}(\vec{S})$ of a given configuration of N spins is made up of two parts: (1) a contribution that arises solely from the inter-spin molecular forces ($= \mathcal{H}_{S \leftrightarrow S}$), and (2) a contribution that is due to the interaction between the spins and any external magnetic fields ($= \mathcal{H}_{S \leftrightarrow H}$). Since S_i is effectively the magnetic moment of the i^{th} spin, we can write $\mathcal{H}_{S \leftrightarrow H} = -H \sum_i S_i$. Although $\mathcal{H}_{S \leftrightarrow S}$ may be written in the form $\mathcal{H}_{S \leftrightarrow S} = -\sum_{ij} J_{ij} S_i S_j$, where J_{ij} represents the interaction between the i^{th} and j^{th} spins, it is in general more open and depends on the specifics of the model. The only natural constraint that can be imposed is that $\mathcal{H}_{S \leftrightarrow S}$ remain invariant under a simultaneous reversal of all magnetic fields and magnetizations; i.e. $\mathcal{H}_{S \leftrightarrow S}$ should be an even function of $\vec{S}$:

$$\mathcal{H}_{S \leftrightarrow S}(S_1, S_2, \dots, S_N) = \mathcal{H}_{S \leftrightarrow S}(-S_1, -S_2, \dots, -S_N). \quad (7.28)$$

Once $\mathcal{H}_{S \leftrightarrow S}$ and $\mathcal{H}_{S \leftrightarrow H}$ are both specified, the basic problem is to once again find a way to compute the sum-over-states appearing in the expression defining the partition function (equation 7.2):

$$Z_N(H, T) = \sum_{\vec{S}} e^{-(\mathcal{H}_{S \leftrightarrow S}(\vec{S}) - H \sum_i S_i) / k_B T}. \quad (7.29)$$

It is important to understand that critical behavior can only exist in the *thermodynamic limit*; that is, only in the limit as the size of the system $N \rightarrow \infty$. Were we to examine the analytical behavior of any observables (internal energy, specific heat, etc) for a *finite* system, we would generally find no evidence of any phase transitions. Since, on physical grounds, we expect the free energy to be proportional to the size of the system, we can compute the *free energy per site* $f(H, T)$ (compare to equation 7.3):[†]

[†]Note that we also expect the thermodynamic limit to be independent of the way in which it is taken. In a three dimensional system, for example, the result should be the same whether we take *length* $\rightarrow \infty$ first, followed by *width* $\rightarrow \infty$ and *height* $\rightarrow \infty$ or take *width* $\rightarrow \infty$ first, followed by *length* $\rightarrow \infty$ and *height* $\rightarrow \infty$.

$$f(H, T) = -k_B T \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N(H, T). \quad (7.30)$$

From this we can calculate any observables of interest. For example, we can immediately find the internal energy per site, $u(H, T)$, specific heat per site, $c(H, T)$ and magnetization, $M(H, T) = N^{-1} \langle \sum_i S_i \rangle$:

$$\begin{cases} u(H, T) &= -T^2 \frac{\partial}{\partial T} \left(\frac{f(H, T)}{T} \right), \\ c(H, T) &= \frac{\partial}{\partial T} u(H, T), \\ M(H, T) &= -\frac{\partial}{\partial H} f(H, T). \end{cases} \quad (7.31)$$

The correlation between sites i and j , C_{ij} , is defined as

$$C_{ij} \equiv \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle. \quad (7.32)$$

It is expected to depend only on the vector distance $\vec{r}_{ij}$ between the sites i and j and, away from the critical temperature T_c , to decay exponentially as $|\vec{r}|$ becomes large; i.e.

$$C_{ij}(|\vec{r}_{ij}|) \sim |\vec{r}_{ij}|^{-\zeta} e^{-|\vec{r}_{ij}|/\xi}, \quad \text{as } |\vec{r}_{ij}| \rightarrow \infty, \quad (7.33)$$

where ζ is some number. The correlation length ξ is a function of both H and T and is expected to diverge at $T = T_c$. It is also expected that its behavior around the critical point follows a power law with critical exponents ν and ν' :

$$\begin{cases} \xi(H=0, T) \sim \left(\frac{T}{T_c} - 1\right)^{-\nu} & \text{as } t \rightarrow 0^+, \\ \xi(H=0, T) \sim \left(1 - \frac{T}{T_c}\right)^{-\nu'} & \text{as } t \rightarrow 0^-. \end{cases} \quad (7.34)$$

7.1.5.2 One Dimensional Ising Model

Consider an Ising model consisting of a one-dimensional N -site lattice with nearest-neighbor inter-spin interactions. Assuming that the inter-spin coupling J_{ij} is the same throughout the lattice -- so that $J_{ij} = J$ for all i and j -- we can write the inter-spin energy $\mathcal{H}_{S \leftrightarrow S}(\vec{S}) = -J \sum_i S_i S_{i+1}$. The energy function $\mathcal{H}$ is then given by

$$\mathcal{H} = -J \sum_{i=1}^N S_i S_{i+1} - H \sum_{i=1}^N S_i, \quad (7.35)$$

where we have also assumed periodic boundary conditions ($S_{N+1} = S_1$).

The partition function may be written using equation 7.29:

$$Z_N(H, T) = \sum_{\vec{S}} e^{\{(J/k_B T) \sum_{i=1}^N S_i S_{i+1} + (H/k_B T) \sum_{i=1}^N S_i\}}. \quad (7.36)$$

We now note that the exponential can be written as a sum of products of terms that involve only neighboring spins:

$$Z_N(H, T) = \sum_{\vec{S}} \mathcal{E}(S_1, S_2) \mathcal{E}(S_2, S_3) \cdots \mathcal{E}(S_N, S_1), \quad (7.37)$$

where $\mathcal{E}(S_i, S_{i+1}) = \exp\{(J/k_B T) S_i S_{i+1} + \frac{1}{2}(H/k_B T)(S_i + S_{i+1})\}$. This decomposition is very convenient since, if we think of $\mathcal{E}(S, S')$ as a 2×2 matrix – called the *transfer matrix* – with elements

$$\mathcal{E} = \begin{pmatrix} \mathcal{E}(+1, +1) & \mathcal{E}(+1, -1) \\ \mathcal{E}(-1, +1) & \mathcal{E}(-1, -1) \end{pmatrix} = \begin{pmatrix} e^{J/k_B T + H/k_B T} & e^{-J/k_B T} \\ e^{-H/k_B T} & e^{J/k_B T - H/k_B T} \end{pmatrix} \quad (7.38)$$

then the sum over spins $S_2, S_3, \dots, S_N$ in equation 7.37 becomes a simple matrix product that is turned into a trace by the remaining sum over S_1 :

$$Z_N(H, T) = \text{Trace } \mathcal{E}^N. \quad (7.39)$$

Since $\mathcal{E}$ is a positive, symmetric matrix, it can be diagonalized:

$$\mathcal{E} = \mathbf{V} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \mathbf{V}^{-1}, \quad (7.40)$$

where λ_i are the eigenvalues of $\mathcal{E}$ (i.e. $\mathcal{E}\mathbf{x}_i = \lambda_i\mathbf{x}_i$), and $\mathbf{V} = (\mathbf{x}_1, \mathbf{x}_2)$ is the 2×2 matrix whose columns consist of $\mathcal{E}$'s eigenvectors $\mathbf{x}_1$ and $\mathbf{x}_2$. Substituting this expression into equation 7.39 yields

$$Z_N(H, T) = \text{Trace} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}^N = \lambda_1^N + \lambda_2^N. \quad (7.41)$$

The eigenvalues are found from the eigenvalue equation

$$\det(M) = \lambda^2 - 2\lambda e^{-J/k_B T} \cosh\left(\frac{H}{k_B T}\right) + 2 \sinh\left(\frac{2J}{k_B T}\right) = 0, \quad (7.42)$$

where

$$M = \begin{pmatrix} e^{J/k_B T + H/k_B T} - \lambda & e^{-J/k_B T} \\ e^{-H/k_B T} & e^{J/k_B T - H/k_B T} - \lambda \end{pmatrix}. \quad (7.43)$$

This yields

$$\left. \begin{matrix} \lambda_1 \\ \lambda_2 \end{matrix} \right\} = e^{J/k_B T} \cosh\left(\frac{H}{k_B T}\right) \pm \sqrt{e^{2J/k_B T} \sinh^2\left(\frac{H}{k_B T}\right) + e^{-2J/k_B T}}. \quad (7.44)$$

Assuming that $\lambda_1 > \lambda_2$, we can rewrite the expression for Z_N as

$$Z_N(H, T) = \ln \lambda_1 + \frac{1}{N} \ln(1 + (\frac{\lambda_2}{\lambda_1})^N) \longrightarrow_{N \rightarrow \infty} \ln \lambda_1. \quad (7.45)$$

In particular, from equation 7.30, we have that the free energy per site is given by

$$\begin{aligned}
 f(H, T) &= -k_B T \lim_{N \rightarrow \infty} \frac{1}{N} \ln Z_N(H, T), \\
 &= -k_B T \ln \lambda_1, \\
 &= -k_B T \ln [e^{J/k_B T} \cosh(\frac{H}{k_B T}) + \sqrt{e^{2J/k_B T} \sinh^2(\frac{H}{k_B T}) + e^{-2J/k_B T}}].
 \end{aligned} \tag{7.46}$$

The magnetization is given by

$$M(H, T) = -\frac{\partial f(H, T)}{\partial H} = \frac{e^{J/k_B T} \sinh(\frac{H}{k_B T})}{\sqrt{e^{2J/k_B T} \sinh^2(\frac{H}{k_B T}) + e^{-2J/k_B T}}}. \tag{7.47}$$

Since M is continuous for all values of H and T , this one-dimensional system does not exhibit a phase transition for any positive temperature.[†]

7.1.6 Mean-Field Approximation

Consider a general Ising Hamiltonian, $\mathcal{H}[\{\vec{S}\}]$, given by

$$\mathcal{H}[\vec{S}] = -\sum_{(i,j)} J_{ij} S_i S_j - H \sum_i S_i, \tag{7.48}$$

where the first sum is over all neighboring sites i and j . The total magnetic field acting on site ' i ' is equal to

$$H_i = H + \sum_j J_{ij} S_j. \tag{7.49}$$

The mean-field approximation consists of replacing H_i with its mean-field value H' , obtained by replacing the spins S_j with an average value $\langle S_i \rangle$:

$$H' = H + Jq \langle S \rangle, \tag{7.50}$$

where we have assumed that $\langle S_i \rangle = \langle S \rangle$ for all i , and $q = |\mathcal{N}|$ is the number of neighbors in each local neighborhood of i .

[†]Despite the analyticity of $M(H, T)$, it could nonetheless be argued that the one-dimensional Ising model harbors a critical point. It can be shown (see [bax82]) that the correlation length $\xi = [\ln(\lambda_1/\lambda_2)]^{-1}$. If $H = 0$, however, then it can also be shown that $\lim_{T \rightarrow 0^+} (\lambda_1/\lambda_2) = 1$ and, thus, that $\xi \rightarrow \infty$ at $H = T = 0$. Since one commonly associates a divergent correlation length with criticality, it is in this sense that $H = T = 0$ may be thought of as a critical point.

The average magnetization can now be found in a straightforward manner:

$$\begin{aligned}
 m \equiv \langle S \rangle &= \frac{1}{Z} \sum_{S=\pm 1} S e^{H'/k_B T} = \frac{e^{H'/k_B T} - e^{-H'/k_B T}}{e^{H'/k_B T} + e^{-H'/k_B T}} \\
 &= \tanh\left(\frac{H + Jqm}{k_B T}\right).
 \end{aligned} \tag{7.51}$$

Suppose the external field $H = 0$. We see from the above equation that when the temperature lies below the Curie temperature $T_c = Jq$, there will exist a nonzero spontaneous magnetization, M_0 , given implicitly by $M_0 = \tanh(JqM_0/k_B T)$. As for the behavior near T_c , we first set $t \equiv (T - T_c)/T_c$, so that $t \rightarrow 0$ as $T \rightarrow T_c$. Using this new variable, the mean-field equation can be written as

$$M_0 = (1 + t) \tanh^{-1}(M_0). \tag{7.52}$$

Since for T just less than T_c , M_0 is small but nonzero, we can approximate $\tanh^{-1}(M_0)$ by $M_0 + M_0^3/3$. Solving this approximate equation for M_0 , we find that

$$M_0 = (-3t)^{1/2} [1 + \mathcal{O}(t)]. \tag{7.53}$$

Comparing to equation 7.12, we thus see that the mean-field value for the critical exponent β exists and is given by

$$\beta = \frac{1}{2}. \tag{7.54}$$

Similar arguments would show that the other critical exponents are given by $\alpha = 0$, $\delta = 3$, $\gamma = 1$ and $\nu = 1/2$ [bax82].

7.1.7 Spin Glasses

Spin glasses are magnetic materials in which the interaction among the constituent magnetic moments, or spins, is random. Real systems typically consist of dilute, weakly interacting populations of magnetic atoms – i.e. *magnetic impurities* – located within nonmagnetic host metals. If μ and μ' are the magnetic moments of any two arbitrary magnetic impurities, and $J(r) \sim r^{-3} \cos(\alpha r)$ an oscillatory range- r dependent coupling between them (with α some constant), the interaction energy is given by $E = -J(r)\vec{\mu} \cdot \vec{\mu}'$. In particular, since r is random, the coupling can be either ferromagnetic ($J(r) > 0$) or anti-ferromagnetic ($J(r) < 0$); in other words, the system is, in general, *frustrated*. “Frustration” arises whenever there are conflicting constraints and makes impossible the simultaneous minimization of pair-interaction energies. Suppose we want to find the minimal energy state of a two-dimensional spin glass. Consider any closed loop consisting of individual link-couplings J_{ij} . It is easy to see that if the product of these couplings is *negative*, there is no way of positioning the spins at the nodes of the loop so as to satisfy all

Much of what is currently known about spin glasses can be traced back to the pioneering work of Edwards and Anderson [edw75]. Their idea was to try to capture the essential properties of real spin glasses with a simple *Ising*-like Hamiltonian of the form:

$$\mathcal{H}_{\text{spin-glass}} = -\sum_{ij} J_{ij} S_i S_j, \quad (7.55)$$

where the sites i and j are on some regular two or three dimensional lattice, the sum is taken over nearest neighbors and the couplings J_{ij} 's are assumed to be independent random variables, obeying, say, Gaussian statistics ($P(J_{ij} = J) \sim \exp[-(J_0 - J)^2/(2\Delta J^2)]$).

We make two important remarks about this Hamiltonian:

(1) While the locations of the spins are not random – indeed, the spins populate sites of a regular lattice – the interactions themselves are completely random. Frustration, too, has been retained. Thus, arguably, two of the three fundamental properties of real spin glass systems are satisfied. What remains to be seen, of course, is the extent to which this simplified model retains the overall physics.

(2) Our second remark is cautionary. While one might at first suspect that $\mathcal{H}_{\text{spin-glass}}$ is equivalent to a Hamiltonian describing spins in a random external field h_{ext} ($\mathcal{H} = \sum_{ij} J' S_i S_j - \sum_i h_{\text{ext},i} S_i$), a little thought will show that the analogy is really a poor one. While both systems harbor an intrinsic randomness, the randomness in spin glasses is due not to any external fields but solely to the internal spin-spin couplings.

Because of the underlying randomness of the spin-spin interactions, Edward and Anderson's "simple" Hamiltonian (equation 7.55) is very difficult to solve. The first to consider a mean-field theory of spin glasses, in which each spin effectively interacts with all other spins in a random manner, were Sherrington and Kirkpatrick [sherr75]. However, even their simplified model proved difficult to solve. It was "solved" only in 1979 by Parisi using his *Replica Method* [par79]. Without discussing the method itself (see [par79],[par80] and [par83] for details and further references), we summarize some of the results of Parisi's solution below.[†]

For high temperatures, the spin-glass system behaves essentially the way conventional *Ising*-spin systems behave; namely, a variety of different configurations are accessible, each with some finite probability. It is only at low enough temperatures that a unique *spin-glass phase* – characterized chiefly by the appearance of a *continuum of equilibrium states* – first appears.

To understand the properties of this new phase, it is instructive to contrast them with what we know about conventional ferromagnetic and anti-ferromagnetic phases. For example, we recall from elementary statistical physics, that ferromagnetic systems – that is, systems whose couplings $J_{ij} = J > 0$, for all i, j – have two

[†]We emphasize that it is very much the properties of Parisi's *Replica* solution that we are about to summarize and not necessarily those of real spin glasses. It has not yet been rigorously proven that Parisi's solution is really the solution to Sherrington-Kirkpatrick's mean-field theory. Moreover, it is still an open question whether the spin glass Hamiltonian $\mathcal{H}_{\text{spin-glass}}$ (equation 7.55) itself describes real spin glasses.

configurations that minimize the energy: one configuration consists of spins that are all equal to $+1$ (or magnetization $M = +1$), the other of spins that are all equal to -1 (or magnetization $M = -1$). As the temperature $T \rightarrow 0$, the system evolves to either one or the other minimal-energy configuration, depending on its initial state. It is important to realize that the fact that there are coexisting minimal energy states is not at all surprising, and in fact could be trivially predicted from the underlying Hamiltonian's symmetry under a global spin-reversal. Now, contrast this behavior with that of spin glasses, for which an infinite number of equilibrium states appear as $T \rightarrow 0$, essentially none of which are related by any underlying symmetry.

In each of the spin-glass equilibrium states $\vec{g}$, the local magnetizations $m_i = \langle S_i \rangle_{\vec{g}}$ are all nonzero; however, the global magnetization per site, $M = \frac{1}{N} \sum_i S_i >_{\vec{g}} \sim 1/\sqrt{N} \rightarrow 0$ as $N \rightarrow \infty$. Unlike a conventional Ising-spin system, where an order parameter (such as global magnetization) can be determined simply by projecting the attractors onto one or a few reference configurations, spin glasses, because of their intrinsic randomness, possess no such preferred references. Consequently some other means of defining an appropriate order parameter must be found.

One possible order parameter, proposed by Parisi [par83], is not so much an order "parameter" as an order "function." Define $q_{\alpha\beta}$ to be the "overlap" between the states α and β :

$$q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N S_{\alpha,i} S_{\beta,i}. \quad (7.56)$$

Then, letting p_α and p_β be the probabilities of states α and β , respectively, the probability that the overlap between α and β is equal to q is given by

$$P(q) = \sum_{\alpha,\beta} p_\alpha p_\beta \delta(q - q_{\alpha\beta}), \quad (7.57)$$

where $\delta(x)$ is the *Dirac-delta function*. Parisi [par83] shows how $P(q)$ can be calculated using his *Replica method*.

For conventional Ising-spin systems, $P_{\text{Ising}}(q)$ takes on the expected simple forms; namely, either $P_{\text{Ising}}(q) = \delta(0)$ in the (high-temperature, zero magnetization) paramagnetic phase or the double-peaked $P_{\text{Ising}}(q) = \delta(q + M^2) + \delta(q - M^2)$ for temperatures below the Curie critical temperature, $T < T_c$.

In contrast, for low enough temperatures, Parisi's solution to Sherrington-Kirkpatrick's spin-glass model predicts that $P_{\text{spin-glass}}(q)$ that not only includes the two delta spikes at $\pm q_M$ but a finite probability for the entire *continuum* of sites $-q_M \leq q \leq q_M$ as well; see figure 7.2. (Note that for high temperatures, it is still true that $P_{\text{spin-glass}}(q) = P_{\text{Ising}}(q) = \delta(0)$). Moreover, these attractors are not arbitrarily distributed, but are arranged in a hierarchical-like manner forming an *ultrametric space* [steing85, chowd86].

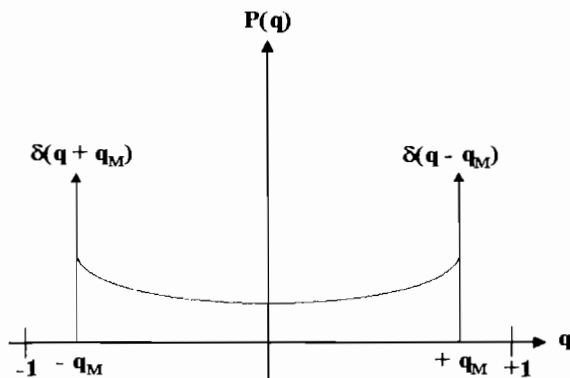


Fig. 7.2 Spin-glass overlap probability $P_{\text{spin-glass}}(q)$ versus overlap q (equation 7.57); $\delta(x)$ is the Dirac-Delta function.

Consider three attractor states, α , β and γ . If the states are arranged ultrametrically, then the probability of having a mutual overlap among these three states is nonzero only in two cases: (1) when $q_{\alpha\beta} = q_{\alpha\gamma} = q_{\beta\gamma}$, corresponding to an equilateral triangle in the state space, or (2) when $q_{\alpha\gamma} = q_{\beta\gamma}$ and $q_{\alpha\beta} > q_{\alpha\gamma}$, corresponding to an isosceles triangle in which the third side is longer than the other two.

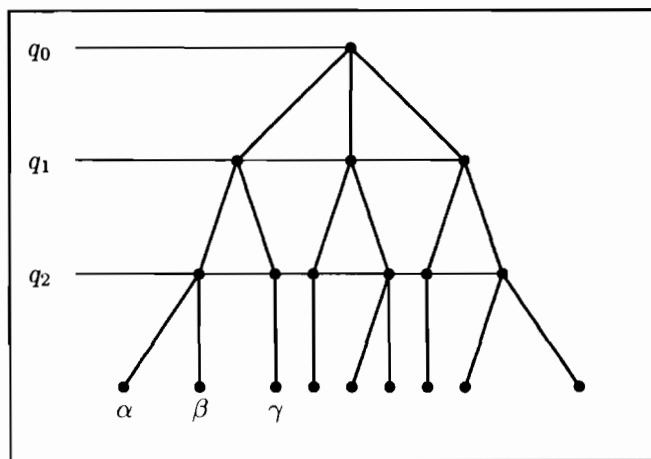


Fig. 7.3 A representation of the (conjectured) ultrametric distribution of spin-glass equilibrium states. The “leaves” of the tree at bottom are identified with the states; overlaps between states are measured by the number of levels it takes to trace the states back to their common “roots”. For the three states α , β and γ , for example, we have that $q_{\alpha\gamma} = q_{\beta\gamma} = q_1$ and $q_{\alpha\beta} = q_2 > q_1$.

A common way of visualizing such spaces is through a kind of hierarchical “tree” (see figure 7.3), whose “leaves” are identified with states and the distances between leaves – measured by counting the number of branches that must be traversed in

order to trace the two given states back to their common “root” – are identified with the overlap between those states. In figure 7.3, we see that $q_{\alpha\gamma} = q_{\beta\gamma} = q_1$ and $q_{\alpha\beta} = q_2 > q_1$, which illustrates the “triangle” rule above.

As for the general relationship between spin glasses and CA systems, we have already seen a close connection between the *zero-temperature limit* of spin glasses and the class of generalized threshold rules in our discussion of Lyapunov functions in section 5.5 (see [goles85b], [goles87b]). The connection between spin-glasses and neural nets (which are themselves related to threshold rules via McColluch and Pitts original neuronal activation rules [mccul43]), was first made by Little ([lit74], [lit78]). There is also a natural equivalence between the energy landscape of spin glasses and the “fitness” landscape of Kauffman’s random Boolean net systems (section 8.6).

There are many excellent reviews of spin glass systems. We recommend the following three sources: the review article by Binder and Young [binder86], the book by Chowdhury [chowd86], and the collection of papers edited by Mezard, et.al. [mez87].

7.2 PCA $\longleftrightarrow$ Spin Model Equivalence

There is a fundamental relationship between d -dimensional PCA and $(d + 1)$ -dimensional Ising spin models. The simplest way to make the connection is to think of the successive temporal layers of the PCA as successive hyper-planes of the next higher-dimensional spatial lattice. Because the PCA rules (at least the set of PCA rules that we will be dealing with) are (1) Markovian (i.e. the probability of a state at time ‘ $t + 1$ ’ depends only on a set of states at time ‘ t ’, and (2) *local*, one can always define a *Hamiltonian* on the higher-dimensioned spatial lattice such that the thermodynamic “weight” of a configuration $\{S_{i,t}\}$ is equal to the probability of a corresponding space-time “history” $\{S_i(t)\}$.

Below, we outline a pedagogical example of PCA $\leftrightarrow$ spin model equivalence; namely, the equivalence between a class of elementary one-dimensional PCA and the Ising lattice gas defined on a two-dimensional triangular lattice. This particular example has been treated in detail by a number of authors, most recently by Domany and Kinzel [domany84] and, in an excellent general review of PCA, by Georges and Le Doussal [geor89]. It will be clear from this discussion how the result generalizes to the case of d -dim PCA $\longleftrightarrow (d + 1)$ -dim spin model equivalence.

Consider a size N one-dimensional lattice with site variables $S_i(t) = \pm 1$, $i = 1, \dots, N$. On even (or odd) time steps, either even-indexed (or odd-indexed) sites evolve according to fixed probabilistic peripheral rules; that is, according to rules that depend only on the values of a given site’s neighboring sites. Such rules are completely specified by a set of four conditional probabilities, $0 \leq \alpha_i \leq 1$, $i = 1, \dots, 4$:

$$\begin{cases} \alpha_1 = P(1 \mid -1, -1), & \alpha_2 = P(1 \mid -1, +1), \\ \alpha_3 = P(1 \mid +1, -1), & \alpha_4 = P(1 \mid +1, +1). \end{cases} \quad (7.58)$$

The conditional probabilities for obtaining $S_i(t+1) = -1$ are given in terms of these four parameters by $P(-1 | S_1, S_2) = 1 - P(1 | S_1, S_2)$.

Now consider an entire temporal history of this PCA. That is, consider the effective two-dimensional lattice that is formed by stacking successive one-dimensional layers on top of one another (see figure 7.4). Because of the Markovian nature of the evolution, the probability of this temporal history is given simply by

$$P(\vec{S}_{t+1}) = \prod_t P(\vec{S}_{t+1} | \vec{S}_t) P(\vec{S}_t) = \prod_i \prod_t P(S_{i,t+1} | S_{i-1,t}, S_{i+1,t}), \quad (7.59)$$

where $P(\vec{S}_{t+1} | \vec{S}_t)$ is the conditional probability (or *transfer matrix*; see equation 7.38 in section 7.1.5.2) to have the one-dimensional PCA state $\vec{S}_{t+1}$ at time ' $t+1$ ' given that it was in state $\vec{S}_t$ at time ' t ', and we have included the time-indices ' t ' and ' $t+1$ ' as subscripts in the expression on the right hand side to emphasize that time is now to be thought of as an additional label in a two-dimensional space-time lattice.

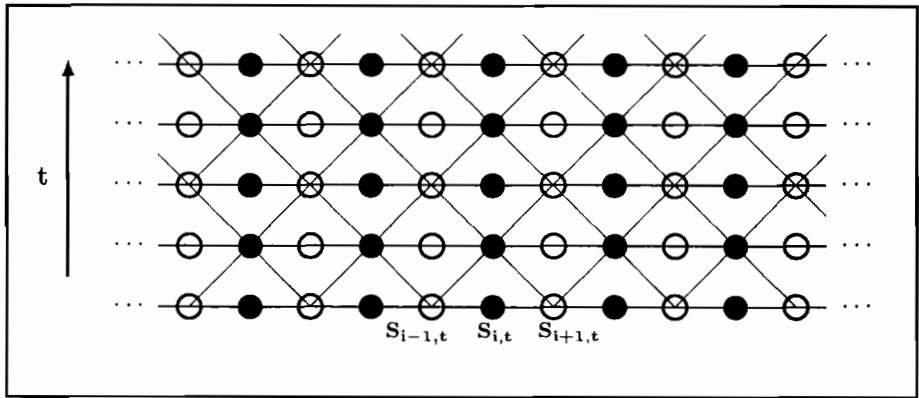


Fig. 7.4 The triangular space-time lattice generated by the temporal evolution of the peripheral PCA system described in the text.

Following Domany and Kinzel [domany84], we can simplify this product expansion considerably by rewriting $P(S_3 | S_1 S_2)$ in exponential form:

$$P(S_3 | S_1, S_2) = \lambda^{-1} \exp\{h_1 S_1 + h_2 S_2 + h_3 S_3 + h_{12} S_1 S_2 + h_{23} S_2 S_3 + h_{13} S_1 S_3 + h_{123} S_1 S_2 S_3\}, \quad (7.60)$$

where the normalization constant λ and coupling constants h_i , h_{ij} and h_{123} (see figure 7.5) are all functions of α_i , $i = 1, \dots, 4$ (equation 7.58). These functions may be obtained in a straightforward manner in three steps [geor89]: (1) Enumerate each of the eight possible conditional probabilities according to equation 7.60; for example, $P(1 | 1, 1)$ is given by

$$P(1 | 1, 1) = \alpha_4 = \lambda^{-1} \exp\{h_1 + h_2 + h_3 + h_{12} + h_{23} + h_{13} + h_{123}\}. \quad (7.61)$$

(2) Multiply all eight equations together to get the normalization constant λ :

$$\lambda = \left(\prod_{i=1}^4 \alpha_i (1 - \alpha_i) \right)^{-1}. \quad (7.62)$$

(3) Follow Enting's [ent77] observation that all of the coupling constants but one $-h^*$, say $-$ can be eliminated by multiplying together the four equations in which h^* appears with a '+' sign. As the reader can easily show, we get the result that

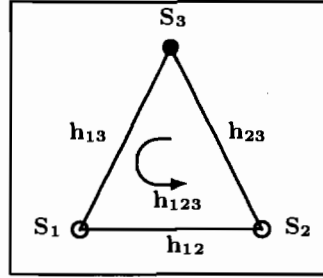


Fig. 7.5 Coupling constants between the spins of an elementary plaquette of the triangular lattice used in defining the Ising Hamiltonian appearing in equation 7.65.

$$\begin{cases} e^{8h_1} = \frac{\alpha_4(1-\alpha_4)\alpha_3(1-\alpha_3)}{\alpha_1(1-\alpha_1)\alpha_2(1-\alpha_2)}, & e^{8h_2} = \frac{\alpha_4(1-\alpha_4)\alpha_2(1-\alpha_2)}{\alpha_1(1-\alpha_1)\alpha_3(1-\alpha_3)}, & e^{8h_3} = \frac{\alpha_1\alpha_2\alpha_3\alpha_4}{(1-\alpha_1)(1-\alpha_2)(1-\alpha_3)(1-\alpha_4)}, \\ e^{8h_{12}} = \frac{\alpha_3\alpha_4(1-\alpha_1)(1-\alpha_4)}{\alpha_2\alpha_3(1-\alpha_2)(1-\alpha_3)}, & e^{8h_{13}} = \frac{\alpha_4(1-\alpha_1)\alpha_3(1-\alpha_2)}{\alpha_1(1-\alpha_4)\alpha_2(1-\alpha_3)}, & e^{8h_{23}} = \frac{\alpha_4(1-\alpha_1)\alpha_2(1-\alpha_3)}{\alpha_1(1-\alpha_4)\alpha_3(1-\alpha_2)}, \\ e^{8h_{123}} = \frac{\alpha_4\alpha_1(1-\alpha_2)(1-\alpha_3)}{(1-\alpha_4)(1-\alpha_1)\alpha_2\alpha_3}, \end{cases} \quad (7.63)$$

The probability of the history $\{S_{i,t}\}$ of the evolution (equation 7.59) can now be written as

$$P[\{S_{i,t}\}] = Z^{-1} \exp\{-\beta\mathcal{H}(\{S_{i,t}\})\}, \quad (7.64)$$

where $\mathcal{H}$ is the Ising Hamiltonian on a triangular lattice:

$$-\beta\mathcal{H}(\{S_{i,t}\}) = (\sum_{j=1}^3 h_j) \sum_{i,t} S_{i,t} + \sum_{\triangle} (h_{12} S_1 S_2 + h_{23} S_2 S_3 + h_{13} S_1 S_3 + h_{123} S_1 S_2 S_3). \quad (7.65)$$

The sum $\sum_{\triangle}$ is taken over each elementary plaquette in the lattice (see figure 7.5). We thus have that *the time evolution of the one-dimensional PCA system is equivalent to the equilibrium statistical mechanics of a spin model on a triangular lattice* ([domany84], [geor89]).[†]

[†]Domany and Kinzel [domany84] point out that this particular PCA system can also be easily

In particular, by averaging over all possible space-time “histories”, all dynamical quantities for the PCA (such as correlation functions) correspond to thermodynamic averages in the associated spin model.

Notice that the associated spin model has the following three properties: (1) it is, in general, anisotropic (i.e. $\alpha_2 \neq \alpha_3$), (2) its set of coupling constants (h_i, h_{ij}, h_{123}) are interdependent (this should be obvious from equation 7.63, which provides a parameterization of each of these seven constants in terms of our original four independent conditional probabilities, α_i (equation 7.58)), and (3) its partition function, Z , can be calculated *exactly*.

In order to show this last point, we first observe that the Boltzman weight of each plaquette, $\mathcal{W}(S_1, S_2, S_3) \equiv \lambda P(S_3 \mid S_1, S_2)$ clearly satisfies the normalization condition

$$\sum_{S_3=\pm 1} \mathcal{W}(S_1, S_2, S_3) = \lambda. \quad (7.66)$$

Summing equation 7.59 over all possible space-time “histories”, $\{\vec{S}_t\}$, we get that

$$1 = \sum_{\{\vec{S}_t\}} P[\{\vec{S}_t\}] = \sum_{\{\vec{S}\}} \prod_{\Delta} P(S_3 \mid S_1, S_2) = \lambda^{-N_{\Delta}} \sum_S \prod_{\Delta} W, \quad (7.67)$$

where N_{Δ} is the number of plaquettes in the lattice. Using the result in equation 7.66, we see that the partition function is given simply by:

$$Z = \lambda^{N_{\Delta}}. \quad (7.68)$$

From equation 7.63, we see that in the deterministic limit, obtained by setting all of our conditional probabilities $\alpha_i = 0$ or 1 ($i = 1, \dots, 4$), all of the coupling constants of the associated spin model go to $\pm\infty$. The different deterministic limits correspond to the different ways in which the zero temperature limit of the spin model can be taken while preserving the relationship among the coupling constants as defined by equation 7.66. A given time-evolution of a deterministic limit of the PCA corresponds to a different ground state of the associated spin model [geor89]. Table 7.1 lists the sixteen possible ground states (along with their elementary rule codes and Wolfram classes) of the *peripheral* PCA of this section.

recast as a problem of *directed percolation* in two-dimensions. Consider a square lattice with a probability p_s of a given site being present and probability p_b of there being a *bond* between any two given sites. Assuming that a single site is “wet” at time $t = 0$ and that “water” can trickle downward through the lattice from a site i to site i' only if the upper site i is “wet” and there exists a bond $b_{ii'}$ between i and i' , the directed percolation problem is to determine the probability of having fully wet sites at time t . A good review of directed percolation may be found in [kinz83].

$(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$	Rule: Rn	Wolfram Class	$(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$	Rule: Rn	Wolfram Class
(0, 0, 0, 0)	0	1	(1, 0, 0, 0)	5	2
(0, 0, 0, 1)	80	2	(1, 0, 0, 1)	85	2
(0, 0, 1, 0)	10	2	(1, 0, 1, 0)	15	2
(0, 0, 1, 1)	90	3	(1, 0, 1, 1)	95	2
(0, 1, 0, 0)	160	1	(1, 1, 0, 0)	165	3
(0, 1, 0, 1)	240	2	(1, 1, 0, 1)	245	2
(0, 1, 1, 0)	170	2	(1, 1, 1, 0)	175	2
(0, 1, 1, 1)	250	1	(1, 1, 1, 1)	255	1

Table 7.1 The sixteen peripheral deterministic elementary rules.

7.3 Critical Behavior of PCA

7.3.1 Peripheral PCA

Consider an isotropic version of the elementary “peripheral” PCA introduced above, this time also with binary site variables $\sigma_i(t) = (1/2)(1 - S_i(t)) \in \{0, 1\}$. Even-indexed (or odd-indexed) sites evolve on either even (or odd) time steps according to a set of rules determined by three conditional probabilities, p_0 , p_1 and p_2 :

$$p_0 = P(1 | 0, 0), \quad p_1 = P(1 | 0, 1) = P(1 | 1, 0), \quad p_2 = P(1 | 1, 1). \quad (7.69)$$

As before, the conditional probabilities for obtaining $\sigma_i(t+1) = 0$ are given in terms of these three parameters by $P(0 | \sigma_1, \sigma_2) = 1 - P(1 | \sigma_1, \sigma_2)$.[†] In the following we set $p_0 = 0$ to make the zero-state an absorbing state.

Figure 7.6 shows the phase diagram of the resulting two-parameter model [domany84]. We see that there are two distinct regions, or phases: an absorbing phase (to the right of the curve), in which the fraction of nonzero sites, $\rho \rightarrow 0$ for almost all initial configurations, and an active phase (to the left of the curve), in which almost all initial states evolve to a stationary state with $\rho \neq 0$. The corners of the phase diagram correspond to deterministic CA: $(p_1, p_2) = (0, 0) \leftrightarrow$ class-2 elementary rule R1, $(0, 1) \leftrightarrow$ class-1 rule R160, $(1, 0) \leftrightarrow$ class-3 rule R90, and $(1, 1) \leftrightarrow$ class-1 rule R250.

Note that the fact that the transition curve ends at $p_1 = 1/2$ and $p_2 = 1$ could be predicted from a simple symmetry property (called *duality* in [kinzel85b]): namely, that any PCA defined by a set of conditional probabilities $\{P(\sigma | \sigma_1 \sigma_2 \sigma_3)\}$ is preserved when each of these probabilities undergoes the duality transformation

$$P(\sigma | \sigma_1 \sigma_2 \sigma_3) \longrightarrow P'(\sigma | \sigma_1 \sigma_2 \sigma_3) = 1 - P(\sigma | \sigma'_1 \sigma'_2 \sigma'_3), \quad (7.70)$$

[†]We have already commented on the equivalence between peripheral PCA and the problem of directed percolation (see footnote on page 343). It is easy to show that the p_1 and p_2 of the isotropic system are given in terms of site- and bond- directed percolation probabilities – p_s and p_b , respectively – by the expressions $p_1 = p_s p_b$ and $p_2 = p_s p_b (2 - p_b)$; see [domany84] and [kinzel85].

where $\sigma' = (\sigma + 1) \bmod 2$. From equation 7.69 we see that (1) the line $p_2 = 1$ is self-dual (that is, it is mapped to itself), and (2) $p_1 \rightarrow p_1' = 1 - p_1$. Thus the phase boundary must end at the point $(p_1)_c = 1/2$ [kinzel85b].

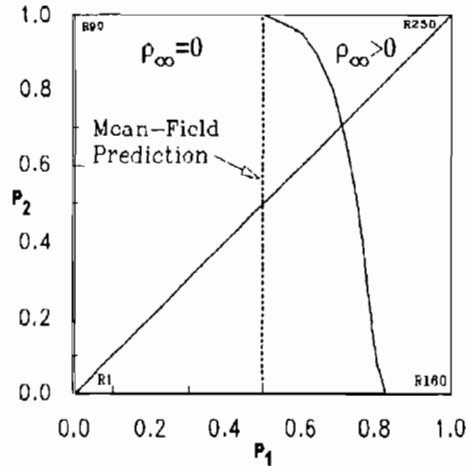


Fig. 7.6. Phase diagram for the peripheral PCA defined in equation 7.69.

7.3.1.1 Critical Exponents

Just as in phase transitions in statistical mechanical systems, observable quantities in PCA systems display singularities obeying simple power laws with universal critical exponents at the transition point. For example, letting n_1 be the number of sites with $\sigma = 1$, ξ be the *correlation length*, and τ be the *correlation time*, Kinzel [kinz85b] finds that for $p \sim p_c$,

$$\begin{cases} n_1(p) & \sim (p - p_c)^\beta, \\ \xi(p) & \sim (p - p_c)^{-\nu_\perp}, \\ \tau(p) & \sim (p - p_c)^{-\nu_\parallel}, \end{cases} \quad (7.71)$$

where $\beta \sim 0.273$, $\nu_\perp \sim 1.100$ and $\nu_\parallel \sim 1.734$.

Another obvious order parameter (equal to zero in the absorbing phase) is the *entropy*, $S = -\sum_{\vec{\sigma}} P_{(\infty)}(\vec{\sigma}) \ln P_{(\infty)}(\vec{\sigma})$, where $P_{(\infty)}(\vec{\sigma})$ is the equilibrium probability to find state $\vec{\sigma}$. Kinzel [kinz85b] finds that, for $p \sim p_c$, S follows the same power law as n_1 : $S \sim (p - p_c)^\beta$.

Note that the critical behavior just described holds true strictly only in the thermodynamic limit; i.e. only when the number of sites $N \rightarrow \infty$. The above results are in fact obtained by extrapolating from finite system calculations. Kinzel

[kinz85b] outlines one simple method based on *transfer-matrix scaling* (valid for one-dimensional systems).

Suppose we have a finite sized system of N lattice sites. Then the time evolution of the probabilities $P(\vec{\sigma}, t)$ is given by

$$P(\vec{\sigma}, t+1) = \sum_{\vec{\sigma}'} \mathcal{T}_{\vec{\sigma}, \vec{\sigma}'} P(\vec{\sigma}', t), \quad (7.72)$$

where $\mathcal{T}_{\vec{\sigma}, \vec{\sigma}'} = P(\vec{\sigma}' | \vec{\sigma})$ is the *transfer matrix* that gives the conditional probability of having state $\vec{\sigma}'$ at time $t+1$ starting from the state $\vec{\sigma}$ at time t . Since $p_0 = 0$, we know from *Frobenius' Theorem* [horn85] that (1) $\mathcal{T}_{0,0} = 0$ and $\mathcal{T}_{0,i} = 0$ for $i \neq 0$, and (2) all other eigenvalues $\lambda_i < \lambda_0$. Since $\sum_{\vec{\sigma}} \mathcal{T}_{\vec{\sigma}, \vec{\sigma}'} = 1$ we also know that the largest eigenvalue of $\mathcal{T}$ is $\lambda_0 = 1$, corresponding to the eigenvector v_0 (with $v_i = 0$ for $i \neq 0$). Asymptotically, for large times t , we therefore have that

$$\vec{P}(t) = \mathcal{T}^t \vec{P}(0) \sim \lambda_0^t \vec{v} \left\{ 1 + \left(\frac{\lambda_1}{\lambda_0} \right)^t + \dots \right\}. \quad (7.73)$$

Since $\lambda_i < \lambda_0$ for all $i > 0$, we see that the relaxation time τ is effectively determined by the second largest eigenvalue, λ_1 : $\tau \sim (-\ln \lambda_1)^{-1}$.

Now, using the fact that the correlation time τ is expected to scale asymptotically for large N as

$$\tau(p - p_c, p_0, \frac{1}{N}) = b^z \tau(b^{-\nu_\perp} (p - p_c), b^{\omega/\nu_\perp} p_0, \frac{b}{N}), \quad (7.74)$$

where b is an arbitrary scale factor, Kinzel [kinz85b] uses the following steps to approximate the critical exponents. First, consider the quantity $Y(N) = \ln[\frac{\tau(p, N)}{\tau(p, N-1)}] / \ln(N/N-1)$, which can be calculated for a line in the parameter space parameterized by p . It can be shown that

$$Y(N) = \begin{cases} \sim N & \text{for } p > p_c, \\ z & \text{for } p = p_c, \\ \sim 0 & \text{for } p < p_c. \end{cases} \quad (7.75)$$

Thus, z and p_c can be approximated by finding the intersection of the functions $Y(N+1)$ and $Y(N)$; the $N \rightarrow \infty$ result is obtained by extrapolation. The other critical exponents may be obtained through scaling of the corresponding partial derivatives of τ and the usual scaling relations.

7.3.1.2 Reduction to a One-Parameter Model

This model can be simplified by reducing it to a single parameter. Vichniac, *et.al.* [vich86b] for example, consider the behavior along the line $p_2 = 1 - p_1$. They point out that this reduction affords p_1 and p_2 a simple interpretation in terms of the familiar Boolean functions AND and XOR (exclusive OR). In particular, for the line $p_2 = 1 - p_1$, we can equate $p_1 = p(\text{XOR})$ and $p_2 = 1 - p_1 = p(\text{AND})$, so that

the reduced rule reads:

$$\sigma_i(t+1) = \begin{cases} \sigma_{i-1}(t) \text{ XOR } \sigma_{i+1}(t) & \text{with prob} = p, \\ \sigma_{i-1}(t) \text{ AND } \sigma_{i+1}(t) & \text{with prob} = 1 - p \end{cases} \quad (7.76)$$

Note that since both AND and XOR yield zero whenever σ_{i-1} and σ_{i+1} are zero, p_0 is equal to zero, which is consistent with the definition of the full model (equation 7.69).

The $p_2 = 1 - p_1$ line crosses Domany and Kinzel's critical curve at $p = p_c \approx 0.785$ (see figure 7.6). Interestingly, Vichniac, *et.al.* find (1) class-1 behavior with $\rho \rightarrow 0$ for $p < p_c$, (2) class-3, or chaotic, behavior with $\rho_\infty \neq 0$ for $p > p_c$, and (3) complex, effectively unpredictable class-4 like behavior for $p = p_c$. This should remind the reader of another instance in section 3.2, albeit within a slightly different context, where the most "complex" (i.e. class-4) rules appear to be situated precisely at a transition-point [vich86b]. There, the idea was to employ a single parameter – namely Langton's λ -parameter [lang90] – to systematically map out the structure of a deterministic rule space. Here, on the other hand, the idea is to map out the behavior of a set of probabilistic rules. The result in both cases, however, is the same: *class-4 rules appears to live precisely on a transition point* (see section 12.8 for a related philosophical discussion of this issue). It is safe to say that much work still remains to be done in order to gain a deeper understanding of the general relationship between class-4 and critical behavior.

We might mention here in passing that while class-1, class-3 and class-4 (but not class-2) can all be obtained from one another with these two simple rules, class-2 behavior can only be obtained if the system is first *quenched* [vich86b]. That is, if the lattice is initially randomly populated with AND and XOR rules according to the prescribed value of p and is then "frozen" for all later times. Such quenched random rules harbor some interesting properties of their own in dimensions $d > 1$, and are the basis of much of Kauffman's findings on random Boolean networks (see section 8.6).

7.3.2 Totalistic PCA

Consider now the class of totalistic PCA, defined by four independent probabilities, $p_1, \dots, p_4$:

$$\begin{cases} p_0 = P(1 | 0, 0, 0), \\ p_1 = P(1 | 0, 0, 1) = P(1 | 0, 1, 0) = P(1 | 1, 0, 0), \\ p_2 = P(1 | 0, 1, 1) = P(1 | 1, 0, 1) = P(1 | 1, 1, 0), \\ p_3 = P(1 | 1, 1, 1). \end{cases} \quad (7.77)$$

As before, we set $p_0 = 0$ to have $\vec{\sigma} = \vec{0}$ as the single absorbing state. Table 7.2 shows the eight deterministic-rule corners of the (p_1, p_2, p_3) -cube. Figure 7.7 shows three slices of the phase-diagram of this system. We see that there always exists

a phase boundary between the (0,0,0) (i.e. rule R1) and (1,1,1) (i.e. rule R254) corners.

p_0	p_1	p_2	p_3	Rule	Class
0	0	0	0	0	1
0	0	0	1	22	3
0	0	1	0	104	2
0	0	1	1	126	3
0	1	0	0	128	1
0	1	0	1	150	3
0	1	1	0	232	2
0	1	1	1	254	1

Table 7.2 The deterministic corners of the (p_1, p_2, p_3) cube of the two-state PCA defined in the text.

The qualitative nature of the phase boundaries, however, is not simply related to the behavioral class of the deterministic rule corners. For example, while figure 7.7-c shows a phase transition to a class-3 rule, figures 7.7-a and 7.7-b show that the boundaries end at the class-3 rule. Similarly, while in figure 7.7-a the phase transition ends at a class-2 rule, there is only the absorbing stationary state close to the class-2 rule in figure 7.7-c.

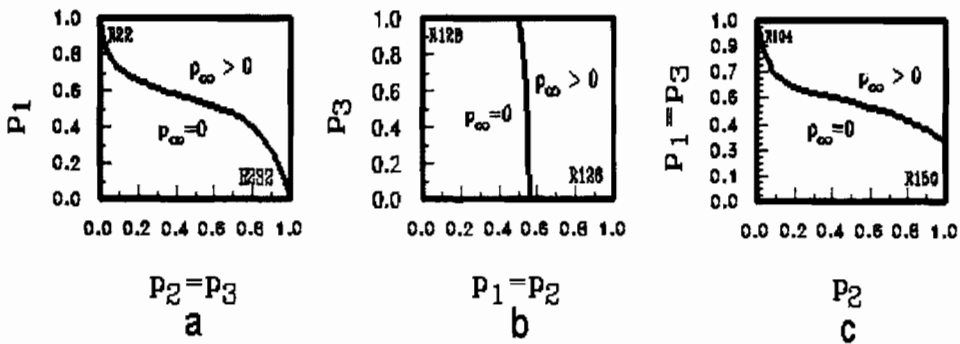


Fig. 7.7 Three sections of the (p_1, p_2, p_3) -phase plot (after [kinzel85b]); see text.

7.4 Mean-Field Theory

Except for a few special cases (most notably, *linear* rules (see below) and the $p_2 = 1$ line for the isotropic peripheral PCA discussed above, which happens to be an endpoint of a disorder line of an exactly solved 2-dim Ising model on a triangular lattice and can be solved exactly [kinzel85b]), phase-diagrams for PCA

must be determined largely through numerical simulation. Nonetheless, mean-field theory often provides a useful approximation, particularly for the time-dependence of the density (or *magnetization*), $\rho(t)$.

In this section we briefly outline a general mean-field theory approach to arbitrary PCA and then apply the formalism to a particular class of one-parameter rules. We then compare the theoretical predictions to numerical simulations on lattices of dimension $1 \leq d \leq 4$.

7.4.1 General Rules

Let us first consider a general probabilistic rule defined on a neighborhood $\mathcal{N}$ consisting of $|\mathcal{N}|$ sites and defined by the set of conditional probabilities $\{P(1 | S_1, S_2, \dots, S_{|\mathcal{N}|})\}$. A little thought will show that these conditional probabilities can always be written in the form

$$P(S'_i | \{S_j \in \mathcal{N}_i\}) = \frac{1}{2} (1 + S'_i \Psi[\{S_j \in \mathcal{N}_i\}]), \quad (7.78)$$

where $\mathcal{N}_i$ is the neighborhood around site i and Ψ is a linear combination of single and multi-spin products ([geor89], [lebo90]). For the (nonisotropic) peripheral PCA rules defined in equation 7.58, for example, Ψ is given by

$$\Psi[S_{i-1}, S_{i+1}] = \psi_0 + \psi_1^{(1)} S_{i+1} + \psi_1^{(2)} S_{i-1} + \psi_2 S_{i-1} S_{i+1}, \quad (7.79)$$

where ψ_0 , $\psi_1^{(1)}$, $\psi_1^{(2)}$ and ψ_2 are given in terms of the original set of four conditional probabilities $\alpha_1, \dots, \alpha_4$ (equation 7.58):

$$\begin{cases} \psi_0 = \frac{1}{2}(\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 - 2), & \psi_2 = \frac{1}{2}(\alpha_1 - \alpha_2 - \alpha_3 + \alpha_4) \\ \psi_1^{(1)} = \frac{1}{2}(-\alpha_1 + \alpha_2 - \alpha_3 + \alpha_4), & \psi_1^{(2)} = \frac{1}{2}(-\alpha_1 - \alpha_2 + \alpha_3 + \alpha_4). \end{cases} \quad (7.80)$$

Multiplying equation 7.78 by S' and summing over $S' = \pm 1$, gives

$$\sum_{S'_i=\pm 1} S'_i P(S'_i | \{S_j \in \mathcal{N}_i\}) = \Psi[\{S_j \in \mathcal{N}_i\}]. \quad (7.81)$$

If we now sum over all space-time histories and make the mean-field substitution of the densities ρ and ρ' for S and S' , respectively, we get the following simple mean-field iterative equation:

$$\rho' = \Psi[\rho]. \quad (7.82)$$

In the case of the peripheral PCA above, for example, this equation appears as

$$\rho' = \psi_0 + (\psi_1^{(1)} + \psi_1^{(2)})\rho + \psi_2\rho^2. \quad (7.83)$$

Notice that in this general case, correlation functions cannot be solved for directly; instead, there is an entire hierarchy of lower-order correlations expressed as functions of higher-order correlations. For example if we take an average of equation 7.79 over all space-time histories, and assume that we have a steady-state so

that $\langle \vec{S} \rangle_{t+1} = \langle \vec{S} \rangle_t$, a simple calculation shows that (for these peripheral PCA), $\langle S_{i,t} \rangle$ is related to the correlation function $\langle S_{i-1,t} S_{i+1,t} \rangle$ according to

$$\langle S_{i,t} \rangle = \frac{\psi_0 + \psi_2 \langle S_{i-1,t} S_{i+1,t} \rangle}{1 - (\psi_1^{(1)} + \psi_1^{(2)})}. \quad (7.84)$$

7.4.1.1 Binary Site Variables

In the case of binary variables $\sigma \in \{0, 1\}$, we can let density $\rho(t)$ at time t represent the probability of finding value $\sigma = 1$ at any site at time t . A simple counting of all possible configurations in an arbitrary neighborhood $\mathcal{N}$ gives us the general mean-field expression for the time-dependence of ρ :

$$\rho(t+1) = \sum_{i=0}^{|\mathcal{N}|} [\rho(t)]^i [1 - \rho(t)]^{|\mathcal{N}|-i} \sum_{\{\text{all } \sigma \text{ s.t. } \sum_{\sigma_k \in \mathcal{N}} \sigma_k = i\}} P(1 | \sigma_1, \sigma_2, \dots, \sigma_{|\mathcal{N}|}). \quad (7.85)$$

For a size $|\mathcal{N}| = 3$ neighborhood, for example, we have that

$$\begin{aligned} \rho(t+1) = & [1 - \rho(t)]^3 P(1 | 0, 0, 0) + \rho(t) [1 - \rho(t)]^2 \sum_{\sigma_1 + \sigma_2 + \sigma_3 = 1} P(1 | \sigma_1, \sigma_2, \sigma_3) \\ & + \rho(t)^2 [1 - \rho(t)] \sum_{\sigma_1 + \sigma_2 + \sigma_3 = 2} P(1 | \sigma_1, \sigma_2, \sigma_3) + \rho(t)^3 P(1 | 1, 1, 1). \end{aligned} \quad (7.86)$$

7.4.2 Linear PCA

A PCA system is called *linear* when all of the conditional probabilities $P(S'_i | \{S_j \in \mathcal{N}_i\})$ can be expressed as a sum of two-spin products [rujan87]:

$$P(S'_i | \{S_j \in \mathcal{N}_i\}) = \frac{1}{2} [1 + \sum_j \psi_1^{(j)} S'_i S_j], \quad (7.87)$$

where $S_i = \pm 1$.

Linear rules have the important property that all single-spin expectations and multi-spin correlations are decoupled. Calculating the expectation $\langle S_k \rangle_{t+1}$, for example, we see that

$$\begin{aligned}
\langle S_k \rangle_{t+1} &= \sum_{\{\vec{S}\}} S_k P(\vec{S}, t+1) \\
&= \sum_{\{\vec{S}\}} S_k \sum_{\{\vec{S}'\}} P(\vec{S}_{t+1} | \vec{S}'_t) P(\vec{S}', t) \\
&= \sum_{\{\vec{S}\}} \sum_{\{\vec{S}'\}} S_k \prod_i P(S_{i,t+1} | S'_t \in \mathcal{N}_i) P(\vec{S}', t) \\
&= \sum_{\{\vec{S}\}} \left(\sum_{\{\vec{S}'\}} \prod_i S'_k P(S'_{i,t+1} | S_t \in \mathcal{N}_i) \right) P(\vec{S}, t) \\
&= \langle \sum_k S'_k P(S'_k | S_t \in \mathcal{N}_k) \rangle_t \\
&= \sum_k \psi_1^{(k)} \langle S_k \rangle_t,
\end{aligned} \tag{7.88}$$

where we have used the relations $\sum_S f(S) = \sum_{-S} f(S)$, $\sum_{S_i} P(S_i | S'_j \in \mathcal{N}_i) = 1$ and equation 7.87. Similar calculations for multi spin products would show that, for linear rules,

$$\langle S_{k_1} S_{k_2} \cdots S_{k_n} \rangle_{t+1} = \sum_{k_1} \sum_{k_2} \cdots \sum_{k_n} \psi_1^{(k_1)} \psi_1^{(k_2)} \cdots \psi_1^{(k_n)} \langle S_{k_1} S_{k_2} \cdots S_{k_n} \rangle_t. \tag{7.89}$$

Another consequence of linearity is that the mean-field approximation becomes exact. From equations 7.82 and 7.88, we can immediately see that the mean-field iterative equation

$$\rho(t+1) = \left[\sum_i \psi_1^{(i)} \right] \rho(t), \tag{7.90}$$

is exact for linear rules.

7.4.3 Totalistic PCA

Consider the set of totalistic PCA, defined by the set of conditional probabilities $\{P_0, \dots, P_{|\mathcal{N}|}\}$, where $P_k = \text{prob}\{\sigma_i(t+1) = 1 | \sum_{j \in \mathcal{N}_i} \sigma_j(t) = k\}$ is the probability that a given site will have value '1' at time $t+1$ given that the sum of its neighbors at time t equals k . Using $\rho(t)$ to estimate the probability of finding value $\sigma = 1$ at any site at time t , the probability that a given site has exactly k neighbors, $p_k(t)$, is given by

$$p_k(t) = \binom{|\mathcal{N}|}{k} [\rho(t)]^k (1 - \rho(t))^{|\mathcal{N}|-k}, \tag{7.91}$$

and, thus,

$$\rho(t+1) = f[\rho(t)] = \sum_{k=0}^{|\mathcal{N}|} P_k \binom{|\mathcal{N}|}{k} [\rho(t)]^k (1 - \rho(t))^{|\mathcal{N}|-k}, \tag{7.92}$$

where $f(x)$ is the *iterative function*.

The possible asymptotic, or equilibrium, values of the density $\rho_\infty \equiv \lim_{t \rightarrow \infty} \rho(t)$ are obtained by solving for the stable fixed points of the equation $\rho = f(\rho)$. Recall that a given solution ρ is stable if $|f'(\rho)| < 1$.

EXAMPLE: Consider the isotropic peripheral PCA defined in equation 7.69:

$$p_0 = P(1 | 0, 0), \quad p_1 = P(1 | 0, 1) = P(1 | 1, 0), \quad p_2 = P(1 | 1, 1).$$

The mean-field equation is given by

$$\rho(t+1) = f[\rho(t)] = p_0[1 - \rho(t)]^2 + p_1\rho(t)[1 - \rho(t)] + p_2[\rho(t)]^2.$$

For the problem with a single absorbing state, $p_0 = 0$, and there are two possible stationary densities: $\rho_1 = 0$ and $\rho_2 = (2p_1 - 1)/(2p_1 - p_2)$. Since $f'(x) = 2p_1(1 - x) + 2x(p_2 - p_1)$, we find that $f'(\rho_1) = 2p_1 < 1 \implies \rho_1$ is stable for $p_1 < 1/2$ and $f'(\rho_2) = 2(1 - p_1) < 1 \implies \rho_2$ is stable for $p_1 > 1/2$. The mean-field critical line is therefore at $p_c = 1/2$ (compare this to the phase diagram in figure 7.6).

7.4.4 Detailed Balance

The question of whether there exists an equilibrium probability distribution ρ_∞ is difficult to answer in general. However, there is one simple scenario for which the answer is easy. Namely, when the system satisfies a condition called *detailed balance*.

To introduce this principle, consider the following equation expressing the Markovian transition between the t^{th} -step probability distribution for state $\vec{S}$, $\rho(\vec{S}, t)$, and $(t+1)^{\text{th}}$ -step probability distribution for state $\vec{S}'$, $\rho(\vec{S}', t+1)$:

$$\rho(\vec{S}', t+1) = \sum_{\vec{S}} P(\vec{S}' | \vec{S}) \rho(\vec{S}, t). \quad (7.93)$$

The sum is taken over all 2^N states, and $P(\vec{S}' | \vec{S})$ is a $2^N \times 2^N$ matrix. Since ρ and P are both probabilities, we know that they must satisfy the following three consistency conditions

$$\left\{ \begin{array}{lcl} P(\vec{S}' | \vec{S}) & \geq & 0 \\ \sum_{\vec{S}} \rho(\vec{S}, t) & = & 1 \\ \sum_{\vec{S}} P(\vec{S}' | \vec{S}) & = & 1 \end{array} \right. \quad (7.94)$$

We also know that if there exists an equilibrium distribution, ρ_∞ , then it must remain invariant under the Markovian transition; i.e. ρ_∞ must satisfy the eigenvector equation

$$\rho_\infty(\vec{S}) = \sum_{\vec{S}'} P(\vec{S} | \vec{S}') \rho_\infty(\vec{S}') \quad (7.95)$$

Now suppose that the system satisfies the condition of *detailed balance*, defined by

$$P(\vec{S} | \vec{S}') f(\vec{S}') = P(\vec{S}' | \vec{S}) f(\vec{S}), \quad (7.96)$$

where f is an arbitrary function depending on a single state. Summing both sides of this equation over $\vec{S}'$ and using the third expression in equation 7.94, we immediately retrieve the requisite eigenvalue equation 7.95. Going back to equation 7.93, this shows that as $t \rightarrow \infty$, the density $\rho(\vec{S}, t) \rightarrow f(\vec{S})$. In particular, if there exists a *Hamiltonian* function $\mathcal{H}[\vec{S}]$ such that

$$P(\vec{S} | \vec{S}') \exp\{-\beta \mathcal{H}[\vec{S}]\} = P(\vec{S}' | \vec{S}) \exp\{-\beta \mathcal{H}[\vec{S}']\}, \quad (7.97)$$

then detailed balance assures us that the Gibbs probability density $\exp\{-\beta \mathcal{H}\}$ is approached asymptotically as $t \rightarrow \infty$.

Notice that the condition of detailed balance is equivalent to *microscopic reversibility*: from equation 7.96, we see that if a given PCA in a stationary state satisfies detailed balance, then a “motion-picture” of the system will appear the same whether the film is run forwards or backwards.

EXAMPLES: (1) *Isotropic Peripheral PCA* – consider the isotropic version of the peripheral PCA defined by equations 7.61 and 7.63; i.e. take $\alpha_2 = \alpha_3 = \alpha_{23}$. In this case, the detailed balance condition is satisfied when the 3-spin coupling constant $h_{123} = 0$. From equation 7.96, we see that this condition translates to

$$\frac{\alpha_1}{1 - \alpha_1} \frac{\alpha_4}{1 - \alpha_4} = \left(\frac{\alpha_{23}}{1 - \alpha_{23}} \right)^2.$$

Thus, the isotropic peripheral PCA effectively describes the parallel 2-step dynamics (following the alternating updating of odd- and even- indexed sites) of the following one-dimensional Ising model:

$$\beta \mathcal{H} = \sum_i (J S_i S_{i+1} + B S_i),$$

where α_1 , α_4 and α_{23} are found from the detailed balance condition above, and the equations

$$\frac{\alpha_1 \alpha_4 (1 - \alpha_1)(1 - \alpha_4)}{[\alpha_{23}(1 - \alpha_{23})]^2} = e^{8h_{12}} = e^{-8J} \quad \text{and} \quad \left(\frac{1 - \alpha_4}{\alpha_1} \right)^2 = e^{8(h_1 + h_2 + h_3)} = e^{-8B}.$$

(2) *General Nearest-Neighbor Rules* [geor89] – in the same way as we derived equation 7.60, we can show that a general nearest-neighbor conditional probability can be

written in exponential form as follows:

$$P(S_3 | S_1, S_0, S_2) = \lambda^{-1} \exp\left\{\sum_i H_i S_i + \sum_{ij} K_{ij} S_i S_j + \sum_{ijkl} K_{ijkl} S_i S_j S_k S_l + L S_0 S_1 S_2 S_3\right\},$$

where the coupling constants are functions of the set of defining conditional probabilities, $\{P(1 | 0, 0, 0), P(1 | 0, 0, 1), \dots, P(1 | 1, 1, 1)\}$.

Taking a product over all sites and simplifying notation somewhat, we get that

$$\prod_i P(S'_i | S_{i-1} S_i S_{i+1}) = \lambda^{-1} \exp\{G_0(\{S\}) + \sum_i S'_i (H_3 + K_{13} S_{i-1} + K_{03} S_i + K_{23} S_{i+1} + G_1(\{S\}))\},$$

where G_0 and G_1 are terms containing only 2-spin and 3-spin products. The detailed balance condition (equation 7.97) then reads

$$\prod_i \frac{P(S'_i | S_{i-1} S_i S_{i+1})}{P(S_i | S'_{i-1} S'_i S'_{i+1})} = \exp\{G_0(\{S\}) - G_0(\{S'\}) + \sum_i [H_3(S'_i - S_i) + (K_{13} - K_{23})S'_i(S_{i-1} - S_{i+1}) + S'_i G_1(\{S\}) - S_i G_1(\{S'\})]\},$$

and is satisfied only if $G_1 \equiv 0$, $K_0 = K_1 = K_2 = L = 0$ and $K_{13} = K_{23}$.

The one-dimensional Hamiltonian $\mathcal{H}$ that assures us of getting the Gibbs measure as $t \rightarrow \infty$ is therefore given by

$$\begin{aligned} -\beta\mathcal{H} &= -G_0 + H_3 \sum_i S_i \\ &= (H_3 - H_0 - H_1 - H_2) \sum_i S_i - (K_{01} + K_{02}) \sum_i S_i S_{i+1} \\ &\quad - K_{12} \sum_i S_i S_{i+2} - K_3 \sum_i S_{i-1} S_i S_{i+1}. \end{aligned}$$

7.4.5 Minimally Diluted Deterministic Rules

Before looking at a few more specific examples, we first follow Bidaux, *et al* ([bidaux89a], [bidaux89b]) in restricting our attention to a class of *minimally diluted deterministic rules* defined for arbitrary lattices on neighborhoods of size $|\mathcal{N}| = 9$. These probabilistic rules are obtained from their deterministic counterparts by prescribing a successor state $\sigma(t+1)$ with probability p (or $1-p$) whenever the deterministic rule prescribes a successor state $\sigma = 1$ (or $\sigma = 0$). We also require that (i) the rules are symmetric (i.e. that $p_{9-k} = p_k$ for all k), and (ii) that there is one absorbing phase defined by an integer k^* (i.e. $p_k = 0$ for all k such that $|9 - 2k| \geq 2k^*$). These rules are convenient to study for two reasons: (1) there is only a single control parameter, p , which simplifies considerably the search for a possible phase transition in the order parameter, ρ . (2) A 9-site allows a consistent sampling to be made of all Cartesian lattices of dimension $1 \leq d \leq 4$. It had been widely believed that all one-dimensional two-state probabilistic CA with a single absorbing state formed a universality class. *Directed percolation*, in fact, has been frequently cited as a prototypical system ([kinzel83], [kinzel85b]). As we shall see below, however, numerical studies of these minimally diluted rules by Bidaux, *et.al.*, strongly suggest that this conjecture is in fact false.

Substituting $|\mathcal{N}| = 9$ into equation 7.92, we obtain the following iterative map for the density ρ :

$$\rho(t+1) = f(\rho(t)) = \sum_{k=0}^9 P_k \binom{9}{k} [\rho(t)]^k (1 - \rho(t))^{9-k}. \quad (7.98)$$

For small enough values of p so that $pf(\rho) < \rho$ for all $0 \leq \rho \leq 1$, $\rho = 0$ will be the only fixed point. As p increases, there will eventually be some density ρ^* for which $pf(\rho^*) > \rho^*$; in this case, we can expect there to be nonzero fixed point densities as well. Qualitatively, the mean-field-predicted behaviors will depend on the shape of the iterative map. If f has a concave downward profile, for example (i.e. if $f'' < 0$ everywhere), then, as p decreases, ρ_∞ decreases continuously to zero at some critical value of $p = p_c$. Note also that the iterative map f_{det} for the deterministic rule associated with its minimally diluted probabilistic counterpart is given by $f_{\text{det}} = f/p$.

Table 7.3 lists the four rules in this minimally-diluted rule-family, along with their corresponding iterative maps. Notice that since rules R_1 , R_2 and R_3 do not have a linear term, $f'(\rho = 0) = 0$ and mean-field-theory predicts a first-order phase transition. By “first order” we mean that the phase transition is *discontinuous*: there is an abrupt, discontinuous change at a well defined critical probability p_c , at which the system suddenly goes from having $\rho_\infty = 0$ as the only stable fixed point to having an asymptotic density $\rho_\infty \neq 0$ as the only stable fixed point (see below).

Rule	$\{p_0, p_1, \dots, p_9\}$	Iterative Map, $f(\rho)$
R_1	$\{0, 0, 0, 0, p, p, 0, 0, 0, 0\}$	$126 p \rho^4 (1 - \rho)^4$
R_2	$\{0, 0, 0, p, p, p, p, 0, 0, 0\}$	$42 p \rho^3 (1 - \rho)^3 (2 - 3\rho + 3\rho^2)$
R_3	$\{0, 0, p, p, p, p, p, p, 0, 0\}$	$6 p \rho^2 (1 - \rho)^2 (6 - 16\rho + 25\rho^2 - 18\rho^3 + 9\rho^4)$
R_4	$\{0, p, p, p, p, p, p, p, p, 0\}$	$3 p \rho (1 - \rho) (3 - 9\rho + 19\rho^2 - 23\rho^3 + 19\rho^4 - 9\rho^5 + 3\rho^6)$

Table 7.3 The four rules in the family of two-state/one-absorbing-state probabilistic PCA defined in the text, along with their corresponding iterative maps (see equation 7.98).

Rule R_4 , on the other hand, has both a linear and quadratic term, so that $f'(\rho = 0) > 0$ in general, and is therefore predicted to have a second order (or *continuous*) phase transition. Although the mean-field predictions are, of course, dimension-independent, they are expected to become exact as the dimension $d \rightarrow \infty$. In practice, it is often found that there exists a critical dimension d_c above which the mean-field critical exponents are recovered *exactly*.

Figure 7.8 shows a plot of the iterative map $f_2(\rho)$ for rule R_2 as a function of ρ for four different values of p : $p = 1$ (top curve), $p > p_c$, $p = p_c$ and $p < p_c$, where $p_c \approx 0.5347$. Notice that all four curves have zero first and second derivatives at the origin. This ensures the existence of some critical value p_c such that for all $p < p_c$, $\rho(t+1) < \rho(t)$ and thus that $\lim_{t \rightarrow \infty} \rho(t) = 0$. In fact, for all $0 \leq p < p_c$ the origin is the only stable fixed point. At $p = p_c$, another stable fixed point $\rho_S \approx 0.373$ appears via a tangent bifurcation. For values of p greater than p_c , f_2 undergoes a

familiar series of period-doubling bifurcations, culminating in chaos.[†]

An *unstable* fixed point, $\rho_U = \rho_U(p)$ appears for $p > p_c$ and defines a “boundary” such that if $\rho(t=0) < \rho_U(p)$ the system decays to zero and if $\rho(t=0) > \rho_U(p)$ then $\rho(t \rightarrow \infty) = \rho_S(p)$, where $\rho_S(p)$ is the stable fixed point for a PCA defined by probability p . Notice that since $\rho_U(p) < \rho_U(p')$ for $p > p'$, the value of the unstable fixed point for $p = 1$, $\rho_U^{(1)} \equiv \rho_U(p=1) \approx 0.1577$, represents a cutoff point for initial densities leading to a nonzero limit for any p ; i.e. if $\rho(t=0) < \rho_U^{(1)}$, then $\rho(t \rightarrow \infty) = 0$. Putting all of this together, we see that if we consider only those initial densities $\rho(t=0) > \rho_U^{(1)}$, then the ‘ ρ_∞ versus p ’ curve for rule R_2 exhibits a typical first-order phase transition at $p = p_c$. The other rules are handled in the same fashion.

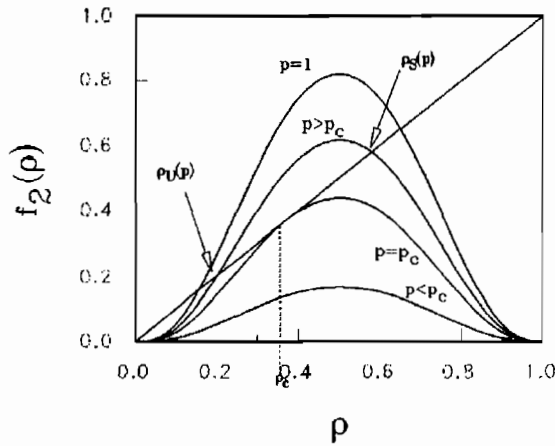


Fig. 7.8 Plot of the iterative map $f_2(\rho)$ as a function of ρ for four different values of p ; see text.

7.4.5.1 Numerical Results

Table 7.4 compares the mean-field-theory prediction for the order of the phase transition and critical probability p_c to numerical results obtained by Biduax, *et.al.* ([bidaux89a], [bidaux89b]) by simulating dynamics on regular lattices of dimension $d = 1$, $d = 2$ and $d = 4$.

We make the following observations:

(1) R_1 does not show any phase transition. This should not be terribly surprising, since, in the deterministic limit, R_1 exhibits either class 2 behavior (i.e. periodicity) or class 4 behavior (spatially separated propagating structures with an ill-defined statistical limit). The density ρ therefore has no well-defined statistical mean for $p = 1$ and the periodicity and/or propagating structures are rapidly destroyed (and thus $\rho \rightarrow 0$) whenever $p < 1$. Moreover, from the above mean-field

[†]See chapter 4 for a general discussion of period-doubling and chaos in one-control-parameter iterative maps.

Rule	MF Theory		$d = 1$		$d = 2$		$d = 4$	
	Order	p_c	Order	p_c	Order	p_c	Order	p_c
R_1	1	≈ 0.9456	no transition		no transition		no transition	
R_2	1	≈ 0.5347	2	≈ 0.721	1	≈ 0.661	1	≈ 0.578
R_3	1	≈ 0.3538	2	≈ 0.427	1	≈ 0.40	1	≈ 0.37
R_4	2	$\approx 1/9$	2	≈ 0.220	2	≈ 0.16	2	≈ 0.125

Table 7.4 Order of phase transition and threshold probabilities versus space dimension for rules $R_1, \dots, R_4$, as determined by mean-field theory and numerical calculation ([bidaux89a], [bidaux89b]).

theory calculations we see that although a stable fixed point does exist away from the origin (suggesting a first-order transition), the threshold $p_c \approx 0.9456$ is very close to the deterministic limit.

(2) *mean-field theory correctly predicts the order of the phase transition for dimensions $d \geq 2$.* mean-field theory also correctly predicts that R_4 undergoes a second-order transition for all dimensions.

(3) *The quantitative agreement between mean-field theory predicted thresholds and numerically calculated values improves with increasing dimension.* Although, as mentioned above, this is to be expected on quite general grounds, the agreement is nonetheless inexact for all dimensions $d \leq 4$; i.e., the “critical” dimension $d_c > 4$ [bidaux89b].

7.5 CA Simulations of Spin Models

7.5.1 Why a “Naive” CA Approach Does Not Work

Suppose we wanted to model an Ising model in the most straightforward possible manner using a CA approach. For argument’s sake, let’s consider modeling a basic Ising model without any external fields. Using binary site variables $\sigma \equiv \frac{1}{2}(1 - S)$ to make any possible connection to conventional CA transparent, our task is to come up with a CA rule ϕ ,

$$\sigma_i(t+1) = \phi[\sigma_i(t), \sigma_j(t) \in \mathcal{N}_i], \quad (7.99)$$

where, as usual, $\mathcal{N}_i$ is the neighborhood around site i , that simulates an Ising spin system with total magnetic energy

$$\mathcal{H}[\vec{\sigma}] = \sum_{\text{NN}(i,j)} (\sigma_i + \sigma_j) \bmod 2. \quad (7.100)$$

From this equation we see that a single spin “flip” $\sigma \rightarrow 1 - \sigma$ induces an energy change $\Delta\mathcal{H}$ equal to

$$\Delta\mathcal{H} = 2(2 - \Delta_i), \quad (7.101)$$

where

$$\Delta_i = \sum_j (\sigma_i + \sigma_j) \bmod 2. \quad (7.102)$$

We can now take one of two approaches: (1) construct a probabilistic CA along lines with the Metropolis Monte Carlo algorithm outlined above (see section 7.1.3.1), or (2) define a deterministic but reversible rule consistent with the microcanonical prescription. As we shall immediately see, however, *neither* approach yields the expected results.

7.5.1.1 Metropolis Prescription

According to the Metropolis algorithm, all negative energy changes are accepted with probability one and all positive energy changes are accepted with a probability equal to the Boltzman weight, $e^{-\Delta\mathcal{H}/kT}$, where $\Delta\mathcal{H}$ is the energy change, k is Boltzman's constant and T is the temperature. Using equations 7.101 and 7.102, we see that this is equivalent to the following PCA rule:

$$\begin{aligned} \sigma_i(t+1) = & \delta_{\Delta_i,0}\{[1 - \sigma_i(t)]p^2 + (1 - p^2)\sigma_i\} + \delta_{\Delta_i,1}\{[1 - \sigma_i(t)]p + (1 - p)\sigma_i\} \\ & + (\delta_{\Delta_i,2} + \delta_{\Delta_i,3} + \delta_{\Delta_i,4})[1 - \sigma_i(t)], \end{aligned} \quad (7.103)$$

where $p = e^{-2/kT}$. In words, the rule states that we are to flip the spin if $\Delta_i = 2, 3$ or 4 ; flip the spin with probability p if $\Delta_i = 1$; and flip the spin with probability p^2 if $\Delta_i = 0$.

Vichniac [vich84] has pointed out that this rule is unfortunately plagued by an unavoidable *feedback catastrophe* that renders it unsuitable as a “simulator” of Ising systems. Suppose the system is in an antiferromagnetic state; i.e. suppose that $\Delta_i = 4$ for all sites i . From equation 7.103, we see that each spin will be flipped on the next iteration step. Thus, the system immediately evolves to the complementary antiferromagnetic state ($\sigma_i = 0$, for all i). If the spin is flipped once again in this new state, however, Δ_i is again equal to 4 and the system will go back to its starting antiferromagnetic state. The result is therefore a continuous oscillation between the two states of maximal energy. Since the Metropolis algorithm is supposed to relax the system towards an equilibrium state, this is a clearly unacceptable situation. To make matters even worse, Vichniac has also shown that this oscillation between maximal energy states is actually an attractor state for many initial conditions and is not merely a result of the special conditions chosen here for illustration.

7.5.1.2 Microcanonical Prescription

What about a microcanonical ensemble based approach? The simplest prescription would be to define a rule that flips the spins only at a constant energy; that is, for $\delta\mathcal{H} = 0$ or $\Delta_i = 2$. The reader may recall that we have already studied some of the behaviors of this rule in section 3.4; it is, in fact, equal to the Fredkin-reversible rule Q2R ([vich84], [vich86a]). From the comments made in our earlier discussion, it

should not surprise us to learn that this “naive” microcanonical approach also falls short as a reliable Ising-spin system simulator. For example, it is easy to see that the microcanonical approach suffers from the same so-called feedback catastrophe as plagued by the Metropolis algorithm. Consider a small cluster of 1-spins in a sea of 0-spins:

0	0	0	0
0	1	1	0
0	1	1	0
0	0	0	0

This configuration has a total energy $\mathcal{H}(t_0) = 8$. Since each $\sigma = 1$ site has two $\sigma = 1$ neighbors and two $\sigma = 0$ neighbors, it gets flipped on the next time step. But each $\sigma = 0$ site has, at most, one $\sigma = 1$ neighbor and will be left unchanged. On the next iteration step, therefore, all of the sites in the cluster will have $\sigma = 0$ and $\mathcal{H}(t_0 + 1) = 0$.

Notice that in both the Metropolis and microcanonical approaches, the underlying mechanism for the feedback catastrophe is the same. The problem arises because the energy change $\delta\mathcal{H}$ induced by a spin-flip is actually valid only if the local neighborhood of a flipped spin remains invariant during the lattice-evolution update. While this invariance holds for any simple asynchronous updating, such as in the usual sequential updating prescribed for by the usual Metropolis algorithm, it does not generally hold for a simultaneous CA-like updating. If we insist on keeping a parallel synchronous dynamics, the feedback catastrophe can therefore only be avoided if the updating proceeds in steps; at each step it being made sure that the neighborhood of local spins remains invariant.

Vichniac [vich84] has shown that for an Ising system with nearest-neighbor interactions, this can be accomplished in one of two ways: either by (1) performing an alternating update of every other spin on a checkerboard pattern, or by (2) enlarging the effective local state-space from two to four states in order to provide for two separate spins at a given site. Hermann [herr86] has carried out a simulation using the first approach. Although the results have been very good at high temperature (i.e. in the paramagnetic phase) the effective simulation “rule” has proven to be somewhat less reliable at low temperatures (in the ferromagnetic phase); see below. The second approach has been exploited by Creutz [creutz86], using both localized and randomly traveling *demons* to assure a proper thermalization. While having only local demons clearly makes the prescription more conventionally CA-like (see below), the randomly-traveling demon variant of the rule has been found to lead to better thermalization.

Another problem with microcanonical-based CA simulations, and one which was not entirely circumvented by Hermann, is the lack of *ergodicity*. Since microcanonical ensemble averages require summations over a constant energy surface in phase space, correct results are assured only if the trajectory of the evolution is ergodic; i.e. only if it covers the whole energy surface. Unfortunately, for low temperatures ($T \ll T_c$), microcanonical-based rules such as Q2R tend to induce states in which only the only spins that can flip their values are those that are located within small

local clusters. Most $\sigma = 1$ spins are completely isolated and are unable to flip; those $\sigma = 1$ spins that are able to flip are typically part of small three- or four- site clusters and give rise to a very few configurations. As a result, most configurations can never be reached. In other words, the system cannot *thermalize* [parad89]. Although Hermann [herr86] “solves” this problem by effectively averaging over many random initial states, the procedure remains questionable since (a) averages must be obtained through summations over states with the same energy and (b) it is not possible to choose random states with an *a priori* given energy [parad89].

7.5.2 Creutz’s Demons

In the previous section we have seen how a “naive” CA approach to modeling a spin system is almost sure to fail. The basic result of that discussion was that if we want our dynamics to remain *synchronous*, we must either give up on simultaneously updating *all* sites of the lattice at a given time step or increase the size of the local state space. Creutz ([creutz83], [creutz84], [creutz86]) has introduced two useful models that exploit both of these strategies by populating the lattice with energy *demons*. Subsequent improvements to the basic model, mostly having to do with making sure that the system thermalizes properly at low temperatures, have been made by Parodi and Ottavi [parod89].

7.5.2.1 Randomly Traveling Demons

A *demon* is essentially an “energy-sack”. In this first – and, of the two, decidedly less CA-like – model, a number of demons are allowed to move freely about the lattice. Whenever a demon moves into a site it helps that site flip its spin in the following manner: if $\Delta\mathcal{H} > 0$ (see equation 7.101), the demon stuffs the additional energy into its sack. If $\Delta\mathcal{H} < 0$, the demon removes the required amount of energy out of its sack and dumps it onto that site. If $\Delta\mathcal{H} = 0$, the spin flips without the demon’s assistance. Ergodicity, and hence a proper thermalization, is assured by having a large enough army of demons stomping around the lattice. Creutz has demonstrated that this simple model works well in both low and high temperature regimes. Unfortunately, the random demon motion cannot easily be accounted for by a conventional CA rule and is therefore not easily implemented by a parallel processing technique. Nonetheless, this model runs an order of magnitude faster than conventional Monte Carlo simulations and does not require high quality random numbers [creutz86].

7.5.2.2 Localized Demons

One obvious way of making the model more amenable to a CA implementation is to permanently attach the demons to each site. In order to accommodate such demons, the state space of each site must also be increased from two to four bits:

$$\sigma_i \longrightarrow \vec{\sigma}_i = (\sigma_i^{(1)}, \sigma_i^{(2)}, \sigma_i^{(3)}, \sigma_i^{(4)}). \quad (7.104)$$

The first bit is the usual Ising spin: $\sigma_i^{(1)} = \sigma_i$. The next two bits, $\sigma_i^{(2)}$ and $\sigma_i^{(3)}$ represent the demon. Since, from equation 7.101, we know that $\Delta\mathcal{H}$ is always even, we let the demon's sack contain only even valued energy bundles, with a maximum value of 6.[†] Letting $\mathcal{H}_{D,i}$ be the total energy of the i^{th} demon, we have that $\mathcal{H}_{D,i} = 4\sigma_i^{(2)} + 2\sigma_i^{(3)}$. The total demon energy, $\mathcal{H}_D$, is therefore equal to

$$\mathcal{H}_D = 2 \sum_i (2\sigma_i^{(2)} + \sigma_i^{(3)}). \quad (7.105)$$

The last bit, $\sigma_i^{(4)}$, encodes the space-time parity of each site and is used to prevent the simultaneous CA-like updating of all lattice sites that we know must somehow be circumvented if the updating is to remain strictly synchronous. At any given time, exactly half of all sites are updated; this is in fact nothing more than Vichniac's [vich84] checkboard updating.

Putting all of this together, Creutz' local demon rule may be written as follows:

$$\sigma_i^{(1)}(t+1) = \left(\sigma_i^{(1)}(t) + \Omega_i(t)\sigma_i^{(4)}(t) \right) \bmod 2, \quad (7.106)$$

where

$$\left\{ \begin{array}{lcl} \Omega_i(t) & = & \begin{cases} 1 & \text{if } 0 \leq \mathcal{H}_{D,i}(t) - \Delta\mathcal{H}_i(t) \leq 6, \\ 0 & \text{else} \end{cases} \\ \mathcal{H}_{D,i}(t+1) & = & \{\mathcal{H}_{D,i}(t) - \Delta\mathcal{H}_i(t)\}\Omega_i(t) + \mathcal{H}_{D,i}(t)(1 - \Omega_i(t)), \\ \sigma_i^{(4)}(t+1) & = & 1 - \sigma_i^{(4)}(t). \end{array} \right. \quad (7.107)$$

A few comments about this algorithm are in order: (1) By construction, the algorithm is set up in such a way that the total energy of the system is exactly conserved at all times:

$$\mathcal{H} = \mathcal{H}_D + \sum_{(i,j)} (\sigma_i^{(1)} + \sigma_j^{(1)}) \bmod 2 = \text{constant}. \quad (7.108)$$

(2) Unlike conventional Metropolis-like Monte Carlo simulations where an effective temperature is defined by coupling the system to some thermal reservoir, here the temperature is a purely statistical parameter that is *deduced* from the observed demon energy:

$$\langle \mathcal{H}_{D,i} \rangle = \frac{\sum_{n=1}^4 n e^{-2(n-1)/k_B T}}{\sum_{n=1}^4 e^{-2(n-1)/k_B T}} \implies T = T(\langle \mathcal{H}_{D,i} \rangle). \quad (7.109)$$

[†]There is nothing sacred about using 6 as the maximum allowable demon energy. However, from the updating algorithm to be defined below in equation 7.106, it can be shown that (1) a single bit would have the undesirable trait of preventing flips of isolated spins surrounded by antiparallel neighbors, and (2) since a two-bit demon will become fully excited only a few percent of the time near the critical temperature, a larger state space is really not essential [creutz86].

(3) The dynamics are not ergodic. Since the rule is symmetric under certain translations of the lattice (for example, any translation along a given axis that is a multiple of two sites), a configuration that is initially symmetric with respect to any set of such translations will remain symmetric throughout the course of the dynamics [creutz86]. Parodi and Ottavi [parod89] have performed extensive numerical simulations of this rule and have in fact found that thermalization is generally poor at low temperatures ($\lesssim .92T_c$). Thermalization can be restored at low temperatures by adding another random process to the dynamics, but only at the cost of again increasing the size of the local state space. Parodi and Ottavi's *Toss Model*, for example, uses a 17-bit linear shift register as a random number generator and can be viewed as a 2^{17+} -state (deterministic and reversible) CA [parod89].

7.6 A Stochastic Version of Conway's Life Rule

An early study of a stochastic CA system was performed by Schulman and Seiden in 1978 using a generalized version of Conway's *Life* rule [schul78]. Though there was little follow-on effort stemming directly from this particular paper, the study nonetheless serves as a useful prototype for later analyses. The manner in which Schulman and Seiden incorporate site-site correlations into their calculations, for example, bears some resemblance to Gutowitz, *et.al.*'s *Local Structure Theory*, developed about a decade later (see section 5.3). In this section, we outline some of their methodology and results.

We begin by recalling that Conway's original deterministic rule is an outer-totalistic (code OT224) $k = 2$ rule defined on the two-dimensional Moore neighborhood:

$$\sigma_{i,j}(t+1) = \delta_{3,\sum' \sigma(t)} + \sigma_{i,j}(t)\delta_{2,\sum' \sigma(t)}, \quad (7.110)$$

where $\delta_{\alpha,\beta}$ is the Kronecker delta and $\sum'$ is a sum over all neighbors of the site (i,j) (excluding the center site itself). Schulman and Seiden generalized this basic model in two ways: (1) they introduced "birth" and "survival" probabilities, $0 \leq P_B^k \leq 1$ and $0 \leq P_S^k \leq 1$, respectively, and (2) they defined an effective "temperature" T to serve as a "decorrelating" agent.

To be more precise, P_α^k is the probability that a site having exactly k living (i.e. $\sigma = 1$) neighbors either survives ($\alpha = S$ and the given site had previously been alive) or is born ($\alpha = B$ and the given site had previously been dead). Conway's deterministic rule, of course, is reproduced by setting $P_B^k = \delta_{k,3}$ and $P_S^k = \delta_{k,2} + \delta_{k,3}$.

The temperature T is defined by

$$P_\alpha^k(T) = \frac{P_\alpha^k(0) + \rho T}{T + 1}, \quad (7.111)$$

where $\rho = \frac{1}{N} \sum_{i,j} \sigma_{i,j}$ is the density of live sites. This definition possesses two useful properties. First, setting $P_B^k(T=0) = \delta_{k,3}$ and $P_S^k(T=0) = \delta_{k,2} + \delta_{k,3}$, we see that the $T = 0$ limit reproduces Conway's deterministic *Life* rule. Second, the

density is conserved at equilibrium. That is, assuming that equilibrium has already been reached under the *Life* rule alone, so that $\rho(t+1) = \rho(t)$, it will still be true that $\langle \rho(t+1) \rangle_T = \rho(t)$, where $\langle x \rangle_T$ is the expectation of x at temperature T , as the reader can easily show by using equation 7.111. This second property is important because it means that T cannot be a driver for the density, but can only alter the pattern of live sites. We also see that in the infinite temperature limit, as $T \rightarrow \infty$, $P_B^k = P_S^k = \rho$ for all k . Schulman and Seiden comment that while there is some similarity between their effective temperature T and the temperature used in the stochastic evolution of dynamical Ising models (see section 7.1.5), the analogy cannot really be carried too far in this case since there is no known conserved energy for Conway dynamics [schul78] (but see the discussion of entropy as it relates to this system, below).

7.6.1 Zero-Temperature Limit

Let us first of all consider the deterministic *Life* rule, or zero temperature limit of our more general stochastic rule. Using the density ρ to represent our state of knowledge of the system at time t , our problem is then to estimate the time-evolution of ρ for $T = 0$.

The simplest approximation to make is simply that the initial distribution of “live” sites is completely random and that any site-site correlations are negligible; i.e. we first take a conventional *Mean-Field* approach (see section 7.4). In this case, the equilibrium density can be written down almost by inspection. The probability of a site having value 1 ($= \rho$) is equal to the probability that it had value 1 on the previous time step multiplied by the probability that it stays equal to 1 (i.e. the probability that a site has either 2 or 3 live neighboring sites) plus the probability that the site was previously equal to 0 multiplied by the probability that it become 1 (i.e. that it is surrounded by exactly 3 live sites). Letting ρ and ρ' represent the density at times t and $t+1$, respectively, simple counting yields[†]

$$\begin{aligned} \rho' &= \rho \left[\binom{8}{3} \rho^3 (1-\rho)^5 + \binom{8}{2} \rho^2 (1-\rho)^6 \right] + (1-\rho) \binom{8}{3} \rho^3 (1-\rho)^5, \\ &= 28\rho^3(\rho-3)(\rho-1)^5. \end{aligned} \tag{7.112}$$

Setting $\rho' = \rho = \rho_e$ at equilibrium, we find that the only real stable nonzero solution for $0 \leq \rho_e \leq 1$ is $\rho_e \approx 0.370$. This uncorrelated approximation actually describes the infinite temperature limit (effectively, $T \gg 1$) rather well, since as the temperature increases, local correlations of the basic *Life* rule steadily decrease.

[†]Note that this equation could just as easily be written in a more general form describing arbitrary rules defined by general vectors P_α^k : if all correlations are neglected, we have that

$$\rho' = \sum_{k=0}^N \rho^k (1-\rho)^{N-k} \left[\rho P_S^k + (1-\rho) P_B^k \right].$$

In order to improve upon the mean-field approximation given in equation 7.112, we must somehow account for possible site-site correlations. Let us go back to the deterministic version of the basic *Life* rule (equation 7.110). We could take a formal expectation of this equation but we first need a way to compute expectation values of Kronecker delta functions. Schulman and Seiden [schul78] provide a simple means to do precisely that. We state their result without proof.

Schulman and Seiden first note that a δ -function can be written as a sum of products of σ 's. Let $L = \{1, \dots, l\}$ and K be any subset of the set L of cardinality k . Thus K can be written as $K = \{\alpha_1, \dots, \alpha_l\}$, where $1 \leq \alpha_i \leq l$, for all i . Given a *delta*-function, $\delta_{k, \sum' \sigma_\alpha}$, where the primed sum is over some l σ 's, we have that

$$\delta_{k, \sum_{i=1}^l \sigma_i} = \sum_K \sigma_{\alpha_1} \cdots \sigma_{\alpha_k} (1 - \sigma_{\alpha_{k+1}}) \cdots (1 - \sigma_{\alpha_l}), \quad (7.113)$$

where the sum is over all subsets K having exactly k elements; this sum contains $\binom{l}{k}$ terms.

By rewriting all of the δ -functions in this manner, the problem of taking the expectation of equation 7.110 has been conveniently reduced to taking expectations of simple products of σ 's. Schulman and Seiden go on to show exactly how such expectations can be expressed as functions of second-order correlation functions (or *cumulants*), $\langle \sigma_1 \sigma_2 \rangle_C \equiv \langle \sigma_1 \sigma_2 \rangle - \langle \sigma_1 \rangle \langle \sigma_2 \rangle$ [schul78]:

$$\begin{aligned} \langle \delta_{k, \sum' \sigma} \rangle &= \binom{8}{k} \rho^k \mu^{8-k} + \left(\sum_{r < s} \langle \sigma_r \sigma_s \rangle_C \right) \cdot \\ &\quad \left[\binom{6}{k-2} \rho^{k-2} \mu^{8-k} - 2 \binom{6}{k-1} \rho^{k-1} \mu^{7-k} + \binom{6}{k} \rho^k \mu^{6-k} \right], \\ \langle \sigma_0 \delta_{k, \sum' \sigma} \rangle &= \binom{8}{k} \rho^{k+1} \mu^{8-k} + \sum_{r=1}^8 \langle \sigma_0 \sigma_r \rangle_C \left[\binom{7}{k-1} \rho^{k-1} \mu^{8-k} - \binom{7}{k} \rho^k \mu^{7-k} \right] + \\ &\quad \sum_{r < s} \langle \sigma_r \sigma_s \rangle_C \rho \left[\binom{6}{k} \rho^k \mu^{6-k} - \right. \\ &\quad \left. 2 \binom{6}{k-2} \rho^{k-1} \mu^{7-k} + \binom{6}{k-2} \rho^{k-2} \mu^{8-k} \right], \end{aligned} \quad (7.114)$$

where $\sum_{r < s} \langle \sigma_r \sigma_s \rangle_C$ is the sum of the cumulants for all pairs from the eight neighbors of the central site, σ_0 is the value of the central site itself, $\mu \equiv 1 - \rho$, and the combinatorial coefficients are equal to zero whenever the value of their lower argument exceeds the value of their upper argument.

Using 7.114, the expectation of equation 7.110 can be written as follows:

$$\begin{aligned} \rho' &= 56\rho^3\mu^5 + 28\rho^3\mu^6 + 4\mathcal{B} (7\rho\mu^6 - 21\rho^2\mu^5) \\ &\quad + 2\mathcal{A} (20\rho^3\mu^3 + 15\rho^3\mu^4 - 30\rho^2\mu^4 - 12\rho^2\mu^5 + 6\rho\mu^5 + \rho\mu^6), \end{aligned} \quad (7.115)$$

where $\mathcal{A} \equiv 4L_1 + 2L_2 + 3L_3 + 4L_4 + L_5 = (1/2) \sum_{r < s} \langle \sigma_r \sigma_s \rangle_C$, $\mathcal{B} \equiv L_1 + L_2 = (1/4) \sum_{r=1}^8 \langle \sigma_0 \sigma_r \rangle_C$, and $L_i = \langle \sigma_0 \sigma_i \rangle_C$ is the cumulate between sites '0' and 'i'.

Equation 7.115, as it stands, cannot yet be used since there is no direct way to iterate the cumulants that appear in $\mathcal{A}$ and $\mathcal{B}$. Since $L_i = \langle \sigma_0 \sigma_i \rangle_C = \langle \sigma_0 \sigma_i \rangle$

$-\langle \sigma_0 \rangle \langle \sigma_i \rangle$, however, we can use equation 7.110 to write

$$\begin{aligned} L_i + \langle \sigma_0 \rangle \langle \sigma_i \rangle &= \langle \sigma_0 \sigma_i \rangle, \\ &= \langle \delta_{3, \sum^{(0)}} \delta_{3, \sum^{(i)}} \rangle + \left\{ \langle \delta_{3, \sum^{(0)}} \sigma_i \delta_{2, \sum^{(i)}} \rangle + \right. \\ &\quad \left. \langle \delta_{3, \sum^{(i)}} \sigma_i \delta_{2, \sum^{(0)}} \rangle \right\} + \langle \sigma_0 \delta_{2, \sum^{(0)}} \sigma_i \delta_{2, \sum^{(i)}} \rangle, \end{aligned} \quad (7.116)$$

where $\sum^{(k)}$ indicates that the sum is to be taken over the eight neighbors of site ' k '. Equation 7.113 then allows us to rewrite this expression as sums of products of random variables. Schulman and Seiden simplify the calculations considerably by treating all cumulants as second-order terms, and then evaluating them only to first order (a procedure that must ultimately be justified by a numerical comparison). When carried out, this procedure yields expressions of the form

$$L'_i + (\rho')^2 = f_i(\rho), \quad (7.117)$$

where $f_i(\rho)$ is a function only of the t^{th} generation density,[†] and ρ' is computed according to the mean-field derived equation 7.112 (i.e. by neglecting cumulants). The calculation thus effectively constitutes a first-order correction to the zeroth-order mean-field calculation performed earlier; it has some of the flavor of a second-order calculation of the more general *Local Structure Theory* [guto87a] discussed in section 5.3.

Unfortunately, in contrast to the uncorrelated estimate of $\rho_e \approx 0.370$, which was previously observed to be in good agreement with high-temperature measurements, the first-order correction actually turns out to be a worse predictor. Using equations 7.117 and 7.115, we find that $\langle \rho_e \rangle \approx 0.19$ for $0.10 < \rho_0 < 0.67$, as compared with the experimentally determined value of $\rho_e \approx 0.029 \pm 0.009$ [schul78]. Schulman and Seiden point out that part of the problem is that as the pure *Life* system evolves, an increasingly large fraction of the lattice becomes devoid of "live" sites. The asymptotic state in fact consists almost entirely of periodic and spatially widely-separated structures. Introducing, for this reason, a *local density* $\rho_L \equiv (\sum_i \sigma_i)/(N - \mathcal{V})$, where $\mathcal{V}$ is the excluded "vacuum" consisting of all sites that have no live neighbors, we do find a better match between the experimentally measured value $\rho_L \approx 0.229 \pm 0.008$ and its theoretically determined analogue $\langle \rho_L \rangle = \langle \rho \rangle / (1 + \langle (1 - \sigma_0) \delta_{0, \sum' \sigma} \rangle) \approx 0.299$, where $\langle (1 - \sigma_0) \delta_{0, \sum' \sigma} \rangle$ is the probability of finding a "vacuum" site [schul78].

[†]By tedious but straightforward calculation, $f_1(\rho)$, for example, may be found to be equal to

$$\sum_{j=0}^3 \binom{4}{j} \binom{4}{3-j}^2 \rho^{6-j} \mu^{6+j} + 2 \sum_{j=0}^2 \binom{4}{j} \binom{4}{2-j} \binom{3}{2-j}^2 \rho^{5-j} \mu^{7+j} + \sum_{j=0}^1 \binom{4}{j} \binom{3}{1-j}^2 \rho^{4-j} \mu^{8+j}.$$

$f_i(\rho)$, $i = 2, \dots, 5$ are given by similar expressions [schul78].

7.6.2 Finite Temperature

Except for using the statistical measure ρ to characterize the temporal evolution, the evolution itself has so far been entirely deterministic. We now take explicit account of temperature, as introduced via equation 7.111:

$$P_{\alpha}^k(T) = \frac{P_{\alpha}^k(0) + \rho T}{T + 1}, \quad (7.118)$$

Let $q(k, \sigma)$ be the probability that a site with value σ has exactly k live neighbors (i.e. that $\sum' \sigma = k$); note that $\sum_k q(k, \sigma) = 1$. Then

$$\langle \rho' \rangle = \sum_{k=0}^N \left[\rho P_S^{(k)} q(k, 1) + (1 - \rho) P_B^{(k)} q(k, 0) \right]. \quad (7.119)$$

Using equation 7.118, it then follows that

$$\langle \rho' \rangle = \frac{\langle \rho'_0 \rangle + \rho T}{T + 1}, \quad (7.120)$$

where $\langle \rho'_0 \rangle$ is defined by

$$\langle \rho'_0 \rangle = \sum_{k=0}^N \left[\rho P_S^{(k)}(0) q(k, 1) + (1 - \rho) P_B^{(k)}(0) q(k, 0) \right]. \quad (7.121)$$

But this last expression is exactly the quantity that we have been calculating in the last section. Up to second-order cumulants, it is the ρ' given in equation 7.115. We therefore have that

$$\langle \rho'_0 \rangle = \Psi_0(\rho) + \mathcal{A}\Psi_{\mathcal{A}}(\rho) + \mathcal{B}\Psi_{\mathcal{B}}(\rho), \quad (7.122)$$

where $\Psi_{\beta}(\rho)$, $\beta = 0, \mathcal{A}, \mathcal{B}$ are polynomials in ρ and can be read off immediately from equation 7.101. The only calculation remaining is the temperature dependence of the coefficients $\mathcal{A}$ and $\mathcal{B}$, which we recall are sums of order-2 cumulants. Schulman and Seiden derive the simple result that $\langle \mathcal{A}(t+1) \rangle = \mathcal{Q}_{\mathcal{A}}(\rho)/(1+T)^2$ and $\langle \mathcal{B}(t+1) \rangle = \mathcal{Q}_{\mathcal{B}}(\rho)/(1+T)^2$, where the polynomials $\mathcal{Q}_{\mathcal{A}}(\rho)$ and $\mathcal{Q}_{\mathcal{B}}(\rho)$ may be deduced directly from the definitions of $\mathcal{A}$ and $\mathcal{B}$ given following equation 7.115 and the quantities calculated in equation 7.117. Combining this result with equations 7.120, 7.121 and 7.122, we obtain an equation whose fixed points provide an estimate for the equilibrium density as a function of temperature, $\rho_e(T)$:

$$\rho_e = \Psi_0(\rho_e) + \frac{\mathcal{Q}_{\mathcal{A}}(\rho_e)\Psi_{\mathcal{A}}(\rho_e) + \mathcal{Q}_{\mathcal{B}}(\rho_e)\Psi_{\mathcal{B}}(\rho_e)}{(1+T)^2}. \quad (7.123)$$

There is a rather wide disparity between experiment and the second-order cumulate prediction for small T , equation 7.123 correctly predicts both the values of equilibrium density for large T and the fact that the system undergoes a sharp

“phase transition” at finite temperature (although the calculated transition temperature T_c does not match the experimentally measured value).[†]

In our opening remarks in this section, we mentioned that an analogy with dynamical Ising models can only be carried so far since there is no known conserved energy for the *Life* rule. However, Schulman and Seiden were able to discover a possible “constant of the motion”, namely a normalized entropy.

If an $M \times M$ lattice is broken up into $m \times m$ patches, the coarse-grained entropy of the system is given by

$$S = \frac{1}{M^2} \log_2 \prod_{i=1}^{(M/m)^2} \binom{m^2}{B(i)}, \quad (7.124)$$

where $B(i)$ is the number of sites with value $\sigma = 1$ in the i^{th} patch. This expression may be used to measure the entropy of the stochastic system directly. It may also be estimated theoretically by noting that the expectation of S is given by

$$\langle S \rangle = \frac{1}{M^2} \sum_{k=0}^{m^2} P(k) \log_2 \binom{m^2}{k}, \quad (7.125)$$

where $P(k)$ is the probability that a given patch contains exactly k “live” sites. If we neglect all correlations then $P(k) = \binom{m^2}{k} \rho^k (1 - \rho)^{m^2 - k}$; otherwise, $P(k) = \langle \delta_{k, \sum_{\alpha} \sigma_{\alpha}} \rangle$, where the sum is taken over all sites within a given patch and the expectation may again be calculated by the method outlined above (i.e. by expanding the δ -function as a sum of products as in equation 7.113 and rewriting in terms of local cumulants L_i). The result is an approximation that takes into account the effect of local correlations. What Schulman and Seiden found, quite unexpectedly, is that if a *normalized entropy* $\langle \tilde{S} \rangle$ – specifically $\langle \tilde{S} \rangle \equiv \langle S \rangle / \langle S \rangle^{(0)}$, where $\langle S \rangle^{(0)}$ is the entropy of a completely random system of density ρ (i.e. given by equation 7.125 with $P(k) = \binom{m^2}{k} \rho^k (1 - \rho)^{m^2 - k}$) – is plotted as a function of time t , it remains approximately constant after an initial transient decrease. This is noteworthy since it remains roughly constant for a time during which the density decreases by a factor of ten. This same behavior is also seen in experimentally measured values. It is tempting to speculate that, after the initial transient phase is over, the temporal evolution induces a certain constant order – an order that is intrinsic to the rule itself – to be built up and is in fact measured by the normalized entropy [schul78].

[†]A similar plot for local density ρ_L would show a closer agreement at low temperature but would leave the transition temperature unchanged [schul78].

Chapter 8

Generalized Models

This chapter consists of a series of mostly self-contained sections discussing several generalized CA models: reversible CA, coupled-map lattices, quantum CA, reaction-diffusion models, immunologically motivated CA models, random Boolean networks, sandpile models (in the context of self-organized criticality), and structurally dynamic CA (in which the temporal evolution of the *value* of individual sites of a lattice are dynamically linked to an evolving lattice structure), and simple CA models of combat (that are increasingly finding their way into the military operations research community).

8.1 Reversible CA

One of the principal themes of this book is the use of CA in modeling real physical systems and dynamics. To this end, it is important to address the question of what fundamental properties of physical systems can be appropriately abstracted from nature and embodied within abstract CA constructs. As observed earlier, some properties such as *homogeneity* and *locality* are automatically built in on the generic level. Another such property, namely the *reversibility* of microscopic dynamics, which plays such a fundamental role in physics, has its analogue in CA dynamics as well.

We recall that reversible CA were first rather informally introduced in section 2.2. The present section attempts to place our current understanding of the general behavior of reversible CA systems on a firmer (and somewhat more formal) ground. All of the subjects that will be briefly touched upon in the following discussion – including the formal mathematical development of invertible and reversible maps, the basic issue of reversibility versus irreversibility in physics, reversible computation and the fundamental role of reversible CA in modeling physical systems – can be explored more fully in Bennett ([benn73], [benn82], [benn85]), Brillouin ([bril50]), Landauer ([land61], [land67], [land82], [land87], [land88]), Margolous ([marg84], [marg87]) and Toffoli ([toff77], [toff87], [toff90]).

8.1.1 *Invertibility versus Time-Reversal Invariance*

The basic laws of physics (at least on the classical level) are all *time-reversal invariant*, which means that the equations of motion, such as Newton's equation,

$$\frac{d\mathbf{p}}{dt} = -\nabla U(\mathbf{x}), \quad (8.1)$$

where $\mathbf{p}$ is the momentum of a particle, say, and $\mathbf{x}$ is its position, retain exactly the same form under a time reversal transformation $t \rightarrow t' = -t$ (provided that the related physical quantities themselves transform in a consistent fashion; i.e. $\mathbf{p} \rightarrow \mathbf{p}' = -\mathbf{p}$ and $\mathbf{x} \rightarrow \mathbf{x}' = \mathbf{x}$). Time reversal invariance implies that if an initial state S_0 has evolved under Newton's laws to a final state S_T at time T , then a possible evolution of that system is that the time-reversed final state S_T will evolve over a time-reversed path to the time-reversed initial state S_0 ; i.e. the initial configuration is recoverable through a backwards evolution according to a time-reversed but essentially unchanged rule. The action of time reversal may thus be imagined as taking a movie of the original motion and then playing it backwards. A system is said to be time-reversal invariant, or reversible, if the backwards motion is itself an allowed solution of the equations of motion.

In the context of CA systems, it turns out that there is a difference between rules that are invertible and rules that are time-reversal invariant. A global CA rule $\Phi: \Sigma \rightarrow \Sigma$, mapping a global state $\sigma \in \Sigma$ to some other global state $\sigma' \in \Sigma$, is said to be *invertible* if for all states $\sigma' \in \Sigma$ there exists exactly one predecessor state $\sigma \in \Sigma$ such that $\Phi(\sigma) = \sigma'$. The state transition graphs G for all such rules must therefore consist entirely of cycles.

A natural question to ask is whether, in going backwards in time, the set of predecessor states can themselves be obtained from (possibly some other) CA rule Φ' . It is certainly not a-priori obvious that if the global map defined by a local process is invertible, its inverse must also be defined by a local process. In 1972, Richardson [rich72] was in fact able to show that the inverse of an invertible CA rule is itself a CA rule. His proof unfortunately did not provide a scheme by which the inverse map could actually be constructed. A trivial example of unequal inverses are the elementary *shift-right* and *shift-left* rules, **R240** and **R170**, respectively.

As suggested above, time-reversal invariance is a stronger property than simple invertibility and means that the dynamics is not only invertible, but that the time-reversed evolution proceeds according to the *same rule* as well. We shall call all invertible CA rules that are also time-reversal invariant, *reversible rules*.[†]

An obvious, but extremely important, property of reversible CA is that all of the information contained in the initial state can be recovered at any time T merely by running the system backwards in time from the state S_T . Thus, just as there exist as many integrals of the motion as there are variables describing a given mechanical system, the dynamics of reversible CA systems results in as many constants (or

[†]It is regrettable that in the literature invertible and time-reversal invariant rules are often both generically labeled 'reversible'. In the present text we shall use different labels accordingly in order to avoid confusion.

integrals) of the motion as there are sites in the lattice.[†]

Pushing the analogy with mechanical systems a little bit further, it is also true that just as only a limited subset of the entire set of integrals of the motion – particularly *additive* quantities, like *energy* – are of any real dynamical significance in mechanical systems, so too, in reversible CA systems, some invariants are more important than others. Indeed, we will see below examples of CA systems where an additive invariant akin to an ‘energy’ generates the evolution much in the same way that a Hamiltonian generates the time evolution in mechanics.

8.1.2 Historical Overview

Invertibility, at least as it pertains to automata systems, really dates back to Moore’s introduction of the *garden-of-eden*[‡] concept [moore62] in 1962. Moore showed that, under certain conditions, if some configuration has more than one predecessor state then there exists a configuration that has none.[§] The converse was proven by Myhill in 1963 [myhill63].

Early systematic searches for elementary one-dimensional invertible CA rules turned up none for neighborhood sizes of 2 and 3 [yama70] and essentially one case (with eight trivial variants that may be obtained from it by reflection or complementation) out of a total of $2^{16} = 65,536$ possibilities for a neighborhood of size four [patt71]:[¶]

$$\begin{array}{llll}
 \underline{0000} \rightarrow \underline{0} & \underline{0100} \rightarrow \underline{1} & \underline{1000} \rightarrow \underline{0} & \underline{1100} \rightarrow \underline{1} \\
 \underline{0001} \rightarrow \underline{0} & \underline{0101} \rightarrow \underline{1} & \underline{1001} \rightarrow \underline{0} & \underline{1101} \rightarrow \underline{1} \\
 \underline{0010} \rightarrow \underline{1(a)} & \underline{0110} \rightarrow \underline{0(a)} & \underline{1010} \rightarrow \underline{0} & \underline{1110} \rightarrow \underline{1} \\
 \underline{0011} \rightarrow \underline{0} & \underline{0111} \rightarrow \underline{1} & \underline{1011} \rightarrow \underline{0} & \underline{1111} \rightarrow \underline{1}
 \end{array} \tag{8.2}$$

Amoroso and Patt [amoro72] observed that, as a subset of the set of all possible rules, the set of nontrivial reversible rules appeared to be exceedingly small.

[†]In the context of classical mechanical systems this is easy to show. Consider a configuration $C = C(\mathbf{q}, \mathbf{p})$ that is described by $2n$ coordinates $\mathbf{q} = (q_1, \dots, q_n)$ and $\mathbf{p} = (p_1, \dots, p_n)$: as C evolves in time, so do the coordinates $(\mathbf{q}, \mathbf{p})$. The general solution of the equations of motion – which can be expressed either as n 2^{nd} -order differential equations (Lagrange’s equations) or $2n$ 1^{st} order differential equations (Hamilton’s equations) – will therefore involve $2n$ arbitrary constants. Assuming the equations do not explicitly involve the time ‘ t ’, one of these constants can always be taken as an additive constant t_0 . Eliminating $t + t_0$ from the $2n$ functions $\mathbf{q} = \mathbf{q}(t + t_0, r_1, \dots, r_{2n-1})$ and $\mathbf{p} = \mathbf{p}(t + t_0, r_1, \dots, r_{2n-1})$, the $2n - 1$ constants $r_1, \dots, r_{2n-1}$ can then be formally expressed as functions of $\mathbf{q}$ and $\mathbf{p}$. As the configuration C evolves along its orbit, these functions $r_1, \dots, r_{2n-1}$ remain constant with values unique to the given orbit.

[‡]We recall that a *garden-of-eden* configuration is any state that has no predecessor state under the prescribed rule Φ .

[§]Technically, Moore proved that a CA is surjective if and only if the restriction of its global map to finite configurations is injective, where a finite configuration means that only finitely many sites of the lattice are non-quiescent.

[¶]The center site is underlined and the maps labeled (a) are the only ones for which the center site actually changes its value; see *Conserved Landscape Permutations* subsection below.

Sears [sears71] had also shown that the set of invertible CA actually constitutes a vanishingly small subset.

Amoroso and Patt [amoro72] had outlined a general procedure for deciding whether or not a given local map defines an invertible global map, but only for one dimensional systems. Although they had originally conjectured that their one-dimensional technique was extendible, in principle, to higher dimensions, it has recently been proven by Kari ([kari89], [kari90]) that, for dimensions $d \geq 2$, there in fact exists no effective procedure for deciding whether or not a CA (defined in terms of a local map) is invertible.[†] The invertibility of CA is thus, in general, undecidable. Given two rules, however, it is always possible, at least in principle, to decide whether they are inverses of one another.

On the issue of computation-universality, Burks [burks71] had conjectured in 1971 that backwards-deterministic CA cannot be computation-universal. Aladyev ([alad72], [alad73]) had apparently ‘proved’ (erroneously, as it turned out) that Burks’ conjecture was correct by showing that computation-universality required the existence of erasable configurations. Coupled with Amoroso and Patt’s earlier result that, except for one-dimensional systems, there was no practical method for even telling whether a CA was in fact invertible, these results did much to dispel any deep interest in reversible CA during the next few years. This all changed in 1976, with a seminal work by Toffoli. (We might mention here, parenthetically, that despite the 1973 appearance of another seminal work by Bennett addressing the issue of reversible computation, the connection to CA systems was not immediately clear).

Toffoli [toff77] managed to prove that an arbitrary d -dimensional CA can be embedded within a $(d+1)$ -dimensional reversible CA. An immediate corollary of this theorem, is that, given that there exists an *irreversible* d -dimensional computation-universal CA – of which, by that time, literally scores had been found – there exists a *reversible* computation-universal CA.

8.1.3 A Sampling of Synthesis Techniques

An important issue concerning reversible CA is their construction. In particular, we are interested in knowing if there is some systematic method by which reversible CA rules can be constructed from scratch. On the one hand – if the desire is to randomly choose a reversible rule out of the set of all possible rules, the outlook for success is very dim. Amoroso and Patt [amoro72], for example, had observed that, within the space of all possible rules, the set of nontrivial reversible rules appeared to be exceedingly small. Sears [sears71] had also shown that the set of invertible CA actually constitutes a vanishingly small subset. On the other hand, if the desire is to simply define some representative samples of reversible rules (or some set of rules that may also possess some additional special features), a number

[†]It had been shown earlier, by Golze [Golze76], that *surjectivity* is, in general, undecidable for CA of dimensionality greater than one – recall that a map $f : X \rightarrow Y$ is surjective if for each $y \in Y$ there exists at least one $x \in X$ such that $f(x)=y$.

of simple synthesis techniques do exist. Margolus [marg88] and Toffoli ([toff80], [toff87]) provide more details.

Before reviewing some of the more common approaches to constructing reversible CA from scratch, it is first of all important to understand why we should expect any difficulty at all in casually defining them. The difficulty stems mainly from the different cardinalities of the site value set and the set of $\mathcal{N}$ -tuples (where $\mathcal{N}$ is the neighborhood size) defining the rule table. That is to say, since a general CA map ϕ maps $\mathcal{Z}_k^{\mathcal{N}} \rightarrow \mathcal{Z}_k$, an obvious but important consequence is that (except for the case when $\mathcal{N} = 1$; see below) in no case is the complete set of neighborhood site values at time ' t ' uniquely determined by a given site value at time ' $t+1$ ', even if the global rule induced by ϕ is itself reversible.

The only way to make the global rule reversible is to make certain that the complete information about any given site that is stored by all neighbors of that site is sufficient to reconstruct that site's old value. Note that only a very careful 'site-value-conspiracy' can achieve this since the information necessary for reconstruction potentially consists of values stored at some sites whose own neighbors are not neighbors of any of the other sites. Having said that, however, we now proceed to show how a number of useful synthesis techniques can in fact be defined as generalizations of the dynamics of the trivial case (we follow Toffoli [toff77]).

A trivial reversible CA consists of a collection of completely isolated systems; each site contains only itself in its neighborhood. Since $\mathcal{N} = 1$, the rule table and site value sets have the same cardinality. In particular, if the function $\phi : \mathcal{Z}_k \rightarrow \mathcal{Z}_k$ is invertible (i.e. if ϕ serves merely to *permute* the elements of the set $\mathcal{Z}_k$) then the global CA system is itself reversible. More formally, writing $\phi = \pi \in \prod_k$, where $\prod_k$ is the set of all possible permutations of set $\mathcal{Z}_k$, we can describe the dynamics by the equation

$$\sigma_i(t+1) = \pi_i(t)\sigma_i(t), \quad (8.3)$$

where $\sigma_i \in \mathcal{Z}_k$, and where we have generalized the permutation function π to be a more general function of site and time; in the trivial case, of course, π is constant for all sites ' i ' and times ' t '.

As it stands, of course, the dynamical system defined by equation 8.3, is reversible+but is clearly not a CA, since the system is, in general, neither space nor time invariant. We can restore this invariance, however, by choosing $\pi_i(t)$ in such a manner that its dependence on ' i ' and ' t ' is only an indirect one – specifically, so that it depends only on the particular state of the neighborhood (or landscape) of site ' i ' (excluding ' i ' itself) at time ' t '.

The resulting system is again a CA, but reversibility is assured of being kept intact only if we can find a bookkeeping mechanism for keeping track of which permutations are used at what sites. That is to say, if some rule ψ required the use of permutation $\pi_i(t)$ for the landscape at site ' i ' and time ' t ' (let's call it $L_i(t)$), then there must be a complementary rule ψ' that, for going backwards in time, requires

[†]The inverse system is given immediately by $\sigma_i(t) = (\pi_i(t))^{-1}\sigma_i(t+1)$, where we are assured of the existence of the inverse permutation π^{-1} by the fact that all permutations have inverses.

the use of the inverse permutation $(\pi_i(t))^{-1}$ at the landscape $L_i(t+1)$. Below we describe three different methods of achieving this last condition: (1) *Conserved Landscape Permutations* (or *Guarded Context Rules*), (2) the *Fredkin-Reversible Construction* (or **Second-Order** Technique), and (3) *Partitioning CA*.

8.1.3.1 *Conserved Landscape Permutations*

Consider Patt's neighborhood size four reversible rule defined by equation 8.2. Note that this rule stipulates that the value of the center site remains unchanged except for two cases: $0010 \rightarrow 1$ and $0110 \rightarrow 0$ (the underline labels the center site); i.e. the center site flips its value only if it is surrounded by the *landscape* $0 \cdot 10$. Moreover, if the value of the center site does change within context of this one landscape, the value flip *conserves the number* of such landscapes. It is in fact easy to see that the inverse local map for this rule is equal to the forward map. Note that despite being rather trivial example, in that most of the sites of the lattice are prohibited from ever changing their values, this need not be true in general. Separated sites can be effectively coupled by using a number of different and overlapping conserved landscapes.

Toffoli [toff75] showed that it is possible to realize such conserved landscape permutations in CA systems of arbitrary dimensionality and site value space size $|Z_k| = k$. In each case, as in the above example, the method defines the inverse along with the forward map.

8.1.3.2 *The Fredkin 'Second-Order' Construction*

We recall, from our earlier discussion of the Fredkin construction in section 3.1.4., that an arbitrary CA evolution that is **first-order** in time - $\sigma_i(t+1) = \phi[\sigma_j(t) \in \mathcal{N}_i]$, where $\mathcal{N}_i$ is the neighborhood around site ' i ' - can be converted into an invertible CA evolution that is **second-order** in time by subtracting the value of the center site at time ' $t-1$ ':

$$\sigma_i(t+1) = \phi[\sigma_j(t) \in \mathcal{N}_i] \ominus_k \sigma_i(t-1), \quad (8.4)$$

where ' $\ominus_k$ ' is subtraction *modulo-k* and $\sigma_i \in Z_k$.

Since equation 8.4 can be trivially solved for $\sigma_i(t-1) (= \phi[\sigma_j(t) \in \mathcal{N}_i] \ominus_k \sigma_i(t+1))$, we see that any pair of *consecutive* configurations *uniquely* specifies the backwards trajectory of the system. Moreover, this statement holds true for arbitrary (and, in particular, irreversible) functions ϕ . An important consequence of this, first pointed out by Fredkin [vich84a], is that a numerical roundoff in digital computers need not necessarily result in a loss of information. In particular, if the computation is of the form given by equation 8.4, where ϕ involves some roundoff error, the resulting dynamics will nonetheless be reversible and no information will be lost throughout the computation.[‡]

[‡] As a simple example of this, consider the real system $x_{t+1} = \mathcal{R}[x_t^3] - x_{t-1}$, where $\mathcal{R}[x_t^3]$ represents a roundoff of the expression x_t^3 to the nearest integer. Then it is easy to show that **from** the third and fourth iterates $x_3 = 25.3$ and $24 = 16191$, for example, the initial seeds $x_0 = 1$ and $x_1 = 1.7$

Note that the fact that the system is second-order in time does not mean the system cannot be recast into the more familiar first-order form. If we replace the original k -valued site variables σ_i with k^2 values of the pairs $(\sigma_i(t), \sigma_i(t-1))$, for example, where the pair $\hat{\sigma}_i(t) \equiv (\sigma_i(t), \sigma_i(t-1))$ can be numbered in any convenient manner, the rule defined in equation 8.4 can be rewritten as

$$\hat{\sigma}_i(t+1) = \hat{\phi} \left[\hat{\sigma}_j(t) \in \hat{\mathcal{N}}_i \right], \quad (8.5)$$

where $\hat{\phi}$ is an appropriate transition rule for the new site variables, $\hat{\phi}$. Thus, provided that the number of original states at a site is squared, it is possible to associate with every CA another reversible CA.

Many second-order reversible rules of the above form allow a pseudo-Hamiltonian prescription. The evolution of such systems may then be defined as any configurational change that conserves an ‘energy function’. We discuss this ‘Hamiltonian’ formulation a bit later in this section.

Margolus [marg84] points out that second-order reversible CA may also be constructed by using operations other than the subtraction *modulo-k* we used in our example. The actual operation could in fact be a function of the neighbor’s values at time ‘ t ’. In the most general case, the neighborhood at time ‘ t ’ can be used to choose a permutation on the set of allowed site values. The permutation is then applied to the site value at time ‘ $t-1$ ’ to obtain its next state.

8.1.3.3 Partitioning CA

Let us partition an arbitrary lattice $\mathcal{L}$ into equal sized finite sets P . We also introduce a new kind of local function, $f: P \rightarrow P$, that maps the entire contents of a given set $p \in \mathcal{P}$ at time ‘ t ’ to another state of the same set of sites at time ‘ $t+1$ ’. We observe that if f is invertible, then the corresponding global map F is invertible. The function f clearly allows an informational exchange among all sites of a given set of the partition but disallows communication between sites contained in different sets (i.e. partition walls act as information barriers). To allow information to spread throughout the lattice, we first choose another partition, P' , such that its set elements ‘overlap’ those of the original partition P , and another function f' that is of the same kind as f but acts on sets of $\mathcal{P}'$, and then keep alternating between applications of the global maps F and F' (acting on partitions P and P' , respectively) on successive iteration steps. Such a system, first introduced by Margolus in his thesis [marg88], in which global invertibility follows immediately from the invertibility of the local maps f and f' and in which information can be transmitted over arbitrary distances through successive applications of f and f' to overlapping partitions, is called a Partitioning CA. Figure 8.1 shows a two-dimensional example where the partitions are given by overlapping (2×2) blocks of sites (shown as square regions bounded by thick and thin lines).

We recall from the previous section that a second-order Fredkin-reversible rule can always be redefined as a conventional first-order one, but only at a cost of

can be recovered. A discussion of reversible computation appears in section 6.4).

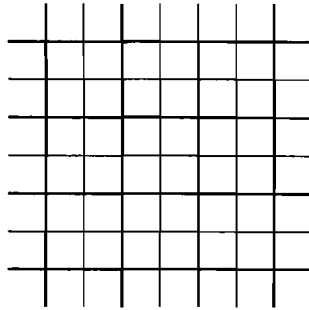


Fig. 8.1 (2×2) -block partitions of a two-dimensional lattice: $\mathcal{P}$ (enclosed by *thick* lines) and $\mathcal{P}'$ (enclosed by *thin* lines).

squaring the size of the state-space. A partitioning CA, for which both spatial and temporal uniformity appears to have been lost, can similarly be recast in a more familiar form, but only if (a) the state space is increased from k to p^k where $p = |\mathcal{P}|$ is the size of the partition sets, (b) two iteration steps are combined into one ‘super-time’ step, and (c) the ‘super-global’ map $\mathcal{F} = \mathbf{F}\mathbf{F}'$ is the composition of global maps F and F' .

An example of a 2-state partitioning CA rule mapping (2×2) blocks to (2×2) blocks is shown in figure 8.2. The rule is rotationally symmetric, so that only one instance of the mapping for a block with a given number of $\sigma = 1$ sites need be given to completely define the rule. The rule is trivially reversible since each initial state is mapped to a unique final state. Observe also that the number of 1’s (shown as solid circles in the figure) and 0’s (shown as clear squares) is conserved, but that this simple conservation law is *not* a consequence of reversibility. Indeed, we could have just as easily defined a rule that conserved the number of 1’s and 0’s as this one but which was not reversible. (We mention here also that, despite its simple appearance, this rule happens to define a universal CA. We will have a chance to discuss reversible computation later on in this section.)

8.1.4 Elementary Reversible CA

Takesue, in a series of papers ([takes87], [takes89], [takes90a], [takes90b]), was the first to undertake a systematic analysis of the ergodic and thermodynamic properties of $r = 1$ one-dimensional reversible CA; he called such systems elementary reversible cellular automata (ERCA). Although much of the discussion below is applicable to more general d -dimensional CA, the focus is mainly on the behavior of ERCA, following [takes89].

ERCA are, in the usual way, obtained from $r = 1$ one-dimensional CA by the Fredkin construction (see section 3.1.4.5). Introducing, for convenience, an ‘additional’ variable $\hat{\sigma}_i(t) \equiv \sigma_i(t-1)$, the evolution of a size N system is determined

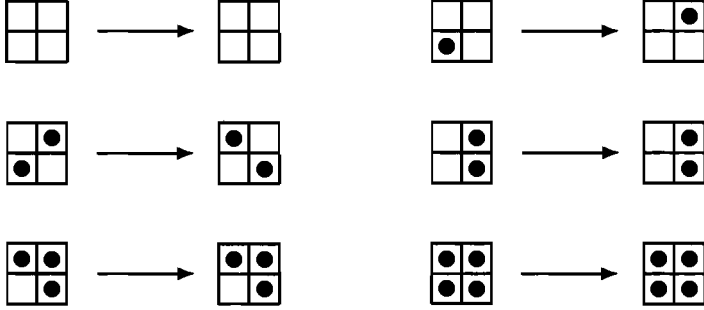


Fig. 8.2 An example of a Partitioning CA reversible rule, f , mapping (2×2) -blocks of two-valued states to (2×2) -blocks: $f : (2 \times 2) \rightarrow (2 \times 2)$. Note that this rule conserves the total number of 1's (indicated by a solid circle) and 0's (indicated by an empty square). The system that evolves under this rule is in fact a universal CA (see Billiard Ball Model, later in this section).

by

$$\begin{cases} \sigma_i(t+1) = \phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)) \oplus_2 \hat{\sigma}_i(t), \\ \hat{\sigma}_i(t+1) = \sigma_i(t), \end{cases} \quad (8.6)$$

where ϕ is an arbitrary $r = 1$ CA rule and $\oplus_2$ is addition modulo two. Observe that the time-reversed evolution is obtained by a simple exchange of the σ and $\hat{\sigma}$ variables:

$$\begin{cases} \sigma_i(t-1) = \hat{\sigma}_i(t), \\ \hat{\sigma}_i(t-1) = \phi(\hat{\sigma}_{i-1}(t), \hat{\sigma}_i(t), \hat{\sigma}_{i+1}(t)) \oplus_2 \sigma_i(t), \end{cases} \quad (8.7)$$

so that ERCA are both reversible and time-reversal invariant.

It is obvious that there are as many ERCA rules as there are possible elementary CA rules. *Reflection*[†] and Boolean *conjugation*[‡] symmetries, however, may be used to reduce the 256 possible ERCA rules into 88 equivalence classes.

We will follow our earlier convention (see section 2.2) of labeling such rules with the code $C[\phi]_R$, where $C[\phi]$ is the standard Wolfram-code for rule ϕ (see equation 2.40). When discussing a generic ERCA we will refer to the rule as ϕ_R to distinguish it from its (generally) irreversible counterpart ϕ .

Defining the Boolean N-vectors $\sigma(t) = (\sigma_1(t), \dots, \sigma_N(t))$ and $\hat{\sigma}(t) = (\hat{\sigma}_1(t), \dots, \hat{\sigma}_N(t))$, the phase space for ERCA is the set of all 4^N possible configurations

$$\Omega_N = \{(\sigma, \hat{\sigma})\} \cong \{0, 1\}^{2N}. \quad (8.8)$$

[†] $\psi(\alpha, \beta, \gamma) = \phi(\gamma, \beta, \alpha)$ is the reflection of rule ϕ .

[‡] $\varphi(\alpha, \beta, \gamma) = \phi(1 - \alpha, 1 - \beta, 1 - \gamma)$ is the Boolean conjugate of ϕ .

The principles of statistical mechanics can be applied to a dynamical system provided that it obeys *Louville's Theorem* (that is, it preserves volumes in phase space) and that its energy remains constant. The first requirement is easy: since all reversible rules ϕ_R define bijective mappings of $\Omega_N \rightarrow \Omega_N$, the phase space volume is trivially preserved in all cases. Reversibility also implies that any size N system must have N dynamical invariants (since the evolution preserves the 'memory' of the initial configuration for all times). Of particular interest, however, are rules allowing the existence of additive invariants -- i.e. those which can be written as a sum over all sites i . By exploiting an analogy with the additive canonical invariants of statistical mechanics, we can at least formally begin to describe the behavior of such rules in purely thermodynamic terms.

As we shall see in the next section, some rules do indeed possess 'energy-like' conserved quantities, although it will turn out that (unlike for more familiar Hamiltonian systems), these invariants do *not* completely govern the evolution of ERCA systems. Their existence nonetheless permits the calculation of standard thermodynamic quantities (such as partition functions).

8.1.5 Additive Invariants

Additive invariants were first studied by Pomeau [pomeau84] and Goles and Vichniac [goles86]. Although, as we shall see below, there are some techniques that can be used to extract a few invariants from particular systems, no general methodology currently exists. A fundamental obstacle appears to be that there is no purely discrete analogue of Noether's Theorem.

8.1.5.1 Noether's Theorem

We recall, from elementary classical mechanics,[†] that symmetry properties of the Lagrangian (or Hamiltonian) generally imply the existence of conserved quantities. If the Lagrangian is invariant under time displacement, for example, then the energy is conserved; similarly, translation invariance implies momentum conservation. More generally, Noether's Theorem states that for each continuous N -dimensional group of transformations that commutes with the dynamics, there exist N conserved quantities.

While it is an easy exercise to prove this theorem for continuous systems, however, its purely discrete analogue, if it exists, has been heretofore unknown: there currently exists no systematic procedure for obtaining conserved quantities from the inherent symmetries of a purely discrete CA-system. It is therefore typically a difficult task to find the conserved quantities of a given system, with most systems generally requiring some special methods or 'tricks'. Indeed, just as for reversibility itself, it is usually much easier to directly synthesize CA systems possessing desired invariants than it is to extract them from a given system [toff90a]. There are a few classes of rules, however, for which it is relatively easy to extract conserved

[†]See, for example, Herbert Goldstein's *Classical Mechanics*, 2nd-edition, Addison-Wesley, 1980

quantities: the class of *Fredkin*-reversible rules, for example.

8.1.5.2 Invariants of Fredkin-Reversible Rules

One simple method for finding additive invariants was suggested by Margolus [marg 87b]. The basic idea, which is quite general and applies to all *Fredkin*-reversible rules of the form $\sigma_i(t+1) = \phi(\sigma_j(t) \in \mathcal{N}_i) \oplus_2 \sigma_i(t-1)$, where $\mathcal{N}_i$ is the set of all neighboring sites of site ' i ', is to simply find some function $\psi = \psi(\sigma_j \in \mathcal{N}_i)$ such that the local product $(1-\phi)\psi$ is identically equal to zero; i.e. choose some ψ that is equal to zero precisely when $(1-\phi)$ is nonzero, and vice-versa. An appropriate 'massage' of the expression $(1-\phi)\psi = 0$ is then likely to reveal an invariant. The following example illustrates the method (we follow Hartman and Tamayo [hart90]).

EXAMPLE: Consider the *Fredkin*-reversible form of the OR rule; i.e. the system

$$\sigma_i(t+1) = (\sigma_{i-1}(t) \text{ OR } \sigma_i(t) \text{ OR } \sigma_{i+1}(t)) \oplus_2 \sigma_i(t-1).$$

Since $1-\phi = 1 - (\sigma_{i-1}(t) \text{ OR } \sigma_i(t) \text{ OR } \sigma_{i+1}(t))$ equals '1' only for $\sigma_{i-1}(t) = \sigma_i(t) = \sigma_{i+1}(t) = 0$, ψ can be any function that yields a '0' for the zero valued neighborhood. Following [hart90], we consider $\psi = (\sigma_{i-1}(t) \text{ XOR } \sigma_{i+1}(t))$.

To simplify the calculation, we first convert to spin variables $\mathbf{a} \rightarrow s = 2\sigma - 1$. Writing $\phi = \sigma_i(t+1) \oplus_2 \sigma_i(t-1) = \frac{1}{2}(1 - s_i(t+1)s_i(t-1))$ and ψ in terms of these spin variables, the (identically vanishing) local product $(1-\phi)\psi$ is given by

$$\frac{1}{4}(1 + s_i(t+1)s_i(t-1))(1 - s_{i+1}(t)s_{i-1}(t)) = 0.$$

Dropping the constant $\frac{1}{4}$, multiplying by $s_i(t+1)s_{i-1}(t)$, and using the fact that the square of all spin variables is equal to one (for example, $s_i(t)s_i(t) = +1$), this equation simplifies to

$$s_i(t+1)s_{i-1}(t) - s_i(t+1)s_{i+1}(t) = -s_{i-1}(t)s_i(t-1) + s_i(t-1)s_{i+1}(t).$$

Summing over all sites ' i ' gives

$$\sum_i \{s_i(t+1)s_{i-1}(t) - s_i(t+1)s_{i+1}(t)\} = - \sum_i \{s_{i-1}(t)s_i(t-1) + s_i(t-1)s_{i+1}(t)\}.$$

We now observe that $\sum_i s_i(t+1)s_{i-1}(t) = \sum_i s_i(t)s_{i+1}(t+1)$ and $\sum_i s_{i+1}(t)s_i(t+1) = \sum_i s_i(t)s_{i-1}(t+1)$ because, in each case, the sum is over exactly the same set of *links*. Substitution of these two expressions into the above equation shows that the quantity $\Phi = \sum_i s_i(t)(s_{i+1}(t+1) - s_{i-1}(t+1))$ is invariant. In terms of the original σ variables, Φ is given by

$$\Phi = 2 \sum_i [2\sigma_i(t-1) - 1] [\sigma_{i+1}(t) - \sigma_{i-1}(t)].$$

Pomeau considered rules of the form given in equation 8.6 with $\phi_i \equiv \phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t))$ defined by

$$\phi_i = \begin{cases} 1 & \text{if } \sigma_{i-1}(t) + \sigma_i(t) + \sigma_{i+1}(t) = q, \\ 0 & \text{else,} \end{cases} \quad (8.9)$$

where q is some constant.[‡] He found that the quantity

$$\Phi(t) = \sum_i \sum_{j=-1}^{+1} \sigma_i(t) \hat{\sigma}_{i+j}(t) - \sum_i (\sigma_i(t) + \hat{\sigma}_i(t)) q \quad (8.10)$$

is invariant under ϕ . To show this, we first write out $\Phi(t+1)$ using equation 8.6:

$$\begin{aligned} \Phi(t+1) &= \sum_i \sum_{j=-1}^{+1} (\phi_i + \hat{\sigma}_i(t)) \sigma_{i+j}(t) - \sum_i (\phi_i + \hat{\sigma}_i(t) + \sigma_i(t)) q, \\ &= \sum_i (\phi_i + \hat{\sigma}_i(t)) \left(\sum_{j=-1}^{+1} \sigma_{i+j}(t) - q \right) - \sum_i \sigma_i(t) q, \end{aligned} \quad (8.11)$$

Since $\phi_i \cdot \left(\sum_j \sigma_{i+j}(t) - q \right)$ is equal to zero (which follows trivially from the definition of ϕ in equation 8.9), $\Phi(t+1)$ is given by

$$\Phi(t+1) = \sum_i \sum_{j=-1}^{+1} \hat{\sigma}_i(t) \sigma_{i+j}(t) - \sum_i (\hat{\sigma}_i(t) + \sigma_i(t)) q. \quad (8.12)$$

Using the symmetry of the neighborhood structure – i.e. site ‘ i ’ is a neighbor of site ‘ j ’ if and only if site ‘ j ’ is a neighbor of site ‘ i ’ – we may exchange σ and $\hat{\sigma}$ in the first summation. Comparing the result to equation 8.10 we see that $\Phi(t+1) = \Phi(t)$. **(QED)**

It is instructive to observe that in terms of conventional spin variables $s_i = 2\sigma_i - 1$ ($s_i = \pm 1$), and written in slightly more general form, Φ takes on the form of the familiar Ising energy

$$\Phi = \frac{1}{4} \sum_{i,j} J_{ij} s_i^t s_j^{t-1} + \sum_i h_i (s_i^t + s_i^{t-1}), \quad (8.13)$$

where $J_{ij} = 1$ if and only if the sites ‘ i ’ and ‘ j ’ are nearest neighbors and $h_i = \frac{1}{4} \sum_j J_{ij} - q$ acts as an external local field. This expression differs from the actual Ising energy only in that it involves spin values at two successive times.

Φ takes on its simplest form for the Q2R CA (see section 3.4), which, we recall, lives on a two dimensional Euclidean lattice and is defined by the rule ϕ_i with $q = 2$.

[‡]Pomeau actually considered the more general form $\phi(\sigma_j \in \{\mathcal{N}_i\}) = \delta(\sum_{j \in \mathcal{N}_i} \sigma_j, q_i)$, where $\mathcal{N}_i$ is the set of all sites in the neighborhood of site ‘ i ’ and $\delta(n, m)$ is the Kronecker delta. This form allows the neighborhood $\mathcal{N}(i)$ to be defined for lattices of arbitrary dimensionality.

In this case, Φ is equal to

$$\Phi = \frac{1}{4} \sum_{i,j} s_i^t s_j^{t-1} \quad (8.14)$$

In both of these cases, Φ represents the energy of two *noninteracting* Ising **spin** systems, one system having spins s over one sublattice and the other spins $\hat{s}$ over the other sublattice. Indeed, the Q2R CA actually provides an efficient microcanonical algorithm for performing parallel simulation of the Ising model (see discussion in section 7.1.5).

Goles and Vichniac extended Pomeau's invariant to two additional cases: (1) where $\phi_i = 1$ if and only if $(\sum_i = q_1 \text{ OR } \sum_i = q_2 \text{ OR } \dots \text{ OR } \sum_i = q_s)$ (where the q_i belong to the same congruence class *modulo* some integer p and $\sum_i \equiv \sum_i \{\sigma_{i-1} + \sigma_i + \sigma_{i+1}\}$), and (2) where Fredkin's construction in equation 8.6 is generalized to systems with ' T ' memory steps - i.e. to cases where $\sigma_i(t) = 1 - \sigma_i(t - T)$ if $\phi_i = 1$ and $\phi_i = 1$ if and only if $\sum_{j=1}^{T-1} (\sigma_{i-1}(t-j) + \sigma_i(t-j) + \sigma_{i+1}(t-j)) = q$.

Takesue [takes87] considers the general class of additive invariants. $\Phi = \Phi(\mathbf{x})$ of the form

$$\Phi(\mathbf{x}) = \sum_i F_{\phi_R}(\sigma_i, \sigma_{i+1}, \hat{\sigma}_i, \hat{\sigma}_{i+1}), \quad (8.15)$$

where $\mathbf{x} = \langle \sigma, \hat{\sigma} \rangle$ is a point in the phase space Ω_N , and F_{ϕ_R} is some appropriately chosen function for an ERCA rule ϕ_R . The choice to have F_{ϕ_R} depend only on two adjacent sites is an arbitrary one, and is made purely for convenience. With this particular form, for example, we can compute the partition function Z of the system, where

$$Z = \sum_{\sigma_1, \hat{\sigma}_1} \sum_{\sigma_2, \hat{\sigma}_2} \dots \sum_{\sigma_N, \hat{\sigma}_N} \prod_i \exp(-\beta E_{i,i+1}), \quad (8.16)$$

and where the 'energy' $E_{i,i+1}(t) = F_{\phi_R}(\sigma_i(t), \sigma_{i+1}(t), \hat{\sigma}_i(t), \hat{\sigma}_{i+1}(t))$ has the natural interpretation of being the energy of each bond $(i, i+1)$ of the lattice. Since this expression for Z is of the same form as for the one-dimensional Ising model, it may be conveniently evaluated using any of the standard methods used in statistical mechanics (the transfer matrix method, for example).

Arbitrarily setting the zero value of energy by $F(0,0,0,0) = 0$, and exploiting the fact that Φ is obtained by a *sum* over sites[†], Takesue is able to explicitly compute all of the additive invariants of the form shown in equation 8.15 for all 47 of 88 representative ERCA rules that possess such invariants [takes89]. He finds, in particular, that 22_R , 36_R , 73_R , and 90_R are the only ERCA rules that have an invariant of the Pomeau variety (equation 8.10). A sampling of some other types of invariants found in other rules is provided in table 8.1 (from [takes89]).

We make several observations:

[†]Which implies that $\Phi(\mathbf{x})$ is determined solely by the set of numbers representing the frequencies of two-site blocks appearing in the phase space point $\mathbf{x}$.

ERCA Rule (ϕ_R)	Additive Invariants $\Phi = \sum F_{\phi_R}$ where $F_{\phi_R} = F_{\phi_R}(\alpha, \beta, \hat{\alpha}, \hat{\beta})$	Other ϕ_R with Φ_i
3_R	$\alpha\hat{\alpha} + \beta\hat{\beta}$	$33_R, 35_R$
	$\alpha\beta\hat{\alpha} + \alpha\hat{\alpha}\beta$	$0_R, 1_R, 2_R$
	$\alpha\beta\hat{\alpha}\hat{\beta}$	$0_R, 1_R, 2_R, 4_R$ $5_R, 6_R, 7_R, 18_R,$ $19_R, 22_R, 23_R, 33_R,$ $35_R, 36_R - 39_R,$ $50_R, 51_R, 54_R, 55_R$
6_R		
	$\alpha + \beta + \hat{\alpha} + \hat{\beta} - (\alpha\hat{\alpha} + \beta\hat{\beta}) - 2\alpha\hat{\beta} - 2\beta\hat{\alpha}$	22_R
	$\alpha\beta\hat{\alpha}\hat{\beta}$	(see rule 3_R)
11_R	$(\alpha\hat{\alpha} + \beta\hat{\beta}) - 2\alpha\beta\hat{\alpha} - 2\alpha\hat{\alpha}\beta + 2\alpha\beta\hat{\alpha}\hat{\beta}$	$9_R, 10_R, 129_R, 139_R$
46_R	$\alpha + \beta - 4\alpha\beta\hat{\beta} - 4\beta\hat{\alpha}\beta + 4\alpha\beta\hat{\alpha}\hat{\beta}$	—
77_R	$\alpha\hat{\beta} - \beta\hat{\alpha} + 2\alpha\beta\hat{\alpha} - 2\alpha\beta\hat{\beta} - 2\alpha\hat{\alpha}\beta + 2\beta\hat{\alpha}\beta$	—
126_R	$\alpha\hat{\alpha} + \beta\hat{\beta} + \alpha\hat{\beta} + \beta\hat{\alpha} - 2\alpha\beta\hat{\alpha} - 2\alpha\beta\hat{\beta}$ $- 2\alpha\hat{\alpha}\beta - 2\beta\hat{\alpha}\beta + 4\alpha\beta\hat{\alpha}\hat{\beta}$	127_R
	$\alpha\hat{\beta} - \beta\hat{\alpha}$	$90_R, 91_R, 94_R, 95_R$ $123_R, 126_R, 127_R, 219_R$ $223_R, 255_R$
219_R	$\alpha + \beta + \hat{\alpha} + \hat{\beta} - 2\alpha\beta - 2\hat{\alpha}\hat{\beta} - (\alpha\hat{\alpha} + \beta\hat{\beta})$ $- \alpha\hat{\beta} - \beta\hat{\alpha} + 2\alpha\beta\hat{\alpha} + 2\alpha\beta\hat{\beta} + 2\alpha\hat{\alpha}\beta$ $+ 2\beta\hat{\alpha}\beta - 4\alpha\beta\hat{\alpha}\hat{\beta}$	...
	$\alpha\hat{\beta} - \beta\hat{\alpha}$	(see rule 126_R)

Table 8.1 A listing of the additive invariants for a few selected ERCA rules [takes89]. The middle column gives the form for $F_{\phi_R} = F_{\phi_R}(\alpha, \beta, \hat{\alpha}, \hat{\beta})$ such that $\Phi = \sum_i F_{\phi_R}$; the last column gives rules that share a given invariant with the rule listed in the first column.

(1) A given ERCA may possess more than one invariant. Conversely, a given invariant may also be shared by more than one ERCA.

(2) The fact that a substantial fraction of the set of ERCA do not have invariants of the form defined in equation 8.15 is not really surprising, as there are many possible alternative forms. One could, for example, consider energy functions F that are functions of values of more than two adjacent sites. For example, Takesue [takes89] points out that a number of rules also possess invariants of the form

$$\begin{cases} \Phi' &= \Phi(t) + \Phi(t+1), \quad \text{and} \\ \Phi'' &= |\Phi(t+1) - \Phi(t)|, \end{cases} \quad (8.17)$$

where $\Phi(t) = \sum_i \{(\sigma_i(t) - \hat{\sigma}_{i+1}(t))^2 + (\hat{\sigma}_i(t) - \sigma_{i+1}(t))^2\}$ and has period two for these rules. Φ' and Φ'' both turn out to be sums of functions of three adjacent sites.

(3) The same equations that are used in constructing the energy function lead to a continuity equation as well. That is, an equation describing the temporal variation of bond energy can be written as the difference between incoming and outgoing flows:

$$E_{i,i+1}(t+1) = E_{i,i+1}(t) + J_i(t) - J_{i+1}(t), \quad (8.18)$$

where $J_i(t)$ is the flow at site ' i ' at time ' t '.[†]

8.1.5.3 Local Conservation Laws

As we have already observed in section 3.1.4.5, CA evolution may conserve locally defined quantities. Moreover, local conservation laws often cause walls to appear that prohibit sites sitting on opposite sides of those walls from exchanging any information. Figure 8.3, which shows the space-time plots of ERCA 18_R, 73_R, and 129_R, provides three such examples.

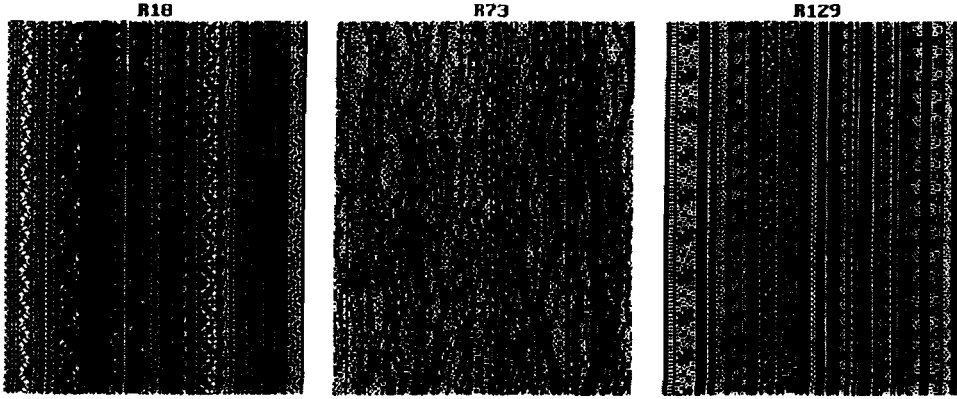


Fig. 8.3. Space-time plots of ERCA 18_R, 73_R, and 129_R.

In the case of ERCA rule 73_R, for example, it is easy to see that once the 3-block

$$\begin{pmatrix} \hat{\sigma}_{i-1} & \hat{\sigma}_i & \hat{\sigma}_{i+1} \\ \sigma_{i-1} & \sigma_i & \sigma_{i+1} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad (8.19)$$

[†]Takesue [takes89a] shows that an arbitrary energy function F of the form given in equation 8.15 can be written in terms of 12 independent parameters b_i , $i = 1, \dots, 12$:

$$\begin{aligned} F(\alpha, \beta, \hat{\alpha}, \hat{\beta}) = & b_1(\alpha + \beta) + b_2(\hat{\alpha} + \hat{\beta}) + b_3\alpha\beta + b_4\hat{\alpha}\hat{\beta} + b_5(\alpha\hat{\alpha} + \beta\hat{\beta}) + b_6\alpha\hat{\beta} + b_7\beta\hat{\alpha} \\ & + b_8\alpha\beta\hat{\alpha} + b_9\alpha\beta\hat{\beta} + b_{10}\alpha\hat{\alpha}\hat{\beta} + b_{11}\beta\hat{\alpha}\hat{\beta} + b_{12}\alpha\hat{\beta}\hat{\alpha}\hat{\beta}. \end{aligned}$$

In terms of these parameters, the flow $J_i(t)$ can be expressed as follows:

$$\begin{aligned} J_i(t) &= J(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t), \hat{\sigma}_i(t)) \\ &= \frac{1}{4} \{ 2\phi_i(t)(1 - 2\hat{\sigma}_i(t))[2b_1 + b_3 + (2b_5 + b_8)\sigma_i(t) + (2b_6 + b_9)\sigma_{i+1}(t) \\ &\quad + (2b_{10} + b_{12})\sigma_i(t)\sigma_{i+1}(t)] + 2(b_6 - b_7)(2\sigma_{i+1}(t)\hat{\sigma}_i(t) - \sigma_i(t) - \sigma_{i+1}(t)) \\ &\quad + (b_8 - b_{10})[2\sigma_i(t)\hat{\sigma}_i(t) + \sigma_{i+1}(t)(1 + 2\sigma_i(t))(1 - \hat{\sigma}_i(t))] \} + \text{constant}, \end{aligned}$$

where $\phi_i(t) = \phi(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t))$.

appears in the evolution, it remains fixed from that time forward. Conversely, if a particular 3-block is not in this local state, it will never evolve into this state. Thus, the quantity

$$\Phi = (1 - \sigma_{i-1})(1 - \hat{\sigma}_{i-1})\sigma_i\hat{\sigma}_i(1 - \sigma_{i+1})(1 - \hat{\sigma}_{i+1}) \quad (8.20)$$

is conserved for all sites ‘ i ’. Whenever rules allow such “walls” to appear, information is clearly prohibited from freely propagating throughout the lattice. In particular, a statistical mechanics cannot be realized even in principle. Table 8.2 (taken from [takes89]) lists a few examples of walls and the ERCA rules under which they evolve.

Wall	ERCA Rules
0	$0_R, 4_R, 12_R$
1	$0_R, 1_R, 2_R, 3_R, 18_R, 19_R, 33_R, 35_R, 50_R, 51_R$
00	$0_R, 4_R, 12_R, 36_R$
11	$0_R, 1_R, 2_R, 3_R, 4_R, 5_R, 6_R, 7_R, 18_R, 19_R, 22_R, 23_R, 33_R, 35_R, 36_R, 37_R, 38_R, 39_R, 50_R, 51_R, 54_R, 55_R$
10	$0_R, 1_R, 2_R, 3_R, 9_R, 10_R, 129_R, 131_R, 139_R$
01	$0_R, 1_R, 129_R$
010	$0_R, 1_R, 9_R, 73_R, 129_R$
101	$0_R, 1_R, 2_R, 3_R, 18_R, 19_R, 131_R, 147_R$
0110	$0_R, 1_R, 4_R, 5_R, 129_R, 133_R$
11 $\rightarrow$ *00*	$4_R, 36_R$
0 $\rightarrow$ *0* $\rightarrow$ *1*	51_R
00 $\rightarrow$ *01* $\rightarrow$ *10*	$51_R, 179_R$
00 $\rightarrow$ *10* $\rightarrow$ *01*	$51_R, 179_R$
0 $\rightarrow$ *0* $\rightarrow$ *1* $\rightarrow$ *1*	255_R
00 $\rightarrow$ *00* $\rightarrow$ *11* $\rightarrow$ *11*	$219_R, 223_R, 255_R$
01 $\rightarrow$ *01* $\rightarrow$ *10* $\rightarrow$ *10*	$126_R, 127_R, 255_R$

Table 8.2 Examples of walls and the ERCA rules under which they evolve; “*” designates an arbitrary site value. Table is from [takes89]

The situation is not much better for rules under which only a local conservation law exists (but no walls are able to form), since the propagation of “energy” is still prohibited. One can show that the flow corresponding to the bond energy for ERCA rule 46_R , for example, is identically equal to zero at all sites. Although no walls form under this rule, since the initial distribution of energy throughout the lattice is effectively fixed at time zero, no propagation can subsequently take place.

Takesue [takes89] has looked for local conservation laws holding true for all blocks $B \leq 6$ sites long. He finds that, for $B \leq 4$, 44 of the 88 ERCA equivalence rule classes possess a local conservation law. Observing that no additional rules supporting local conservation laws appear if site blocks of sizes 5 and 6 are examined, Takesue conjectures [takes89] (but does not prove) that there exists a threshold size

of block, determined by the interaction range, such that if a given ERCA rule does not possess a local conservation law for that block, it does not have *any* local conservation laws.

8.1.6 Thermodynamic Behavior

Takesue [takes87] defines the energy of an ERCA as a conserved quantity that is both additive and propagative. As we have seen above, the additivity requirement merely stipulates that the energy must be written as a sum (over all sites) of identical functions of local variables. The requirement that the energy must also be propagative is introduced to prevent the presence of local conservation laws. If rules with local conservation laws spawn information barriers, a statistical mechanical description of the system clearly cannot be realized in this case. ERCA that are candidate thermodynamic models therefore require the existence of additive conserved quantities with no local conservation laws. A total of seven such ERCA rules qualify.[†]

The seven ERCA rules that have one or more additive conserved quantities and no local conservation laws are listed in table 8.3, along with their ‘energy’ functions.

Rule (ϕ_R)	Associated ‘Energy’ Functions $F_{\phi_R}(\alpha, \beta, \hat{\alpha}, \hat{\beta})$
26_R	$(\alpha - \hat{\beta})^2 + (\hat{\alpha} - \beta)^2 (= F_1)$
90_R	$(\alpha - \hat{\beta})^2 + (\hat{\alpha} - \beta)^2 (= F_1),$ $\alpha\hat{\beta} - \hat{\alpha}\beta \text{ \{or\} } (\hat{\alpha} - \beta)^2 - (\alpha - \hat{\beta})^2 \text{ } (= F_2)$
$91_R, 123_R$	$1 + \alpha\hat{\alpha} + \beta\hat{\beta} - \{1 - 2(1 - \alpha)(1 - \hat{\beta})\}\{1 - 2(1 - \hat{\alpha})(1 - \beta)\} (= F_3),$ $\alpha\hat{\beta} - \hat{\alpha}\beta \text{ \{or\} } (\hat{\alpha} - \beta)^2 - (\alpha - \hat{\beta})^2 \text{ } (= F_2)$
77_R	$\alpha\hat{\beta}(1 - 2\hat{\alpha} - 2\beta) - \hat{\alpha}\beta(1 - 2\alpha - 2\hat{\beta}) (= F_4)$
$94_R, 95_R$	$\alpha\hat{\beta} - \hat{\alpha}\beta \text{ \{or\} } (\hat{\alpha} - \beta)^2 - (\alpha - \hat{\beta})^2 \text{ } (= F_2)$

table 8.3 ‘Energy’ functions F_{ϕ_R} , evaluated for all ERCA rules ϕ_R that have additive invariant but no local conservation laws [takes87].

Notice that there are only four distinct energy functions, $F_1, \dots, F_4$. Moreover, a given rule may possess more than one energy function and, conversely, a given energy function may be invariant under more than one rule.

8.1.6.1 Realizability of the Canonical Distribution

Given a size N lattice (thought of now as a heat-bath), consider some subsystem of size n . An interesting question is whether the energy distribution of the subsystem, $P_n(E)$, is equal to the canonical distribution of a thermodynamic system in equilibrium. That is, we are interested in comparing the actual energy distribution

[†]They qualify at least so far as not having any local invariants on blocks of size $B \leq 6$ [takes89]. Takesue has also numerically verified that energies propagate indefinitely for these rules.

to the well-known canonical distribution

$$P_n(E) \propto \rho_n(E)e^{-\beta E}, \quad (8.21)$$

where $\rho(E)$ is the density of states (or the fraction of all states that have energy E in all possible states of the subsystem of size n), and β is the effective inverse temperature.

The density of states may be found directly by computing $\rho_n(E) = \mathcal{N}(E)/4^n$, where $\mathcal{N}(E)$ is the number of states with energy E .

8.2 Coupled-Map Lattices

A generic CA system, in which space, time and the local state space are all discretized, is actually but one example of an entire hierarchy of a larger class of spatially-extended dynamical systems. Perhaps the simplest conceptual generalization that can be made of CA is to take away the constraint that the local state variables σ must be purely discrete and allow them to be real-valued. Such systems, in which $\sigma \in R^n$ but space and time remain discrete, are called coupled-map lattices (CMLs), and were first studied by Kaneko [kaneko84] and Waller and Kapral [kapral84]. Kaneko has since studied the behavior of such systems extensively, and has compiled an impressive array of findings; we recommend that the interested reader consult any or all of his papers that are listed in the reference section. An excellent recent survey of the phenomenology of spatio-temporal chaos also appears in [crutch87].

As mentioned above, CMLs are simple generalizations of generic CA systems. Confining ourselves for the time being to one-dimension for simplicity, we begin with a one-dimensional lattice of real-valued variables $\sigma_i(t) \in R$ whose temporal evolution is given by

$$\sigma_i(t+1) = F(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)), \quad (8.22)$$

where $F : R^3 \rightarrow R$ is, for the moment, an arbitrary continuous function. Some early examples of CMLs used a simple diffusive coupling of the center site to its neighbors ([kaneko84], [kapral84]):

$$\sigma_i(t+1) = f(\sigma_i(t)) + D \{ \sigma_{i+1}(t) - 2\sigma_i(t) + \sigma_{i-1}(t) \}, \quad (8.23)$$

where D is the “diffusion constant”. Since the second factor on the RHS of this equation represents the “average” of the value-flux moving into site i from neighboring sites, it is reasonable to restrict D to the range $[0, 1/2]$. Yamada and Fujisaka [yama83] showed, however, that this simple diffusive map can yield unbounded solutions for $D \in [0, 1/2]$. They instead considered the following system:

$$\sigma_i(t+1) = f(\sigma_i(t)) + D \{ f(\sigma_{i+1}(t)) - 2f(\sigma_i(t)) + f(\sigma_{i-1}(t)) \}, \quad (8.24)$$

which the reader is invited to show remains bounded for $D \in [0, 1/2]$ whenever $0 \leq \sigma_i(0) \leq 1, i = 1, 2, \dots, N$ and $0 \leq f(x) \leq 1$ for any $x \leq 1$.

More general models couple the action of a given function at the center site to other sites with another (possibly different) coupling dynamics and individual coupling constants. For example, one generic form is given by

$$\sigma_i(t+1) = F(\sigma_i(t)) + \epsilon_{-1}G(\sigma_{i-1}(t)) + \epsilon_0G(\sigma_i(t)) + \epsilon_{+1}G(\sigma_{i+1}(t)), \quad (8.25)$$

where now $F : R \rightarrow R$, $G : R \rightarrow R$ defines the coupling dynamics and $\vec{\epsilon} = (\epsilon_{-1}, \epsilon_0, \epsilon_{+1})$ is the *coupling kernel*. Table 8.4 shows the conventional nomenclature for some typical choices of values $\vec{\epsilon}$.

ϵ_{-1}	ϵ_0	ϵ_{+1}	Coupling Name
ϵ	ϵ	ϵ	Simple-Diffusive
ϵ	0	ϵ	Additive
$\epsilon/2$	$-\epsilon$	$\epsilon/2$	Laplacian
$1/3$	$-2/3$	$1/3$	Totalistic
$\pm\epsilon$	$\mp\epsilon$	0	Uni-Directional

Table 8.4 Some typical choices for the coupling kernel $\vec{\epsilon}$.

The function F is typically chosen to be one of the simple one-dimensional maps exhibiting chaos, such as the *logistic map* ($F(x) = \alpha x(1-x)$) or *circle map* ($F(x) = \omega + x + k \sin(2\pi x)$); for a discussion of the behavior of these and other maps see chapter 4. In the following, we will assume mostly that $G = F$. In the case where $F(x) = \alpha x(1-x)$, for example, the resulting CML system is effectively defined by two control parameters: the logistic map's own α and the global CML's coupling constant ϵ . Recalling the rich variety of period-doubling dynamics latent within the local map $f(x)$ itself, we may anticipate a similarly rich landscape of dynamical behavior in the CML. An obvious question, for example, is how the local period-doubling structure is altered by the local coupling.

8.2.1 Stability of Homogeneous Solutions

Let us begin by considering the stability of homogeneous solutions and/or initial-conditions; i.e. by considering the stability of a simple-diffusive CML when $\sigma_i(0) = \sigma^*$ for all sites ' i ', where σ^* is a fixed point of the local logistic map $F(\sigma) = \alpha\sigma(1-\sigma)$.

Following Waller and Kapral [kapral84], we first recast equations 8.23 and 8.24 as maps of *normal modes*, where the m^{th} normal mode of the i^{th} site variable is defined by

$$\eta_m(t) = \frac{1}{N} \sum_{j=1}^N \sigma_j(t) \exp(-2\pi i j m / N). \quad (8.26)$$

The corresponding normal mode map $\eta_m(t) \rightarrow \eta_m(t+1)$ is obtained by substituting the Fourier-expanded variables $\sigma_j(t) = \sum_{m=1}^N \eta_m(t) \exp(2\pi i j m / N)$ into equations 8.23 and 8.24, multiplying by $\exp(-2\pi i j m / N)$ and summing over $j = 1, 2, \dots, N$. Using the orthogonality relation $\sum_{j=1}^N \exp(2\pi i j (m-s)/N) = N \delta_{ms}$, where δ_{ms}

(= 1 if and only if $m = s$) is the Kronecker-delta function, we get either

$$\eta_m(t+1) = \{a - 4D \sin^2(\pi m/N)\} \eta_m(t) - \alpha \sum_{s=0}^{N-1} \eta_s(t) \eta_{m-s}(t), \quad (8.27)$$

for equation 8.23, or

$$\eta_m(t+1) = \alpha \{1 - 4D \sin^2(\pi m/N)\} \left\{ \eta_m(t) - \sum_{s=0}^{N-1} \eta_s(t) \eta_{m-s}(t) \right\}, \quad (8.28)$$

for equation 8.24. Notice that in equation 8.27 the diffusion does *not* couple the normal modes, whereas in equation 8.28 it does.

Now let us consider the stability of the two systems around fixed points of $f(\sigma)$, and therefore around homogeneous solutions of the CML. From chapter 4 we recall that $\sigma^* = 0$ is a stable fixed point for $a \leq 1$ and $\sigma^* = 1 - 1/\alpha$ is a stable fixed point for $1 < \alpha \leq 3$. Let us see whether our diffusive coupling leads to any instability.

To this end, let us add a small perturbative term to $\sigma_i(t)$, and substitute $\sigma_i(t) = \sigma^* + \delta\sigma_i(t)$ into equation 8.26. We get

$$\eta_m(t) = \sigma^* \delta_{m0} + \delta\eta_m(t), \quad (8.29)$$

where

$$\delta\eta_m(t) \equiv \frac{1}{N} \sum_{j=1}^N \delta\sigma_j(t) \exp(-2\pi i j m/N). \quad (8.30)$$

Substituting equation 8.29 into equation 8.27 and retaining only those terms that are linear in $\delta\eta_m(t)$ we get

$$\delta\eta_m(t+1) = a \{1 - 4D \sin^2(\pi m/N)\} (1 - 2\sigma^*) \delta\eta_m(t), \quad (8.31)$$

whose solution, in terms of $\eta_m(0)$, is given by

$$\delta\eta_m(t) = \{\alpha[1 - 4D \sin^2(\pi m/N)](1 - 2\sigma^*)\}^t \delta\eta_m(0). \quad (8.32)$$

The analogous result for equation 8.28 is given by

$$\delta\eta_m(t) = \{\alpha(1 - 2\sigma^*) - 4D \sin^2(\pi m/N)\}^t \delta\eta_m(0). \quad (8.33)$$

We see from both equations 8.32 and 8.33 that the most unstable mode is the 0th mode and that $\sigma_i(t) = 1 - 1/\alpha$ is stable for $1 < \alpha \leq 3$ and $\sigma_i(t) = 0$ is stable for $0 \leq \alpha \leq 1$. In other words, the diffusive coupling does not introduce any instability into the homogeneous *system*. The only instabilities present are those already present in the uncoupled local dynamics. A similar conclusion would be reached if we were to carry out the same analysis for period p solutions. The conclusion is that if the uncoupled sites are stable, so are the homogeneous states of the CML. Now what about inhomogeneous states'?

8.2.2 Temporal Evolution of Inhomogeneous Initial States

Consider a simple-diffusive CML driven by the logistic map:

$$\begin{cases} \sigma_i(t+1) = f(\sigma_i(t)) + D \{f(\sigma_{i+1}(t)) - 2f(\sigma_i(t)) + f(\sigma_{i-1}(t))\}, \\ f(\sigma) = \alpha\sigma(1-\sigma). \end{cases} \quad (8.34)$$

Figures 8.4-a through 8.4-d show amplitude plots of this CML ($\sigma_i(t)$ vs i) for $\alpha = 3.5$ (i.e. period-4 of $f(\sigma)$) for increasing values of the diffusion constant: $D = 0$ (8.4-a), $D = 0.1$ (8.4-b), $D = 0.25$ (8.4-c) and $D = 0.5$ (8.4-d). In each case the initial condition is randomly chosen, and the amplitudes of each site are shown for four successive time steps after the system has been first allowed to evolve for 300 transient steps. The size of the system is $N = 50$.

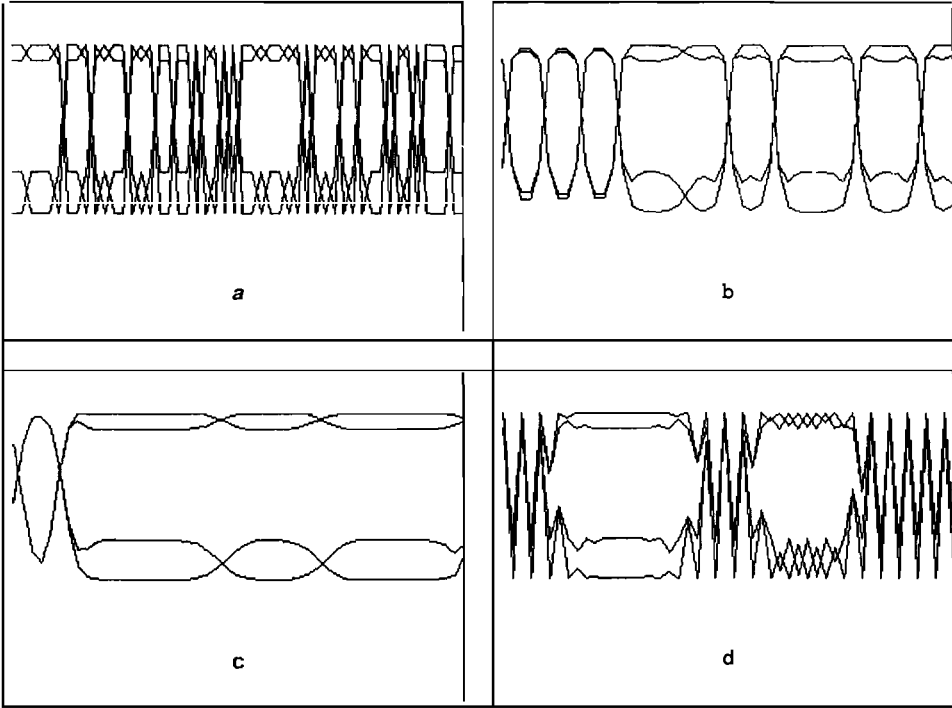


Fig. 8.4 Amplitude plots of $\sigma_i(t)$ vs i for $\alpha = 3.5$ (i.e. period-4 of $f(\sigma)$) for increasing values of the diffusion constant: $D = 0$ (a), $D = 0.1$ (b), $D = 0.25$ (c) and $D = 0.5$ (d).

Notice that as D increases, the spatial pattern initially appears to smooth out gradually (figures 8.4-b, 8.4-c), but then attains a rather jagged appearance at $D = 1/2$ (figure 8.4-d). We see that simple diffusion can indeed induce a spatial instability. A more careful numerical investigation in fact shows that spatial instabilities can occur whenever D is greater than about ~ 0.492 , although their emergence generally appears to be initial-state dependent.

8.2.3 Period-Doubling

A natural question is how does the local period-doubling behavior of the logistic map translate to its CML-version incarnation? Without loss of generality, let us consider the Laplacian-coupled version of the logistic-driven CML:

$$\begin{cases} \sigma_i(t+1) = (1-\epsilon)f(\sigma_i(t)) + \frac{\epsilon}{2}\{f(\sigma_{i+1}(t)) + f(\sigma_{i-1}(t))\}, \\ f(\sigma) = \alpha\sigma(1-\sigma). \end{cases} \quad (8.35)$$

We know that as α is increased, f undergoes a sequence of period-doubling bifurcations on its way towards chaos.

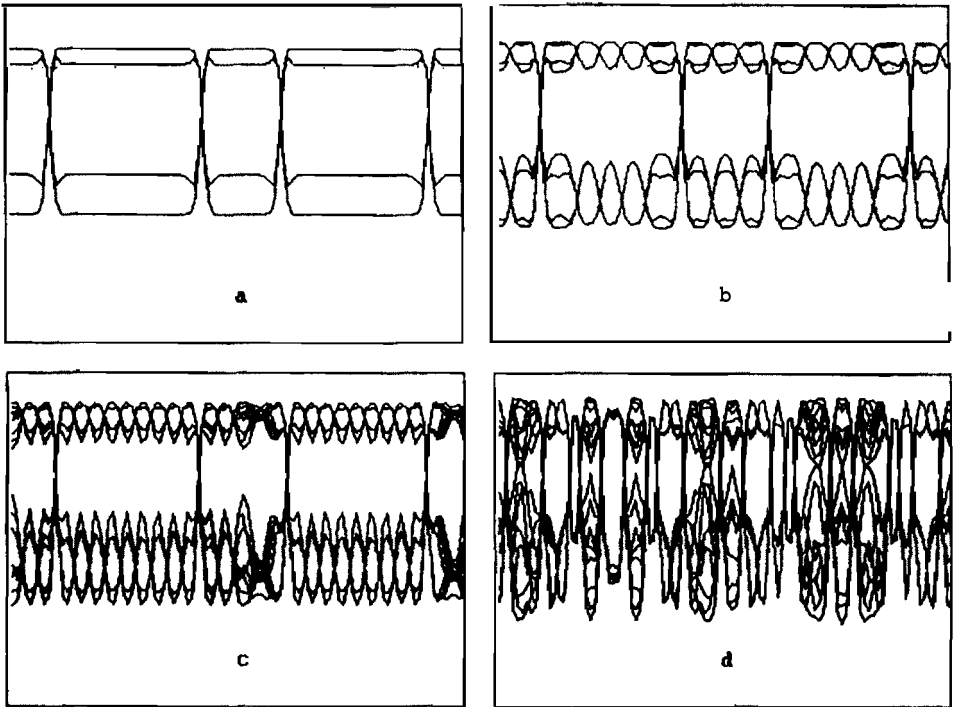


Fig. 8.5 Amplitude plots of $\sigma_i(t)$ vs i for the CML defined in equation 8.35; see text.

It turns out that, in the CML, the local temporal period-doubling yields *spatial domain structures* consisting of phase coherent sites. By domains, we mean physical regions of the lattice in which the sites are correlated both spatially and temporally. This correlation may consist either of an exact translation symmetry in which the values of all sites are equal or possibly some combined period-2 space **and** time symmetry. These coherent domains are separated by domain walls, or **kinks**, that are produced at sites whose initial amplitudes are close to unstable fixed points of $f^\pi(\sigma^*) = \sigma^*$, for some period- π . Generally speaking, as the period of the local map

doubles with α (or ϵ), the spatial wavelength of the CML systematically decreases as well.

Figures 8.5-a through 8.5-d show amplitude plots of $\sigma_i(t)$ vs i for the CML defined in equation 8.35. The size of the system is $N = 100$, the initial state is taken to be a simple sinusoid, $\sigma_i(0) = 0.5 + 0.4 \sin(2\pi i/N)$, and, in each case, 16 time steps are overlapped after the system is first allowed to evolve for 500 transient steps. The lattice coupling constant is fixed at $\epsilon = 0.3$ and the logistic nonlinearity $\alpha = 3.5, 3.57, 3.65$ and 3.71 in figures 8.5-a, 8.5-b, 8.5-c and 8.5-d, respectively. The kink-antikink structures are clearly evident. Notice that as long as α is not too large, the kinks remain fixed in position; as the local nonlinearity increases, however, the domains begin to move and give rise to increasingly complex spatial patterns with characteristic wavelengths.

8.2.4 Kink Diffusion

One of the most striking “higher-level” behaviors observed in CMLs is the diffusion of the kinks/anti-kinks that separate the different domains, a behavior that should remind the reader of our earlier discussion of the diffusion of local kinks induced by the deterministic elementary CA rule **R18** [grass84a] (see section 3.1.2). Before looking at some examples, let us see how this comes about.

As discussed above, an increase in the local nonlinearity α gradually leads to chaos through a period-doubling of the kinks. When α is relatively small ($\lesssim 3.68$), the positions of the domains separated by kinks remains fixed and a chaotic motion is strictly confined to each domain. As a result, domains of varying sizes coexist in this regime, while the actual distribution of their sizes depends on the initial state of a given system [kaneko89]. As α increases, the domain boundaries begin to move in space, with larger-sized domains being the first to become unstable. Some of these larger domains produce patterns with a characteristic wavelength. In particular, if the lattice-coupling is small ($\epsilon < 0.15$), a *zigzag* structure (whose spatial wavelength equals two sites) is typically formed [kaneko88b]. This zigzag structure is characterized by the condition that

$$\zeta(\sigma_{i-1}(t), \sigma_i(t), \sigma_{i+1}(t)) = (\sigma_{i+1}(t) - \sigma_i(t)) (\sigma_i(t) - \sigma_{i-1}(t)) < 0, \quad (8.36)$$

or the condition $(\sigma_{i+1}(t) - \sigma^*)(\sigma_i(t) - \sigma^*) < 0$ where σ^* is an unstable fixed point of the logistic map f .[‡] Regions of two different phases, where a phase is defined by a given *sign* of ζ , are separated by a local defect, or kink (see figures 8.6 and 8.7). Kaneko has identified the following four regimes of behavior, listed in order of increasing α [kaneko88a]:

[‡]Similar zigzag structures have been observed in two-dimensional systems, where they appear as a checkerboard pattern [kapral85].

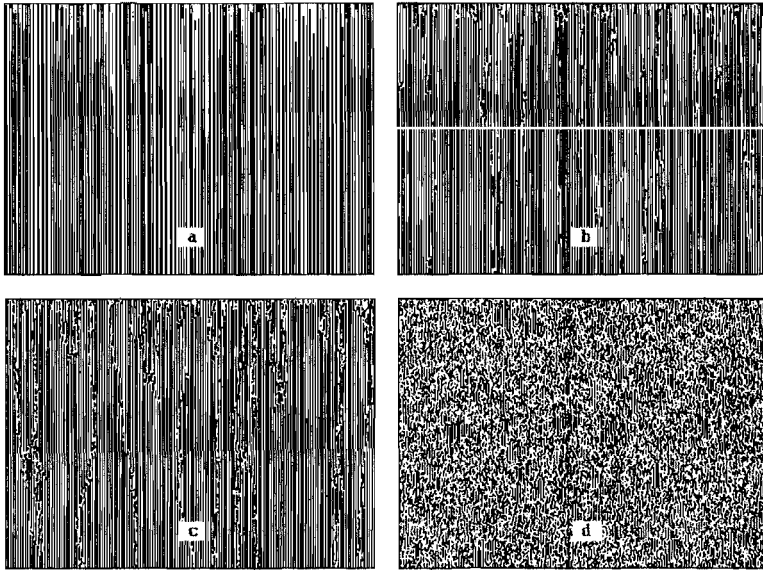


Fig. 8.6 Examples of Kaneko's four regimes of CML behavior, listed in order of increasing α [kaneko88a].

Regime I Frozen Pattern: a basic zigzag structure is first formed in space. If there is no defect present, the temporal change of this zigzag region is period-2. The temporal change of the domain boundary is chaotic (i.e. it has a positive Lyapunov exponent).

Regime II Defect Diffusion: the zigzag pattern is modulated quasi-periodically in time. The chaos in the domain boundary is still localized but it can now move about in space. For $\epsilon \sim 0.1$, the phase change Regime I $\rightarrow$ Regime II occurs at about $\alpha \sim 3.82$.

Regime III - Defect Turbulence: the zigzag pattern is modulated chaotically in time, but the entire pattern is still confined to a single region of space. Defects are still localized but change chaotically in time and can move in space. For $\epsilon \sim 0.1$, the phase change Regime II $\rightarrow$ Regime III occurs at about $\alpha \sim 3.88$.

Regime IV - Fully Developed Turbulence: zigzag regions become unstable; spontaneous pair-creation of defects becomes possible even if starting from defect-free zigzag patterns. For $\epsilon \sim 0.1$, the phase change Regime III $\rightarrow$ Regime IV occurs at about $\alpha \sim 3.92$.

Note that in Regimes II and III, pair-creation of defects does not take place; rather the defect population gradually dwindles by pair-annihilation during collisions. Numerical simulations suggest that the average number of defects decreases

with time t as $t^{-1/2}$, as should be expected for a random-walk motion [kaneko88a].

Figure 8.7 shows an example of several such random-walk pair-annihilations for a size $N = 400$ system obeying periodic boundary conditions. In the figure, $\epsilon = 0.1$, $\alpha = 3.91$ (i.e. Regime 111) and a site $\sigma_i(t)$ is shown whenever $0.75 \leq \sigma_i(t) \leq 0.95$; every 16th time step is plotted from $t = 0$ to $t = 16 \cdot 400$.

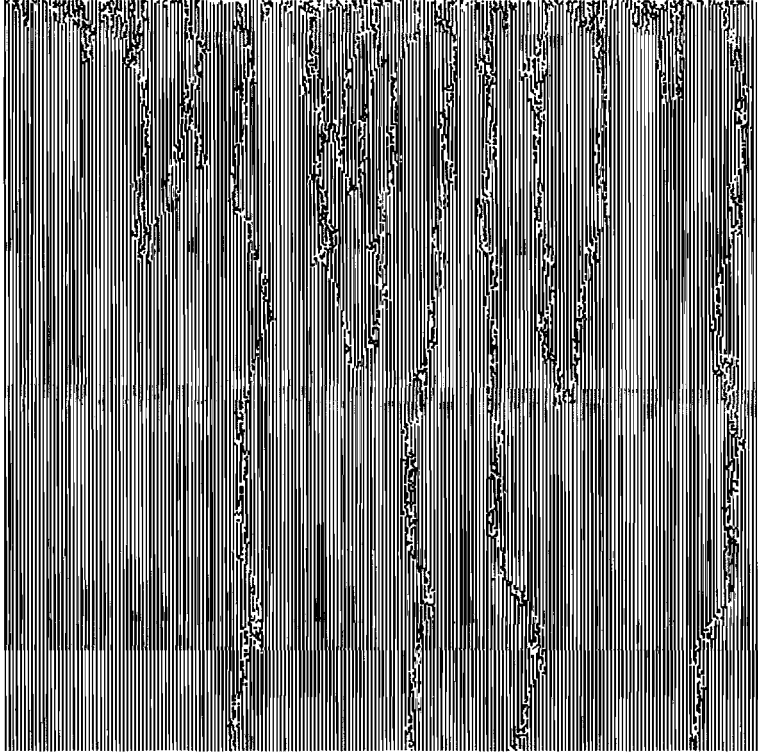


Fig. 8.7 An example of random-walk pair-annihilations for a size $N = 400$ system obeying periodic boundary conditions.

It should be pointed out that, unlike the kink-diffusion observed for the elementary rule **R18** [grass84a], where the kink-motion is very much coupled to the underlying chaotic space-time CA pattern, the “randomness” of the CML’s defect random-walk is due solely to the chaotic motion of the defect itself and not to the randomness of the underlying zigzag pattern. The diffusion process in a CML system consists of the interaction of the chaos of a defect with the motion of the zigzag region. If the period of the motion of the zigzag region is equal to two (Regime I), for example, there are effectively too many constraints to allow the defect to move. On the other hand, if the motion of the zigzag region is quasi-periodic or chaotic, the interaction leads to a movement of a defect.

8.2.5 Quantitative Measures: An Overview

Many of the conventional measures used in studying dynamical systems – power spectra, entropy, Lyapunov exponents, etc. – can in fact be used to quantify the difference among Regimes I-IV ([kaneko89a], [kaneko89c]).

8.2.5.1 Power Spectra

One of the most common ways of characterizing complexity is by taking Fourier transforms. The spatial power *spectrum* of a time series of σ_i , for example, is defined by

$$S(k) = \langle \left| \frac{1}{N} \sum_{j=1}^N \sigma_j(t) e^{2\pi i k j} \right|^2 \rangle_T, \quad (8.37)$$

where $\langle \dots \rangle_T$ represents a long time average.

As the nonlinearity increases and we go through the various regimes, we note the following characteristic behavior of $S(k)$: (1) In regime I, $S(k)$ is typically composed of many peaks, each corresponding to the various sizes of domains that are allowed to exist. (2) As the nonlinearity is increased, the number of distinct peaks diminishes, with each peak still located at the wavenumber corresponding to the size of a given domain. (3) In regime III, the peak at $k = 1/2$ begins to grow with broad-band noise (due to the chaotic defect) appearing at $k \sim 0$. (4) As the system approaches regime IV, the peak at $k = 1/2$ and the broad-band noise at $k \sim 0$ begin coexisting, with the broad-band noise increasing as the nonlinearity increases. (5) Once the system has entered regime IV, individual peaks disappear and the power spectrum consists entirely of a monotonically decaying pattern; this pattern is fit roughly by a Gaussian of the form $S(k) \propto \exp(-\text{constant} \cdot k^2)$ [kaneko89].

We can similarly consider the behavior of the temporal power spectrum of a pattern, $P(\omega)$, defined by

$$P(\omega) = \langle \left| \sum_{n=t_0}^{t_1} \sigma_j(n) e^{2\pi i n \omega} \right|^2 \rangle \quad (8.38)$$

Regimes I-III are each characterized by peaks immersed in broad-band noise. In regime IV the peaks are replaced by a Lorentzian band noise around [kaneko89].

8.2.5.2 Pattern Distribution

Domains were defined above as any physical regions of the lattice in which the sites are correlated both spatially and temporally. More precisely, let us define a domain of size D as a spatial sequence of m sites, $\sigma_{i-h}, \sigma_{i-h+1}, \dots, \sigma_i, \dots, \sigma_{i+m}$, where $h+m+1 = D$, such that the quantity $(\sigma_j - \sigma^*)$, where σ^* is an unstable fixed point of the logistic map, takes on the same sign for each site σ_j in the sequence. In this way we can effectively “discretize” the continuous-valued lattice sites by the

prescription

$$\begin{cases} \sigma_i(t) = 0 & \text{if } \sigma_i(t) < \sigma^*, \\ \sigma_i(t) = 1 & \text{else.} \end{cases} \quad (8.39)$$

By sampling over the entire lattice and many iterations we can then estimate the probability distribution function of the domain sizes D , $Q(D)$.

In Regime I, for example, there are many possible domain sizes and, consequently, $Q(D) \neq 0$ for many different D 's; moreover, the maximum domain size increases with the total lattice size [kaneko89]. Regimes II and III, on the other hand, allow only a relatively few domain sizes so that $Q(D) \neq 0$ for only a few domain sizes D . In addition, there appears to be a cutoff size D_c (which does not depend on lattice size) such that $Q(D > D_c) = 0$. In the case of fully developed turbulence in Regime IV, $Q(D) \propto \exp(-\text{constant} \cdot D)$, which is indicative of the random generation of domains.

Note that the quantity $(1 - Q(D))$ can be thought of as a “disorder parameter” distinguishing the different regimes of behavior. Numerical measurements of this disorder parameter around the transition point at which the zigzag pattern collapses spontaneously (i.e. around $\alpha_c \approx 3.92$) suggest a critical-like behavior [kaneko89a]:

$$1 - Q(D) \approx (\alpha - \alpha_c)^\beta. \quad (8.40)$$

The exponent β decreases from 1.6 to 1.0 as the system size increases from $N = 2$ to $N = 100$. Kaneko suggests that this may result from an effective increase in the number of possible pathways for the zigzag collapse, and thus that the change of β with size may be regarded as a path from the dynamical systems theory to statistical mechanical phase transition problems [kaneko89a].

8.2.5.3 Entropy

The discretized symbol-sequence defined in equation 8.39 suggests that we might use two other familiar measures of “complexity” to characterize the various dynamical regimes of behavior; namely, the pattern entropy and dynamical entropy.

Pattern Entropy: The pattern entropy, S_p , is a purely static measure, and is defined by

$$S_p = \sum_D Q(D) \log Q(D). \quad (8.41)$$

It has the interesting behavior of first being large (almost constant) for Regime I; decreasing to a small value as the nonlinearity is increased and the system enters Regimes II and III; and again increasing to a large value in Regime IV [kaneko89a, kaneko89b]. Kaneko has also observed that around the zigzag collapse transition point (i.e. $a = a_c$), $S_p \propto (a - \alpha_c)^{\beta'}$, where $\beta' \approx \beta$ (see equation 8.40).

Dynamical Entropy: In order to capture the *dynamics* of a CML pattern, Kaneko has constructed what amounts to $\pm$ mutual information between two successive patterns at a given time interval [kaneko93]. It is defined by first obtaining an estimate, through spatio-temporal samplings, of the probability transition matrix $T_{D,D'} \equiv$ transition from domain of size D to a domain of **size** D' . The dynamical entropy, S_d , is then given by

$$S_d = \sum_{D,D'} Q(D) T_{D,D'} \log T_{D,D'}. \quad (8.42)$$

It should be clear from this definition and equation 8.41 defining S_p above that $S_p \geq S_d$. If the pattern is such that it spatially complex from temporally static, there are no transitions between domain sizes; the result is a positive S_p but vanishing S_d . If $T_{D,D'}$ is independent of D (which is approximately true in the fully turbulent regime) then $S_d = S_p$. It turns out that S_d is nonvanishing and large precisely when the CML system has entered the regime of fully developed turbulence; S_d vanishes for Regimes I and II. At the onset of defect turbulence, the dynamical entropy increases as $S_d \propto (\alpha - \alpha_c)^\delta$, where $\delta \approx \beta$ (see equation 8.40) [kaneko89a].

Other measures have also proved useful: full *spatio-temporal* power spectra [kaneko89a]; *Lyapunov Spectra*, which can be calculated from the eigenvalues of products of Jacobi matrices ([kaneko86], [kaneko89]); and the *Kolmogorov-Sinai* entropy, an interesting feature of which is its decrease with increasing nonlinearity in Regime II [kaneko89b].

Table 8.5 summarizes some of the behaviors of the measures introduced in the sections above for each of the four regimes for the case where the diffusive coupling is of medium size:[†]

Regime	Spatial Power Spectra $S(k)$	Pattern Distribution $Q(D)$	Pattern Entropy S_p	Dynamical Entropy S_d
I	many peaks	$Q(D) \neq 0$ for many D 's	large	0
II	few prominent peaks	$Q(D_1), Q(D_2) \neq 0$ $Q(D) = 0$ otherwise	small	0
III	few peaks and broad-band noise at $k = 0$	$(1 - Q(1))$ $\propto (\alpha - \alpha_c)^\beta$	$\propto (\alpha - \alpha_c)^{\beta'}$	$\propto (\alpha - \alpha_c)^\delta$
IV	smooth decay	$\propto \exp(-\text{const} \cdot k)$	large	large, $S_d \approx S_p$

[†]See Table III in [kaneko90]

8.2.5.4 Concluding Comments

We conclude this section with a few general observations about the zigzag regime (see [crutch87]): (i) For small diffusive-couplings, zigzag structures typically start to form at the domain boundary and propagate inward at a constant speed. (ii) Zigzags appear in a wide variety of different CML systems. In some lattices they are confined to relatively small parameter ranges; in others they are more readily observed. Generally speaking, whenever the diffusive coupling is large, one finds that the zigzag structures are modulated either quasi-periodically or chaotically. (iii) spatial instabilities whose characteristic wavelengths are *different* from two also exist, of course, and these exhibit a similar quasiperiodic route to chaos. (iv) in some parameter regimes, as we have seen, the kinks in the zigzag regions propagate as stable “particle-like” structures. In two dimensions, a brownian motion of a chaotic “string” has been observed, separating two out-of-phase zigzag regions. Crutchfield and Kaneko [crutch87] compare this diffusive motion to the spatial diffusion found for a particle in a periodic potential well [huber80] and suggest that it is also reminiscent of the dislocations observed in low Reynolds number Couette flow [donn80]. Brownian motion has also been observed in liquid convection and in video feedback ([crutch84a], [crutch84b]). The study of such localized chaotic defect motion may shed light on some localized dynamical disorder observed in some real physical systems [kaneko88b].

8.2.6 Spatio-Temporal Intermittency

We recall from our earlier discussion of chaos in one-dimensional continuous systems (see section 4.1) that period-doubling is not the only mechanism by which chaos can be generated. Another frequently occurring route to chaos is intermittency. But while intermittency in low dimensional dynamical systems appears to be constrained to purely temporal behavior [pomeau80], CMLs exhibit a spatio-temporal intermittency in which laminar eddies are intermixed with turbulent regions in a complex pattern in space-time.

Figures 8.8-a through 8.8-d show a few snapshots illustrating intermittent behavior. We have used the logistic-equation driven CML (equation 8.34) and set $D = 0.25$ and $\alpha = 3.83$. Each figure shows 16 times overlapped after a certain number of iterations have elapsed (100 iterations in figure 8.7-a, 200 in figure 8.7-b, 300 in 8.7-c, and 500 in 8.8-d). Notice how, depending on the time of the snapshot, some regions are periodic and others are turbulent. Islands of order tend to come and go as time progresses; i.e. the local order is intermittent.

In their study of CMLs exhibiting a Pomeau-Manneville intermittency, Crutchfield and Kaneko [crutch87] have observed the following general behavior:[‡]

[‡]Note that while their observations were made specifically for a CML driven by a circle map (see equation 8.43), and for a specific set of circle-map parameters chosen so that the local map is locked in period-2 motion ($k = 0.2$ and $w = 0.55$), the authors are quick to point out that the observations apply to any driving local function that itself exhibits intermittent behavior.

Localized Kink Regime: when the diffusive coupling is too small for kinks to move, the initial kinks separating domains remain locked in position. The behavior is analogous to that of class c2 elementary CA.

Transition Regime: the kinks become unstable and are able to propagate but remain localized; global intermittent pattern cannot yet be formed. The patterns are reminiscent of class c4 behavior.

Saturation Dynamics: the burst and laminar regions form geometric structures very reminiscent of class c3 behavior of elementary CA. The distribution of laminar clusters appears to follow an exponential law. If a temporal sequence of values for a given site were recorded for a system in this phase, the result would be a temporally-intermittent time series; i.e. bursting regions in which site values alternate between high and low values and punctuated by intervals of time during which the behavior is fairly regular and the spatial pattern is close to uniform.

Fully Developed Turbulence: burst regions spread throughout the entire lattice so that it becomes very difficult to discern **any** laminar regions.

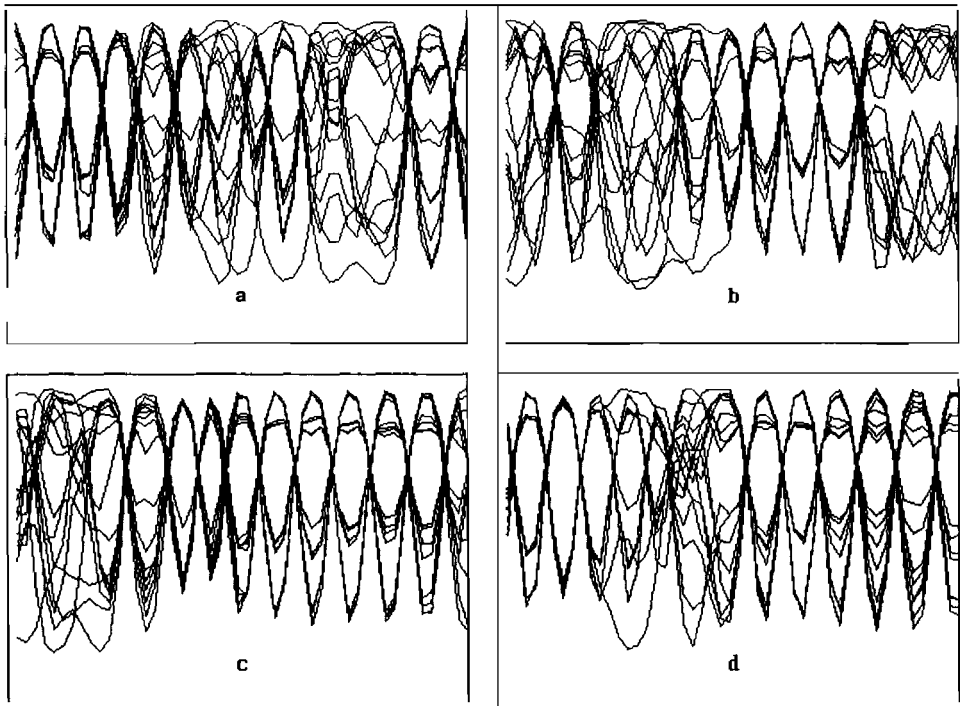


Fig. 8.8 Amplitude plots of $\sigma_i(t)$ vs i for the CML defined in equation 8.35; see text.

We should contrast the so-called Pomeau-Manneville intermittency [pomeau80] with intermittency via pattern competition [kaneko87]. We have commented earlier

how the logistic-map driven CML undergoes an instability at some spatial wavenumber k , developing a stable spatial pattern with that wavenumber. As the nonlinearity parameter α increases, that pattern becomes unstable via chaotic bursts, which propagate intermittently in space and time. Although the detailed mechanism responsible for this type of intermittency has not yet been firmly established, it has been observed to exist in relatively large regions of parameter space [crutch87] and there is evidence to suggest that it is characterized by low temporal frequency noise [kaneko87].

8.2.7 Soliton Turbulence

Let us consider the same Laplacian coupled CML **as** in the previous sections, but with f equal now equal to the one-dimensional circle map; i.e. consider

$$\begin{cases} \sigma_i(t+1) = (1-\epsilon)f(\sigma_i(t)) + \frac{\epsilon}{2}\{f(\sigma_{i+1}(t)) + f(\sigma_{i-1}(t))\}, \\ f(\sigma) = w + \sigma + \frac{k}{2a} \sin(2\pi\sigma) \mod 1, \end{cases} \quad (8.43)$$

where the frequency parameter w and nonlinearity factor k both take on a constant value for all sites i . Although this CML harbors a rich variety of diverse behaviors (see [kaneko87]), we will only focus on its interesting ability to generate soliton turbulence in this section.

Let us first recall a few facts about the one-dimensional circle map. Much in the same way **as** the logistic map is the prototypical map exhibiting period-doubling, the circle map is the prototypical map describing a route to chaos through quasiperiodicity and mode locking. While k clearly controls the degree of nonlinearity in the system, w effectively determines the so-called winding number $w = \lim_{n \rightarrow \infty} (f^n(\sigma_0) - \sigma_0)/n$, or the rate of rotation. A phase, or mode, locking occurs precisely when $w = p/q$ for some relatively prime integers p and q . We see that when $k = 0$, $w = w$; i.e. that if $k = 0$ we have a mode-locking whenever w is a rational number. Since the rationals constitute a set of measure zero on $[0, 1]$, however, we also see that almost all maps are quasiperiodic for $k = 0$. **As** the value of k increases, the measure of the set of values of w for which $w = p/q$ steadily increases until, at $k = 1$, the set of values of w for which the motion is quasiperiodic has measure zero. This occurs because the set of values of w for which w is irrational forms a Cantor set.

At the risk of oversimplifying, there are essentially three different dynamical regimes of the one-dimensional circle map (we have not yet formed our CML): (I) $|k| < 1$ – for which we find mode-locking within the so-called *Arnold Tongues* (see section 4.1.5) and the w is irrational; (II) $k = 1$ – for which the non mode-locked w intervals form a self-similar Cantor set of measure zero; (III) $|k| > 1$ – for which the map becomes noninvertible and the system is, in principle, ripened for chaotic behavior (the real behavior is a bit more complicated since, in this regime, chaotic and nonchaotic behavior is actually densely interwoven in $k - w$ space).

When the circle map is used to drive the CML as in equation 8.43, the spatial-diffusion coupling generally induces the independent oscillations represented by each circle map to synchronize. In some parameter regions, kink/anti-kink pair annihilations lead, asymptotically, to a simple homogeneous state. In other regimes, the CML exhibits complex, aperiodic “turbulent” behavior that is sustained by continuous kink/anti-kink collisions. In still other regimes, there is a billiard-ball-like chaos induced by meandering isolated kinks [crutch87].

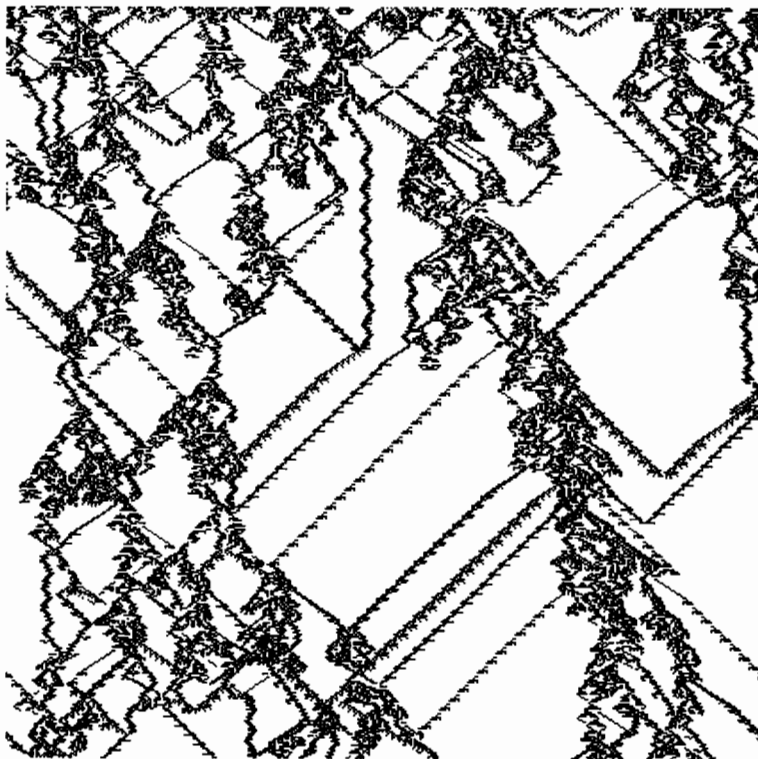


Fig. 8.9 An example of soliton turbulence. The size of the system is $N = 400$, the coupling $\epsilon = 0.4$; $w = 0.3$, $k = 1.2$; see text.

Figure 8.9 shows an example of such a billiard-ball chaos, or “soliton turbulence.” The size of the system is $N = 400$, the coupling $\epsilon = 0.4$; $w = 0.3$, $k = 1.2$. The actual plot is of the spatial derivative $\mathcal{D}_{i,i+1}(t) \equiv |\sigma_{i+1}(t) - \sigma_i(t)|$; a site i at time t is colored black whenever $0.05 \leq \mathcal{D}_{i,i+1}(t) \leq 1$ and t is a multiple of four (i.e. every fourth time step is shown).

The emergent soliton structures are obviously very reminiscent of the “propagating structures” normally associated with one-dimensional class **c4** elementary CA, as well as the “glider”-like structures appearing in Conway’s *Game of Life* (section 3.4.4). There are two noteworthy differences between these systems, however (aside from the fact that we are looking at the spatial derivative here as opposed to a

binary state plot): (1) there appears to be a much greater variety in the type of soliton that can be created, and (2) the emission of solitons occurs in a largely unpredictable fashion (as compared, say, with the regularly timed emissions of gliders from a glider-gun in the *Game of Life*).

It is interesting to note that the parameter regime within which these solitons emerge appears to lie just on the edge of the transition between homogeneous asymptotic states and fully developed global turbulence. This is consistent with Langton's observation that class **c4** rules appear to exist precisely "on-the-edge" of the transition between periodic class **c2** and chaotic class **c3** elementary rules (see section 3.2 and [lang90]).

8.2.8 CA Approximation of Coupled-Map Lattices

In a series of papers ([chate88b], [chate89a], [chate89b], [chate90]), Chate and Manneville explore the transition to turbulence via spatiotemporal intermittency in coupled map lattices (CMLs) by approximating them by n -state deterministic CA.[†] In addition to providing a systematic way of studying the approach to criticality in CMLs, such approximations have two additional virtues: (1) they provide some insight into the interrelationship among criticality, continuous and discrete systems and deterministic and probabilistic rules; (2) since, as we shall see, varying the CML's spatial coupling is effectively equivalent to traversing a path in the abstract CA rule-space, a discrete CA approximation also provides a natural ordering to an a-priori order-less rule space. While this should remind the reader of the "natural" ordering of the elementary CA rule-space provided by Langton's λ -parameter (see section 3.2), there is a difference. The λ parameter is entirely "intrinsic" – or static – in the sense that it is derived entirely from the abstract template of the rule itself. In the present case of rule-paths constructed via CA approximations of CMLs, the rule ordering is "extrinsic" – or *dynamic* – since it is derived from a separately defined, and more importantly, non-unique, local rule.

In this section, we follow Chate and Manneville's analysis of the following one-dimensional CML system:

$$x_i(t+1) = (1 - \epsilon)f[x_i(t)] + \frac{\epsilon}{2}(f[x_{i-1}(t)] + f[x_{i+1}(t)]), \quad (8.44)$$

where ϵ is the spatial coupling and f is taken to be a tent-map-like local function defined by (see figure 8.10-a)

$$f(x) = \begin{cases} sx & \text{if } 0 \leq x \leq 1/2, \\ s(1-x) & \text{if } 1/2 \leq x \leq 1, \\ \zeta(x - x^*) + x^* & \text{if } x > 1 \end{cases} \quad (8.45)$$

where $s > 2$, $|\zeta| \leq 1$ and $x^* \equiv (s+2)/4$. This simple form for f was chosen because it satisfies the "minimal" requirements necessary to observe spatiotemporal

[†]A similar scheme was used by Oono and Kohmoto [oono85].

intermittency [chate88a]:[†] (1) the existence of a non-chaotic asymptotic state, (2) the stability of this non-chaotic state with respect to infinitesimal perturbations but with the possibility of instability under localized finite perturbations introduced via the coupling, and (3) the possibility of transient chaotic behavior.

The behavior off (the details of which may be found in [chate88a] and [chate88b]) is in fact characterized by two distinct dynamical regions: (1) A laminar region ($x > 1$), in which the dynamics is trivial - once $x(t) > 1$, $x(t') > 1$ for all t' . The laminar region thus acts as a necessary ‘(absorbing state.’ (2) A chaotic, or turbulent, region ($x < 1$), for which there exists a critical ϵ_c such that for $\epsilon < \epsilon_c$ the CML evolves into a homogeneous laminar state and for $\epsilon > \epsilon_c$, the system exhibits sustained regimes of spatiotemporal intermittency and is characterized by stationary statistical values [chate89a].

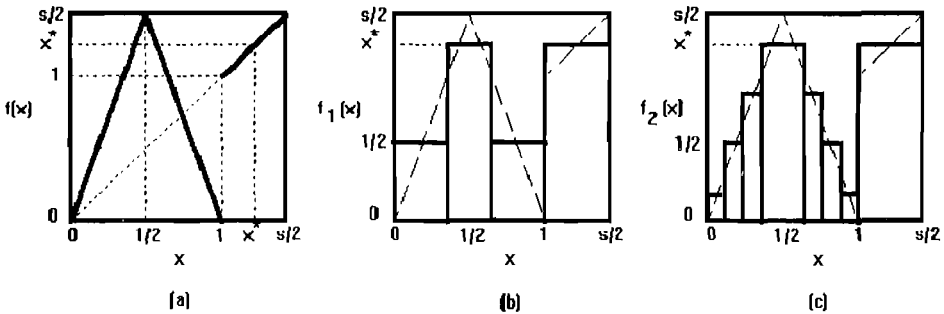


Fig. 8.10 First and second order approximations (f_1 and f_2) of Chate and Manneville's [chate88a] tent-map-like local CML function f (equation 8.45).

The average density of turbulent sites ($x > 1$), for example, is the same whether the averaging is performed over space, time or both. While the transition region also exhibits scaling properties characteristic of continuous phase transitions,[†] and it has been conjectured that the system is in the same universality class as directed percolation [Pomeau86], it *does not* appear to be universal [chate90]. The critical exponents characterizing the distribution of laminar ‘clusters’ at the transition threshold for $\zeta = 1$, for example, are different for $s = 2.1$ and $s = 3$ and do not agree with the corresponding value for directed percolation. Indeed, the two CA approximation schemes about to be outlined below were both motivated, in part, by this observed inequality [chate90].

The Chate and Manneville approximation schemes consist of finding sets of increasingly finer piece-wise linear step-function approximations of the continuous

[†]The same f has also been used as a model for spatiotemporal intermittency in Rayleigh-Benard convection ([cili88], [davi89]).

[†]These properties include (1) a continuous decrease in the average density of turbulent sites as the threshold is approached from above (with exponent β); (2) divergence of the average transient time; (3) algebraic distributions of the sizes and durations of laminar ‘clusters’ at the threshold (with exponents $\zeta_{\perp}$ and $\zeta_{\parallel}$). Houliik, Webman and Jensen [houl90] discuss the critical behavior of this map from a mean-field theoretic perspective.

CML f ([chate89a], [chate89b]. When f is replaced by another *discrete* function $\tilde{f}$, taking on one of a finite site of distinct values, the CML defined by $\tilde{f}$ and equation 8.44 effectively becomes a k -state CA defined on the same lattice and local neighborhood structure. Of course, we are entirely free to choose any $\tilde{f}$ that we desire, *provided* that it preserves the critical dynamical features of the original function; in particular, $\tilde{f}$ must preserve the absorbing character of the laminar state.

The first method is based on considering the pre-images of the laminar state. Let $\zeta = 1$ and consider the first-order approximation, f_1 . Since $f_1(x)$ must preserve the absorbing character of the laminar state, we can let $f_1(x) = x^*$ for all $x > 1$. To preserve the character of the turbulent region, we take a cue from the fact that, in the CML system, the chaos is really *transient* since an arbitrary initial state in the turbulent region eventually winds up in the laminar region. Because this happens after a finite number of steps, it can be modeled by considering the *preimages* of the laminar state. From equation 8.45 we see that the preimage of the laminar region $I_L = (1, s/2]$ consists of the two intervals $I_1 = (1/s, 1 - 1/s)$ and $I_2 = I_L$:

$$f^{-1}(I_L) = I_1 \cup I_L. \quad (8.46)$$

Let $\bar{I}_1 = [0, 1/s] \cup [1 - 1/s, 1]$ be the complementary set of I_1 on the unit interval $[0, 1]$. Then, the first-order step-function approximation of f can be written

$$f_1(x) = \begin{cases} x^* & \text{if } x \in I_1 \cup I_L, \\ 1/2 & \text{if } x \in \bar{I}_1. \end{cases} \quad (8.47)$$

The second order approximation, f_2 , is essentially a refinement of f_1 and may be found from f_1 by considering the pre-images of I_1 . We first define the interval I_2 as the pre-image of I_1 under f : $I_2 \equiv f^{-1}(I_1)$, and let $\bar{I}_2$ be the complement of I_2 in $\bar{I}_1$: $\bar{I}_2 \equiv \bar{I}_1 - I_2 = [0, s/2] - (I_L \cup I_1 \cup I_2)$. The “refined” function f_2 is then given by taking the values of f_1 at the midpoints of the subintervals of $[0, s/2]$, delimited by the partition (I_L, I_1, I_2) ; see figure 8.10-b.

We can continue to construct increasingly finer approximations of the original function f by iterating the above steps. Thus, the p^{th} order approximation will use the intervals

$$\begin{cases} I_p &= f^{-1}(I_{p-1}), \\ \bar{I}_p &= \bar{I}_{p-1} - I_p = [0, s/2] - \bigcup_{i=0}^p I_i, \end{cases} \quad (8.48)$$

and will take on 2^p different values of f at all midpoints of the $(2^{p+1} - 1)$ p^{th} order subintervals of $[0, s/2]$. As can be inferred from the above construction, the subintervals eventually form a fractal set $I_\infty = \lim_{p \rightarrow \infty} I_k$ of dimension $d(s) = \log 2 / \log[s/(s-2)]$; for $s = 3$, this is the conventional *Cantor Set* with fractal dimension $d = \log 2 / \log 3$. Thus, at p^{th} order, the original one-dimensional CML is approximated by a 2^p -state CA with a single absorbing state. Since to each choice

of s and ϵ in the original CML there corresponds a unique approximating CA, the original problem of studying the transition to turbulence via spatiotemporal intermittency as ϵ is varied is thus effectively equivalent to studying the same transition but for a *sequence of CA rules*.

While this first method provides some insights into the dynamical processes underlying the spatiotemporal intermittency regimes of the original CML (see below), it suffers from two drawbacks: (i) the approximating function f_p does *not* converge to f as $p \rightarrow \infty$, and (ii) the number of required p^{th} -order CA states (and thus the number of local configurations that must be examined in order to construct the CA rule-table) quickly diverges with p . In [chate90], Chate and Manneville consider a somewhat simpler step-function approximation of f , in which the turbulent part of the phase-space ($0 \leq x \leq 1$) is divided into $2p - 1$ equal-sized patches having p different heights; the laminar part is also divided in steps with heights that match those previously defined. As the reader can easily show, the two methods yield equivalent approximations at lowest order.

8.2.8.1 First Order Approximation

The first order (i.e. $p = 1$) approximation of the CML system defined by equation 8.44 (using either of the two methods defined above) is given by an elementary $k = 2$, $r = 1$ CA. Since there are only 32 such rules, the particular CA rule corresponding to a CML system with parameters ϵ and s may be found directly by calculating the outcome of each of the five possible local states.[†] Looking at the first-order step function $f_1(x)$ in equation 8.47, we can identify the absorbing state $x = x^*$ with the CA state $\sigma = 0$, and $x = 1/2$ with $\sigma = 1$.

For example, if $(f_1[x_{i-1}(t)], f_1[x_i(t)], f_1[x_{i+1}(t)]) = (0, 1, 1)$ or $(1, 1, 0)$, equation 8.44 gives $x_i(t+1) = g(\epsilon, x^*) = 1/2 - \epsilon/4 + \epsilon x^*/2$. Setting $x^* = (s+2)/4$, the corresponding binary entries for $(0, 1, 1)$ and $(1, 1, 0)$ in the approximating CA rule-table are then given by

$$(0, 1, 1), (1, 1, 0) \longrightarrow \begin{cases} 0 & \text{if } \frac{1}{r} < g(\epsilon, (s+2)/4) < 1 - \frac{1}{r} \text{ or } g(\epsilon, (s+2)/4) > 1, \\ 1 & \text{else.} \end{cases} \quad (8.49)$$

The other rule-table entries are found in a similar manner.

Table 8.6 traces the evolution of the approximating CA rules as ϵ increases from 0 to 1 for $2 \leq s \leq 3$. We see that as ϵ increases, only 7 of the 32 possible rules are actually “visited.” Nonetheless, even at this crude first order approximation, a remnant of the CML’s transition to spatiotemporal intermittency remains. In particular, there is a threshold value of ϵ , $\epsilon_c = 2 - 4/s$, that acts as a boundary point below which the approximating CA-rule is simple-periodic (class 1 or 2) and above which it is complex (class 3 or 4). The surprising fact is not that the CML’s transition appears to be approximated by the CA-rule path – after all, allowing for finite-length computer words, the CML itself is essentially just a very-high order CA

[†]We impose the *quiescence* condition, $\vec{0} \rightarrow 0$, and left-right symmetry.

ϵ	Rule	Dynamics (Class)
$(0, 2/s - 4/s^2)$	32	Periodic (2)
$(2/s - 4/s^2, 1 - 2/s)$	36	Periodic (2)
$(1 - 2/s, 4/s - 8/s^2)$	4	Periodic (2)
$(4/s - 8/s^2, 2 - 4/s)$	76	Periodic (2)
$(2 - 4/s, 2/s)$	94	Complex (3)
$(2/s, 1 - 2/s + 4/s^2)$	90	Complex (3)
$(1 - 2/s + 4/s^2, 1)$	122	Complex (3)

Table 8.6 Effective CA rules corresponding to the CML defined in equation 8.44 for $0 \leq \epsilon \leq 1$ and $2 \leq s \leq 3$.

approximation of the ideal system – but that the qualitative nature of that transition appears to be already well captured in the lowest-order CA approximation.

8.2.8.2 Higher Order Approximations

As might be expected, as the order of the approximation, p , is increased, an increasingly large set of the features of the original CML system is recovered. As mentioned above, the number of CA rules also grows very quickly with the order of the approximation. Fortunately, since we are generally only interested in the qualitative picture of the rule-path as ϵ is varied, it is not necessary to look at (or even define) each and every rule that appears on that path. Chate and Manneville in fact report their conclusions based on numerical simulations of the approximating CAs for two values of s , $s = 2.1$ and $s = 3$. We briefly summarize some of their findings.

s -Dependence: First, in contrast to the unique seven CA-rule path found for all values of s for $p = 1$, the CA-rule paths become s -dependent for all orders $p > 1$. For $s = 2.1$, for example, the corresponding CA rules are all either class 1 or class 2, and thus fail to display any spatiotemporal intermittency behavior. For larger values of s – in particular, for $s = 3$ – a threshold coupling ϵ_c appears, separating, as in the $p = 1$ case, trivial/periodic behavior (for $\epsilon < \epsilon_c$) from complex dynamics (for $\epsilon > \epsilon_c$).

Chate and Manneville point out, however, that despite not accounting for the CML's spatiotemporal intermittency for lower values of s , the fact that the CA-approximations for low and high s values have intrinsically “different” behaviors suggests that different underlying processes may actually be responsible for the spatiotemporal disorder for $s = 2.1$ and $s = 3$: a *quasi-deterministic* process for $s \sim 3$ and a *quasi-probabilistic* one for $s \sim 2$. Moreover, this fundamental behavioral difference may provide an important clue as to the lack of universality of the transition ([chate89a], [chate89b]). The quasi-deterministic process is simply an interplay between trivial/periodic class 1/2 rules and complex rules in Wolfram classes 3 and 4. Because of the absence of class 3 and 4 rules in the CA-rule paths for $s = 2.1$, Chate and Manneville ([chate89], [chate90a]) hypothesize that

-- much like the case in directed percolation -- complex spatiotemporal behavior results essentially from a *probabilization* between rules of class 1 or 2 only.[†]

Threshold Convergence to CML Values: How close the value of ϵ_c gets to the spatiotemporal intermittency threshold for the CML, $\epsilon_{c,CML} \sim 0.360$ depends on the approximation method. Because f_p does not converge to f when it is constructed using the pre-images of the laminar state (method I), ϵ_c remains close but does not converge to $\epsilon_{c,CML}$. Method II, on the other hand, assures us that $f_p \rightarrow f$ as $p \rightarrow \infty$ so that we may expect the difference between ϵ_c and $\epsilon_{c,CML}$ to eventually vanish.

Criticality: For $s = 3$ (and other *large* values of s) there appears a transition region consisting of very complex, apparently unpredictable, rules. These rules exhibit most of the characteristics that are typically associated with class 4 rules, such as having irregular, sometimes very long, transients when starting from random states. Chate and Manneville liken this transition region to a *critical surface* in the CA-rule space; “critical-rules” lying on this surface being analogous to critical points in statistical mechanics ([chate90a], [chate90b]). Chate and Manneville further suggest a possible connection -- via the concept of *marginal stability* -- between critical rules and *self-organized criticality*[‡]. A system is said to be *marginally stable* when it is in such a state for which any local perturbation is *just* able to propagate to infinity in space and time. Since the spatiotemporal intermittency transition region represents a threshold *beyond which* disorder can propagate unabated, it can be looked at as representing a marginally stable state.

8.3 Quantum Cellular Automata

Despite having seen ample evidence of the success that CA have in modeling a variety of real physical systems we have thus far only briefly touched upon the possibly much more fundamental role they may play in the *microphysical* domain. Although we will leave the philosophical discussion of (and speculations on) this theme to a later chapter, we note here that despite the well-known *fermion doubling* problem encountered in quantum lattice field theories -- a problem that many cite as reason enough to eliminate any discrete or CA-based theory from serious consideration as a viable fundamental field theory (see [svozil87]) -- there remains a strong belief that a ‘true’ fundamental theory can only be formulated within a totally discrete dynamical framework (see [chew87], [fred90], [jour85] and [noyes87]). Moreover, from a more practical standpoint, as CA get increasingly smaller in size, it will no longer be reasonable to ignore quantum effects; indeed, as the computing scale gets smaller and smaller, quantum effects may well dominate the system behavior

[†]See sections 3.1.4.3 and 7.3 for discussions of the “probabilization” of deterministic rules. The connection between CMLs and probabilistic CA is elucidated further in [chate88a], which provides a detailed discussion of the reduction of the minimal CML defined in equation 8.44 to a probabilistic CA.

[‡]See discussion of Bak, *et.al.*’s sand pile model in section 8.7.

[feyn82]. It is of more than passing interest, therefore, to explore the behavior of microphysically relevant generalizations of simple CA models.

One such obvious generalization is provided by a *quantum CA* (QCA) system, in which the time-evolution of ‘classical’ site variables ‘ σ ’ is replaced by quantum-dynamical transitions between k -component site *state amplitudes* $|\sigma\rangle$. This chapter summarizes the behavior of two simple one-dimensional quantum models: *QCA-I*, developed by Grossing and Zeilinger (see [gross88a], [gross88b], [gross88c] and [gross88d]) and *QCA-II*, introduced by Ilachinski (see [ilach88a] and [ilach88b]).

Conventional CA are defined by assigning to each of the ‘ N ’ linearly connected sites, a time-dependent variable $\sigma_i(t)$ ($i=0,1,\dots,N$), belonging to a finite commutative ring $\mathcal{R}_k$ (usually represented by the integers modulo ‘ k ’, $\mathcal{Z}_k$). These site values, or *colors*, evolve iteratively according to a range- r mapping $\phi: \mathcal{Z}_k^{2r+1} \rightarrow \mathcal{Z}_k$:

$$\sigma_i(t+1) = \phi[\sigma_{i-r}(t), \dots, \sigma_i(t), \dots, \sigma_{i+r}(t)]. \quad (8.50)$$

Although the two quantum models are defined somewhat differently, both QCA-I and QCA-II start with the same basic premise, endowing the *classical* system with two characteristically quantum features. They both (1) replace each site variable with a quantum state containing all ‘ k ’ classical site-color possibilities, and (2) introduce a quantum transition operator ‘ $\hat{\Phi}$ ’, defining mixed color $\rightarrow$ mixed color transitions. Only in QCA-II, however, is $\hat{\Phi}$ also *unitary*; see discussion below.

8.3.1 QCA-I

Focusing on strictly local (i.e. nearest neighbor) interactions, Grossing and Zeilinger [gross88a] consider the following unitary evolution operator U , approximated to first order by:

$$U = \exp\{-iHt/\hbar\} \simeq 1 - iHt/\hbar, \quad (8.51)$$

where, using periodic boundary conditions and assuming $|\delta| \ll 1$, the Hamiltonian H is (for small ϵ) given by

$$H = \begin{pmatrix} \ddots & \ddots & \ddots & & & 0 \\ & \epsilon & 0 & \epsilon^* & & \\ & & \epsilon & 0 & \epsilon^* & \\ & & & \epsilon & 0 & \epsilon^* \\ 0 & & & & \ddots & \ddots & \ddots \end{pmatrix}. \quad (8.52)$$

Using $\delta \equiv \epsilon t/\hbar$, the corresponding evolution operator and rule for QCA-I then become, respectively,

$$U = \frac{1}{\sqrt{N}} \begin{pmatrix} \ddots & \ddots & \ddots & & & 0 \\ & i\delta & 1 & i\delta^* & & \\ & & i\delta & 0 & i\delta^* & \\ & & & i\delta & 0 & i\delta^* \\ 0 & & & & \ddots & \ddots & \ddots \end{pmatrix} \quad (8.53)$$

and

$$\sigma_j(t) = \frac{1}{\sqrt{N}}(\sigma_j(t) + i\delta\sigma_{j-1}(t) + i\delta^*\sigma_{j+1}(t)), \quad (8.54)$$

where N is a normalization factor assuring that $\sum_j |\sigma_j(t)|^2 = 1$ for all times t . Notice that, unless δ is vanishingly small (or the off-diagonal elements somehow manage to conspire in just the right way), $UU^\dagger \neq 1$; i.e. the evolution is in general non-unitary.

Under the scheme presented here, therefore, unitary, reversible quantum mechanics is possible only if the locality requirement is relaxed (see [gross88d] for a brief discussion of how this finding relates to other notions of reversibility). Choosing instead to maintain an analogy with classical CA systems by studying rules that are strictly local, Grossing and Zeilinger use equation 8.54 to define their quantum CA, thus leaving δ as an independent parameter.

The qualitative behavior of this system is most conveniently studied by looking at space-time maps of the normalized probability values $p_j(t) = |\sigma_j(t)|^2$, using grey shades to represent different probabilities. For simplicity, δ is set equal to $\delta_c(1+i)$, and the effects of varying magnitudes of the off-diagonal terms is observed by varying δ_c .

8.3.1.1 General Properties

Consider the evolution of initial states in which only a single site has nonzero amplitude. Figure 8.11 shows grey-scale plots (or *probability maps*) for a system with 125 sites evolving according to equation 8.54 with $\delta = \delta^* = \delta_c = 0.05, 2$ and 20 ; in each case the number of time steps plotted is 600. We make a few general observations.

Probability maps typically exhibit striped wave-like interference patterns. It is easy to show why striped patterns (i.e. patterns for which, at a given time step, the site probabilities alternate between low and high values), emerge for all systems with $\delta_c \geq \sqrt{2}$. Assume that $|\sigma_j(t)| \neq 0$. At time ' $t+1$ ' we then have

$$|\sigma_j(t+1)|^2 = \frac{1}{N}, \quad |\sigma_{j-1}(t+1)|^2 = |\sigma_{j+1}(t+1)|^2 = \frac{2}{N}\delta_c^2, \quad (8.55)$$

followed, at time ' $t+2$ ', by

$$|\sigma_j(t+2)|^2 = \frac{2}{N} \left| \frac{1}{2} - 2\delta_c^2 \right|^2, \quad |\sigma_{j\pm 1}(t+2)|^2 = \frac{4}{N'}\delta_c^2, \quad |\sigma_{j\pm 2}(t+2)|^2 = \frac{2}{N'}\delta_c^4. \quad (8.56)$$

For $\delta_c > \sqrt{2}$, we therefore see that

$$|\sigma_j(t+1)|^2 > |\sigma_{j\pm 2}(t+1)|^2 > |\sigma_{j\pm 1}(t+2)|^2, \quad (8.57)$$

resulting in the characteristic striped pattern of these systems. We note that although the above reasoning does not preclude striped patterns from emerging for $\delta_c < \sqrt{2}$, such patterns are general only local.

As δ_c increases, periodic "ellipse-like" structures emerge whose periods increase with δ_c . What is not shown in the figures, is that as the systems evolve for large

δ_c	General Behavior
~ 0.02	striped waves
~ 0.08	separated interference patterns
~ 0.20	melting interference patterns
~ 0.50	ripples
~ 20	elliptical disks
≥ 4000	"final state" disk

Table 8.7 Classes of behavior in QCA-I [gross88b].

times, the ellipses eventually flatten out and form "plane wave surfaces". Table 8.7 summarizes Grossing and Zeilinger's characterization of the general classes of behavior as a function of δ_c [gross88b].

Now consider what happens if we allow several sites to have non vanishing amplitude at time zero (see figure 8.12). In general, there appear to be three distinct phases of the evolution: (1) a complex transient period during which recognizable large-scale structures first emerge, (2) an intermediate period during which periodic ellipse-like structures appear, followed by (3) a final and stable "plane-wave" pattern.

Both the complexity and the sensitivity to initial states of the patterns generally increases as the number of initial sites with nonzero amplitude increases. As the number of nonzero sites increases, it also becomes increasingly likely that a change in the value of one of those sites (or a move in its location either to the left or right) will significantly alter the resulting pattern.

In general, patterns having more than one nonzero site appear to obey the following two simple rules:

Relative Initial Point Location Rule: if the number of zero sites between nonzero sites is odd the resulting pattern is typically symmetrical and consists of "melting ellipses"; if the number is even, the pattern is distorted or dies out [gross88b].

Constancy in Time Criterion: if the initial state is such that the location of sets of initially nonzero sites is rotationally symmetric with respect to the axis of the torus defined by periodic boundary conditions, the resulting pattern becomes stable after a few time steps and remains conserved for all later times.

8.3.1.2 A Conservation Law

QCA-I systems possess an interesting conservation law. Consider the ellipse-like structures appearing in figures 8.11-b,c and 8.11-b,c. Although, as stated above, these "ellipses" cannot be considered as being truly periodic structures since they eventually flatten out producing plane-waves, there is nonetheless a definite – and, as it turns out, *fixed* – period of time that elapses between the centers of neighboring "ellipse-like" patterns. Moreover, this period remains invariant under changes to either the size of the system or the number of initially nonzero sites.

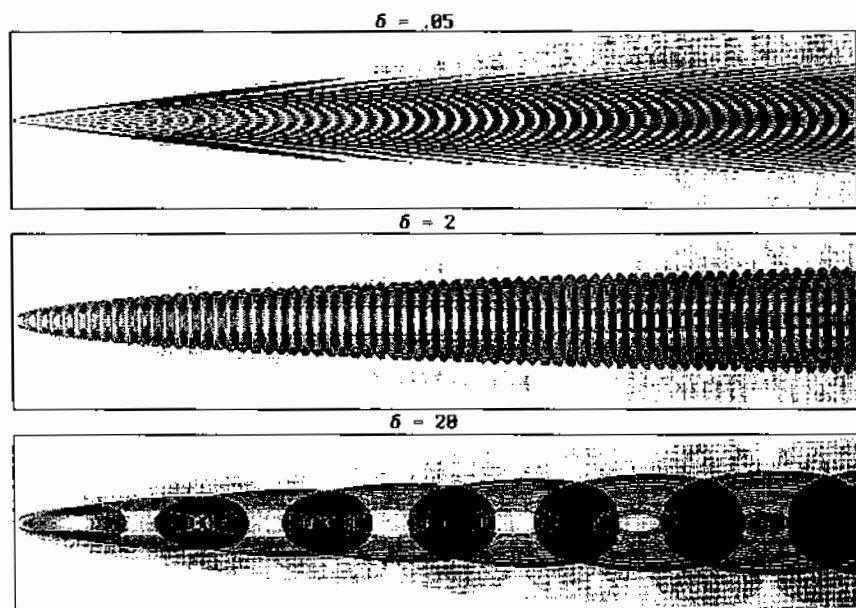


Fig. 8.11 QCA-I Model (Grossing and Zeilinger [gross88b]); see text.

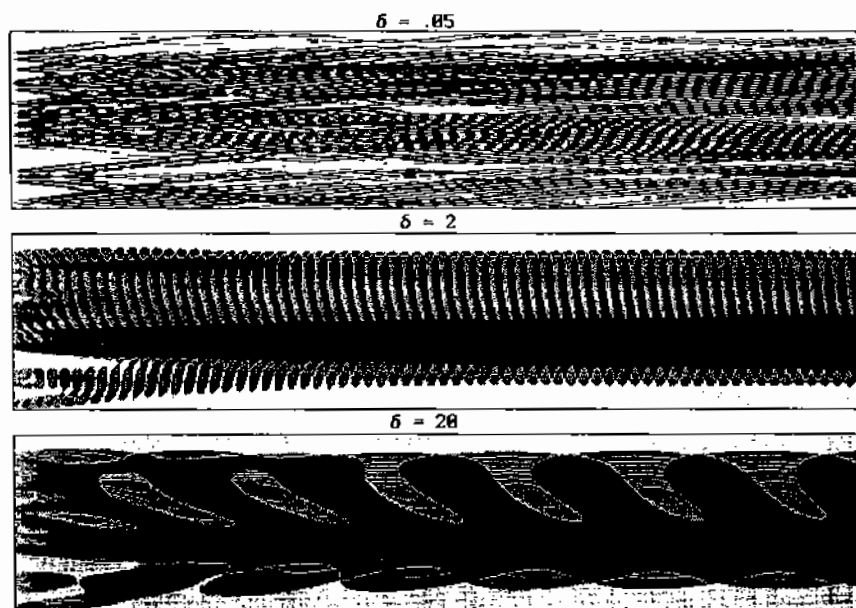


Fig. 8.12 QCA-I Model (Grossing and Zeilinger [gross88b]); see text.

Changing a size 400 system to a size 50 system, for example, effectively speeds-up the decay into a plane wave state but otherwise leaves the period unchanged. Likewise, although patterns starting from two different initial states consisting of either 10 or 20 randomly positioned nonzero sites typically have different appearances, the periodicity of the resulting global structures is exactly the same.

Grossing and Zeilinger have studied this periodicity “invariance” quantitatively, as a function of δ [gross88c]. Generalizing the parameter δ (which they call a *mixing parameter*) to have possibly non-equal real and imaginary components, we write δ as

$$\delta = \delta_c + i\delta'_c = \delta_R e^{i\phi}, \quad (8.58)$$

where $\phi = \tan^{-1}(\delta'_c/\delta_c)$.

Plotting the periodicity ($= \Delta$) of the resulting patterns as a function of δ_R for a variety of phase angles ϕ , Grossing and Zeilinger found that for $\delta_R \gtrsim 1$ and a given value of ϕ ,

$$\Delta = k(\phi) \cdot \delta_R, \quad (8.59)$$

where $7/2 \leq k(\phi) \leq 5$ is a constant depending only on the phase angle ϕ . This constant $k = 7/2$ for $\phi = 0, \pi/2, \pi, \dots$ and $k = 5$ for $\phi = \pi/4, 3\pi/4, \dots$ [§]

Calling $\omega = 1/\Delta$ the *characteristic frequency* of the quantum CA, the general conservation law that holds for QCA-I systems may then be written as

$$\delta_R \cdot \omega = \text{constant}. \quad (8.60)$$

8.3.2 QCA-II

QCA-II, like QCA-I, uses *locality* as a key ingredient to achieving a quantum-dynamical analogue of a classical (or c-) CA system. Unlike QCA-I's evolution operator, however, the QCA-II time-evolution operator is both local and *unitary*. Interestingly enough, the imposition of these two requirements has two consequences: (1) the evolution operator acting on a given site depends on the neighboring site values only *implicitly*, and (2) only a very limited subset of c-CA rules have a direct quantum analogue. Moreover, in a way to be described below, the quantum (or q-) dynamics actually has the c-dynamic evolution embedded within it.

Formally, to each site ‘ i ’ is assigned a k -dimensional complex *color* vector space $\mathcal{C}_i^{(k)}$, spanned by the color eigenvectors $|\sigma^{(0)}\rangle, |\sigma^{(1)}\rangle, \dots, |\sigma^{(k-1)}\rangle$, so that a general state $|\sigma_i(t)\rangle$ is a linear superposition of the $|\sigma^{(j)}\rangle$'s:

[§]Note that no such regularity has been found for $\delta_R < 1$, except for a rapid rise of Δ to infinity for extremely small values of δ_R [gross88c]. The irregular behavior for $\delta_R \leq 1$ is in sharp contrast to the distinct linear relationship between Δ and δ_R for $\delta_R > 1$. The regime of smaller δ_R 's just might deserve a closer look.

$$\begin{cases} |\sigma_i(t)\rangle = \sum_{j=0}^{k-1} \alpha_i^{(j)}(t) |\sigma^{(j)}\rangle, & \text{where} \\ \sum_{j=0}^{k-1} |\alpha_i^{(j)}(t)|^2 = 1 & \forall i, t. \end{cases} \quad (8.61)$$

The physical interpretation of such a state rests in the understanding that upon a color measurement at site ‘ i ’ and time ‘ t ’, there is a probability $|\alpha_i^{(j)}(t)|^2 \equiv |\langle \sigma_i(t) | \sigma^{(j)} \rangle|^2$ of finding the color ‘ j ’.

The global state of the system at any time ‘ t ’, $|\Sigma(t)\rangle$, is the tensor product of the individual site states, and is therefore a vector in a k^N -dimensional tensor product space $\mathcal{C}$.[†]

$$|\Sigma(t)\rangle \equiv \prod_{i=1}^N \otimes |\sigma_i(t)\rangle. \quad (8.62)$$

The time-evolution operator $\hat{\Phi}_i$ acts on each site state $|\sigma_i\rangle$,

$$|\sigma_i(t+1)\rangle = \hat{\Phi}_i |\sigma_i(t)\rangle \quad (8.63)$$

and is, like its classical counterpart, a function of the site-states in the r -neighborhood of site ‘ i ’. It is required to satisfy the following two conditions:

1. $\hat{\Phi}_i$ transforms a state in color eigenstate ‘ j_1 ’ to color eigenstate ‘ j_2 ’ with a probability ‘ p_{j_1, j_2} ’ equal to the probability that a *measurement* of the states in the r -neighborhood of the center-site will reveal them to be such that the ‘classical’ rule ‘ ϕ ’ would have evolved ‘ $j_1 \rightarrow j_2$ ’.
2. $\hat{\Phi}_i$ is *unitary*.

The first condition assures the existence of a classical evolution embedded within the dynamics defined by $\hat{\Phi}$. Specifically, if the member sites of the range- r neighborhood about a given site ‘ i ’ happen to be all in color eigenstates (with $|\sigma_i\rangle = |\sigma^{(j_1)}\rangle$), then $\hat{\Phi}_i |\sigma_i = \sigma^{(j_1)}\rangle = |\sigma'_i = \sigma^{(j_2)}\rangle$ with probability=1, where ‘ j_2 ’ is such that $\phi[\sigma_i = \sigma^{(j_1)}] \rightarrow \sigma'_i = \sigma^{(j_2)}$.[‡] In this way, the probabilistic content of the model is *intrinsically generated* by the dynamics of superposition states and is not some arbitrarily chosen external parameter. That is to say, since $p_{j_1, j_2} = p_{j_1, j_2}(\{\alpha^{(j)}\})$ are fixed functions of state-amplitudes, the dynamics, from the quantum viewpoint, remains strictly deterministic.

The second condition is clearly necessary to achieve any consistent (i.e. probability conserving) quantum dynamics. It has the additional effect of *restricting* the number of classical rules for which a quantum analogue can be constructed (see ‘ $k=2$ ’ example below).

[†]Although, as discussed below, each site-state evolves according to an operator which is a function of its neighboring site-states, the sites nonetheless evolve *independently* of each other. The use of a tensor product description is thus justified.

[‡]The variables ‘ σ_i ’, without a ket, represent classical variables belonging to Z_k .

The full quantum dynamics then takes the general form

$$|\Sigma(t+1)\rangle = \prod_{i=1}^N \hat{\Phi}_i |\sigma_i(t)\rangle, \quad (8.64)$$

where, generally, $\hat{\Phi}_i = \hat{\Phi}_i[|\sigma_j(t)\rangle \in \mathcal{N}'_i]$, where $\mathcal{N}'_i$ is the neighborhood around site 'i' (excluding the center site 'i'); see below.

8.3.2.1 $k=2$ Systems

Consider the QCA-II q-analogue of elementary range $r=1$, $k=2$ c-CA rules. The QCA-II color space $\mathcal{C}_i^{(2)}$ is spanned by $|\sigma^{(0)}\rangle$ and $|\sigma^{(1)}\rangle$, which may be written in the obvious color representation as $|\sigma^{(0)}\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and $|\sigma^{(1)}\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. A general state $|\sigma_i(t)\rangle$ is then written as $|\sigma_i(t)\rangle = \alpha_i^{(0)}(t) |\sigma^{(0)}\rangle + \alpha_i^{(1)}(t) |\sigma^{(1)}\rangle$. The most general action of $\hat{\Phi}_i$, satisfying condition (1) above, is therefore given by

$$\begin{cases} \hat{\Phi}_i |\sigma^{(1)}\rangle &= p_{11}^{1/2}(i) e^{i\beta} |\sigma^{(1)}\rangle + p_{10}^{1/2}(i) e^{i\gamma} |\sigma^{(0)}\rangle \\ \hat{\Phi}_i |\sigma^{(0)}\rangle &= p_{01}^{1/2}(i) e^{i\delta} |\sigma^{(1)}\rangle + p_{00}^{1/2}(i) e^{i\epsilon} |\sigma^{(0)}\rangle, \end{cases} \quad (8.65)$$

where the phases ' β , γ , δ , ϵ ' are real constants, and the ' $p_{jk}(i)$ ' are, for the moment, unspecified functions of lattice position 'i'.

Demanding that $\hat{\Phi}_i$ be unitary as well leads to the explicit matrix form:

$$\hat{\Phi}_i = \begin{pmatrix} p^{1/2}(i) & e^{-i\delta}[1-p(i)]^{1/2} \\ -e^{i\delta}[1-p(i)]^{1/2} & p^{1/2}(i) \end{pmatrix}, \quad (8.66)$$

in which a single phase ' δ ' remains free and $p \equiv p_{11}$. Insofar as the qualitative behavior is independent of ' δ ', it will subsequently be taken as zero.

Observe that $\hat{\Phi}$ is completely defined by the probability of a $|\sigma^{(1)}\rangle \rightarrow |\sigma^{(1)}\rangle$ transition. That is, the underlying classical rule *must* be of the following form:

1. *assuming* ' $\sigma_i = 1$ ', we are free to define the list of all $2r$ -tuples for which $\phi[\sigma_i = 1] \rightarrow [\sigma'_i = 1] : \mathcal{L}_{11}(i) \equiv \{(\sigma_{i-r}^{(k)}, \dots, \sigma_{i-1}^{(k)}, \sigma_{i+1}^{(k)}, \dots, \sigma_{i+r}^{(k)})\}$, $k = 1, 2, \dots, n$.
2. Define $\mathcal{S}^{(2r)}$ to be the set of *all possible* $2r$ -tuples (excluding the center-site). Then our choice for the set $\mathcal{L}_{11}(i)$ *fixes the corresponding set* $\mathcal{L}_{01}(i)$, listing those $2r$ -tuples for which $\phi[\sigma_i = 0] \rightarrow [\sigma'_i = 1] : \mathcal{L}_{01}(i) \equiv \mathcal{S}^{(2r)} - \mathcal{L}_{11}(i)$.

If we choose to have $\phi[1] = [1]$ for $(\sigma_{i-1}, \sigma_{i+1}) = (1, 0)$, for example, then we *must* have $\phi[0] = [1]$ precisely for $(\sigma_{i-1}, \sigma_{i+1}) \in \{(0, 1), (0, 0), (1, 1)\}$ in order to get probability conserving quantum transitions.

Observe that the *classical* evolution is reproduced whenever all ' $2r$ ' neighboring sites of a selected site are in color eigenstates (*i.e.* whenever $|\alpha_i| \in \{0, 1\}$). In this

case the q-operator $\hat{\Phi}$ takes on the following effectively classical form:

$$\hat{\Phi}^{(classical)} \equiv \begin{pmatrix} \phi & 1-\phi \\ 1-\phi & \phi \end{pmatrix}, \quad (8.67)$$

where the c-rule $\phi \in \{0, 1\}$.

Finally, using the physical interpretation of the quantum site-state coefficients ' α_i ', we can write down an explicit form for the probability functions ' p '. Since ' ϕ ' is defined by the list $\mathcal{L}_{11}$, we must simply write down the probability that a measurement of the ' $2r$ ' states around a given site ' i ' will yield a $2r$ -tuple which is an element of $\mathcal{L}_{11}$. We therefore get sums of products of absolute squares, with individual list elements ' $\sigma^{(0)}$ ' contributing the terms $|\alpha^{(0)}|^2$ and list elements ' $\sigma^{(1)}$ ' contributing $|\alpha^{(1)}|^2$:

$$p(i) = \sum_{j \in \mathcal{L}_{11}(i)} \prod_{\substack{k=i-r \\ (k \neq i)}}^{i+r} \{ \sigma_k^{(j)} |\alpha_k^{(1)}(t)|^2 + (1 - \sigma_k^{(j)}) |\alpha_k^{(0)}(t)|^2 \}. \quad (8.68)$$

Table 8.8 lists all non-trivial (independent) ' $k = 2, r = 1$ ' rules for which a q-dynamics exists.

rule #	class	p_{11}
57	2	$ \alpha_{i-1}^{(0)} ^2 \alpha_{i+1}^{(1)} ^2$
108	2	$1 - \alpha_{i-1}^{(1)} ^2 \alpha_{i+1}^{(1)} ^2$
156	2	$1 - \alpha_{i-1}^{(1)} ^2 \alpha_{i+1}^{(0)} ^2$
54	3	$ \alpha_{i-1}^{(0)} ^2 \alpha_{i+1}^{(0)} ^2$
60	3	$ \alpha_{i-1}^{(0)} ^2 \alpha_{i+1}^{(1)} ^2 + \alpha_{i-1}^{(0)} ^2 \alpha_{i+1}^{(0)} ^2$
105	3	$ \alpha_{i-1}^{(0)} ^2 \alpha_{i+1}^{(1)} ^2 + \alpha_{i-1}^{(1)} ^2 \alpha_{i+1}^{(0)} ^2$
150	3	$ \alpha_{i-1}^{(1)} ^2 \alpha_{i+1}^{(1)} ^2 + \alpha_{i-1}^{(0)} ^2 \alpha_{i+1}^{(0)} ^2$

Table 8.8 A list of all (independent) elementary 1-dimensional ' $k = 2, r = 1$ ' rules supporting a QCA-II quantum dynamical analogue of the form defined by equations (5.4) and (5.7). Two additional rules, **51** and **204**, both of class-2, yield $p_{11} = '0'$ and ' 1 ', respectively, so that their q-behavior remains essentially classical. (p_{11} is the $\sigma = 1 \rightarrow \sigma' = 1$ transition probability which defines the quantum operator $\hat{\Phi}$).

Although the above formalism, whose only real characteristically quantum feature is amplitude superposition, defines a very 'simple' toy model[§], the dynamics is far from trivial. Consider, for example, a system consisting of '3' points (linked in a periodic manner), the sites of which evolve according to the q-analog of the following c-rule:

$$' \phi[\sigma_i(t) = 1] \longrightarrow \sigma_i(t+1) = 1' \iff (\sigma_{i-1}(t), \sigma_{i+1}(t)) = (1, 0). \quad (8.69)$$

[§]The model is, in fact an excellent example of a *minimalist quantum theory*, as discussed in [dres86].

The quantum operator $\hat{\Phi}$ is then defined by the probability

$$p_i = |\alpha_{i \oplus 32}^{(1)}(t)|^2 |\alpha_{i \oplus 31}^{(0)}(t)|^2, \quad (8.70)$$

where ' $\oplus_3$ ' is addition *modulo-3*. We find that the global state $|\Sigma(0)\rangle$, a vector in the $2^3=8$ dimensional space $\mathcal{C}$:

$$|\Sigma(0)\rangle = \begin{pmatrix} \alpha_0^{(1)} & \alpha_1^{(1)} & \alpha_2^{(1)} \\ \alpha_0^{(1)} & \alpha_1^{(1)} & \alpha_2^{(0)} \\ & \cdot & \\ & \cdot & \\ \alpha_0^{(0)} & \alpha_1^{(0)} & \alpha_2^{(0)} \end{pmatrix}, \quad (8.71)$$

evolves, upon a *single iteration*, into $|\Sigma(1)\rangle = \prod_{i=1}^3 \otimes \hat{\Phi}_i |\sigma_i(0)\rangle =$

$$\begin{pmatrix} (p_0^{1/2} \alpha_0^{(1)} + (1-p_0)^{1/2} \alpha_0^{(0)}) (p_1^{1/2} \alpha_1^{(1)} + (1-p_1)^{1/2} \alpha_1^{(0)}) (p_2^{1/2} \alpha_2^{(1)} + (1-p_2)^{1/2} \alpha_2^{(0)}) \\ (p_0^{1/2} \alpha_0^{(1)} + (1-p_0)^{1/2} \alpha_0^{(0)}) (p_1^{1/2} \alpha_1^{(1)} + (1-p_1)^{1/2} \alpha_1^{(0)}) (p_2^{1/2} \alpha_2^{(0)} - (1-p_2)^{1/2} \alpha_2^{(1)}) \\ \cdot \\ \cdot \\ (p_0^{1/2} \alpha_0^{(0)} - (1-p_0)^{1/2} \alpha_0^{(1)}) (p_1^{1/2} \alpha_1^{(0)} - (1-p_1)^{1/2} \alpha_1^{(1)}) (p_2^{1/2} \alpha_2^{(0)} - (1-p_2)^{1/2} \alpha_2^{(1)}) \end{pmatrix}. \quad (8.72)$$

Despite having a simple physical interpretation, it is clear that quantum states generally have very complex formal representations.

8.3.2.2 $k=3$ Systems

In the color representation $|\sigma^{(2)}\rangle \equiv \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $|\sigma^{(1)}\rangle \equiv \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ and $|\sigma^{(0)}\rangle \equiv \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$,

the imposition of the two operator conditions leads to

$$\hat{\Phi}^{(k=3)} = \begin{pmatrix} p_{22}^{1/2} & p_{21}^{1/2} & -(1-p_{22}-p_{21})^{1/2} \\ (1-p_{22}-p_{21})^{1/2} & \eta & (p_{22}+p_{21}-\eta^2)^{1/2} \\ -p_{21}^{1/2} & (1-p_{21}-\eta^2)^{1/2} & \eta \end{pmatrix}, \quad (8.73)$$

where $\eta = \eta(p_{22}, p_{21})$ is chosen to make $\hat{\Phi}$ unitary:

$$\eta = (1-p_{22}-p_{21})^{1/2} p_{21}^{1/2} \frac{(1-p_{22}^{1/2})}{1-p_{22}}. \quad (8.74)$$

Note that $\hat{\Phi}$ in this case is completely specified by the *two* transition probabilities

' p_{21} ' and ' p_{22} ':

$$p_{2\beta}(i) = \sum_{j \in \mathcal{L}_{2\beta}(i)} \prod_{\substack{k=i-r \\ (k \neq i)}}^{i+r} \left\{ \sum_{s=0}^2 \delta_{\sigma_k^{(j)}, s} |\alpha_k^{(s)}(t)|^2 \right\}, \quad (8.75)$$

where $\mathcal{L}_{2\beta}(i)$ is an explicit list of all $2r$ -tuples for which $\phi[\sigma_i=2] \rightarrow [\sigma'_i=\beta]$, $\beta \in \{1, 2\}$, ' $\delta_{i,j}$ ' is the *Kronecker delta* and $p_{21} + p_{22} \leq 1$ always.

Since $\eta = 0$ whenever p_{22} or p_{21} are zero, the corresponding *classical* behavior of eigenstates $|\sigma^{(1)}\rangle$ and $|\sigma^{(0)}\rangle$ must always involve a color change. In particular, the matrix form of the classical evolution is given by

$$\hat{\Phi}^{(classical)} \equiv \begin{pmatrix} \delta_{2,\phi} & \delta_{1,\phi} & \delta_{0,\phi} \\ \delta_{0,\phi} & 0 & 1 - \delta_{0,\phi} \\ \delta_{1,\phi} & 1 - \delta_{1,\phi} & 0 \end{pmatrix}, \quad (8.76)$$

where $\phi = \phi[\sigma_{i-r}, \dots, \sigma_{i+l}] \in \{0, 1, 2\}$. The formal extension to higher dimensions and other lattice structures is straightforward.

8.3.2.3 General Properties

When ' $k = 2$ ', $\hat{\Phi}$ is diagonalized by the matrix $\mathcal{U} \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}$. Although this makes a formal solution for the state at site ' k ' at time ' t ' straightforward, in principle:

$$|\sigma_k(t)\rangle = \mathcal{U} \begin{pmatrix} \prod_{j=0}^{t-1} [p_j^{1/2} + i(1-p_j)^{1/2}] & 0 \\ 0 & \prod_{j=0}^{t-1} [p_j^{1/2} - i(1-p_j)^{1/2}] \end{pmatrix} \mathcal{U}^{-1} |\sigma_k(0)\rangle, \quad (8.77)$$

where ' p_j ' is evaluated at the site ' k ' at time ' $t = j$ ', the *range-dependence* of ' p_j ' assures that the behavioral evaluations of quantum systems are at least as difficult to come by as that of their classical counterparts.

It is instructive to first of all consider the case when $p_j \equiv p$ for all sites ' k ' and times ' j ' (i.e. a quantum model which retains the dynamical form of equations 8.66 and 8.73 but in which $p(i)$ are *externally* chosen and fixed in time and space). In this crude approximation to the fully range-dependent q-model, it is easy to calculate $\mathcal{W}[\sigma^{(1)}; t] \equiv$ the probability of finding the color ' $\sigma^{(1)}$ ' at time ' t '. Choosing an initial q-state with equal color amplitudes ($|\sigma(0)\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$), for example, we find that

$$\begin{aligned} \mathcal{W}[\sigma^{(1)}; t] &\equiv |\langle \sigma(t) | \sigma^{(1)} \rangle|^2 = \frac{1}{8} |(\mathcal{P}^t + \mathcal{P}^{*t}) + i(\mathcal{P}^{*t} - \mathcal{P}^t)|^2 \\ &= \frac{1}{2} + \frac{1}{2} \sin 2\theta t, \end{aligned} \quad (8.78)$$

where $\mathcal{P} \equiv p^{1/2} + i(1-p)^{1/2}$ and $\theta \equiv \tan^{-1} \sqrt{p^{-1} - 1}$. This typically quantum-like oscillatory probabilistic behavior appears to shape much of the qualitative development of the fully dynamic model as well.

Ilachinski [ilach88] has performed numerical investigations of a variety of systems, including all ' $k=2, r=1$ ' rules listed in table (8.8) and an extensive sampling of systems evolving according to ' $k=3, r=1$ ' and ' $k=2, r=2$ ' rules. We make the following general observations:

1. Suppose we start from an initial state in which all sites are in color eigenstates $|\sigma^{(0)}\rangle$, except for a single site at ' i_0 ' which is in the state $|\sigma_{i_0}\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

Since $\hat{\Phi}$ becomes a $(0,1)$ -matrix for all sites except for those in the immediate $r=1$ neighborhood around ' i_0 ' (see equation 8.66), the eigenstates *outside* of this neighborhood get mapped into color-eigenstates corresponding to the classical colors to which ϕ itself would map a given color. Site-locations of superposition states propagate outward from ' i_0 ', developing threshold patterns unique to each given rule.[†] Figure 8.13 shows threshold maps of the evolution of the q-analogs of CA rules R57, R156 and R105, each starting from an initial state with a single mixed color-state.

2. Recognizable regularity in probability patterns, starting from randomly selected initial site-states, generally appears only when the measurement threshold is significantly less than certainty.

3. Occasionally, such as in the post-transient q-development of rule R57, which consists of very well defined wave-like space-time *bands* within which the probability of measuring color ' $\sigma^{(1)}$ ' at individual sites is exceedingly high ($\sim 50\%$ of all sites have $\mathcal{W} > .98$)[†] a particular rule will yield patterns in which there is an almost *classical-like certainty* of measuring a selected color. It is generally true, that the color-probability distribution tends to be more heavily weighted toward this *near-classical* regime.

4. There is a qualitative universality in the quantum behavior of class-3 rules, whose threshold plots typically consist of strong local oscillation patterns. Although clearly a manifestation of the fundamental additivity of probability amplitudes, the majority of patterns also possess distinctive *local regularities* by which evolutions defined by particular rules can be uniquely identified: characteristic features of the

[†]We should emphasize the characteristic difference between classical and quantum ST-developments. Classically, of course, it is easy to directly show the true state of each site; in the quantum case, however, each state consists of all ' k ' classical color possibilities. We may take one of at least two options: either (1) use a grey-scale map as we had done earlier for the QCA-I model, or (2) use a *threshold probability map*, whereby a site is colored black if and only if the probability of observing a given color at that site exceeds some selected threshold value. It turns out that, for QCA-II systems, the second option is more convenient. A quantum space-time (or q-ST) plot therefore represents only a possible sequence of color measurements (*modulo* a chosen confidence level of observing the selected color ' $\sigma^{(1)}$ ' (when ' $k=2$ ', of course, it also represents the threshold value of the *average color* measured at given sites).

[†]We might also mention that, for this rule, the region of *color-indeterminacy*, somewhat arbitrarily defined as the set of sites having $.4 < \mathcal{W} < .6$, takes on a similarly regular band-pattern.

classical ST patterns are *locally reproduced* in the quantum evolution (with varying degrees of measurement certainty). This local reproduction is particularly strong for *class-2* rules. Thus, the band-pattern of rule **R57** mimics the periodic classical pattern, the vertical strips characterizing the classical evolution of rules **R108** and **R156** show up distinctly in their quantum analogs, and, although the quantum evolution of each of the $k=2$, $r=1$ *class-3* rules consists of similar local probability oscillations, each nonetheless maintains a unique oscillation pattern.

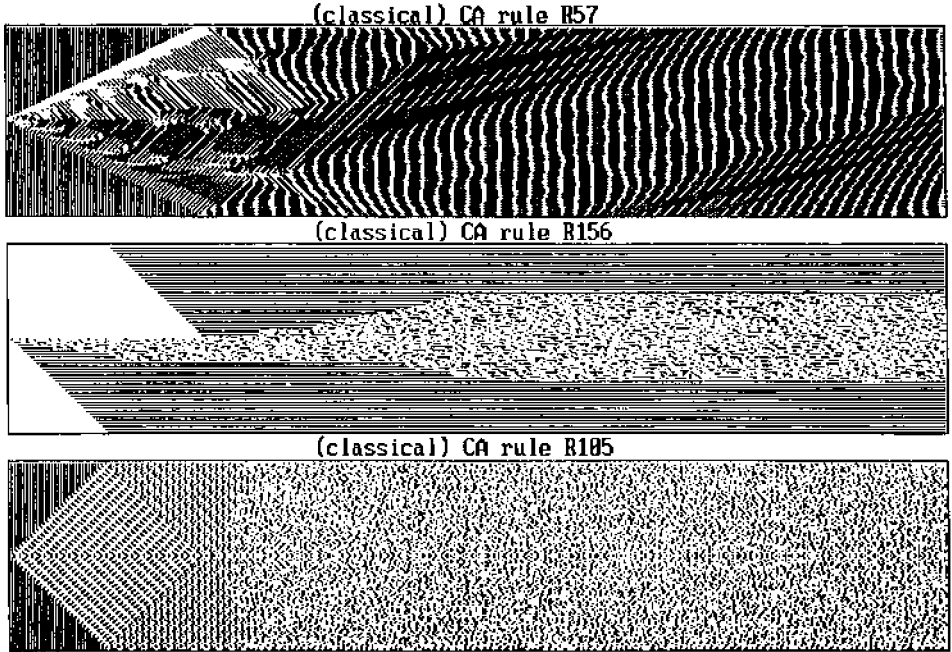


Fig. 8.13 QCA-II Model (Ilachinski [ilach88a]); see text.

5. Quantum patterns for $k=2$, $r=2$ systems also typically appear random except for local patches of regularity. Color measurements within these regions tend to reveal, with high probability ($\mathcal{W} = 0.9$), local color patterns that mimic their classical counterparts. ' $k=3$ ' patterns display a much smaller degree of regularity, even at relatively low threshold values. A typical sequence of color measurements for these systems will only very minimally resemble the classical evolution.

6. Much of the regularity in classical systems can often be best discerned directly by observing their spatial power spectra (see section 6.3). We recall that in the simplest cases, the spectra consist of few isolated discrete peaks; in more complex chaotic evolutions, we might get white noise patterns (such as for elementary additive rules). A discrete fourier transform (f_ν) of a typical quantum state is defined in the most straightforward manner:

$$f_\nu \equiv \frac{1}{N} \sum_{i=0}^{N-1} e^{-i2\pi\nu i/N} |\alpha_i^{(1)}|^2. \quad (8.79)$$

For classical evolutions, we merely substitute ' σ_i ' for $|\alpha_i^{(1)}|^2$. Looking at plots of $N |f_\nu|^2$ vs. ν/N , it is clear that although the quantum dynamics generally appears to preserve the characteristic structure of the classical spectrum, particular structural details tend to be *washed-away* [ilach88b]. If high or low frequency components are heavily favored in the classical evolution, for example, they will similarly be favored in the quantum model; discrete peaks, however, will usually disappear. White-noise spectra, of course, will remain so in the quantum model.

We conclude this section with a short 'philosophical' aside. It is the opinion of the authors of this book, that the single greatest lesson to be taken away from even a cursory examination of CA systems – indeed, the one deep “truth” behind all CA systems – is their constant reminder that complex dynamical behavior need not always be a result of a complex dynamical origin. By demonstrating the existence of self-organized behavior, CA provide a powerful conceptual paradigm for thinking about possible origins of real physical complexity. Except for a few isolated speculations about their possible relevance to the complexities in real microphysics, however, have thus far remained effectively unexplored. Models such as the two defined in this chapter, and others incorporating similar intrinsically quantum-like features, should give us a hint as to whether the paradigm is deep enough to begin probing truly fundamental physics (see chapter 12 for an in-depth exploration of this theme).

8.4 Reaction-Diffusion Systems

In this section we introduce several CA models of prototypical *reaction-diffusion* systems. Such systems, the first formal studies of which date back to Turing[†], often exhibit a variety of interesting spatial patterns that evolve in a self-organized fashion.

A large class of *reaction-diffusion* reactions may be expressed by the (deceptively simple) equation

$$\frac{\partial \mathbf{s}}{\partial t} = \Psi(\mathbf{s}) + \Gamma \nabla^2 \mathbf{s}, \quad (8.80)$$

where $\mathbf{s}(\mathbf{x}, t)$ is a vector that describes the state of the system, $\Psi(\mathbf{s})$ is a reaction term that describes the kinetics of the medium, and $\Gamma \nabla^2$ defines the diffusion. In general, $\Psi(\mathbf{s})$ is either some polynomial or rational function of $\mathbf{s}$, and the (diagonal) diffusion matrix $\Gamma = \text{diag}(\Gamma_1, \dots, \Gamma_N)$ defines the manner in which the chemicals diffuse with different diffusion coefficients. Since most systems of interest are typically much too complicated to be solved analytically, one must usually resort to numerical solution. Two excellent reviews of the mathematical theory behind reaction-diffusion equations are given by Kuramoto [kura84] and Fife [fife79].

[†]Turing studied certain problems of embryology in the 1950s. His model, in which the initial symmetry of a system is, under certain circumstances, broken by the action of reacting and diffusing chemicals, leads to the emergence of spatial structures resulting from non-homogeneous patterns of certain chemical substances called *morphogens* [turing52].

8.4.1 *The Belousov–Zhabotinskii Reaction*

One of the most famous reaction-diffusion systems – widely regarded as the prototypical example of oscillating chemical reactions – is the so-called *Belousov–Zhabotinskii* (or *BZ*) reaction. Although the specifics of the reaction have changed somewhat from Belousov’s original experiments in the 1950’s in the (old!) Soviet Union ([belous58], [winf84]) and Zhabotinskii’s subsequent modifications ([zhabo64], [zaik70]), all of the different variants of the basic reaction produce a similar set of often striking spatial patterns. In its present incarnation, the BZ model involves the reaction of bromate ions with an organic substrate (typically malonic acid) in a sulfuric acid solution with cerium (or some other metal-ion catalyst). When this mixture is allowed to react exothermally at room temperature, interesting temporal and spatial oscillations (i.e. chemical waves) result ([winf85a], [winf85b], [zaik70]). The system oscillates, changing from yellow to colorless and back to yellow about twice a minute, with the oscillations typically lasting for over an hour (until the organic substrate is exhausted).

There exist many different CA models exhibiting BZ-like spatial waves. One of the simplest, and earliest, described in the next section, is a model proposed by Greenberg and Hastings in 1978 [green78], and based on an earlier excitable media model by Weiner and Rosenbluth [weiner46].[†] One of the earliest and simplest *mathematical* models of the BZ reaction, called the *Oregonator*, is due to Field and Noyes [field74].

The BZ reaction has proven to be an incredibly rich source of complex dynamical behavior. Since a thorough discussion of most of the following phenomena would take us too far afield from the focus of this book, we mention only in passing that, in addition to its oscillatory behavior, the BZ reaction has also been observed to give rise to *chemical chaos* [schmitz77], *birhythmicity* [roux83] and has been used as a prototype system in studies on *coupled oscillators* ([marek75], [crow89]). A nice overview discussion of some of these behaviors may be found in [epstein90].

8.4.2 *Greenberg–Hastings Model*

Citing a number of earlier – and, in their opinion, unnecessarily complicated – research efforts to duplicate the characteristic spatial patterns of BZ-like reactions,[§] Greenberg and Hastings wanted to construct a model that reproduced such patterns in the *simplest possible manner*, doing away with the need for extensive computation as the only means by which the desired results can be obtained. Previous studies,

[†]Weiner and Rosenbluth had used a discrete diffusion model with excitable kinetics to study phenomenologically observed spatial phenomena in cardiac muscle tissue.

[§]Greenberg and Hastings cite papers by Balkhovskii [balak65], Gul’kho and Petrov [gul72], Reshodko and Bures [resh75], and Winfree [winf74]. The authors assert that Winfree’s heuristic explanation of the appearance of spiral spatial patterns in terms of the interaction of diffusion and the local dynamics near the core of the spirals left the precise mechanism of the formation of such spirals unclear, particularly in view of the complicated nature of the differential equations used to describe them.

they maintained, tended to obscure rather than elucidate the simplicity of the actual mechanisms responsible for the oscillatory behavior.

The Greenberg-Hastings model [green78] uses the two-dimensional von-Neumann neighborhood and assumes that each site is populated by variables σ that take on one of three values: $\sigma_{i,j} \in \{0, 1, 2\}$. It is important to have at least three values since the dynamics of excitable media are typically characterized by the following three states and/or phases: (1) a globally stable equilibrium state, (2) a transient excited state that is induced by some stimulus exceeding a prescribed threshold level, and (3) a refractory period, during which the medium no longer responds to stimulus and gradually returns to its resting state.

The sites are updated according to

$$\sigma_{i,j}(t+1) = \mathcal{R}(\sigma_{i,j}(t)) + \mathcal{D}(\sigma_{i,j}(t), \sigma_{i-1,j}(t), \sigma_{i+1,j}(t), \sigma_{i,j-1}(t), \sigma_{i,j+1}(t)), \quad (8.81)$$

where the ‘reaction’ ($= \mathcal{R}$) and ‘diffusion’ ($= \mathcal{D}$) terms are given by, respectively,

$$\begin{aligned} \mathcal{R}(\sigma) &= \begin{cases} 2 & \text{if } \sigma = 1, \\ 0 & \text{else,} \end{cases}, \\ \mathcal{D}(\sigma_0, \sigma_1, \sigma_2, \sigma_3, \sigma_4) &= \begin{cases} 1 & \text{if } (\sigma_1 = 1 \text{ or } \sigma_2 = 1 \text{ or } \\ & \sigma_3 = 1 \text{ or } \sigma_4 = 1) \text{ and } \sigma_0 = 0, \\ 0 & \text{else.} \end{cases} \end{aligned} \quad (8.82)$$

Heuristically, the dynamics proceed as follows: the reaction term makes all *active* ($\sigma = 1$) and *refractory* ($\sigma = 2$) sites cycle to their respective successor states. The diffusion term defines the manner in which ‘activity’ (defined by sites with value $\sigma = 1$) diffuses through the lattice.

Specifically, a given site becomes ‘active’ on the next time step if at least one of its neighbors is already active; otherwise it becomes quiescent ($\sigma = 0$). Once a given site has become active, it becomes *refractory* ($\sigma = 2$) on the next time step. Refractory sites are both insensitive to the values of neighboring sites and incapable of activating them. Upon becoming *refractory*, sites attain the quiescent state on the next time step.

A prominent feature of the spatial patterns that typically emerge from random initial states – very reminiscent of the patterns observed in BZ reactions – is a collection of outwardly winding *spiral* waves, centered on a variety of local ‘singularities’. These are clearly evident in figure 8.14-a and 8.14-b, for example, which show a snapshot views of a 320×200 lattice after 50 and 500 iteration steps, respectively, starting from a random initial state consisting of 5% *active* and 5% *refractory* sites. Notice that the spirals are not truly circular-wave-like, but rather are square-like, retaining and showing-off the symmetry of the neighborhood structure of the underlying lattice.

The spirals are composed of active wavefronts propagating over regions of quiescent sites. Simple singularities around which long-wavelength spirals form include local configurations of the form $\begin{pmatrix} \cdots, 0, 1, \cdots \\ \cdots, 2, 2, \cdots \end{pmatrix}$, $\begin{pmatrix} \cdots, 2, 0, \cdots \\ \cdots, 1, 1, \cdots \end{pmatrix}$, $\begin{pmatrix} \cdots, 1, 2, \cdots \\ \cdots, 0, 0, \cdots \end{pmatrix}$

and $\begin{pmatrix} \dots, 1, 0, 2, \dots \\ \dots, 2, 0, 1, \dots \end{pmatrix}$, where ‘ $\dots$ ’ represent arbitrary site values.

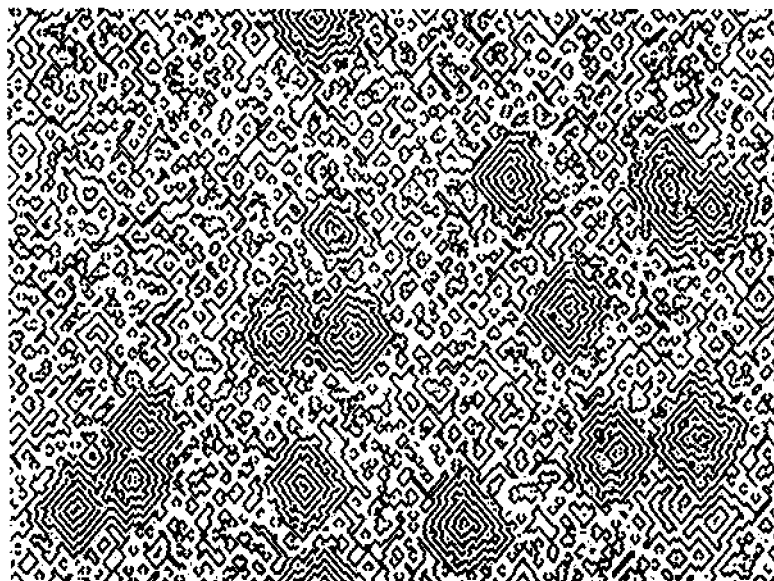


Fig. 8.14-a Greenberg-Hastings model of the BZ-reaction; 320×200 lattice after 50 iteration steps, starting from a random initial state consisting of 5% active and 5% *refractory* sites.

More complex singularities that generate shorter wavelength waves sometimes result from collisions between these simple singularities. In general, each singularity defines some region that is covered by the traveling waves emanating from them. A stationary boundary forms between regions generated from different singularities. After some transient period, a steady state is reached in which waves continually propagate from the singularities to the boundaries (see figure 8.14-b).

8.4.3 Hodgepodge Rule

Another rule exhibiting the characteristic spiral structures induced by BZ-like reactions is the *Hodgepodge* rule, introduced recently by Gerhardt and Schuster [gerh89]. The model is based on a heterogeneous catalytic reaction first investigated empirically by Jaeger *et.al.* ([jaeger81], [jaeger85]).[†] Gerhardt and Schuster's motivation was to investigate whether the complex temporal oscillation patterns of the CO_2 production are correlated with the formation of spatial structures on the catalyst, as caused by various local interactions between different ‘catalytic agents’

[†]Namely, the oxidation of carbon monoxide catalyzed by palladium crystals incorporated into a zeolite matrix.

[gerh89].[†] Much to their surprise, they found that their CA model not only fairly-well describes the CO oxidation, but also gives rise to the same circular and spiral wave structures seen in many BZ-like systems.

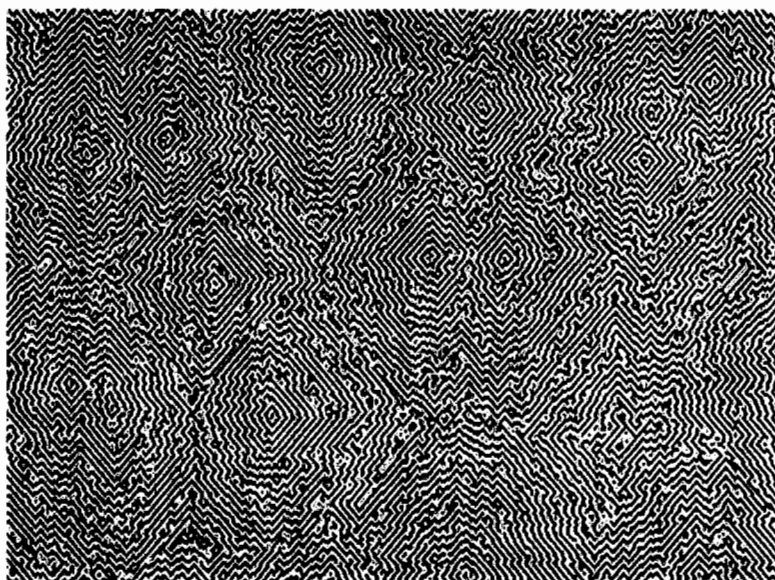


Fig. 8.14-b Greenberg-Hastings model of the BZ-reaction; 320×200 lattice after 500 iteration steps, starting from a random initial state consisting of 5% active and 5% refractory sites.

The *Hodgepodge* rule can be defined on the von Neumann or Moore neighborhoods (and arbitrary-sized extensions of them). Like the Greenberg-Hastings model discussed in the previous section, the Hodgepodge rule associates the values of sites with three different site *types*. Under the Hodgepodge rule, however, the number of what Greenberg and Hastings had called *active* sites is increased from one to an arbitrarily specified value. Site variables σ therefore take on any of N different values, $\sigma \in \{0, 1, 2, \dots, N\}$.

Choosing to describe their rule in terms of a spread of a disease, Gerhardt and Schuster interpret σ as follows. Cells whose value $\sigma = 0$ are labeled as *healthy* cells; cells with value $\sigma = N$ are labeled as *ill* cells; cells with intermediate values $1 < \sigma < N$ are called *infected*. The temporal evolution of the system, parameterized by constants μ_K , μ_I and ν (see below), is then defined in terms of these three different ‘infection’ states.

Healthy Cells: In analogy to the catalytic reaction in the chemical system, in

[†]Their assumption was that the formation of spatial structures on the catalyst is caused purely by local interactions between different catalytic agents in the form of heat transfer and CO diffusion [gerh89].

which a catalytic agent in the palladium phase can be exited either by heat transfer from neighboring particles *developing* into the palladiumoxide phase or by neighboring particles already *in* the palladiumoxide phase, healthy cells are assumed to become *infected* if a certain number of either infected or ill cells are in their neighborhood. Introducing parameters $0 < \mu_K \leq N$ and $0 < \mu_I \leq N$ to control the infection/ illness efficacy rate, we thus have that

$$\sigma_{ij}(t+1) = \left\lceil \frac{K_{ij}(t)}{\mu_K} \right\rceil + \left\lceil \frac{I_{ij}(t)}{\mu_K} \right\rceil \quad \text{for } \sigma_{ij}(t) = 0, \quad (8.83)$$

where $[x] \equiv \text{least integer } m < x$ and $K_{ij}(t)$ and $I_{ij}(t)$, respectively, give the number of ill and infected cells neighboring cell ' ij ' at time ' t ':

$$\begin{aligned} K_{ij}(t) &= \{\text{Number of } (r, s) \mid (r, s) \in \mathcal{N}_{ij} \text{ and } \sigma_{rs} = N\}, \\ I_{ij}(t) &= \{\text{Number of } (r, s) \mid (r, s) \in \mathcal{N}_{ij} \text{ and } 0 < \sigma_{rs} < N\}. \end{aligned} \quad (8.84)$$

Infected Cells: Infected cells are assumed to gradually, and linearly, approach the ill state as a function of the *average degree of infection* in their neighborhood. Define $S_{ij}(t)$ as the average degree of infection of sites neighboring site ' (i, j) ' at time ' t ':

$$S_{ij}(t) = \frac{1}{I_{ij}(t)} \sum_{(r,s) \in \mathcal{N}_{ij} \mid 0 < \sigma_{rs}(t) < N} \sigma_{rs}(t). \quad (8.85)$$

The evolution of infected cells is then determined by

$$\sigma_{ij}(t+1) = \min(S_{ij}(t) + \nu, N), \quad \text{for } 0 < \sigma_{ij}(t) < N, \quad (8.86)$$

where $\min(x, y)$ is equal to the smaller of the two values x and y , and ν is some fixed integer. Gerhardt and Shuster interpret the local averaging process as a heat transfer between neighboring catalytic units [gerh89].

Ill Cells: Once a site becomes *ill*, it immediately (i.e. on the next time step) reverts back to being healthy:

$$\sigma_{ij}(t+1) = 0, \quad \text{for } \sigma_{ij}(t) = N. \quad (8.87)$$

This can be interpreted as the reduction of a catalytic unit after the palladiumoxide phase has been reached.

As an example, consider a system of size 20×20 , and take $N = 100$, $\mu_K = 2$ and $\mu_I = 3$. What happens if we vary the parameter ν between the value 1 and, say, 20? Gerhardt and Schuster found that when this system evolves from a random initial state (using the Moore neighborhood for updates), some combination of four basic behavioral types emerges [gerh89]. Behavioral types – which appear to depend most strongly on the value of the parameter ν – are characterized by both the *manner* in which the *fraction of sites that are infected* ($\equiv f_I$) varies as a function of *time* and the *kind of transition-wave spatial patterns* that develop:

- *Type 1* – $f_I \sim 1$ for all times ‘ t ’, with small deviations away from the maximal infection coverage occurring at irregular intervals; transition waves travel only a short distance before dying out; type-1 behavior typically appears for $2 \leq \nu \leq 4$.
- *Type 2* – $f_I = f_I(t)$ is characterized by a saw-tooth-like pattern of peaks of various amplitudes, with the peaks appearing at almost regular intervals; transition waves travel outward from a central focus to the boundary, with widely differing radii; type-2 behavior typically appears for $3 \leq \nu \leq 8$.
- *Type 3* – $f_I = f_I(t)$ oscillates, with nearly regular periods, between $f_I = 1$ and $f_I \lesssim 0.1 - 0.3$, with the lower amplitudes all having nearly the same value; transition waves are similar to those of type-2 in that they spread out from local foci, but here appear to be much more regular; type-3 behavior typically appears for $7 \leq \nu \leq 20$.
- *Type 4* – $f_I \sim 0.75$ for all times ‘ t ’, with only small deviations; transition waves cover the entire lattice in the form of *spirals*; type-4 behavior typically appears for $13 \leq \nu \leq 20$; see figure 8.15 for an example of a type-4 spatial pattern.

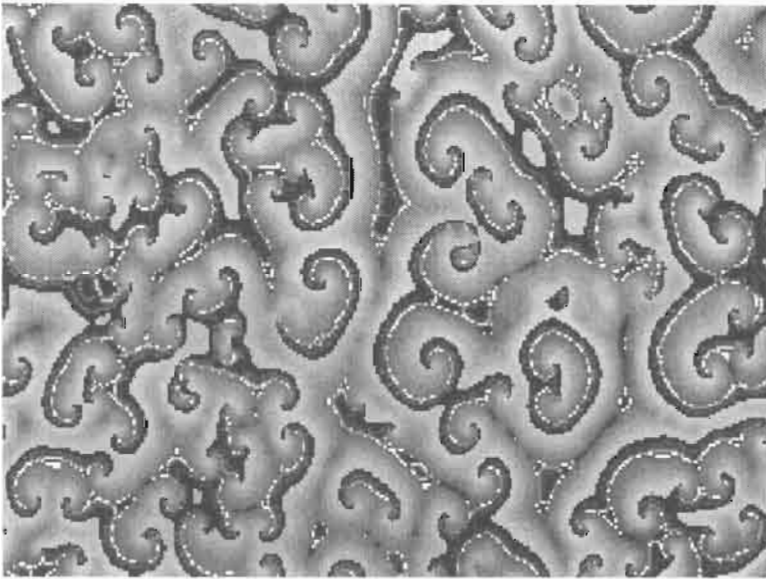


Fig. 8.15 Screenshot from a run of Gerhardt and Schuster's *Hodgepodge* CA rule.

Note that a given value of ν does not define the behavioral type, as there is considerable overlap with transitions between individual types of behavior fairly common. For example, the system can switch back and forth between type-3 and type-4 behavior for $\nu = 15$.

8.5 Applications to Immunology

Although immunology is not, at first sight, as obvious or as “natural” a choice for CA simulation as are lattice gases and spin systems, in recent years a number of authors have nonetheless developed interesting immunologically motivated CA models (see, for example, [kaufm91], [pand91] and [stew91]). This discussion follows recent reviews by Stauffer ([stauff90b], [stauff91a] and [stauff92]). For background information on immunology, the interested reader can consult [perel88].

A properly functioning immune system helps protect the body against bacterial and viral infections. It consists of several different types of cells. When a foreign element such as a virus (or antigen) ($= V$), enters the body, it is recognized by the body’s white blood cells which then trigger the immune system to produce antibodies ($= A$) to neutralize the invading antigens. Because antigens may come in a variety of shapes, antibodies must also be appropriately shaped, or “fitted,” to a particular antigen, analogously to the way a key is fitted into a lock.

In addition to antibodies, the immune system also consists of bone-marrow derived lymphocytes, or B cells, and T cells that come from the thymus gland, both of which (indirectly) produce antibodies. These cells, in turn, may be helped by helper cells ($= H$) and suppressed by suppressor cells ($= S$). Helper cells may be alarmed as to the presence of antigens by macrophages ($= M$) that eat the antigens and leave parts of their meal on their cell surface.

The immune system can malfunction either by attacking itself or the body (which happens in auto-immune diseases such as multiple sclerosis) or by being weakened itself in some way (such as what occurs as a result of the AIDS virus).

We now describe two simple CA models of (1) a normal immune response, and (2) an auto-immunity malfunction due to AIDS. The general idea, first outlined by Atlan [atlan89], is simple enough. We merely discretize the concentrations of each type of cell (high concentration $\longleftrightarrow 1$; low concentration $\longleftrightarrow 0$) and assume that these concentrations interact in some local deterministic manner. The result is (perhaps a grossly simplified) mean-field-like model of a body being invaded by a homogeneous concentration of cells. In the case where an infection spreads throughout a body in minutes or hours and the body’s immune response proceeds on the order of days, the approximation may not be that far-fetched. In the case of more slowly growing localized clusters of cancer-cells, say, an even more CA-like model on a full lattice might be appropriate.

8.5.1 Normal Immune Response

The normal immune response is modeled using antibodies A , B cells, helpers H , suppressors S and antigens, or viruses, V . Each of these concentrations can be either *high* ($= 1$) or *low* ($= 0$). The dynamics is defined as follows:

$$\begin{cases} A &= B \cdot H \cdot V, \\ B &= (B + V) \cdot H, \\ H &= H + (1 - S) \cdot V, \\ S &= H + S, \\ V &= V \cdot (1 - A). \end{cases} \quad (8.88)$$

We can interpret these equations in the following way. The first line assures us that antibodies will be present only when B cells, helper cells and antigens are all present. The second line states that B cells will grow if antigens and/or B cells are present and if helped by helper cells. The third line indicates that helper cells arise either if other helper cells are present or, if no suppressor cells are present, if there are any antigens. The fourth line yields suppressor cells if suppressor cells are already present and/or there are any helper cells. The last line implies that the antigen remains if there are no antibodies or vanishes if antibodies are present. Since concentrations cannot exceed '1,' it is understood that, in the above equations, $1 + 1 = 1$.

Consider, for example, the case where a virus is present in an otherwise untouched virgin system ($ABHSV = 00000$). Application of the above "rules" results in the destruction of the virus in two iterations:

$$ABHSV = 00001 \longrightarrow 00101 \longrightarrow 01110. \quad (8.89)$$

Notice that the system is left with high concentrations of B, H and S cells. Thus, if a virus is reintroduced into the same system after the original infection has been eliminated, it is immediately destroyed:

$$ABHSV = 01111 \longrightarrow 11110 \longrightarrow 01110. \quad (8.90)$$

More generally, it is easy to show that by starting from any of the $2^5 = 32$ possible states, the above equations eventually yield only one of five possible fixed points: $ABHSV = 00000$, 01100 , 01110 , 01000 or 01001 . The first three fixed points are healthy and correspond to the *virgin* state, the *vaccinated* state and the *immune* state. Systems found in any of these three states are immunologically sound in the sense that any added antigens are immediately destroyed and the system is returned into the immune state. The remaining two fixed points correspond to immunologically impaired systems: in both these cases, the system is unable to eliminate antigens.

In order to generalize this basic model to a full lattice we need only define the interaction between neighboring lattice sites. For example, we can assume that an antibody or antigen is present at a site (i, j) at time t if at least one of that site's five nearest neighbors contained an antibody or antigen, respectively, at time $t - 1$. However, Stauffer ([stauff91a], [stauff92]) reports that such systems are uninteresting; when seeded with small concentrations of antigens they eventually all reach the fixed immune state (01110). More interesting results may be found by using analogs of local majority rules, wherein an antigen or antibody is assumed to exist at a given site only if a majority of neighboring sites contain those types of cells, respectively [neum89].

8.5.2 Immune Disease: AIDS

A normally functioning immune system immediately recognizes invading antigens and mounts an appropriate response. Helper T cells play an important coordinating role by both increasing their own numbers after recognizing the initial attack and signaling B cells into action to destroy the invaders. T cells also signal cytotoxic cells (which are another type of suppressor T cell) to kill the antigens. The immune response is switched off when the growth of helper T cells is reduced by the suppressor action of the T cells.

Now suppose the body's immune system malfunctions and begins attacking the body itself. A typical scenario might involve *killer* cells K attacking helper and/or suppressor cells. Chowdbury and Stauffer [chowd90] developed a simple five-cell model using two types of helper cells (H_1 and H_2), two type of suppressors (S_1 and S_2) and one killer cell (K):

$$\begin{cases} K &= K + H_1 + H_2 > S_2 + S_2, \\ H_1 &= H_1 + H_2 > S_1, \\ H_2 &= K + H_1, \\ S_1 &= H_1 + H_2, \\ S_2 &= H_1, \end{cases} \quad (8.91)$$

where, in the equations for K and H_1 , the right hand side is to be interpreted as a Boolean operation. That is, in the case for H_1 , for example, H_1 is set equal to 1 if $H_1 + H_2$ is greater than S_1 .

Chowdbury and Stauffer found that this model yields only three fixed points: *healthy* ($KH_1H_2S_1S_2 = 00000$), *immune* (01111) and *sick* (11111). If placed on a square lattice as discussed above, the entire system becomes *sick* after a short time.

In patients infected with HIV (human immunodeficiency virus), the helper cell population is weakened to the point where the immune system is no longer able to function properly. The body thus becomes susceptible to otherwise nonlethal diseases such as pneumonia.

A recent example of a CA model of the immune response in AIDS is Pandley's four-cell model using interactions among macrophages ($= M$) containing parts of the virus on their surface, helper T cells ($= H$), cytotoxic T cells ($= C$) and the virus ($= V$) ([pand89], [pand91]):

$$\begin{cases} C &= H \cdot M \cdot V, \\ H &= (M + H) \cdot (1 - V), \\ M &= M + V, \\ V &= (H + M + V) \cdot (1 - C). \end{cases} \quad (8.92)$$

The first equation states that cytotoxic cells grow only if helper cells, macrophages and the virus are all present. The second equation implies that, when the virus is not present, helper cells grow if macrophages and/or helper cells are present. The third equation implies that macrophages grow both when the virus is present and there is already a concentration of macrophages. The last equation describes the

growth of the virus, in the absence of cytotoxic cells, due to the presence of helper cells, macrophages and the virus itself.

It is easy to show that equations 8.92 has two fixed points – $(CHMV) = (0000), (0011)$ – and one limit cycle of period two – $(CHMV) = (0111) \rightarrow (1011) \rightarrow (0010) \rightarrow (0111)$.

Now consider a “latticized” version of this model. Populate a square lattice – which may represent a tissue sample in which the modeled immune reactions are assumed to occur – with each of the four cell types C, H, M and V and initialize the system so that a fraction p_0 of each cell type is in its *high* (i.e. = 1) concentration state. Assign the value 1 to each site (i, j) if the sum of the concentrations of its nearest neighbors that are of the same cell type as site (i, j) is nonzero. After all sites have been assigned “new” values in this manner, update the system according to equations 8.92.

Stauffer [stauff92] reports that the concentration of cells in this system quickly saturates. For low initial concentrations p_0 , the viral population wins over the population of cells of the immune system and the system can be said to develop AIDS. For larger p_0 , the population of helper T cells becomes greater than that of the virus and the immune system wins.

More complex models must carefully consider additional factors such as the receptor structure of helper T cells and allow for, what in reality, is a less than perfect “lock and key” match between antibody and antigen. For the latter case, Stauffer [stauff92] describes two schemes in which more than one type of antibody fits a given antigen and more than one type of antigen corresponds to a given antibody.

8.6 Random Boolean Networks

Consider a directed graph of size N with adjacency matrix A_{ij} ,[†]. We will say that $\mathcal{G}_{N,\kappa}$ represents a size N directed graph of connectivity κ if each site of the graph has *in-degree* equal to κ ; i.e. $\sum_{j=1}^N A_{ji} = \kappa$ for all sites ‘ i ’. A size N *Random Boolean Network* with connectivity κ – or (N, κ) -net – generalizes the basic binary ($k = 2$) CA model by evolving each site variable $x_i \in \{0, 1\}$ of $\mathcal{G}_{N,\kappa}$ according to a randomly selected Boolean function of κ inputs:

$$x_i(t+1) = \mathcal{F}^{(\kappa)}(\{x_j(t)\} \mid A_{ji} = +1). \quad (8.93)$$

Since there are two choices for every combination of states of the κ inputs at each site, $\mathcal{F}^{(\kappa)}$ is randomly selected from among 2^{2^κ} possible Boolean functions of κ inputs.

This model was first introduced by Kauffman [kauff69] in a study of cellular differentiation in a biological system (binary sites were interpreted as elements of an ensemble of genes switching on and off according to some set of random rules). Since its original conception, however, related models have found wide application in an

[†]See section 2.1.3 for a general overview of matrix terms and notation.

increasingly large domain of diverse problems. As we shall see below, such models of strongly disordered systems nonetheless exhibit remarkable and unexpected order. In the following, we follow Kauffman ([kauff84], [kauff84]). Further details may be found in [kauff93].

8.6.1 Overview of the Dynamics of (N, κ) Nets

Since we will be dealing with finite graphs, we can analyze the behavior of random Boolean nets in the familiar fashion of looking at their *attractor* (or *cycle*) state structure. Specifically, we choose to look at (1) the number of attractor state cycles, (2) the average cyclic state length, (3) the sizes of the basins of attraction, (4) the stability of attractors with respect to minimal perturbations[†], and (4) the changes in the attractor states and basins of attraction induced by mutations in the lattice structure and/or the set of Boolean rules.

Table 8.9 lists some properties of random Boolean nets as a function of N for the cases $\kappa = 1$, $\kappa = 2$, $\kappa > 5$ and $\kappa = N$.

κ	State Cycle Length	Number of State Cycle Attractors	Stability with respect to minimal perturbations
1	$\exp(\frac{1}{8} \log^2 N)$	$(\frac{1}{\sqrt{e}})^{N(1+O(1))}$	low
2	$\sqrt{N}$	$\sqrt{N}$	high
> 5	$2^{\beta N-1}$, $\beta > 1$	$\sim \frac{1}{2} N \log[(\frac{1}{2} \pm \alpha)^{-1}]$	low
N	$2^{\frac{N}{2}-1}$	$\frac{N}{e}$	low

Table 8.9 State cycle length and the number of state cycles for random boolean nets of size N and connectivity κ ; $\alpha = p_\kappa - 1/2$, where p_κ is the mean internal homogeneity of all Boolean functions on κ inputs (see text).

8.6.1.1 $\kappa = 1$

In this case, each site can have many identical outputs but receives only a single input. There are four possible Boolean functions with one input: two yield fixed values of 0 or 1, independent of input (these two *static* functions, $\mathcal{F}_0$ and $\mathcal{F}_1$ are always among the 2^{2^1} possible Boolean functions), the third inverts the input ($\mathcal{F} \equiv -$) and the fourth is the identity ($\mathcal{F} \equiv +$). We will discuss behavior arising only from the latter two *active* functions. Exact results for the analytically tractable case of allowing a distribution of all four Boolean functions have been derived by Flyvbjerg and Kjaer [flyvb88].

Figure 8.16 shows a portion of typical $(N, 1)$ -net. The arrows indicate inputs to given sites and '+' and '-' represent the two active Boolean functions at the sites toward which the arrows are pointing. Note that the structure degenerates into subnets of dynamically independent loops with outwardly radiating 'tails'. An input signal cannot enter a loop since the site by which it would enter the loop

[†]Minimal perturbations are of the form $x_i \rightarrow x_i \oplus 1$, for randomly chosen 'i'.

would have to have *two* inputs, one external and one internal. Similarly, a subnet can have at most one loop since the direction of propagation along a branch is determined by the loop from which it originates. The overall behavior is therefore a product of the behaviors of many isolated subsystems.

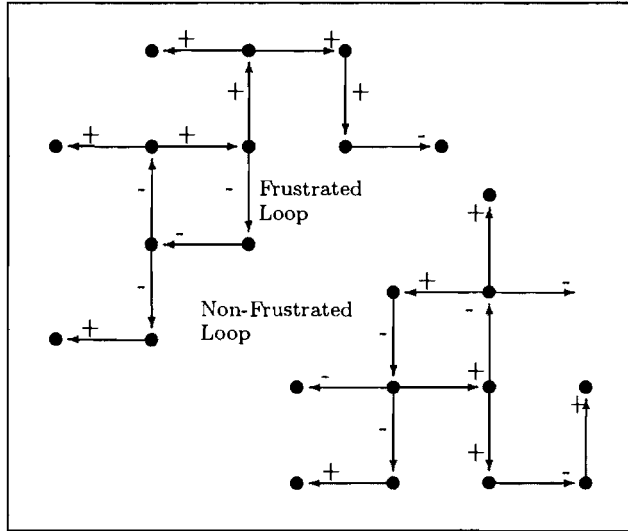


Fig. 8.16 Typical random Boolean network with connectivity $\kappa = 1$. Arrows indicate inputs to given sites; '+' and '-' represent the Boolean functions at the sites toward which the arrows are pointing.

The dynamics are fairly simple to describe. Consider the behavior of the tails. Since signals propagate along the direction of the arrows from the first site of a given tail to the last, the value of the i^{th} site at time t is a function only of the value of the first site at time $(t - i)$. Starting from a random initial state, the transient behavior lasts only as long as it takes for the signal to propagate entirely through a given tail. The maximum transient length of the system is therefore equal to the longest tail in the graph. Since all signals that propagate along the tails originate in the one loop of a given subnet, the stationary state is effectively determined by the loop. In particular, the period of a subnet is equal to the period of its loop.

Frustrated Loops. The period of a loop depends on whether or not it is 'frustrated'. Consider the parity of the number of value inversions contained in a loop. If it is odd, the loop is said to be *frustrated*. In this case, a signal propagating around the loop has to go around *twice* before the loop returns to its initial state. Letting l be the number of site in a loop, the period of the loop is therefore equal to $2 \times l$ for configurations with no symmetries, or an odd factor of $2l$ for certain special cases. In particular, a frustrated loop cannot have fixed points.

In the case of an unfrustrated loop, a signal that propagates around a loop once

returns to its original value. The period of the loop, in this case, is equal to either l or to some factor of l . In particular, the period is 1 if the initial value of each site is the output that corresponds to the value of its input site. It therefore follows that unfrustrated loops have two fixed points.

Table 8.9 shows that while the number of attractors increases exponentially, the average cycle length increases rather slowly as a function of N . Random Boolean nets with connectivity one are also generally only moderately stable with respect to minimal perturbations.

8.6.1.2 $\kappa = 2$

Nets with connectivity two exhibit a remarkable collective spontaneous order. As we can see in table 8.9, both the number and size of attractors increases only as $\sqrt{N}$. A net of size $N = 10^3$, for example, settles down into one of only about 100 different attractors, consisting, on average, of about 100 states. The dynamics therefore effectively shrinks the total phase space down to about 10^{-2998} of the original volume.

Attractor states are typically stable with respect to $\sim 80 - 95\%$ of the possible minimal perturbations, and *mutations* (by which sites are deleted or Boolean functions of single sites are altered) affect the dynamical behavior only slightly.

The remarkably ordered behavior of $(N, 2)$ -nets derives principally from the appearance of a connected *frozen core* of sites, each element of which remains frozen in a fixed state. This frozen core creates percolating ‘walls’ of constancy that effectively partition the net into a dynamically static subset and (dynamically) isolated islands of sites that continue evolving but are incapable of communicating through the frozen core.

Kauffman [kauff86b] describes two related mechanisms responsible for the formation of such percolating walls: (1) *forcing structures* and (2) *internal homogeneity clusters*. An important point to keep in mind is that these two mechanisms, described below, currently represent the *only* established means by which the ordered behavior of $\kappa = 2$ nets can (in part) be deduced.

Forcing Structures: Consider the Boolean ‘OR’ function.[†] Note that the value of ‘ σ_1 OR σ_2 ’ is fixed as 1 whenever either σ_1 or σ_2 is equal to 1. Kauffman calls any function with the property that at least one value of at least one of its inputs fixes its output, a *canalizing function* [kauff84]. The Boolean functions ‘OR’ and ‘AND’, for example, are both canalizing functions, but the ‘EXCLUSIVE OR’ function is not.

Now, consider some subgraph of a random Boolean net with connectivity two (or greater), all of whose nodes are populated with a canalizing function that forces the output to be ‘1’ in the event of at least one 1-valued input. The population of canalizing functions guarantees the propagation of the value ‘1’ down through all descendants of the original 1-valued site. In particular, if the subgraph contains loops, the loops will be forced into fixed states with all sites having value ‘1’. Such

[†] $(0 \text{ OR } 0) = 0$, $(0 \text{ OR } 1) = 1$, $(1 \text{ OR } 0) = 1$, and $(1 \text{ OR } 1) = 1$.

(canalizing) subgraphs are called *forcing loops* or *descendent forcing structures*. Observe, also, that these subgraphs clearly provide ‘walls of constancy’ since their fixed states cannot ever be changed by perturbing the outside inputs.

More generally, forcing structures generated out of subgraphs containing a variety of different canalizing functions form a large interconnected web that *percolates* through the entire system [kauff84]. Sites of the web attain fixed values, and form walls of constancy through which isolated, but otherwise dynamically active, islands cannot communicate. The precise nature of the emergent forcing structures due to percolation is essentially a mathematical problem in the theory of *random directed graphs*.

For the analytically tractable case of random *undirected* graphs it can be shown that a ratio of forcing connections to site number equal to $1/2$ represents a *percolation threshold* below which only small, unconnected forcing structures are present and above which fully connected forcing structure begin to emerge [palmer85]. Numerical results for random directed graphs suggest that when the number of forcing connection exceeds the site number, large connected extended forcing structures likewise emerge.

It is easy to see that nets with connectivity $\kappa = 1$ allow only canalizing functions. As we have just seen in the above discussion of the dynamics for that case, such nets are composed of subnets, and yield relatively short periods. In the case of the $2^{2^2} = 16$ possible Boolean functions for $\kappa = 2$ inputs, 10 are canalizing for both inputs (including the two trivial constant mappings), and 4 are canalizing for one. The fraction of Boolean functions that are canalizing is actually maximum for $\kappa = 2$, and decreases rapidly for increasing κ . In fact, Gelfand and Walker [gelf84] provide an upper bound for the fraction of Boolean functions on κ inputs that are canalizing, and show that

$$\frac{4\kappa 2^{\kappa-1}}{2^{2^\kappa}} = \frac{4\kappa}{2^{2^{\kappa-1}}} \longrightarrow 0 \text{ as } \kappa \rightarrow \infty. \quad (8.94)$$

Internal Homogeneity Clusters: Walker and Ashby [walker66] first showed that increasing the *sameness* of the entries – or the internal *homogeneity* – of a Boolean function’s rule table tends to decrease the cycle length.

Let $P^{(\kappa)} = P^{(\kappa)}(\mathcal{F})$ be the fraction of the 2^κ elements of the rule table for a κ -input Boolean function $\mathcal{F}$ that yield a ‘1’. Then the internal homogeneity of that Boolean function is given by the deviation of $P^{(\kappa)}$ from $1/2$. Derrida and Stauffer [derrida86a], Weisbuch and Stauffer [weis87] and De Arcangelis ([arcan88], [arcan88]) report that, for two and three dimensional lattices with nearest neighbor coupling, there exists a critical P_c , such that for $P^{(\kappa)} > P_c$, a net evolves into (1) a connected “frozen web” of fixed points with value ‘1’ and (2) isolated pockets of activity, or *islands* that are cut off from one another by the frozen web, but whose dynamics remains otherwise unconstrained. For $P^{(\kappa)} \sim 1/2$, on the other hand, percolating webs of sites fixed at the value ‘1’ do not form. The critical value P_c therefore defines a point at which a kind of “phase transition” occurs. P_c generally

depends on the type of lattice, and increases for increasing neighborhood size.

Note that it is not required that the favored value of each site be ‘1’. Exactly the same argument as given above would hold true if, say, half of the sites yielded ‘1’ with probability $P^{(\kappa)} > P_c$ and the other half yielded ‘0’ with probability $P^{(\kappa)} > P_c$.

Define the *internal homogeneity* of a Boolean function, $\mathcal{I}$, to be the greater of the number of ‘1’ or ‘0’ values that occur in the rule table for that function [gelf84]. The OR function, for example, has three ‘1’ and one ‘0’ value and thus has $\mathcal{I} = 3$. The corresponding $P(\mathcal{F}) = 3/4$. Defined in this way, we see that $P(\mathcal{F}) \geq 1/2$ for all Boolean functions $\mathcal{F}$. It can be shown [gelf84] that the average value of P (averaged over all κ -input Boolean functions) is given by

$$\langle P \rangle = 2^{-2^\kappa} \sum_{\mathcal{F}} P(\mathcal{F}) = \frac{1}{2} + 2^{-(2^\kappa+1)} \binom{2^\kappa}{2^{\kappa-1}}. \quad (8.95)$$

For random Boolean networks, P_c effectively defines the dividing line between ordered and chaotic behavior. Kauffman [kauff86b] calls the large percolating frozen webs that appear for $P^{(\kappa)} > P_c$ *homogeneity clusters*. They are distinguished from forcing structures (see discussion above) by noting that while forcing structures require only that a *single* value at each site suffices to force one or more descendent sites into a forced state, homogeneity clusters may instead arise from the more general circumstance of a *joint* activity of two sites forcing the activity of a single descendent site.

8.6.1.3 $\kappa > 5$

Although number of distinct attractors is $< N/e$, the average length of an attractor increases exponentially with N . The exponential rate of growth is relatively small for small connectivities, and increases to $N/2$ for $\kappa \rightarrow N$. Generally speaking, $(N, \kappa > 5)$ nets show complex behavior but have relatively few distinct cycles. The stability of the cycles with respect to minimal perturbations is also generally low.

8.6.1.4 $\kappa = N$

Since each site of an $(N, \kappa = N)$ -net receives inputs from all other sites of the net, this case represents a *maximally disordered system*: at each time step, each site is replaced by a random choice among the 2^N possible states.

Table 8.9 shows that while the number of cycles grows only linearly with N , the average cycle length increases exponentially as $2^{\frac{N}{2}-1}$. Moreover, it can easily be shown that attractor states are *unstable* with respect to almost all minimal perturbations and that mutations of Boolean functions totally disrupt such states.

Derrida and Flyvberg [flyvb88] and Derrida and Bessis [derrida88] have examined the “overlap” between two attractors by looking at the probability that two randomly chosen initial states evolve toward the same attractor. These studies find that the distribution is very similar to that found in certain spin-glass models.

Since, in this case, the state of each site depends on the states of *all* other sites, including itself, the specification of each Boolean function requires that all

$\mathcal{N} = 2^N$ entries of the rule table be filled in. Each configuration can be interpreted as being the binary representation of some whole number between 0 and $\mathcal{N} - 1$. This suggests that the behavior of $(N, \kappa = N)$ -nets is equivalent to the behavior of a random mapping of a finite set of $\mathcal{N}$ integers to itself.

8.6.2 Random Mappings

Random maps have been studied by a large number of different authors, including Kruskal [krus54], Rubin and Sitgreaves [rubin54], Pittel [pittel83] and Kolchin [kolc86].

Consider an order ' N ' system and a random function ' ϕ ', which maps each of the $\mathcal{N} \equiv 2^N$ possible binary states Σ_i to unique successor states $\Sigma_j = \phi(\Sigma_i)$ with probability $p[\phi] = 1/\mathcal{N}^{\mathcal{N}}$. We can immediately compute the asymptotic N -dependence of the cyclic structure of the corresponding state transition graph G_ϕ [†]:

8.6.2.1 Average Cycle Length

Suppose the initial state is Σ_0 , and consider the sequence of iterates

$$\Sigma_0 \rightarrow \phi(\Sigma_0) = \Sigma_1 \rightarrow \phi^2(\Sigma_0) = \Sigma_2 \rightarrow \cdots \rightarrow \Sigma_{a-1}, \quad (8.96)$$

where state Σ_{a-1} is reached in $a - 1$ steps and the states $\Sigma_0, \dots, \Sigma_{a-1}$ are all different. Then the probability of having at least one cycle of length ' $l = a$ ' is given by the product of the probability that each state ' i ' is different from the $i - 1$ preceding ones times the probability that $\Sigma_a = \Sigma_0$:

$$p[a] = \sum_{i=1}^{\mathcal{N}-a+1} p[\phi^{a+i-1}(\Sigma_0) = \phi^i(\Sigma_0) \ \& \ \phi^{j < a+i-1}(\Sigma_0) \neq \phi^i(\Sigma_0)], \quad (8.97)$$

where ϕ^j is the j^{th} functional iterate of the initial argument. We see that

$$p[\phi^{\mathcal{N}}(\Sigma_0) = \Sigma_0 \text{ and } \phi^{m < \mathcal{N}}(\Sigma_0) \neq \Sigma_0] =$$

$$\begin{aligned} & p[\phi^{\mathcal{N}}(\Sigma_0) = \Sigma_0] \cdot \prod_{i=1}^{\mathcal{N}-1} p[\phi^i(\Sigma_0) \neq \Sigma_0] \\ &= \frac{1}{\mathcal{N}} \left(1 - \frac{1}{\mathcal{N}}\right) \left(1 - \frac{2}{\mathcal{N}}\right) \cdots \left(1 - \frac{(\mathcal{N}-1)}{\mathcal{N}}\right) \\ &= \frac{1}{\mathcal{N}} \prod_{j=1}^{\mathcal{N}-1} \left(1 - \frac{j}{\mathcal{N}}\right). \end{aligned} \quad (8.98)$$

Thus,

$$p[a] = \frac{1}{\mathcal{N}} \sum_{i=a}^{\mathcal{N}} \prod_{j=1}^{i-1} \left(1 - \frac{j}{\mathcal{N}}\right). \quad (8.99)$$

[†]Recall, from section 2.2.1 that G_ϕ is defined by having a link from ' i ' to ' j ' if and only if $\phi(\Sigma_i) = \Sigma_j$

Observing that $\prod_{j=1}^{i-1} (1 - \frac{j}{\mathcal{N}}) \sim e^{-i^2/2\mathcal{N}} \{1 + \mathcal{O}(\frac{i}{\mathcal{N}})\}$, we have the following asymptotic result:

$$\begin{aligned} p[a]_{\mathcal{N} \rightarrow \infty} &\longrightarrow \frac{1}{\mathcal{N}} \int_a^\infty \exp\{-y^2/2\mathcal{N}\} dy \\ &= \frac{1}{\mathcal{N}} \left\{ \left(\frac{\pi\mathcal{N}}{2}\right)^{1/2} - \sqrt{2\mathcal{N}} \int_0^{a/\sqrt{2\mathcal{N}}} e^{-t^2} dt \right\} \\ &= \left(\frac{\pi}{2\mathcal{N}}\right)^{1/2} \left[1 - \Phi\left(\frac{a}{\sqrt{2\mathcal{N}}}\right)\right], \end{aligned} \quad (8.100)$$

where $\phi(y) \equiv \frac{2}{\sqrt{\pi}} \int_0^y \exp\{-t^2\} dt$ is the probability integral. We therefore find that the average cycle length

$$\begin{aligned} \langle a \rangle &= \sum_{i=1}^{\mathcal{N}} a p[a] \longrightarrow \int_0^\infty x \left(\frac{\pi}{2\mathcal{N}}\right)^{1/2} \left[1 - \Phi\left(\frac{x}{\sqrt{2\mathcal{N}}}\right)\right] dx \\ &= \sqrt{2\mathcal{N}\pi} \int_0^\infty y \left[1 - \Phi(y)\right] dy \\ &= \sqrt{\frac{\pi}{8}} \mathcal{N}^{1/2} = \sqrt{\frac{\pi}{8}} 2^{N/2}. \end{aligned} \quad (8.101)$$

8.6.2.2 Average Number of Length- a Cycles

$\mathcal{N}p[a]$ = the average number of points belonging to length- a cycles, so that the average number of a -cycles is given by $N(a) \equiv \mathcal{N}p[a]/a$. Thus,

$$\begin{aligned} N(a) &= \frac{1}{a} \prod_{j=1}^{a-1} \left(1 - \frac{j}{\mathcal{N}}\right) \\ &= \frac{1}{a} \frac{(\mathcal{N}-1)(\mathcal{N}-2) \cdots (\mathcal{N}-a+1)}{\mathcal{N}^{a-1}}. \end{aligned} \quad (8.102)$$

Using the approximation $(\mathcal{N})_a/\mathcal{N}^a \sim \exp\{-a^2/2\mathcal{N}\}$, valid for large $\mathcal{N}$ and $(\mathcal{N}-a)$, we see that $N(a) \sim 1/a$ whenever $a \ll \mathcal{N}$ but falls off much more rapidly when $a \gtrsim \sqrt{\mathcal{N}}$.

8.6.2.3 Average Cycle Number

$N_c = \sum_{i=1}^{\mathcal{N}} N(a)$. Thus

$$\begin{aligned} N_c &\sim \int_1^\infty \frac{1}{x} e^{-x^2/2\mathcal{N}} dx \\ &\sim \frac{1}{2} \int_1^\infty \frac{1}{y} e^{-y^2/2\mathcal{N}} dy \\ &\sim -\frac{1}{2} Ei\left(-\frac{1}{2\mathcal{N}}\right) \end{aligned}$$

$$\sim \ln \mathcal{N} = (\log_e 2) N, \quad (8.103)$$

where $Ei(x) \equiv \int_{-x}^{\infty} e^{-t}/t \, dt$ is the exponential Integral.

8.7 Self-Organized Criticality

The power spectra $S(f)$ for transport phenomena in many diverse physical systems – including transistors, superconductors, highway traffic and river flow ([bak88a],[carl90]) – has been experimentally observed to diverge at low frequencies with a power law $f^{-\beta}$, with $0.8 < \beta < 1.4$. Moreover, $S(f)$ obeys this power-law behavior over very large time scales. Commonly referred to as the $1/f$ -noise (or *flicker-noise* noise) problem, there is currently no general theory that adequately explains the ubiquitous nature of $1/f$ noise.

The mechanism of *Self-organized criticality*, a concept first introduced by Bak, Taug and Wiesenfeld [bak87a], may possibly provide a fundamental link between such *temporal scale invariant* phenomena and phenomena exhibiting a *spatial scale invariance* – familiar examples of which are given by fractal coastlines, mountain landscapes and cloud formations [mandel82].

Bak, *et. al.* argue that spatially extended dynamical systems evolve spontaneously into minimally stable critical states and that this self-organized criticality is the common mechanism responsible for a variety of fractal phenomena. They suggest that $1/f$ noise is actually not noise at all, but is instead a manifestation of the intrinsic dynamics of self-organized critical systems. ‘Self-organized’ refers to the fact that the system, after some initial transient period, naturally evolves into a critical steady state without any tuning of external parameters. This stands in marked contrast with the critical points at phase transitions in thermodynamic systems that can only be reached by a variation of some parameter (temperature, for example). ‘Criticality’ refers to the fact that the steady state shows correlations on all length scales and is characterized by spatial and temporal power-law distribution functions. Other than the absence of any control parameters, the resulting behavior is thus strongly reminiscent of the critical point in thermodynamic systems undergoing a second-order phase transition.

In this section we introduce Bak, *et. al.*’s *Sandpile Model*, a simple CA model mimicking the flow of sand in a sandpile by a nonlinear relaxational diffusion process when the system is locally perturbed above some threshold value. Details may be found in [bak87a], [bak87b], [bak88a], [bak88b], [bak89a], [bak89b], [bak90], [liu90], [mcnam90] and [weisen89].

8.7.1 Sandpile CA Model

Heuristically, the sandpile CA tries to reproduce the essential dynamics of building up a sandpile from scratch by adding grains (or units) of sand slowly and randomly to a given area. At first the pile is flat with additions of sand inducing only minor local rearrangements of that pile. As the pile grows in size, however, it gets steeper

and steeper, with additions of sand sometimes causing minimal restructuring to take place and sometimes causing avalanches to occur. These avalanches themselves get larger and larger as the slope of the pile increases, until, finally, a statistically stationary state is reached for which the sandpile's slope can no longer be increased and any further addition of sand induces rearrangements to take place on all possible length scales and time scales. The system thus organizes itself into a critical state and stays in that state for as long as units of sand are slowly added. The same critical state would be reached if the sandpile is allowed relax after starting with a very large slope. Given that we have reached a steady state, the basic question to be answered, therefore, is *what is the distribution of sandslides that is induced by the addition of a single grain of sand?*

8.7.2 One Dimensional Sandpiles

Consider, first of all, a one dimensional sandpile CA. It is defined as follows. Each site of a one dimensional lattice represents a position at which units of sand may be placed. The number of units of sand at site ' i ' at time ' t ' is given by $\sigma_i(t)$. Let $\eta_i(t)$ represent the *local slope*, defined as the difference between the number of units of sand on neighboring sites:

$$\eta_i(t) \equiv \sigma_i(t) - \sigma_{i+1}(t). \quad (8.104)$$

The dynamics, which consists of two operations, is most conveniently expressed in terms of this local slope value. Start with an arbitrary initial pile of sand, $\eta(t=0)$. If the local slope at any site i exceeds an arbitrarily chosen threshold value η_c , the system is allowed to relax by continually applying a *relation rule* $\phi_{\text{relax}} = \phi_{\text{relax}}(\eta)$ that effectively slides one unit of sand 'downhill' (i.e. to the right) according to (see figure 8.17)

$$\eta(t+1) = \phi_{\text{relax}}(\eta(t)) : \begin{cases} \eta_j(t+1) &= \eta_j(t) \text{ for all } j \neq i-1, i, i+1, \\ \eta_{i-1}(t+1) &= \eta_{i-1}(t) - 1, \\ \eta_i(t+1) &= \eta_i(t) - 2, \\ \eta_{i+1}(t+1) &= \eta_{i+1}(t) + 1. \end{cases} \quad (8.105)$$

After all local slopes of the pile are again less than η_c , one unit of sand is added to a random site i . In terms of the local slope variable, this amounts to applying the *addition rule* ϕ_{add}

$$\eta(t+1) = \phi_{\text{add}}(\eta(t)) := \begin{cases} \eta_j(t+1) &= \eta_j(t) \text{ for all } j \neq i-1, i, i+1, \\ \eta_{i-1}(t+1) &= \eta_{i-1}(t) + 1 \\ \eta_i(t+1) &= \eta_i(t) - 1. \end{cases} \quad (8.106)$$

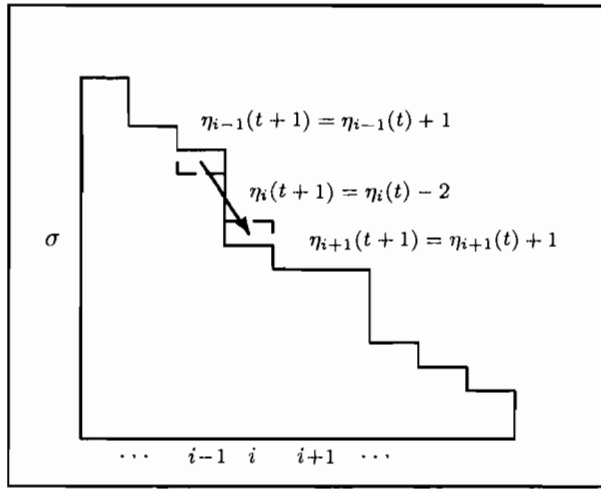


Fig. 8.17 One dimensional *sandpile CA*; σ_i gives the number of units of sand at site ' i ' at time ' t ', $(\dots, i-1, i, i+1, \dots)$ label column number, and $\eta_i(t)$ is the difference between the amount of sand on neighboring sites ($= \sigma_i(t) - \sigma_{i+1}(t)$). The figure depicts the rule for the case when the local slope exceeds a specified threshold and causes a grain of sand to slide downhill. See text for complete rule.

The complete dynamics are then specified by the rule $\Phi = \Phi(\eta)$:

$$\eta(t+1) = \Phi(\eta(t)) = \begin{cases} \phi_{\text{relax}}(\eta(t)) & \text{if there exists } i \text{ such that } \eta_i(t) > \eta_c, \\ \phi_{\text{add}}(\eta(t)) & \text{else.} \end{cases} \quad (8.107)$$

Note that equations 8.105 and 8.106 effectively define a simple discrete diffusion process in one dimension; the presence of a threshold condition also makes the diffusion process a nonlinear one (see below).

Boundary conditions are set by putting a 'wall' on the left hand side of the pile ($\eta_0(t) = 0$ for all t) and allowing sand to fall off an 'edge' on the right hand side ($\eta_N(t+1) = \eta_N(t) - 1$, $\eta_{N+1}(t+1) = \eta_{N+1}(t) + 1$, whenever $\eta_N(t)$ exceeds the threshold η_c). The net effect of these two conditions is to have an overall flow of sand from left to right.

8.7.2.1 Resultant Dynamics

The rather simple dynamics of this one dimensional system can actually be solved exactly. The result is that for any initial configuration the system evolves towards a *minimally stable state* η_0 , all of whose local slope values $\eta_i = \eta_c$. Once this minimally stable state is reached, the addition of a unit of sand to any site results in that one unit sliding from site to site until it finally falls off the 'edge' on the right side, again leaving the pile in the state η_0 . The minimally stable state is thus both sensitive to local perturbation and robust because it is ultimately left unchanged by any perturbation. If the sand is added completely randomly, the resulting flow

is random white noise (i.e. it has a power spectrum equal to $1/f^0$). In order to obtain more interesting dynamics and phenomena – in particular, in order to do away with the robustness of the minimally stable state – we must look at similar systems defined for two or more spatial dimensions.

8.7.3 *d*-Dimensional Sandpiles

The one dimensional rules given in equations 8.105 and 8.106 can be readily generalized to a d dimensional Euclidean lattice. Let $\eta(\mathbf{r}, t)$ be the d dimensional analogue of the one dimensional local slope at lattice point $\mathbf{r}$ at time ' t '.[†] Addition of sand is then generated by the rule

$$\phi_{\text{add}}^{(d)} : \begin{cases} \eta(\mathbf{r}, t+1) &= \eta(\mathbf{r}, t) + d, \\ \eta(\mathbf{r} - \mathbf{x}_i, t+1) &= \eta(\mathbf{r} - \mathbf{x}_i, t) - 1, \end{cases} \quad (8.108)$$

where $\mathbf{x}_i$ is a unit vector linking each lattice point to its nearest neighbor in the positive $x_1, x_2, \dots, x_d$ directions.

If $\eta(bfr) > \eta_c$ then the system relaxes according to

$$\phi_{\text{relax}}^{(d)} : \begin{cases} \eta(\mathbf{r}, t+1) &= \eta(\mathbf{r}, t) - 2d, \\ \eta(\mathbf{r} \pm \mathbf{x}_i, t+1) &= \eta(\mathbf{r} \pm \mathbf{x}_i, t) + 1. \end{cases} \quad (8.109)$$

In two dimensions, for example, $\phi_{\text{add}}^{(d-2)}$ and $\phi_{\text{relax}}^{(d-2)}$ are given by

$$\phi_{\text{add}}^{(d-2)} : \begin{cases} \eta(x-1, y, t+1) &= \eta(x-1, y, t) - 1, \\ \eta(x, y-1, t+1) &= \eta(x, y-1, t) - 1, \\ \eta(x, y, t+1) &= \eta(x, y, t) + 2, \end{cases} \quad (8.110)$$

and

$$\phi_{\text{relax}}^{(d-2)} : \begin{cases} \eta(x \pm 1, y, t+1) &= \eta(x \pm 1, y, t) + 1, \\ \eta(x, y \pm 1, t+1) &= \eta(x, y \pm 1, t) + 1, \\ \eta(x, y, t+1) &= \eta(x, y, t) - 4. \end{cases} \quad (8.111)$$

At first sight it might seem as though we should expect the same sort of dynamics as for the one-dimensional case. Namely, that the system will evolve towards a robust least stable state for which $\eta(x, y) = \eta_c$ for all sites x and y . It turns out that this naive expectation is false. Consider a perturbation of an arbitrary site while the system is in the least stable state. The perturbation will cause the

[†]The physical meaning of η is not the natural d dimensional analogue of slope. Although the local slope for systems in $d \geq 2$ dimensions is a vector quantity, the model discussed above assumes it to be a scalar. We should point out that despite its name, the *sandpile model* was originally conceived with a more general purpose in mind; namely, as serving as a simple computational aid in the study of typical behaviors of spatially extended dynamical systems with many degrees of freedom. It is only for its one-dimensional incarnation that the sandpile metaphor is most naturally appropriate. Nonetheless, stricter generalizations of the one-dimensional sandpile model to $d > 1$ dimensions, called *vector avalanche automata* and obeying a threshold relaxation that depends on a (locally conserved) gradient of a scalar field, have also been found to display a self-organized criticality (albeit with different scaling exponents). See [mcnamb90].

neighboring sites to become unstable, which will in turn cause their neighbors to become unstable, and so on, until the entire lattice is made to feel the effects of the initial perturbation. The final state of this avalanche is a statistically stationary (self-organized) critical state η^* , consisting of locally connected domains; it is *not* the least stable state. A perturbation of a single site within a domain leads to a chain reaction affecting all of the sites within that domain.

8.7.3.1 Spatial Power-Law Distribution

The most important property of the self-organized critical state is the presence of locally connected domains of *all sizes*. Since a given perturbation of the state η^* can lead to anything from a trivial one-site shift to a lattice-wide avalanche, there are no characteristic length scales in the system. Bak, *et al.* [bak87] have, in fact, found that the distribution function $D(s)$ of domains of size s obeys the power law

$$D(s) = s^{-\beta}, \quad (8.112)$$

where $\beta \approx 1$ for domains up to size $s = 500$ for a 50×50 two dimensional system and $\beta \approx 1.35$ for a three dimensional $20 \times 20 \times 20$ lattice.

Note that while the power-law distribution is reminiscent of that observed in equilibrium thermodynamic systems near a second-order phase transition, the mechanism behind it is quite different. Here the critical state is effectively an attractor of the system, and no external fields are involved.

8.7.3.2 Temporal Power-Law Distribution

The fact that there are no characteristic length scales immediately implies a similar lack of any characteristic time scales for the fluctuations. Consider the effect of a single perturbation of a random site of a system in the critical state. The perturbation will spread to the neighbors of the site, to the next nearest neighbors, and so on, until, after a time τ and a total of f sand slides, the effects will die out. The distribution of the life-times of the avalanches, $D(t)$, obeys the power law

$$D(t) \approx t^{-\alpha} \quad (8.113)$$

where $\alpha \approx 0.43$ in two dimensions and $\alpha \approx 0.90$ in three dimensions.

1/f Noise

It is not hard to see that, given a power-law distribution of lifetimes (equation 8.113), the power spectrum $S(f)$, defined by

$$S(f) = \int \langle F(t_0 + t)F(t_0) \rangle_{t_0} \exp(2\pi i f t) dt, \quad (8.114)$$

where $F(t)$ is the instantaneous energy dissipation rate at time ' t ', and $\langle \dots \rangle_{t_0}$ represents an average over all times t_0 , also obeys a power law. We follow [bak87b].

First, to find $F(t)$, let $f(\mathbf{x}, t)$ represent the dissipation of energy at site $\mathbf{x}$ at time ' t '. Since the dynamics specified by equations 8.109 yields an energy dissipation of

one unit, we have that $f(\mathbf{x}, t) = \delta(\mathbf{x}, t)$. The growth rate of a given domain is equal to the instantaneous energy dissipation rate $F(t) = \int f(\mathbf{x}, t) d\mathbf{x}$. A domain of size $s = \int F(t) dt$ (integrated over the duration of a single avalanche) therefore represents *total dissipated energy* resulting from a single perturbation.

Now consider the case where the system is perturbed randomly in space and time and $F(t)$ represents a superposition of many avalanches (occurring simultaneously and independently).[†] The total power spectrum is the (incoherent) sum of individual contributions for single relaxation event due to single perturbations. Consider the relaxation due to a single perturbation in a given domain. The resulting correlation function $C(t) = \frac{s}{\tau} \exp(-\frac{t}{\tau})$ yields a contribution to $S(f)$ equal to $S(f; s, \tau) = s/(1 + 4\pi f^2 \tau^2)$. The total power spectrum is then given by

$$\begin{aligned} S(f) &= \sum S(f; s, \tau), \\ &\approx \int \frac{s}{1 + 4\pi f^2 \tau^2} D(\tau) d\tau, \\ &\approx f^\gamma = f^{\alpha-2}. \end{aligned} \tag{8.115}$$

One of the virtues of having such a simple dynamical model (and a major theme of the subject of this book) is the possibility of capturing the truly essential ingredients of certain observed dynamical or physical properties of more complex systems. Flicker noise is a good case in point. The shear breadth of phenomena that purportedly show $1/f$ -noise suggests that *if there is a common underlying mechanism responsible for its appearance*, then that mechanism is likely to be independent of the physical details of any given system. Therefore, an extremely useful place to start looking for such a mechanism is in the dynamical behavior of simple dynamical systems that capture the generic properties of a wider classes of more realistic physical systems.

Wiesenfeld, *et. al.* [wiesen89] compare the simplicity of the ‘independent relaxation time’ interpretation of $1/f$ -noise fluctuations in the sandpile CA model to other recent models yielding $1/f$ noise:

Intermittency:[†] Manneville [mann80] showed that for the special case of a generic intermittency threshold in which the tangent point lies at the endpoint of the interval (in the case of a one dimensional iterative map of an interval to itself), the resulting chaotic dynamics has a power spectrum $S(f) \sim 1/(f(\log f)^2)$ for low f . Miracky, *et. al.* were able to modify the map to obtain an exact $1/f$ behavior [mirack87]. Because the result depends on the fine-tuning of an external parameter, however, it does not so much explain the generic appearance of flicker noise phenomena as beg the obvious question, “why do systems typically sit at whatever

[†]The notion that $1/f$ noise results from a distribution of relaxation times, operating simultaneously and independently, was first proposed by A. van der Ziel, *Physica* **16** (1950) 359.

[†]see section 4.1 for a general discussion of one-dimensional iterative maps and intermittency.

parameter value is required to induce $1/f$ noise?”

Coupled Logistic Map arrays:[†] Keeler and Framer [keeler87] showed that an array of coupled logistic maps displayed *robust intermittency* (persisting over a whole parameter interval) and a low-frequency power spectrum dependence of the form $f^{-\beta}$ (with relatively large β). In contrast to the absence of any characteristic length scales in the critical state of the sandpile CA model, however, Keeler and Farmer show that the logistic array displays a “stable natural wavelength”. Wiesenfeld, et. al. [wiesen89] suggest that an experiment that tests the correlations between spatial and temporal fluctuations could be used to decide between these two approaches.

Hierarchical Structures:[§] Huberman and Kerzberg [huber85c] show that $1/f$ noise can result from certain hierarchical structures, the basic idea being that diffusion between different levels of the hierarchy yields a hierarchy of time scales. Since the ‘hierarchical dynamics’ approach appears to be (on the surface, least) very different from the sandpile CA model, it is an intriguing challenge to see if the two approaches are related on a more fundamental level.

8.8 Structurally Dynamic Cellular Automata

In this section we investigate the behavior of *structurally dynamic cellular automata* (SDCA). This is an abstract model system in which the topological structure of the underlying lattice is dynamically coupled to the local site value configuration. The coupling is defined to treat *geometry* and *value configurations* on an approximately equal footing: the structure is altered locally as a function of individual site neighborhood value-states and geometries while local site-connectivity supports site-value evolution precisely as in conventional nearest-neighbor CA-models defined on random lattices. More detailed discussions appear in [adam94], [halp90], [ilach87], and [ilach88]. Majercik [maj94] has studied (a hierarchy of) SDCA models as models of computation, and defines a class of CA-universal SDCA.

In addition to providing a natural framework for a CA-like analysis of the generation, transmission and interaction of *topological disturbances* in the lattice, the model allows for the study of true *geometric self organization*, and not merely geometric analogs such as organized space-time patterns of value-configurations which clearly owe their existence to a regularity of structure of the background lattice. Immediate applications can be made to simulations of *crystal growth*, *pattern formation* of random cellular structures [rivier86] and neural network models incorporating a *synaptic plasticity* in their dynamics [mals86]. More ambitiously, SDCA are seen to embody a necessary property of truly self-modifying systems: the events themselves are dynamically coupled to, and therefore continually modify, the spatial arena on which their transformations are defined. In view of the recent proposals that the topology and dimension of a discrete space-time may be self-generated dynamic

[†]See section 4.1.4 for a discussion of the one-dimensional logistic map.

[§]See section 12.3.2 for a discussion of complexity in hierarchical structures.

constructs, such systems could prove to be of fundamental physical importance (see discussion in chapter 12). Hossbacher [hass98] has recently used a generalized version of the basic SDCA model to describe fluids in which the particle flow is coupled to a dynamical geometry (i.e. chemical self-assembly).

8.8.1 The SDCA Model

Conventional CA models are defined on particular lattice-networks, the sites of which are populated with discrete-valued dynamic elements evolving under certain local transition functions. Such a network with N sites is simply a general (undirected) graph G of size N and is completely defined by the $(N \times N)$ connectivity matrix

$$\ell_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are linked;} \\ 0 & \text{otherwise.} \end{cases} \quad (8.116)$$

Using the graph metric function $D_{ij} = \min_{paths} [\#links(i, j; path)]$, we can write a general r -neighborhood CA *value-transition rule* ' f ' in the form

$$\sigma_i^{t+1} = f[\{\sigma_j^t \mid j \in S_r^G(i)\}], \quad (8.117)$$

where $S_r^G(i) = \{j \mid D_{ij} \leq r\}$ is the radius- r *graph sphere* about the site- i . Extending the conventional dynamic arena, consisting of $\sigma_i^t \in \{0, 1\}$, $i=1, \dots, N$, to include the *vertex-interconnectivity*, ℓ_{ij}^t , our task is to explore evolutionary properties of the more general system

$$\begin{cases} \sigma^{t+1} &= F_1[\{\sigma^t\}, \{\ell^t\}] \\ \ell^{t+1} &= F_2[\{\sigma^t\}, \{\ell^t\}], \end{cases} \quad (8.118)$$

in which the changing *value* states and *geometries* are explicitly coupled. The complete system at time- t must now be specified by the state-vector

$$|G>_t = |\sigma_1^t, \dots, \sigma_N^t; \quad \{\ell_{ij}^t\}>. \quad (8.119)$$

The time-evolution of $|G>$ then proceeds according to the following transition rules: (i) *value* processors of the general form given above and familiar from CA simulations and (ii) *link* processors, which can be divided into site *couplers*, linking previously unconnected vertices and site *decouplers*, which disconnect linked points. Because the topology can be altered only by either a deletion of *existing links* or an addition of links between pairs of vertices ' i ' and ' j ' with $D_{ij} = 2$, the dynamics is *strictly local*.

To be more precise, we first restrict the general value-transition rule F_1 to (maximally symmetric) *totalistic* (T) and *outer-totalistic* (OT) type. Since the underlying lattice is a fully dynamic object, $|G>$ will, in general, tend towards having a complex local geometry with an unspecified local *directionality*. The most general rules which can therefore be applied are those which are completely invariant under all rotation and reflection symmetry transformations on local neighborhoods. T (OT) value rules are then specified by listing particular *sums* $\{\alpha\}$ (*outer-sums*

$\{\alpha_0\}, \{\alpha_1\}$ corresponding to center site values '0' and '1' respectively) for which the value of the center site becomes '1'. Formally,

$$\sigma_i^{t+1} = \phi_{\{\alpha\}}\left(\sum_j \ell_{ij}^t \sigma_j^t, \sigma_i^t\right), \quad (8.120)$$

where

$$\phi_{\{\alpha\}}(x, a) = \begin{cases} \sum_{\alpha} \delta(x + a, \alpha) & \longleftrightarrow \text{totalistic} \\ a \sum_{\alpha_1} \delta(x, \alpha_1) + (1 - a) \sum_{\alpha_0} \delta(x, \alpha_0) & \longleftrightarrow \text{outer-tot.}, \end{cases} \quad (8.121)$$

and $\delta(x, y)$ is the *Kronecker delta*. Note that $\sum_j \ell_{ij}^t \sigma_j^t$ sums the values of all sites 'j' linked to 'i' at time 't'. The action on the state $|G\rangle$ is represented by

$$\hat{\phi}_{\{\alpha\}}^i |\sigma\rangle_t = |\sigma_1^t, \dots, \sigma_i^{t+1} = \phi_{\{\alpha\}}(\sum_j \ell_{ij}^t \sigma_j^t, \sigma_i^t), \dots, \sigma_N^t\rangle, \quad (8.122)$$

where we distinguish the *operator* $\hat{\phi}^i$ acting on the global value state from the actual local transition *function* ϕ which transforms each site value.

Local geometry altering rules are constructed by direct analogy: for any two selected sites i and j we restrict attention to site values of vertices contained within a 1-*sphere* of either site; that is, to all $k \in S_1(i, j) = S_1(i) \cup S_1(j)$. *Link* operators, whose action on the state is represented by –

$$\begin{aligned} \text{decouplers : } \quad \hat{\psi}_{\{\beta\}}^{ij} |\ell_{ij}^t\rangle &= |\ell_{11}^t, \dots, \ell_{ij}^{t+1} = \psi^{ij}, \dots, \ell_{NN}^t\rangle \\ \text{couplers : } \quad \hat{\omega}_{\{\varepsilon\}}^{ij} |\ell_{ij}^t\rangle &= |\ell_{11}^t, \dots, \ell_{ij}^{t+1} = \omega^{ij}, \dots, \ell_{NN}^t\rangle, \end{aligned} \quad (8.123)$$

either *link* or *unlink* two sites 'i' and 'j' depending on whether the actual sum of values in $S_1(i, j)$ matches any of those given in the $\{\beta\}$ or $\{\varepsilon\}$ lists, which completely define *decouplers* and *couplers*, respectively.

In order to construct classes of rules analogous to the two types of value-rules defined above, we partition the local neighborhood into 3 disjoint sets (figure 8.18): $S_1(i, j) = V_{ij} \cup A_{ij} \cup B_{ij}$, where

$$\begin{cases} V_{ij} &= \{i, j\}, \\ A_{ij} &= \{k \mid k \in C_1(i) \cap C_1(j)\} \text{ where } C_1(i) = S_1(i) - \{i\}, \\ B_{ij} &= S_1(i) \cup S_1(j) - V_{ij} - A_{ij}. \end{cases} \quad (8.124)$$

The action of link operators is then conveniently expressed as a function of the sums within the individual partitions. Defining $\nu_{ij} = \sigma_i + \sigma_j$, $a_{ij} = \sum_{k \in A_{ij}} \sigma_k$, and $b_{ij} = \sum_{k \in B_{ij}} \sigma_k$, we get

$$\text{decouplers : } \psi_{\{\beta\}}^{ij} = \psi_{\{\beta\}}^{ij}(\nu_{ij}, a_{ij}, b_{ij}) \quad \text{where,}$$

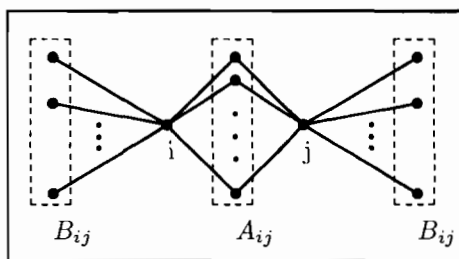


Fig. 8.18 Neighborhood partitioning. In the same way as *outer* sites can be considered separately for value transitions, we may, for topology transitions, distinguish between those sites belonging to *both* i and j ($\in A_{ij}$) and those belonging to *one* of the two sites but not both ($\in B_{ij}$). In this way we obtain the analogous *totalistic* (**T**), *outer-totalistic* (**OT**), and an additional type called *restricted totalistic* (**RT**).

$$\psi_{\{\beta\}}^{ij}(x, y, z) = \begin{cases} \{1 - \sum_k \delta(x + y + z, \beta_k)\} \ell_{ij} & \mathbf{T} \\ \{1 - \sum_k \delta(x, \beta_{1,k}) \delta(y + z, \beta_{2,k})\} \ell_{ij} & \mathbf{OT} \\ \{1 - \sum_k \delta(x, \beta_{1,k}) \delta(y, \beta_{2,k}) \delta(z, \beta_{3,k})\} \ell_{ij} & \mathbf{RT}, \end{cases} \quad (8.125)$$

$$\text{and couplers: } \omega_{\{\varepsilon\}}^{ij} = \omega_{\{\varepsilon\}}^{ij}(\nu_{ij}, a_{ij}, b_{ij}) \quad \text{where,}$$

$$\omega_{\{\varepsilon\}}^{ij}(x, y, z) = \begin{cases} \delta(D_{ij}, 2) \sum_k \delta(x + y + z, \varepsilon_k) & \mathbf{T} \\ \delta(D_{ij}, 2) \sum_k \delta(x, \varepsilon_{1,k}) \delta(y + z, \varepsilon_{2,k}) & \mathbf{OT} \\ \delta(D_{ij}, 2) \sum_k \delta(x, \varepsilon_{1,k}) \delta(y, \varepsilon_{2,k}) \delta(z, \varepsilon_{3,k}) & \mathbf{RT}. \end{cases} \quad (8.126)$$

In the above expressions, **RT** stands for *restricted totalistic* rules which maximally subdivide the local neighborhood. The inclusion of an ℓ_{ij} in the expressions for ψ assures that only those sites already *linked* can be decoupled and the $\delta(D_{ij}, 2)$ in the equations defining ω are put in to make sure that only sites separated by distance=2 may be dynamically coupled.

The various type-specific *sums* appearing above are indexed with the following conventions:

1. **T** – rules are defined by the ‘ k ’ overall sums of values in $S_1(i, j)$ for which the particular action is to be taken. (Ex – define ‘ ψ ’ by *unlinking* ‘ i ’ and ‘ j ’ if the total sum = 1(= β_1), 3(= β_2) or 5(= β_3). Equation (4.10) then states that $\ell_{ij}^{n+1} = 0$ if and only if $\ell_{ij}^n = 1$ and $\nu_{ij}^n + a_{ij}^n + b_{ij}^n \in \{1, 3, 5\}$.

2. **OT** – rules are specified by giving ‘ k ’ 2-tuples $(\beta_{1,k}, \beta_{2,k})$, and $(\varepsilon_{1,k}, \varepsilon_{2,k})$, where $\{1, k\}$ labels the sum ‘ $\sigma_i + \sigma_j$ ’ and $\{2, k\}$ labels the corresponding *outer sum* = $\sum_{s \in S_1(i, j) - \{i, j\}} \sigma_s$. (Ex – *link* ‘ i ’ and ‘ j ’ if $\sigma_i + \sigma_j = 0$ and outer sum = $\{3, 4\}$, so that ‘ ω ’ is defined by listing the two 2-tuples $(\varepsilon_{1,1}=0, \varepsilon_{2,1}=3)$ and $(\varepsilon_{1,2}=0, \varepsilon_{2,2}=4)$).

3. **RT** – rules are completely specified by giving the ‘ k ’ 3-tuples of values $(x = \sigma_i + \sigma_j, y = \text{sum in } A, z = \text{sum in } B)$, for which the link operation between ‘ i ’

and ‘ j ’ is to be performed. (Ex –define ‘ ψ ’ by *unlinking* ‘ i ’ and ‘ j ’ for the following values of partitioned sums: $(0, 0, 1)$, $(0, 0, 2)$, $(0, 1, 1)$, $(1, 1, 1)$; we then have that $(\beta_{1,1}=0, \beta_{2,1}=0, \beta_{3,1}=1)$, $(\beta_{1,2}=0, \beta_{2,2}=0, \beta_{3,2}=2)$, $(\beta_{1,3}=0, \beta_{2,3}=1, \beta_{3,3}=1)$, and $(\beta_{1,4}=0, \beta_{2,4}=1, \beta_{3,4}=1)$).

Global transition operators are obtained by applying individual value and link operators to all *sites* and *site-pairs* in the graph G :

$$\begin{cases} \hat{\Phi}_{\{\alpha\}}|\sigma\rangle &= \prod_i \hat{\phi}_{\{\alpha\}}^i|\sigma\rangle, \\ \hat{\Psi}_{\{\beta\}}|\ell\rangle &= \prod_{n<ij} \hat{\psi}_{\{\beta\}}^{ij}|\ell\rangle, \quad \text{and} \\ \hat{\Omega}_{\{\varepsilon\}}|\ell\rangle &= \prod_{nn<ij} \hat{\omega}_{\{\varepsilon\}}^{ij}|\ell\rangle, \end{cases} \quad (8.127)$$

where the products for $\hat{\Psi}$ and $\hat{\Omega}$ need to be taken only over *nearest* and *next nearest* pairs respectively. Given the full *value-topology* transition rule Γ , defined by

$$|G\rangle_{t+1} = (\hat{\Omega}\hat{\Psi}\hat{\Phi})|G\rangle_t = \Gamma|G\rangle_t, \quad (8.128)$$

the fundamental problem is to understand the generic behavior of accessible graphs- G emerging from all possible initial structures and value configurations. We emphasize that the lattice *fully* participates in the dynamics and that, in general, no embedding is implied – it is the abstract *connectivity* itself whose evolution we are attempting to trace.

8.8.2 An Example

The application of the rather cumbersome expressions defining transition rules is in practice extremely straightforward, as we demonstrate with the following example: Consider a graph G defined as a (5×5) lattice with some distribution of values $\sigma=1$ at time ‘ $t=1$ ’ (see figure 8.19). We are interested in one *global* update of the system $|G\rangle_{t=1} \xrightarrow{\Gamma} |G\rangle_{t=2}$ with rules specified by

$$\begin{aligned} (\text{value}) \quad \Phi_{\{\alpha\}} : \quad \{\alpha\}_{totalistic} &= \{1, 3, 5\}, \\ (\text{topology}) \quad \Psi_{\{\beta\}} : \quad \{\beta\}_{outer-tot.} &= \{(\beta_{1,1}=1, \beta_{2,1}=3), (\beta_{1,2}=1, \beta_{2,2}=4)\}, \\ \Omega_{\{\varepsilon\}} : \quad \{\varepsilon\}_{outer-tot.} &= \{\varepsilon_{1,1}=1, \varepsilon_{2,1}=3\}. \end{aligned} \quad (8.129)$$

We evolve the system by systematically sweeping through...

1. All *sites*, setting $\sigma_i=1$ only at those ‘ i ’ for which the sum of the values at ‘ i ’ and its neighbors is equal to ‘2’ at $t=1$. By *neighbors* of any point ‘ i ’ we will always mean the set of vertices *linked* to ‘ i ’: (a, b) , (h, m) and (x, y) , for example, are all *neighbors* at $t=1$.

Writing out a few *value-changing* terms explicitly, we find that

$$\sigma_c^{t=2} = \phi(\sigma_b^{t=1} + \sigma_c^{t=1} + \sigma_d^{t=1} + \sigma_h^{t=1}) = \phi(3) = 1, \quad \text{and}$$

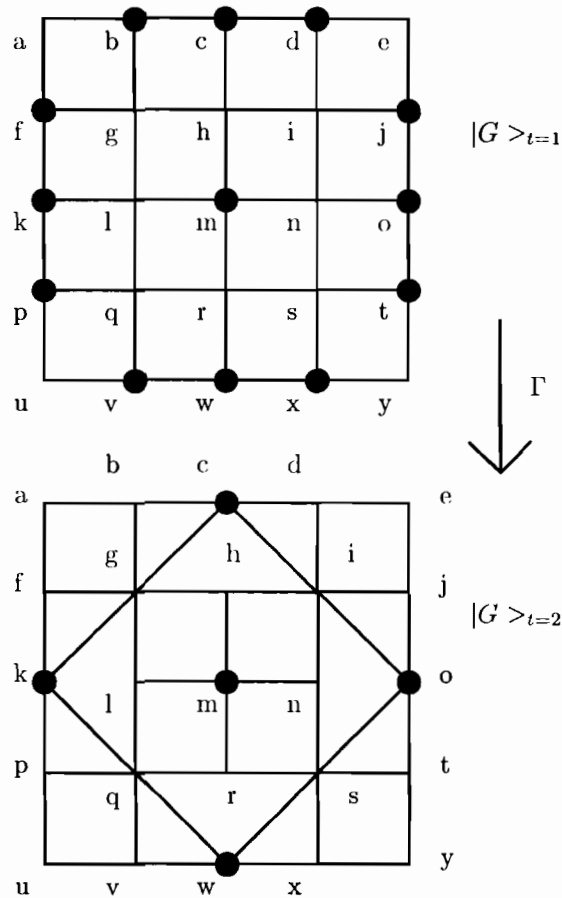


Fig. 8.19 Sample dynamic update of a (5 x 5) lattice from $t=1$ to $t=2$, obeying a **T**-type value-rule with $\sigma \rightarrow \sigma'$ for local sums = 1, 3, 5 (i.e. $\alpha \in \{1, 3, 5\}$), and **OT**-type link rules: (i) *link* for $\{\varepsilon_{1,1}=1, \varepsilon_{2,1}=3\}$ and (ii) *unlink* for $\{\beta_{1,1}=1, \beta_{2,1}=3\}$ and $\{\beta_{1,2}=1, \beta_{2,2}=4\}$. Solid sites indicate that $\sigma=1$.

$$\sigma_b^{t=2} = \phi(\sigma_a^{t=1} + \sigma_b^{t=1} + \sigma_c^{t=1} + \sigma_g^{t=1}) = \phi(2) = 0. \quad (8.130)$$

2. All *linked pairs* of sites 'i' and 'j', removing those links only if the 2-tuple $(\alpha, \beta) \in \{(1, 3), (1, 4)\}$, where $\alpha = \sigma_i + \sigma_j$ and ' β ' is the sum of values of the *neighbors* of 'i' and 'j' at $t=1$. For the points 'c' and 'h', for example, we have $(\alpha, \beta) = (1, 3)$, so that the link ℓ_{ch} is no longer present in $|G>_{t=2}$:

$$\begin{aligned} \ell_{ch}^{t=2} &= \psi(\sigma_c^{t=1} + \sigma_h^{t=1}, \sigma_b^{t=1} + \sigma_d^{t=1} + \sigma_g^{t=1} + \sigma_i^{t=1} + \sigma_m^{t=1}) \ell_{ch}^{t=1} \\ &= \psi(1, 3)(1) = 0. \end{aligned} \quad (8.131)$$

3. All *next-nearest neighbors* 'i' and 'j', *linking* them only if the 2-tuple $(\alpha, \beta) = \{(1, 3)\}$. By *next-nearest neighbor* we mean those pairs which are themselves *unlinked* but which *share at least one other linked neighbor*: (a, g) , (h, r) and (w, y) , for example, are all *next-nearest neighbors* at $t=1$. For 'c' and 'g' we find

$$\begin{aligned}\ell_{cg}^{t=2} &= \omega(\sigma_c^{t=1} + \sigma_g^{t=1}, \sigma_b^{t=1} + \sigma_d^{t=1} + \sigma_f^{t=1} + \sigma_h^{t=1} + \sigma_i^{t=1}) \delta(D_{cg}, 2) \\ &= \omega(1, 3)(1) = 1.\end{aligned}\quad (8.132)$$

Notice that although $\ell_{dn}^{t=1} = 0 \rightarrow \ell_{dn}^{t=2} = 1$, it is *hidden by overlap* with the remaining links $\ell_{di}^{t=2} = 1$ and $\ell_{in}^{t=2} = 1$. For this reason, not all link changes can always be observed directly in the following figures.

Other sites and links are updated in precisely the same manner. Had the *link-rules* been of *totalistic*-type, only *one* sum would have to be considered: the sum of the values of the points in question along with their neighbors' values. Had they been, instead, of *restricted totalistic*-type, *three* sums would have to be considered: the sum of the values of the sites in question, the sum of the values of their *common* neighbors (neighborhood *A* in figure 8.18) and the sum of the values of the points that are neighbors of one of the considered points, but not of the other (neighborhood *B* in figure 8.18). The final state $|G>_{t=2}$ emerges after the above process has been applied concurrently to *all pairs, neighbors and next-nearest neighbors* in $|G>_{t=1}$.

We conclude this section with a few general comments:

1. As defined above, Γ consists of three operators acting simultaneously on the state $|G>$. More generally, one may prescribe any of 10 possible time-orderings to the operators Ω , Ψ and Φ . That is, specify certain *intermediate* state dependencies, so that, for example $\Gamma_1|G>\equiv(\Omega\Psi)(\Phi|G>)$ would in general be expected to yield results different from, say, $\Gamma_2|G>\equiv\Omega(\Phi(\Psi|G>))$. While we will be solely concerned with the *synchronous* time ordering defined above, we do not expect the qualitative results to depend critically on this choice.

2. A given rule Γ is completely defined by the set of *sums* $\{\alpha\}$, $\{\beta\}$ and $\{\varepsilon\}$. Alternatively, by generalizing our encoding scheme for *value rules* (equation 2.4), we can conveniently summarize a chosen transition rule by a vector-code

$$\vec{C} = (c[\phi], c[\psi], c[\omega])_{a,b}, \quad \text{where} \quad (8.133)$$

$$c[\phi] = \begin{cases} \sum_{\alpha} 2^{\alpha} & \leftrightarrow \mathbf{T} \\ \sum_{\alpha_0} 2^{2\alpha_0} + \sum_{\alpha_1} 2^{(2\alpha_1+1)} & \leftrightarrow \mathbf{OT}, \end{cases} \quad (8.134)$$

$$c[\psi] = \begin{cases} \sum_k 2^{\beta_k} & \leftrightarrow \mathbf{T} \\ \sum_k 2^{3\beta_{2,k} + \beta_{1,k}} & \leftrightarrow \mathbf{OT} \\ \sum_k 2^{3(\beta_{2,k} + \alpha\beta_{3,k}) + \beta_{1,k}} & \leftrightarrow \mathbf{RT}, \text{ and} \end{cases} \quad (8.135)$$

Rule type	ϕ	ψ	ω
T	2^{d+1}	2^{2d}	2^{2d-1}
OT	2^{2d+2}	$2^{6(d-1)}$	$2^{3(2d-3)}$
RT		$2^{3(a+1)(2d-1)}$	$2^{3(a+1)(2d+1)}$

Table 8.10 Numbers of possible rules for each of the three types of transition rules. d =maximum allowable degree and a =maximum sum to be used from partition A_{ij} . *Ex-* for $d=5$, we have $N_\phi=4096$, $N_\psi=2^{24} \sim 2 \times 10^7$ and $N_\omega = 2^{21} \sim 2 \times 10^6$. We thus have $N_T=N_\phi N_\psi N_\omega \sim 10^{17}$ possible outer-totalistic type Γ 's.

$$c[\omega] = \begin{cases} \sum_k 2^{\varepsilon_k} & \leftrightarrow \mathbf{T} \\ \sum_k 2^{3\varepsilon_{2,k} + \varepsilon_{1,k}} & \leftrightarrow \mathbf{OT} \\ \sum_k 2^{3(\varepsilon_{2,k} + b\varepsilon_{3,k}) + \varepsilon_{1,k}} & \leftrightarrow \mathbf{RT}, \end{cases} \quad (8.136)$$

where $a=\max\{\beta_{2,k}\}+1$, $b=\max\{\varepsilon_{2,k}\}+1$, and must be specified only for **RT**-type topology rules. The Γ appearing in the above example, therefore, can be summarized by $c[\phi]=42$, $c[\psi]=2^{3(3)+1} = 1024$ and $c[\omega]=2^{3(4)+1} + 2^{3(3)+1} = 9216$. Note that ' Ψ ' and ' Ω ' are chosen always to be of the *same type*.

3. Computer simulations of these systems require that some measures be taken to prevent possible memory overflows, such as would happen in cases either of *pure coupling*, where links are continually added and none deleted, or in isolated regions of a graph where for a few sites more neighbors are added than are allowed by memory. We thus introduce *working* link transition rules

$$\tilde{\psi}^{ij} \equiv \begin{cases} \psi^{ij} & \longleftrightarrow d'_i \text{ or } d'_j > \delta \equiv d_{min} \\ 1 & \longleftrightarrow \text{else,} \end{cases} \quad (8.137)$$

$$\tilde{\omega}^{ij} \equiv \begin{cases} \omega^{ij} & \longleftrightarrow d'_i \text{ or } d'_j < \Delta \equiv d_{max} \\ 0 & \longleftrightarrow \text{else,} \end{cases} \quad (8.138)$$

where $d_i=\text{degree}(i)$ (i.e. number of neighbors of i). In words: make a sweep of the lattice, temporarily storing the *candidates* to *add* and *delete* for each point. If, for any point i , the *updated* degree is greater than δ then proceed with deleting the stored deletion-candidates, otherwise *do not* delete; similarly, provided that the *updated* degree is less than Δ proceed with addition. Thus, it is sufficient that *one* of two points allow a dynamic link change between them for that change to be enacted. In the following, the complete constrained dynamics will be quoted as $\tilde{C}_{(a,b)}^{[\delta,\Delta]}$. If constraints play no role in the actual evolution of specific examples, they will be left out of the definition.

4. Because each dynamic update involves three separate types of processing, the number of possible rules is extraordinarily large (see table 8.1). Unlike pure value transitions, however, the fraction of the total number which yield interesting behavior (i.e. neither immediately explosive, where the number of links increases without bound, nor immediately degenerative, where an initial graph rapidly dwindles to a few isolated links) appears to be manageably smaller.

5. We point out that, though it is the intrinsic *geometrical* patterning whose generic behavioral properties we are trying to deduce, one may approach these systems from an alternative point of view: maintain the emphasis on unraveling the *value* configurational behavior, and interpret the presence of $[\Psi, \Omega]$ as background operators inducing *nonlocal* spatial connectivities. Whereas the systems defined above are completely abstract entities, in that locality is strictly defined by the link structure, the alternative scheme would be to embed the discrete networks in some specified manifold, and to study the effects of dynamically allocated non-local communication channels.

8.8.3 Emerging Patterns and Behaviors

Consider patterns that emerge from simple value seeds starting from ordered 2-dimensional Euclidean lattices.[¶] A single non-zero site may represent a small local disturbance that then propagates outward, restructuring the lattice. With appropriately chosen Γ s one can induce a rich spectrum of different time evolutions only slightly perturbed by very few concurrent link changes to ones in which the initial geometry becomes radically altered.

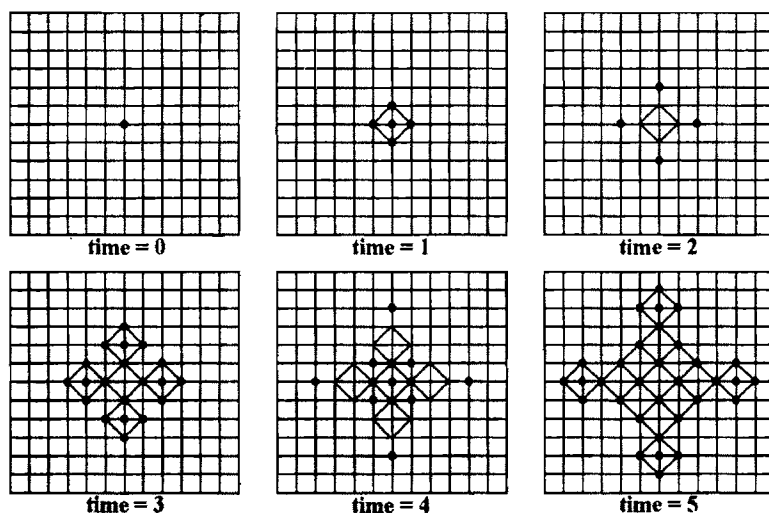


Fig. 8.20 First five iterations of an SDCA system starting from a 4-neighbor Euclidean lattice seeded with a single non-zero site at the center. The global transition rule Γ consists of totalistic-value and restricted totalistic topology rules: $\vec{C} = (26, 69648, 32904)_{[3,3]}$ (see text for rule definitions). Solid sites have $\sigma = 1$.

Figure 8.20 shows the first five iterations of a system starting from a four neighbor lattice with a single non-zero site at its center. The link structure is given

[¶]The graphical representation of developing 1-dimensional systems, in which link additions must be shown as arcs to avoid overlap with existing links, is needlessly confusing and is not considered.

explicitly and the solid circles represent sites with $\sigma = 1$. Notice how the link additions *follow* the emerging corrugated boundary surface of the value configuration. Remember that link additions are more than passive markers indicating particular correlations between local value configurations and structure; their presence directly influences all subsequent value development in their immediate vicinity.

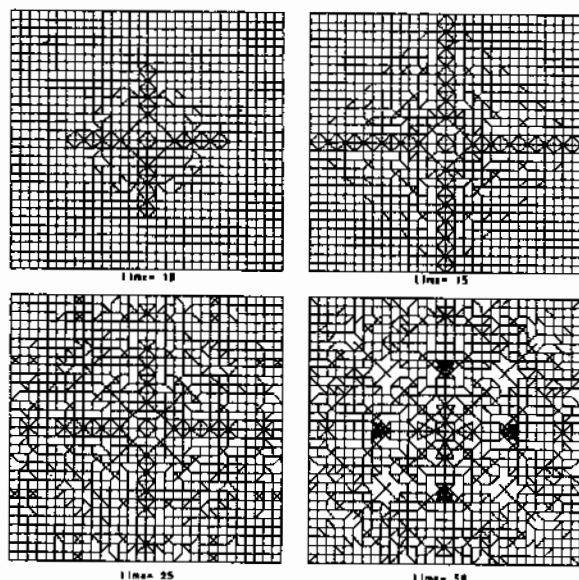


Fig. 8.21 Several further time frames in the structural evolution of the same system shown in the preceding figure. The values have been suppressed for clarity. The boundaries of the original lattice *do not* extend beyond the region shown so that the development is strictly confined to a 31×31 graph.

Figure 8.21 (in which site values are suppressed for clarity) shows the continued development of this system. Though boundary effects begin to appear by $t = 25$, the characteristic manner in which this particular Γ restructures the initial graph is clear:

- There is a high degree of geometrical organization (the symmetry of the initial state is trivially preserved by the totally symmetric Γ).
- The lattice remains connected.
- The distribution of link changes made throughout the lattice remains fairly uniform (i.e. there is an approximate uniformity in the probability of appearance of particular local value states which induce a structural change).
- Link-lengths do not get arbitrarily large.

The last point implies that for a system embedded in the plane, communication

channels remain approximately local. The global pattern emerges as a consequence of local ordering. On the other hand, Γ s for which link-lengths get arbitrarily large are also easy to find.

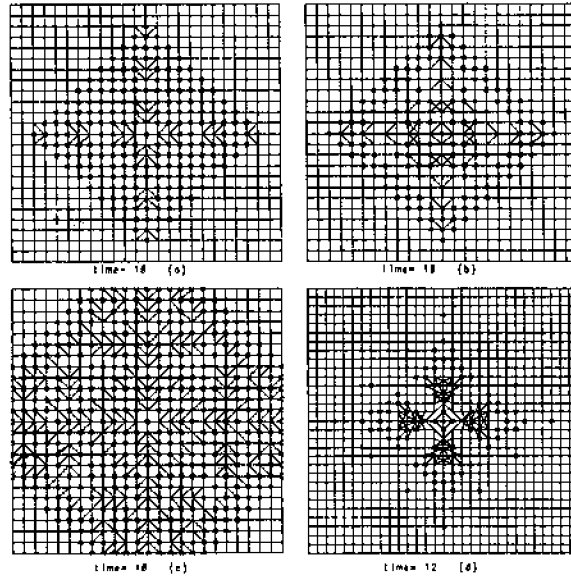


Fig. 8.22 Snapshot views of four typical developing states starting from a single non-zero site at the center of a 4-neighbor graph. Γ s are as follows: (a) OT $c[\phi] = 1022$ and RT coupler $c[\omega] = 16$, $b = 1$; (b) T $c[\phi] = 22$ and RT coupler $c[\omega] = 32$, $b = 2$; (c) OT $c[\phi] = 1022$ and RT coupler $c[\omega] = 8$, $b = 1$; (d) T value and OT topology rules $\tilde{C} = (682, 19634061312, 133120)_{[2,8]}$.

Some other varieties of behavior are shown in figure 8.22 and 8.23. Figures 8.22-a and 8.22-b are representative of the class of link rules for which the induced structural change is only minimal. Such systems evolve essentially as a CA system on a mildly perturbed underlying lattice. Other rules may have a much stronger effect on the lattice and can significantly alter the manner in which the pure value propagation proceeds in the absence of any link operators.

Figure 8.22-c shows an example of a link rule that accelerates the outward propagation of the value configuration. Compare the diameter of this pattern to that in the earlier figures, both shown at equal times. The outwardly oriented links that emerge from sites along the boundary surface become conduits by which non-zero values rapidly propagate. Had the underlying lattice topology been suppressed in this figure, and attention focused exclusively on the developing value state, we could have interpreted the result as showing an effective increase in information propagation speed due to non-local connectivities (see comment 5 of the previous section).

Figure 8.22-d, on the other hand, gives an example in which the link dynamics lags behind the value development. In this example, the boundary proceeds outward

essentially unaffected by changes in geometry which are themselves confined to the interior parts of the lattice (at least at this early stage of this system's development).

Figure 8.23 shows snapshot views of a few system undergoing a slightly more complex evolution. Figure 8.23-b, for example, shows a rule in which the outward value propagation rapidly deletes most links from the original lattice but leaves a complex – but structurally stable – geometry at the origin of the initial disturbance. Figure 8.23-c, on the other hand, shows a typical state of a system whose global connectivity becomes progressively more complicated.

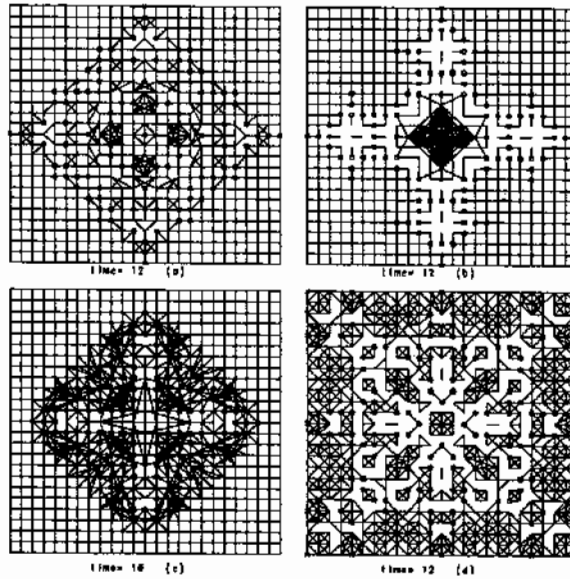


Fig. 8.23 Four more examples of states emerging from simple seeds. Figure (a,b,c) start from 4-neighbor graphs and (d) from an 8-neighbor graph ($\equiv$ 4-neighbor with diagonals). Γ 's are as follows: (a) T value and RT topology rules $\vec{C} = (42, 69648, 32904)_{[3,3]}$; (b) T value and OT topology rules $\vec{C} = (42, 589952, 8192)_{[2,8]}$; (c) T value and topology rules $\vec{C} = (42, 128, 4)_{[0,10]}$; (d) T $c[\phi] = 682$ and RT topology rules defined explicitly by $\Psi_{(104),(114),(124),(103),(113),(123)}$ and $\Omega_{(111),(215)}$.

A typical evolution starting from an initial state in which all sites are randomly assigned $\sigma = -1$ with probability $p = 1/2$ is shown in figure 8.24. Notice the rapid development of complex local connectivity patterns, the appearance of which points to a geometrical self-organization.

In general, structural behaviors emerging from random value states under typical Γ 's can be grouped into four representative categories:

Category 1: Initial states decay into structurally much simpler final states in which most links have been destroyed so that the graph G consists essentially of a large number of small local subgraphs.

Category 2: Evolution leads to periodic but globally connected geometries. Systems in this category arise either because of a specific class-2 Φ s remaining unchanged by the coupling to the lattice or class-3 Φ s coupling with $\{\Psi, \Omega\}$ in such a way as to induce a lattice structure that supports a periodic state.

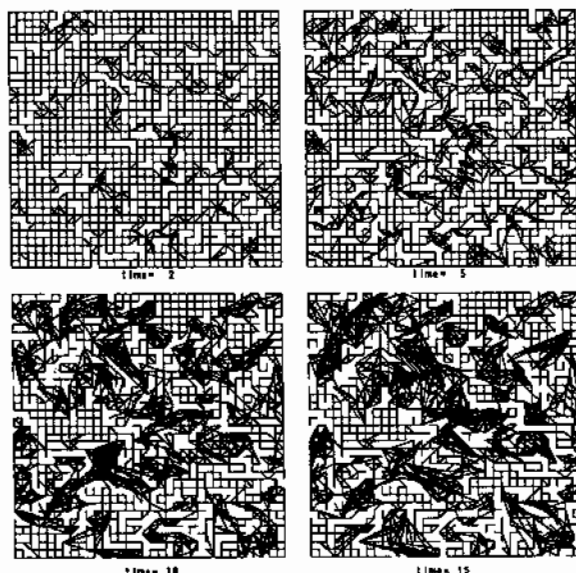


Fig. 8.24 Evolution of a 35×35 lattice whose sites are initially randomly seeded with $\sigma = 1$ with probability $p = 1/2$. The development proceeds according to T value and OT topology rules defined by code $\vec{C} = (84, 36864, 2048)$. The constraints are $[\delta = 0, \Delta = 10]$. The appearance of localized substructures is evidence of a geometrical self-organization.

Category 3: Systems exhibiting a proloner growth in complexity. Defining $\langle d \rangle \equiv \text{average degree} = \text{average number of neighbors per site}$ and an *effective dimensionality* $D_{\text{effec}} \equiv \text{ratio of the number of next-nearest to nearest neighbors}$, both of these measures increase in value in category 3 SDCA systems and appear to be bounded only by imposing an upper constraint Δ . Because the site value density responds to the changing local neighborhood structure, it is possible that what at first appears to be an explosive growth in fact eventually leads to a more sedate, if not stasis, behavior at some larger $\langle d \rangle \gg \Delta$. Certainly Φ s that yield $\rho^{(\sigma)}$ s that remain fairly constant over a large range of $\langle d \rangle$ (such as the $\oplus_2$ rule) when coupled with link rules that themselves become progressively less active with increasing $\langle d \rangle$, may induce evolutions leading to only mild changes within specific ranges of the local structural parameters.

Category 4: Category 4 includes a remarkable set of rules whose action appears to lead to a *sustained* global dynamics during which the value of D_{effec} remains almost constant. That is, particular combinations of Ψ and Ω effectively induce a

structural equilibrium: though large numbers of link changes continue to be made, so that the detailed structure of the graph continues to change, the average ration of the number of next-nearest to nearest neighbors stays approximately constant over long period of time. Simulations have, unfortunately, been run for too short a time and on graphs containing too few sites to permit making a conclusive statement. Nonetheless, it is conjectured that as $N \rightarrow \infty$, there are a large set of category-4 Γ s that maintain an average D_{effec} arbitrarily close to a desired value D^* . Category-4 behavior, of course, can always be artificially induced either by imposing severe $[\delta, \Delta = \delta]$ constraints, or, as is typically the case for category-3 Γ s, by impeding growth with some desired Δ .

The evolution of systems starting from random initial value states is generally difficult to follow visually, particularly for Γ s that induce many structural changes, and must therefore be studied indirectly. The simplest way is to chart the time-development by recording selected statistical measures. A more detailed account is given in [ilach88].

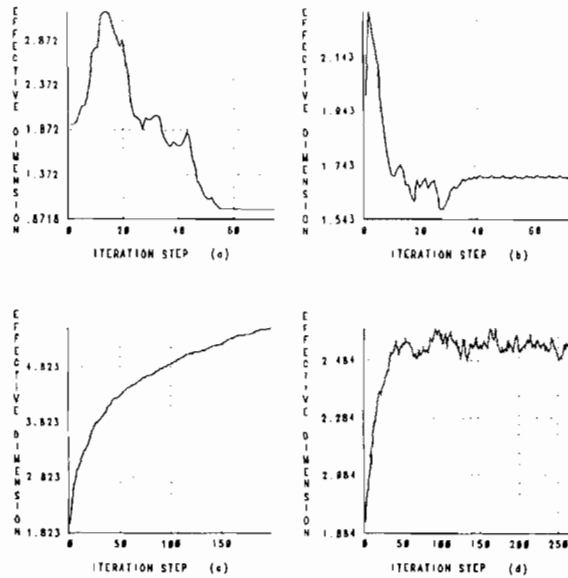


Fig. 8.25 Time development of the effective dimensionality D_{effec} for each of the four categories of behavior (see text): (a) T type Γ defined by $\vec{C} = (42, 128, 4)$; (b) T value and OT topology rules $\vec{C} = (64, 9216, 1024)$; (c) T value and OT topology rules $\vec{C} = (682, 512, 512)_{[0,10]}$; (d) T value and RT topology rules defined explicitly by $\vec{\beta} \in \{(011), (110), (121), (233), (243)\}$ and $\vec{\epsilon} \in \{(120), (010), (021), (224)\}$.

Figure 8.25 shows examples of rules in each of the four categories defined above. The initial structure in each case is 35×35 4-neighbor Euclidean lattice, so that $D_{\text{effec}}^{t=0} \sim 2$. Figure 8.23-a gives an example of a category-1 behavior, in which a short period of initial growth is followed by a decay into an essentially disconnected states. The final state is characterized by $\langle d \rangle < 1$ and is stable. Figure 8.25-b

shows a system that starts from the same initial state as in figure 8.25-a but whose Γ leads to a periodic structural state. Just the right number of links have been deleted to permit regions with isolated activity to emerge.

Figure 8.25-c shows category-3 behavior in which D_{effec} steadily increases. The apparent leveling off seen toward the end of the run is due both to a decreased overall activity level and the increasingly greater felt effect of a $\Delta = 10$ constraint. The system in figure 8.25-d clearly exhibits category-4 behavior, characterized by a continued development within a relatively narrow interval of values of D_{effec} . Note that the evolution in this last figure here is almost pure (i.e. unconstrained) and is not an artifact of strictly imposed dynamic conditions.

8.9 Mobile CA

In the previous section we considered a generalized CA rule structure in which the underlying lattice structure becomes an integral part of the CA dynamics. We conclude this chapter by briefly mentioning one other obvious, and no less significant, generalization in which the lattice sites are allowed to move. Normally, of course, site values are fixed and the only “movement” is that of information as a temporal consequence of the site value updates. When we “see” a glider move across the screen in Conway’s *Life* rule,[†] it is really the higher-order configurations of 1’s and 0’s that we are referring to, and not the actual lattice sites on which they are defined. One context in which it is natural to use mobile sites is in the modeling of land combat.

8.9.1 Models of Combat

If one abstracts the essentials of what happens on a battlefield, ignoring the myriad layers of detail that are, of course, required for a complete description, one sees that much of the activity involves the same kind of simple nearest-neighbor interactions that define cellular automata (see [ilach97a]). Woodcock, Cobb and Dockery [wood88] in fact show that highly elaborate patterns of military force-like behavior can be generated with a small set of cellular automaton-like rules. Ilachinski [ilach99] has taken this idea a step further to develop a “conceptual laboratory” in which one can explore self-organized emergent behavior on a notional battlefield using simple user-defined mobile CA (see **An Artificial-Life CA Model of Combat** in Chapter 11).

In Woodcock, *et al.*’s model, each combatant – or automaton – is endowed with a set of rules with which it can perform certain tasks. Rules are of four basic varieties:

Situation Assessment, such as the determination of whether a given automaton is surrounded by friendly or enemy forces.

Movement, to define when and how a given automaton can move; certain kinds

[†]See section 3.4.4.

of movement can only be initiated by threshold and/or constraint criteria.

Combat, which governs the nature of the interaction between opposing force automata; a typical rule might be for one automaton to "aim fire" at another automaton located within some specified fight radius.

Hierarchical Control, in which a three-level command hierarchy is established; each lower-level echelon element keys on those in the next higher echelon on each time step of the evolution.

These basic rules can then be augmented by additional rules to (1) simulate the impact that terrain barriers such as rivers and mountains have on the movement of military forces; (2) provide a capability for forces to respond to changing combat conditions (for example, a reallocation of firepower among three types of weapons: aimed firepower, area firepower and smart weapons firepower), and (3) replace entities lost through combat attrition. Figure 8.26 shows a schematic of three sample rules. A further extension involves relating notional features of battlefield geometry to the structure of real battlefields [dock93].

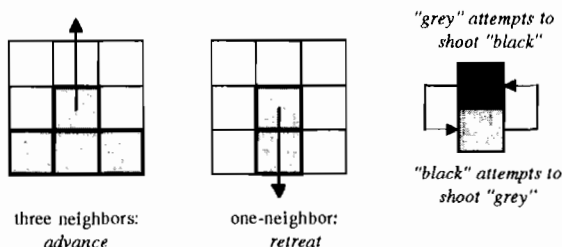


Fig. 8.26 Three sample rules in Woodcock, et. al.'s CA combat model.

One can argue that CA are ideal for studying combat because they force the user to focus on very basic processes. Woodcock, et. al. stress that the goal of CA-based model of combat is not to codify a body of rules that comes as close as possible to the actual behavioral rules obeyed by real combatants; rather, the goal lies in "finding the simplest body of rules that both can generate nontrivial global combat-like phenomena and provide a new understanding of the combat process itself by extracting the maximum amount of behavioral complexity from the least complicated set of rules." [wood88] Additional details are discussed in chapters 3.1 and 3.2 of reference [dock93].

8.10 Appendix: Origins of Irreversibility — The Kac Ring Model

While no one debates the validity of Boltzman's equation (equation 9.32) – one good reason for this is that there has been no experimental evidence suggesting that the theory is wrong – it is in a very important sense laced with a fundamental

paradox: while the laws of mechanics are fundamentally *reversible* (i.e. are symmetric in time), Boltzman's equation contains the first derivative with respect to time and therefore harbors an explicit *irreversibility*. Indeed, Boltzman's H-theorem states that entropy increases in time, a result which is somehow derived from the laws of mechanics that are themselves reversible. Moreover, Boltzman's equation is inconsistent with Poincare's *Recurrence Theorem*, which asserts that the state of every finite mechanical system approaches the initial state arbitrarily closely after a sufficiently long time [arnold78].[†] Yet, although such a return obviously requires the entropy to decrease back to its initial value, it is not permitted by Boltzman's equation, even as an approximation. Despite these and other arguments that there is a clear inconsistency between Boltzman's equation and basic mechanics, however, the fact remains that there is no experimental evidence suggesting that Boltzman's equation is incorrect. What of the origin of irreversibility then?

A simple model that illustrates the mathematical origins of irreversibility was first introduced by Kac in 1956 [kac56] and has come to be known as *Kac's Ring Model*.

Consider a circular ring with N equally spaced fixed sites, m of which are marked in some fashion; say, with a cross 'x' (see figure 8.27).

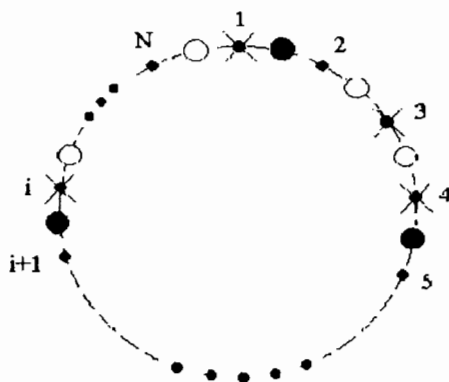


Fig. 8.27 Kac ring model: black and white balls move on a circular ring through points $1, 2, \dots, N$. If a ball moves across a point marked with a cross ('x'), it changes color.

Between each site there sits either a black or white ball. During a discrete time step, all balls simultaneously move clockwise one unit by crossing over their neighboring sites. A given ball changes its color if and only if it crosses a marked site. The problem is to find the distribution of "colors" at time t given some initial distribution at $t = 0$. Since the balls are essentially idealized scattering objects and individual sites are "scattering centers" we should, along with Boltzman, expect equilibrium to be approached as a result of "collisions" (i.e. color changes). Equilibrium is here understood as the state with an equal number of black and white balls. What this model so elegantly illustrates – the elegance of the argument

[†]The time required for such a return is called the *Poincare Recurrence Time*.

stemming from the model's subtle simplicity – is not so much the fact that equilibrium is eventually reached but the precise *manner* in which equilibrium is reached; more precisely, it underscores exactly what assumptions are needed to ensure that equilibrium is approached.

Aside from Kac's original paper mentioned above, a very nice concise discussion of the Kac ring model can be found in Wannier's text [wann66]. More detailed discussions, including a careful comparison between the approaches to equilibrium in *classical mechanical* and *quantum mechanical* versions of the model, are given by Dresden in [dres62], [dres72] and [dres87].

Before exploring the behavior of this system, we mention its two most obvious properties, consistent with what we expect of any "Newtonian" mechanical system: (1) *reversibility* – since, if at any time the direction of motion of the balls is suddenly reversed, the pattern of colors will be the same as before, and in the same positions; (2) *periodicity* – since each ball returns to its original position and color after two complete clockwise (or counterclockwise) cycles (i.e. the Poincare Recurrence Time is $2N$).

Perhaps our first instinct is to take the most direct approach. Namely, to simply write down and solve a set of "Newtonian" equations-of-motion describing the scattering dynamics in terms of basic system variables. While this naive, intuitive approach might be attractive, we show below that it turns out to be both "right" and "wrong".

"Newtonian" Approach: Let $N_b(t)$ and $N_w(t)$ represent the number of black and white balls at time t , respectively. Let $n_b(t)$ and $n_w(t)$ be the number of black and white balls having a marked site directly ahead of them at time t . The "Newtonian" equations of motion are then given by

$$\begin{cases} N_b(t+1) &= N_b(t) - n_b(t) + n_w(t), \\ N_w(t+1) &= N_w(t) + n_b(t) - n_w(t). \end{cases} \quad (8.139)$$

We also have two constraints. We require that the total number of balls and number of marked sites both remain fixed for all time:

$$\text{for all times } t, \quad \begin{cases} N_b(t) + N_w(t) &= n, \\ n_b(t) + n_w(t) &= m. \end{cases} \quad (8.140)$$

By themselves, equations 8.139 and 8.140 are insufficient to determine $N_b(t)$ and $N_w(t)$. An additional condition is needed. A simple choice would be a Boltzman Stosszahlansatz-like assumption that the color of a ball is uncorrelated with the property that the site ahead of it is marked. In particular, introducing the parameter $\mu \equiv m/n$, we assume that

$$\frac{n_b(t)}{N_b(t)} = \frac{n_w(t)}{N_w(t)} = \mu. \quad (8.141)$$

With this additional condition, equations 8.139 yield

$$\begin{aligned} N_b(t) - N_w(t) &= (1 - 2\mu) [N_b(t-1) - N_w(t-1)], \\ &= (1 - 2\mu)^t [N_b(0) - N_w(0)]. \end{aligned} \quad (8.142)$$

Assuming $\mu < 1/2$, this “solution” implies a monotonic approach to equilibrium with time. From a purely “statistical” point of view, this is certainly correct: the difference in number between the two different balls decreases exponentially toward a state in which neither color is preferred. In this sense, the solution is consistent with the spirit of Boltzman’s H-theorem, expressing as it does the idea of *motion towards disorder*. But the equation is also very clearly wrong. It is wrong because it is obviously inconsistent with the fundamental properties of the system: it violates both the system’s reversibility and periodicity. While we know that the system eventually returns to its initial state, for example, this possibility is precluded by equation 8.142. As we now show, the problem rests with equation 8.141, which must be given a *statistical interpretation*.

Statistical Approach: It is convenient to introduce the variables ϵ_i and η_i :

$$\epsilon_i = \begin{cases} +1 & \text{if there is no marker at site } i, \\ -1 & \text{if there is a marker at site } i. \end{cases} \quad (8.143)$$

and

$$\eta_i(t) = \begin{cases} +1 & \text{if the ball between sites } i-1 \text{ and } i \text{ is white at time } t, \\ -1 & \text{if the ball between sites } i-1 \text{ and } i \text{ is black at time } t. \end{cases} \quad (8.144)$$

In terms of these new variables, the scattering-dynamics are embodied by the equation

$$\eta_i(t+1) = \epsilon_{i-1}\eta_{i-1}(t). \quad (8.145)$$

Iteration yields the full “mechanical” solution:

$$\eta_i(t) = \epsilon_{i-1}\epsilon_{i-2}\epsilon_{i-3} \cdots \epsilon_{i-t}\eta_{i-t}(0), \quad (8.146)$$

where all indices should be taken *modulo* N .

Now, by definition, $N_b(t) = \frac{1}{2} \sum_i [1 + \eta_i(t)]$ and $N_w(t) = \frac{1}{2} \sum_i [1 - \eta_i(t)]$. From equation 8.146 we then have

$$\begin{aligned} N_b(t) - N_w(t) &= \sum_{i=1}^N \eta_i(t), \\ &= \sum_{i=1}^N \epsilon_{i-1}\epsilon_{i-2}\epsilon_{i-3} \cdots \epsilon_{i-t}\eta_{i-t}(0). \end{aligned} \quad (8.147)$$

We cannot progress any further at this point without assuming something about the distribution of markers. It is this distribution that effectively determines the

mechanical properties of our system. Since we do not particularly care about the exact distribution of markers, let us embed the model in an ensemble of other Kac ring models and consider an *average over all markers*. We have

$$\langle N_b(t) - N_w(t) \rangle = \sum_{i=1}^N \langle \epsilon_{i-1} \epsilon_{i-2} \epsilon_{i-3} \cdots \epsilon_{i-t} \eta_{j-t}(0) \rangle, \quad (8.148)$$

where $\langle \cdots \rangle$ denotes a probabilistic average over an ensemble of models. If we now assume that all marker positions are equally probable, so that the average of any t consecutive ϵ_j factors is independent of the first factor ϵ_{i-1} , we have that

$$\langle N_b(t) - N_w(t) \rangle = \langle \epsilon_1 \epsilon_2 \epsilon_3 \cdots \epsilon_t \rangle [N_b(0) - N_w(0)]. \quad (8.149)$$

For simplicity, let $\mu = m/n$ be the probability that a site contains a marker, and assume it is the same for all sites.[†] Let the probability that there are s markers among t sites be given by $p(s, t)$. The ensemble average may then be written as

$$\langle \epsilon_1 \epsilon_2 \epsilon_3 \cdots \epsilon_t \rangle = \sum_{s=0}^t (-1)^s p(s, t). \quad (8.150)$$

But $p(s, t)$ is simply the binomial distribution. More precisely, if $t \leq N$, $p(s, t) = \frac{t!}{s!(t-s)!} \mu^s (1-\mu)^{t-s}$. If $N < t \leq 2N$, a certain number of ϵ_j factors occur twice and so yield a factor ‘1’. In this case $p(s, t) = \frac{(2N-t)!}{s!(2N-t-s)!} \mu^s (1-\mu)^{2N-t-s}$. If $t > 2N$, the solution repeats periodically. Our “statistical approach” solution (equation 8.148) thus becomes

$$\langle N_b(t) - N_w(t) \rangle = (1 - 2\mu)^{N - |N-t|} [N_b(0) - N_w(0)]. \quad (8.151)$$

We make a few remarks about this solution. First, notice that for times $t \leq N$, this solution matches our “Newtonian” result given in equation 8.142. For large times, however, the behavior is periodic, as required by Poincaré’s recurrence theorem. Second, we see that, for $\mu < 2$, equilibrium is approached monotonically in the limit $t \rightarrow \infty$. In particular, we see that *two* processes are actually needed to ensure an approach to equilibrium: (1) *an ensemble average over site markers*, and (2) *the limit of an infinite system*. The derivation also suggests the true mathematical origin of irreversibility. Irreversibility turns out to not be due to the underlying mechanics, which remains strictly reversible, but to an averaging over a set of “disturbances” (i.e. markers) that are *external to the underlying mechanics*. It is this subtle interplay between a reversible underlying mechanics and external influence that helps explain a part of the seeming paradox introduced as motivation for this section. Lest the reader leave this section thinking that no mystery remains, however, we should be quick to point out that the general relation between this “external averaging” and Boltzman’s *Stosszahlansatz*, as embodied in equations 8.141, is tenuous at best and is still hotly debated. See [wann66] for additional details.

[†]While Kac [kac56] did not originally make this assumption, the conclusions remain the same.

Chapter 9

CA Models of Fluid Dynamics

This chapter is organized into two main parts. To give the reader an appreciation of real fluids, and the kinds of behaviors that it is hoped can be captured by CA models, the first part provides a mostly physical discussion of continuum fluid dynamics. The basic equations of fluid dynamics, the so-called *Navier-Stokes* equations, are derived, the *Reynolds Number* is defined and the different routes to turbulence are described. Part I also includes an important discussion of the role that conservation laws play in the kinetic theory approach to fluid dynamics, a role that will be exploited by the CA models introduced in Part II.

Perhaps the single most successful practical application of CA as *computing devices* that has been made thus far has been made in the field of fluid mechanics. Despite still being in their infancy, CA models of fluid dynamics, or *lattice gases* (LG), have already amply demonstrated that they can reproduce many of the essential features of thermodynamical and hydrodynamical behavior ([livi88], [monaco89], [doolen90], [doolen91]). Moreover, as the inherent parallel-processing dynamics of lattice gases is increasingly well exploited to build fast dedicated CA hardware for their simulation (such as the Connection Machine [hill85], RAP1 [clouq87], and CAM-8 [toff91]; see **Appendix A**), fluid behavior that was heretofore analytically intractable is becoming computationally analyzable. In terms of providing a practical technological benefit to the design of ships or airplanes, for which having accurate predictions of fluid flow near and around obstacles such as airplane wings is absolutely crucial, the importance of rapid LG “computers” cannot be overstated. As Weisbuch has suggested [weis91], such computers can play the role of “numerical wind tunnels.”

9.1 Continuum Fluid Dynamics

A mathematical description of continuum fluid dynamics can proceed from two fundamentally different points of view: (1) A *macroscopic*, or “top-down” ([hass87], [hass88]), approach, in which the equations of motions are derived as the most

general equations that define mass, energy and momentum conservation laws and obey the usual spatial invariances (translational, rotational and Galilean), or (2) A microscopic, or “bottom-up” ([hass87], [hass88]), approach, in which a molecular dynamics is derived from the microscopic properties of a fluid and the aggregate properties of the fluid are treated statistically. In this second approach, the various transport coefficients (viscosities, sound velocity, etc.) are all derived from the microscopic properties of the fluid (such as the inter particle potential).

There are many excellent fluid dynamics texts available. Lucid discussions of the “top-down” approach, with a strong emphasis on experimental observations, may be found in the texts by Batchelor [bat67] and Tritton [tritt88]. For the “bottom-up” approach, the reader is encouraged to consult the statistical mechanics texts by Balescu [bal75] and Huang [huangk63]. An excellent general introduction to the mathematical theory of fluid dynamics is the book by Chorin and Marsden [chor90], while Landau and Lifshitz’ classic text [landau59] remains one of the best overall references.

We begin our discussion with the “top-down” approach. Let Γ be a two or three dimensional region filled with a fluid, and let $\vec{v}(\vec{x}, t)$ be the velocity of a “particle” of fluid moving through the point $\vec{x} = (x, y, z)$ at time t . Note that $\vec{v}(\vec{x}, t)$ is a vector-valued field on Γ , and is to be identified with a macroscopic fluid cell. The fact that we can make this so-called *continuum assumption* – namely that we can simultaneously speak of a “velocity of a particle of fluid” and think of a particle of fluid as a “macroscopic cell” – is not at all obvious, of course, and deserves some attention.

In fact, we are assuming that a particular length scale exists such that a fluid cell can be defined that is *simultaneously* both small enough to justify our treating it as a mathematical point, and large enough so that it possesses whatever macroscopic properties are normally associated with the fluid in bulk. We are also assuming that the velocity field $\vec{v}$ is smooth enough to allow standard calculus operations to be performed on it. Physically, of course, if we go all the way down to the molecular level, the continuum assumption is patent nonsense. It is made plausible, however, if we think of the various macroscopic thermodynamic properties of an ideal gas. While the velocities of the individual molecules may be quite large, for example, the bulk flow velocity – or, more precisely, the *average molecular velocity* – is not. Likewise, the temperature, being essentially the average energy of the Brownian motion of the individual molecules, is also well defined in a statistical sense. All of the other “usual” macroscopic quantities – density, pressure, viscosity, etc. – are defined in the same way. Since such averaging processes make sense only if they are performed over a large number of molecules, our ideal “fluid cell” must be such that (i) it is large enough to contain a large number of molecules, and (ii) it appears “point-like” with respect to the bulk fluid flow. In the end, it is worth remembering that the continuum assumption is just that, namely an assumption. Its validity must ultimately be justified through experimental verification of the predictions of fluid behavior made by the equations that are themselves derived

from this assumption.[†]

9.1.1 Continuity Equation

We first derive the so-called continuity equation, which is a direct consequence of the conservation of mass. If ρ is the density, or mass per unit volume, then the total mass of a fluid contained in Γ is equal to $M = \int_{\Gamma} \rho \, d\Gamma$. Letting $dS = \hat{\mathbf{n}} \, dS$ be an element of the surface, with $\hat{\mathbf{n}}$ a unit vector perpendicular to the surface, the mass flow per unit time through the surface element is $\rho \vec{v} \cdot dS$. The total fluid flow out of the volume Γ is then given by

$$\text{rate of loss of mass from } \Gamma = \int_S \rho \vec{v} \cdot \hat{\mathbf{n}} \, dS. \quad (9.1)$$

Since a continuity of flow implies that the fluid flow through the surface must equal the loss of fluid in the enclosed volume, we have that

$$\int_S \rho \vec{v} \cdot \hat{\mathbf{n}} \, dS = -\frac{\partial}{\partial t} \int_{\Gamma} \rho \, d\Gamma = \int_{\Gamma} \nabla \cdot (\rho \vec{v}) \, d\Gamma, \quad (9.2)$$

or that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0, \quad (9.3)$$

which is known as the *continuity equation*. If the fluid is *incompressible*, $\rho = \text{const}$, and the continuity equation reduces to

$$\nabla \cdot \vec{v} = 0. \quad (9.4)$$

9.1.2 Euler's Equation

We next consider the consequences of Newton's second law of motion; i.e. the consequences of the fact that the rate of change of momentum of a fluid cell must equal the total force that is acting on it.

There are two possible kinds of force acting on a fluid cell: *internal stresses*, by which an element of fluid is acted on by forces across its surface by the rest of the fluid, and *external forces*, such as gravity, that exert a force per unit volume on the entire volume of fluid. We define an *ideal fluid* to be a fluid such that for any motion of the fluid there exists a *pressure* $p(\vec{x}, t)$ such that if S is a surface in the fluid with unit normal vector $\hat{\mathbf{n}}$, the stress force that is exerted across S per unit area at $\vec{x}$ at time t is equal to $-p(\vec{x}, t)\hat{\mathbf{n}}$. An ideal fluid is therefore one for which the only forces are internal ones, and are orthogonal to S ; i.e. there are no tangential forces.[‡]

[†]See [tritt88] for an expanded discussion of this point.

[‡]This means, in particular, that all fluid "rotations" (and the ubiquitous "vortices" that form behind the oars of a rowboat, for example) are disallowed in an ideal fluid. We will shortly consider a more realistic fluid.

Using the pressure of an ideal fluid, we see that the total force acting on a volume of fluid due to the rest of the fluid is given by $-\int_S p d\mathbf{S}$. Applying *Stokes Theorem*, we then have that

$$-\int_S p d\mathbf{S} = \int_{\Gamma} \nabla p d\Gamma. \quad (9.5)$$

Observing that the fluid-dynamical analogue of $\vec{F} = m\vec{a}$ is the equation

$$-\nabla p = \rho \frac{d\vec{v}}{dt}, \quad (9.6)$$

Euler's Equation for an ideal, dissipationless fluid is obtained by applying the chain-rule to the total-derivative $d\vec{v}/dt (= \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v})$ and substituting into equation 9.6:

$$\frac{\partial \vec{v}}{\partial t} = -\vec{v} \cdot \nabla \vec{v} - \frac{1}{\rho} \nabla p. \quad (9.7)$$

9.1.2.1 Momentum Flux Tensor

Since in real fluids, some of the energy of fluid flow is typically converted into heat by viscous forces, it is convenient to generalize equation 9.7 so that it allows for dissipation. Consider the momentum of fluid flowing through the volume $d\Gamma (= \rho \vec{v})$. Since its time rate of change is given by $\partial(\rho \vec{v})/\partial t = (\partial \rho/\partial t)\vec{v} + \rho(\partial \vec{v}/\partial t)$, we can use equations 9.3 and 9.7 to rewrite this expression as follows:

$$\frac{\partial(\rho \vec{v})}{\partial t} = -\vec{v} \cdot \nabla (\rho \vec{v}) - \rho(\vec{v} \cdot \nabla)\vec{v} - \nabla p, \quad (9.8)$$

or, in component form,

$$\frac{\partial(\rho v_i)}{\partial t} = -\sum_k \frac{\partial}{\partial x_k} \Pi_{ik}, \quad (9.9)$$

where

$$\Pi_{ik} \equiv p\delta_{ik} + \rho v_i v_k \quad (9.10)$$

is the *momentum flux tensor*. Equation 9.9 is the generalized *Euler's Equation*. The physical interpretation of Π_{ik} is most easily seen by integrating equation 9.9 and again applying *Stokes Theorem*:

$$\frac{\partial}{\partial t} \int_{\Gamma} (\rho v_i) d\Gamma = - \int_{\Gamma} \sum_k \frac{\partial}{\partial x_k} \Pi_{ik} d\Gamma = - \int_S \sum_k \Pi_{ik} dS. \quad (9.11)$$

We see that the time rate of change of the i^{th} component of momentum ($= \rho v_i$) in volume Γ (on the LHS) is equal to the surface integral of the i^{th} component of momentum ($= \sum_k \Pi_{ik} dS$) flowing through dS (on the RHS); i.e., Π_{ik} is the i^{th} component of momentum flowing in the k^{th} direction.

9.1.3 Navier-Stokes Equations

While the general form of the generalized Euler's equation (equation 9.9) allows for dissipation (through the term Π_{ik}), the expression for the momentum flux density as yet contains no explicit terms describing dissipation. Viscous stress forces may be added to our system of equations by appending to Π_{ik} a (momentarily unspecified) tensor σ' . Formally, we write

$$\Pi_{ik} = p\delta_{ik} + \rho v_i v_k - \rho \sigma'_{ik} = \sigma_{ik} + \rho v_i v_k, \quad (9.12)$$

where $\sigma_{ik} = p\delta_{ik} - \rho \sigma'_{ik}$ is the *generalized stress tensor* and σ'_{ik} is the *viscosity stress tensor*.

The form of σ'_{ik} can be deduced by making a few simplifying assumptions: (1) we suppose that the gradient of the velocity is changing slowly enough that $\sigma'_{ik} \propto \alpha \partial v_i / \partial x_k$, for some constant α ; (2) σ'_{ik} is equal to zero when $\vec{v} = 0$; and (3) since a rotation cannot impart a net momentum transfer to the fluid, σ'_{ik} must also vanish under all rotations. The unique form that satisfies these three properties is given by ([hass87], [hass88]):

$$\sigma'_{ik} = \alpha \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} \right) + \beta \delta_{ik} \sum_j \frac{\partial v_j}{\partial x_j}, \quad (9.13)$$

where α and β are unspecified coefficients; this quantity is more conventionally written in the form ([hass87], [wolf86c])

$$\sigma'_{ik} = \mu \left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3} \delta_{ik} \sum_j \frac{\partial v_j}{\partial x_j} \right) + \zeta \delta_{ik} \sum_j \frac{\partial v_j}{\partial x_j}, \quad (9.14)$$

where μ is the *kinematic shear viscosity* and ζ is the *kinematic bulk viscosity*.

The incompressible Navier-Stokes equations are obtained by substituting the above form for σ'_{ik} into the generalized Euler equation (equation 9.9) and by using the incompressibility condition ($\sum_i \partial v_i / \partial x_i = 0$; equation 9.4) and Euler's equation ($\partial v_i / \partial t = -\sum_k v_k (\partial v_i / \partial x_k) - \frac{1}{\rho} (\partial p / \partial x_i)$; equation 9.7):

$$\begin{aligned} \frac{\partial(\rho v_i)}{\partial t} &= -\sum_k \frac{\partial}{\partial x_k} \Pi_{ik}, \\ &= -\sum_k \frac{\partial}{\partial x_k} \left\{ \rho v_i v_k + p \delta_{ik} - \rho \mu \left[\frac{\partial v_i}{\partial x_k} + \frac{\partial v_k}{\partial x_i} - \frac{2}{3} \delta_{ik} \sum_j \frac{\partial v_j}{\partial x_j} \right] - \rho \zeta \delta_{ik} \sum_j \frac{\partial v_j}{\partial x_j} \right\}, \\ &= -\sum_k \left\{ \rho v_k \frac{\partial v_i}{\partial x_k} + \delta_{ik} \frac{\partial p}{\partial x_i} + \left(\frac{2}{3} \rho \mu \delta_{ik} - \rho \zeta \delta_{ik} \right) \frac{\partial}{\partial x_k} \sum_j \frac{\partial v_j}{\partial x_j} \right\}. \end{aligned} \quad (9.15)$$

If we set $\zeta = (2/3)\mu$,[†] the last two terms cancel and the incompressible Navier-Stokes equations take their conventional form [tritt88]:

$$\begin{cases} \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{v}, \\ \nabla \cdot \vec{v} = 0, \end{cases} \quad (9.16)$$

where $\nu = \mu/\rho$, and is known as the *kinematic viscosity*. Any external forces $\vec{F}_i$ that may be acting on the body of fluid as a whole (such as gravity), can be added by appending appropriate terms of the form $\vec{F}_i/\rho$ on the LHS of the first of the two equations in equation 9.16.

To obtain physically meaningful solutions, a set of appropriate boundary conditions must also be specified. One obvious requirement is that no fluid should pass through the boundary (i.e. wall) itself. Thus, if we choose a reference frame in which the boundaries are at rest, we require that $\vec{v} \cdot \hat{n} = 0$, where $\hat{n}$ is the unit normal to the surface. Another condition, the so-called *no-slip* condition ([tritt88], [feyn64]), is the requirement that the fluid's tangential velocity vanishes at the surface: $\vec{v} \times \hat{n} = 0$.

The first equation in equation 9.16 is a three-dimensional nonlinear partial differential equation for the velocity field $\vec{v}$. In general, due to its nonlinearity, it is extremely difficult to solve. While it is true that for small velocities, the Navier-Stokes equations can be linearized and, at least when the geometry of boundaries and/or obstacles is relatively “simple,” even be solved analytically, as velocities become larger, instabilities appear and make it increasingly difficult to obtain any kind of analytical results. Indeed, for some problems, it is nontrivial to obtain even numerical approximations. Since turbulent flow typically involves a complicated nesting of eddies and vortices (see below), literally ranging in scale from the macroscopic to the molecular, part of the difficulty stems from the need to simultaneously take into account these widely differing length scales, and therefore to use either extremely small or variable-sized meshes for numerical finite-difference calculations. On the purely theoretical side, it is also worth observing that while, for three-dimensions, it is known that smooth solutions depending continuously on the initial conditions exist for a *short time*, it remains an open problem as to whether solutions of the incompressible Navier-Stokes equations actually exist for *all time* [tem77].[‡]

Before discussing the onset, and nature, of fluid turbulence, it is convenient to first recast the Navier-Stokes equations into a *dimensionless* form, a trick first used by Reynolds in his pioneering experimental work in the 1880's. In this form, the Navier-Stokes equations depend on a single dimensionless number called *Reynolds number*, and fluid behavior from smooth, or laminar, flow to chaos, or turbulence,

[†]While we are free to assume that this relationship holds between μ and ζ , we can only do so at a cost; in this case, the cost being that the pressure must itself be reinterpreted since it is no longer the thermodynamic pressure. In practice, μ is much easier to measure than is ζ [tritt88].

[‡]Solutions are known to exist for all time in two-dimensions [chor90].

can be traced as a function of $\mathcal{R}$ alone.

9.1.4 *Reynold's Number*

A particular fluid flow "problem" must have an associated *characteristic length* L and *characteristic velocity* V . These values may be more or less arbitrarily specified, with the only constraint being that they represent some typical scales. For example, if the problem involves a flow past a sphere, L could be the diameter of the sphere and V could be the velocity of the fluid at infinity. The characteristic length and characteristic velocity also fix a characteristic time scale $T \equiv L/V$.

Now suppose we reduce our real variables $\vec{x}$, $\vec{v}$ and t according to these characteristic scales:

$$\vec{v}' = \frac{\vec{v}}{V}, \quad \vec{x}' = \frac{\vec{x}}{L}, \quad t' = \frac{t}{L/V}. \quad (9.17)$$

We first observe that the compressibility condition (equation 9.4) remains unchanged:

$$\nabla' \cdot \vec{v}' = 0. \quad (9.18)$$

Next, we substitute these dimensionless variables into the incompressible Navier-Stokes equations (equation 9.16). In Cartesian coordinates, the i^{th} component of the first equation reads

$$\begin{aligned} \frac{\partial(v'_i V)}{\partial t'} \frac{\partial t'}{\partial t} + V \sum_j v'_j \frac{\partial(v'_i V)}{\partial x'_j} \frac{\partial x'_j}{\partial x_j} &= -\frac{1}{\rho} \frac{\partial \rho}{\partial x'_i} \frac{\partial x'_i}{\partial x_i} + \nu \sum_j \frac{\partial^2(v'_i V)}{\partial (x'_i L)^2}, \\ \text{or} \quad \frac{V^2}{L} \left(\frac{\partial v'_i}{\partial t'} + \sum_j v'_j \frac{\partial v'_i}{\partial x'_j} \right) &= \frac{V^2}{L} \frac{\partial}{\partial x'_i} \left(\frac{p}{\rho V^2} \right) + \frac{V}{L^2} \nu \sum_j \frac{\partial^2 v'_i}{\partial (x'_i)^2}. \end{aligned} \quad (9.19)$$

In vector notation, we see that

$$\frac{\partial \vec{v}'}{\partial t'} + (\vec{v}' \cdot \nabla') \vec{v}' = -\nabla p' + \frac{1}{\mathcal{R}} (\nabla')^2 \vec{v}', \quad (9.20)$$

where $p' = p/(\rho V^2)$ and $\mathcal{R}$ is the *Reynold's Number*:

$$\mathcal{R} = \frac{\rho L V}{\mu} = \frac{L V}{\nu}. \quad (9.21)$$

Whatever boundary conditions are appropriate for a given problem may, of course, themselves be easily transcribed into the new coordinate system.

What this transcription into dimensionless variables means *physically* is very interesting. It means that, if expressed in terms of the dimensionless variables $\vec{v}'$, $\vec{x}'$ and t' , any two fluid "problems" will have essentially the same "flow solutions" whenever their Reynolds numbers are equal. This is of considerable practical importance, of course, since it implies that the air flow past an airplane wing, for example,

can be determined from measurements performed on an appropriately scaled-down model sitting in a wind-tunnel. It is important to remember, however, that we are still dealing with *incompressible* fluids. In the case where the compressibility of a fluid cannot be neglected, there is another dimensionless parameter – the so-called *Mach number*, $\mathcal{M} = V/c$, where $c = \text{speed-of-sound}$ – that must also be taken into account. In general, the flows can be expected to be the same in two situations only when *both* their Mach numbers and Reynolds numbers are equal.

In order to give the Reynolds number a physical interpretation, we can look at the “typical” magnitudes of individual terms of the Navier-Stokes equation. Since $|\vec{v} \cdot \nabla \vec{v}| \sim V^2/L$ and $|\nu \nabla^2 \vec{v}| \sim \nu V/L^2$, we see that

$$\frac{|\vec{v} \cdot \nabla \vec{v}|}{|\nu \nabla^2 \vec{v}|} \sim \frac{VL}{\nu} = \mathcal{R}. \quad (9.22)$$

In other words, $\mathcal{R}$ can be thought of as a “gauge”, measuring the relative importance of the purely inertial forces (as embodied by the $\vec{v} \cdot \nabla \vec{v}$ term) and the viscous forces (as embodied by the term $\nu \nabla^2 \vec{v}$, which provides the mechanism by which energy may be dissipated).

9.1.5 Fluid Flow as a Function of Reynolds Number

Turbulence is generally understood to refer to a state of *spatiotemporal chaos*; that is to say, a state in which chaos exists on all spatial and temporal scales. If the reader is unsatisfied with this description, it is perhaps because one of the many important open questions is how to rigorously define such a state. Much of our current understanding actually comes from hints obtained through the study of simpler dynamical systems, such as ordinary differential equations and discrete mappings (see chapter 4), which exhibit only *temporal chaos*.[†] The assumption has been that, at least for scenarios in which the velocity field fluctuates chaotically in time but remains relatively “smooth” in space, the underlying mechanisms for the onset of chaos in the simpler systems and the onset of the “temporal” turbulence in fluids are fundamentally the same.

Before we discuss some conjectures as to the onset of turbulence, let us first of all get a qualitative feel for the different stages of behavior as the Reynolds number is increased. Consider, for example, the viscous flow around a circular cylinder ([feyn64], [bat67]).

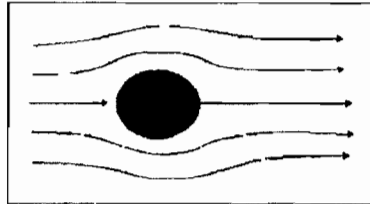
For very low Reynolds numbers, $\mathcal{R} \ll 1$, the flow lines wrap smoothly around the cylinder, as shown in figure 9.1.

Increasing $\mathcal{R}$ to values > 1 ($\sim 10 - 20$) induces a distinct change in behavior: a circulation appears, in the form of two symmetrically positioned vortices behind the cylinder (see figure 9.2). It is believed that the circulation pattern appears suddenly at some threshold value of $\mathcal{R}$. Also notice that the fluid velocity at any given point in space is still constant.

An altogether different behavior emerges for slightly larger values of $\mathcal{R}$ ($\sim 40 -$

[†]See also our discussion of spatiotemporal chaos in coupled-map lattices in section 8.2.

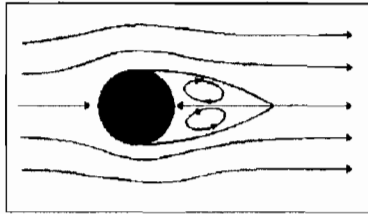
100). In this new regime, the velocity at any point begins to change with time, albeit in a cyclic manner. In particular, at least one of the two vortices that were previously confined to a region immediately behind the cylinder gets long enough that it effectively “breaks off” and moves down stream.



Reynolds Number $\sim 10^{-2}$

Fig. 9.1 Schematic “snapshot” of the laminar flow of an incompressible viscous fluid past a cylinder; the Reynolds number is $\mathcal{R} \sim 10^{-2}$.

Meanwhile, the flow near the cylinder curls towards the cylinder and forms a new vortex that takes the place of the original. As time goes on, the vortices on either side of the cylinder take turns breaking off and traveling down stream. A snapshot of this behavior is shown schematically in figure 9.3. This stream of successively broken-off vortices is known as a *von Karman vortex street* [tritt88].



Reynolds Number ~ 10

Fig. 9.2 A local “circulation” first appears for $\mathcal{R} \sim 10$.

A little bit of physical intuition as to how the vortices form in the first place may help in explaining the behavior as $\mathcal{R}$ is increased still further. We know that $\vec{v} = 0$ at the cylinder’s surface. We also know that the velocity increases rapidly as we get further from that surface. Therefore vortices are due to this rapid local velocity variation. If the variation is small enough, there is enough time for the vorticity to diffuse out of the region just outside the cylinder’s surface and create a large von Karman vortex street of vorticity down stream [feyn64].

At a certain critical point, however, the velocity is great enough so that there is insufficient time for the vortices to diffuse into a larger region. By the time $\mathcal{R} \sim 10^3$, the vorticity begins to fill in a tiny band – the so called *boundary layer* – within which the flow is effectively chaotic. As $\mathcal{R}$ is increased beyond this threshold, the chaotic region grows, reaching ever farther downstream. At still larger $\mathcal{R} \sim 10^5$, there finally appears a fully formed *turbulent boundary layer* (see figure 9.4).

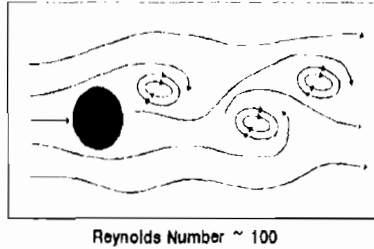


Fig. 9.3 A so-called *von Karman Vortex Street* forms behind a cylinder for $\mathcal{R} \sim 100$.

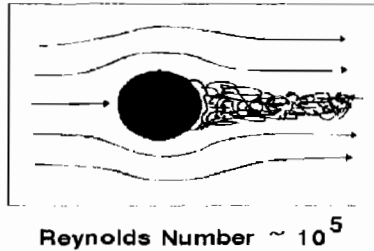


Fig. 9.4 A “turbulent boundary layer” forms behind a cylinder for $\mathcal{R} \sim 10^5$.

We should stress that while it is well known that turbulence exists for $\mathcal{R} \gg 1$, this fact is an *experimental* observation. No rigorous proof that such behavior follows from the actual Navier-Stokes equations has yet been found.

9.1.6 Routes to Turbulence

There have been a number of proposed scenarios, or “routes”, for how laminar flow for small $\mathcal{R}$ transitions into fully developed turbulence as $\mathcal{R}$ is increased. Four of the most frequently cited routes are the *Landau-Hopf route* [landau44], the *Ruelle-Takens-Newhouse route* ([ruelle71], [newh78]), the *Pomeau-Manneville route* ([pomeau80], [eckman81]) and the *Feigenbaum route* ([feig80b], [feig80c]). We briefly discuss each in turn.

9.1.6.1 Landau-Hopf Route

Landau proposed in 1944 that turbulence arises essentially through the emergence of an ever increasing number of quasi-periodic motions resulting from successive bifurcations of the fluid system [landau44]. For small $\mathcal{R}$, the fluid motion is, as we have seen, laminar, corresponding to a stable fixed point in phase space. As $\mathcal{R}$ is

increased, however, the fixed point becomes unstable and gives rise to a periodic motion, characterized by some frequency f_1 .[†] A further increase in $\mathcal{R}$ results in the loss of stability of this periodic motion, giving rise to a quasi-periodic motion, characterized by f_1 and f_2 , where f_2 is incommensurate with (i.e. rationally independent of) f_1 . This process continues as $\mathcal{R}$ increases, resulting in increasingly large set of frequencies that is needed to characterize the motion as successive stages of oscillatory motion are destabilized:

$$\vec{v}(t) = \vec{v}(f_1 t) \longrightarrow \vec{v}(f_1 t, f_2 t) \longrightarrow \vec{v}(f_1 t, f_2 t, f_3 t) \longrightarrow \cdots \quad (9.23)$$

Landau then identifies “turbulence” as the limit state consisting of an infinite number of incommensurate frequencies.

Now, there are some immediate problems with this formulation. For example, if correct, it implies that chaotic behavior can exist only in systems that have a large number of degrees of freedom (since the phase space dimension must be greater than the dimension of the attractor). Yet it is well known that chaos requires no more than three degrees of freedom [berge84]. Indeed, it has been experimentally observed that the power spectra of fluids does *not* develop an ever increasing set of discrete frequencies, but instead rather abruptly turns into broad noisy bands [swin78]. The Landau-Hopf route also ignores the possibility of *phase-locking*, in which nearby frequencies can interact with one another and thereby effectively reduce the number of independent frequencies needed to describe the motion [gucj83]. In short, it is now believed that the Landau-Hopf route probably does not adequately describe the onset of turbulence.

9.1.6.2 Ruelle-Takens-Newhouse Route

This route, due to Ruelle and Takens [ruelle71], assumes that the onset to turbulence starts out exactly as in the Landau-Hopf scenario, namely by an increase in frequency components. Unlike that scenario, however, Ruelle and Takens suggested

[†]Whenever a stable fixed point becomes unstable and gives rise to a limit cycle when a parameter crosses some critical value, the phenomenon is called a *Hopf bifurcation* ([hopfe44], [mars76]). For example, consider the system

$$\frac{dr}{dt} = -(\alpha r + r^3), \quad \frac{d\theta}{dt} = \omega.$$

The solution is given by

$$r^2(t) = \frac{\alpha r_0^2 e^{-2\alpha t}}{r_0^2(1 - \exp(-2\alpha t)) + \alpha}, \quad \theta(t) = \omega t,$$

where $r_0 = r(t=0)$ and $\theta(t=0) = 0$. It is easy to see that as α decreases from positive to negative values the system trajectory undergoes an abrupt qualitative change: for $\alpha \geq 0$ the trajectory approaches a *fixed point* at the origin, while for $\alpha < 0$, it spirals towards a *limit cycle* with radius $r(t \rightarrow \infty) = \sqrt{\alpha}$.

that turbulence can come about after only a *finite* number Hopf bifurcations:[†]

$$\text{fixed point} \longrightarrow \text{limit cycle} \longrightarrow 2 - \text{torus} \longrightarrow \text{strange attractor} = \text{turbulence.} \quad (9.24)$$

There is experimental evidence to support the Ruelle-Takens route. Swinney and Gollub [swin78], for example, in their investigation of *Couette flow*,[‡] showed that the power spectrum undergoes only a few well-defined transitions: from periodicity to quasi-periodicity and from quasi-periodicity directly into a chaotic flow. Measurements of so-called *Rayleigh-Benard* flow, in which a fluid contained between thermally conducting horizontal plates that are heated from below undergoes convective rolls, are also consistent with the Ruelle-Takens route [berge84].

9.1.6.3 Pomeau-Manneville Route

In 1980, Pomeau and Manneville [pomeau80] found that some of their numerical solutions to the Lorentz model displayed one of two interesting types of behavior, depending on the value of a single parameter, r :[§] periodic behavior for $r < r_c$ and a periodic behavior that is intermittently interjected with chaotic behavior for $r > r_c$.[¶] They called this kind of behavior *intermittency*, and hypothesized three possible underlying mechanisms that may be responsible (type-I, type-II and type-III intermittency; see [schus88]). Each effectively depends on the particular way in which a stable and unstable fixed point merge. Type-I intermittency, for example, which is the responsible mechanism in the Lorentz system, is an *inverse tangent* bifurcation, with two fixed points merging as shown in figure 9.5.

How does this relate to fluid turbulence? The idea is that there exists a critical value of the Reynolds number, $\mathcal{R}_c$, such that intermittent turbulent behavior can appear in the system for $\mathcal{R} > \mathcal{R}_c$. Moreover, if the behavior of the Lorenz system correctly identifies the underlying mechanism, it may be predicted that, as $\mathcal{R}$ changes, (1) the duration of the intermittently turbulent behavior will be random, and (2) the mean duration of the laminar phases in between will vary as

[†]Ruelle and Takens originally conjectured that a strange attractor can form after *four* Hopf bifurcations. Newhouse, Ruelle and Takens [newh78] later showed that only *three* Hopf bifurcations are actually needed. See [schus88] for an expanded discussion.

[‡]Couette flow refers to the fluid flow between two concentric cylinders with either one or both of the cylinders rotating with some given angular velocity ω . It can be shown that the Reynolds number for this system is given by $\mathcal{R} = r_{\text{inner}}\omega(r_{\text{outer}} - r_{\text{inner}})/\nu$.

[§]The system that Pomeau and Manneville studied was first introduced by Lorentz in his pioneering study of chaos in the atmosphere [lorenz63]. It is a set of three coupled ordinary differential equations:

$$\begin{cases} dx/dt &= \sigma(x - z), \\ dy/dt &= -xz + rx - y, \\ dz/dt &= xy - bz. \end{cases}$$

Lorentz found that when $r = 28$, $\sigma = 10$ and $b = 8/3$, (i) the trajectories are attracted to a bounded region in space, (ii) the motion appears chaotic, and (iii) there is a great sensitivity to initial conditions.

[¶]Pomeau and Manneville found $r_c \sim 166$ [pomeau80].

$$|\mathcal{R} - \mathcal{R}_c|^{-1/2} \text{ [schus88].}$$

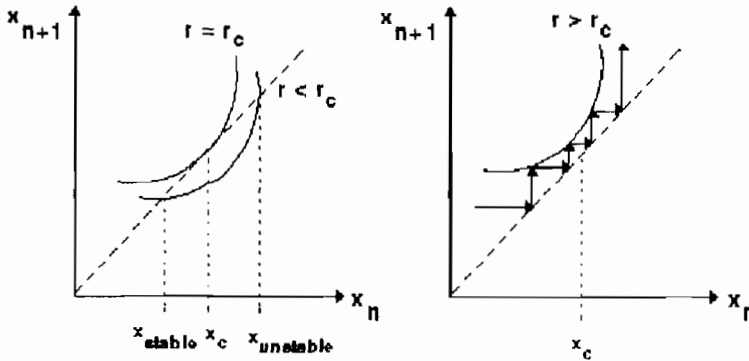


Fig. 9.5 Schematic representation of Type-I intermittency. The plot on the LHS shows a return map for the system as it appears just below and precisely at the critical parameter value r_c . The plot on the RHS shows the return map for $r > r_c$. Note how, for $r > r_c$, $x = x_c$ appears to first “attract” then “repel” trajectories.

Both type-I intermittency [berge80] and type-II intermittency [dubois3] has been observed in a Rayleigh-Benard experiment.[†] Generally speaking, however, only a relatively small subset of experiments appear to be consistent with this particular route.

9.1.6.4 Feigenbaum Route

This route should already be familiar to us from our discussion of the logistic map in chapter 4. From that chapter, we recall that the Feigenbaum route calls for a sequence of period-doubling bifurcations (*pitchfork* bifurcations versus the *Hopf* bifurcations of the Landau-Hopf route) such that if subharmonic bifurcations are observed at Reynolds numbers $\mathcal{R}_1$ and $\mathcal{R}_2$, another can be expected at $\mathcal{R}_3$ determined by

$$\mathcal{R}_3 \sim \mathcal{R}_2 - \frac{\mathcal{R}_1 - \mathcal{R}_2}{\delta}, \quad (9.25)$$

where $\delta = 4.6692 \dots$ is the *Feigenbaum constant*. This behavior has been frequently observed in a variety of experiments, including Rayleigh-Benard convection [lib80].

9.1.7 Kinetic Theory: Boltzman's Equation

Let us now shift our focus and consider the “bottom-up”, or kinetic theory, approach to fluid dynamics. Kinetic theory describes fluids by assuming that they are made up of a large number of individual atoms or molecules, each subject to the laws of

[†]As of this writing, there has been no experimental evidence of Type-III intermittency in a Rayleigh-Benard or any other fluid system.

Newtonian mechanics. Since it is impossible to completely specify the initial state of such a system, kinetic theory contents itself with describing a “smoothed” version of the system. The smoothed version is simply one where all exact state-information below some characteristic length and time is replaced by a probabilistic description.

To be more precise, let us assume, as Boltzman first did in 1872 [boltz72], that we have N perfectly elastic billiard balls, or hard-spheres, inside a volume V , and that a complete statistical description of our system (be it a gas or fluid) at, or near, its equilibrium state is contained in the one-particle phase-space distribution function $f(\vec{x}, \vec{v}, t)$:

$$f(\vec{x}, \vec{v}, t) d^3x d^3v = \begin{array}{l} \text{the number of hard-spheres with positions in} \\ \text{volume element } d^3x \text{ around } \vec{x}, \text{ and velocities in} \\ \text{the velocity-space element } d^3v \text{ around } \vec{v} \text{ at time } t. \end{array} \quad (9.26)$$

Integrating over all of phase space must give us back the total number of hard-spheres in our system: $\int f(\vec{x}, \vec{v}, t) d^3x d^3v = N$.

The goal of kinetic theory is to find the time-evolution equation for $f(\vec{x}, \vec{v}, t)$, with the ultimate aim being to obtain the equilibrium properties of the system through the limiting form of $f(\vec{x}, \vec{v}, t)$ as $t \rightarrow \infty$.

In general, the distribution function changes in time because of the underlying motion of the hard-spheres. Consider first the nonphysical case where there are no collisions. Phase-space conservation, or *Louville's Theorem* [bal75], assures us that

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = 0. \quad (9.27)$$

This equation expresses the change in f that is due solely to independent collisionless motions of the hard-spheres alone.

Now let us add the possibility of collisions. Before we proceed, we make the following two assumptions: (1) *only binary collisions occur*; i.e. we rule out situations in which three or more hard-spheres simultaneously come together (which is a physically reasonable assumption provided that the gas is sufficiently dilute), and (2) Boltzman's *Stosszahlansatz*,[‡] or his “molecular chaos” assumption that the motion of the hard-spheres is effectively pairwise uncorrelated; i.e. that the pair-distribution function is the product of individual distribution functions:

$$f^{(2)}(\vec{x}, \vec{v}_1, \vec{v}_2, t) = f(\vec{x}, \vec{v}_1, t) f(\vec{x}, \vec{v}_2, t). \quad (9.28)$$

The molecular chaos assumption is made purely for mathematical convenience. We should be quick to point out that while it is certainly possible that some specially prepared systems might initially possess this property, it completely ignores the (almost) inevitable correlations that will develop in time.[†]

[‡]“Assumption for calculating the number of collisions.”

[†]See [bal75] for an interesting discussion of this point, and its relation to the so-called BBGKY-hierarchy (a set of equations allowing one to solve for the rate of change of the n^{th} order distribution function $f^{(n)}$ in terms of $f^{(n)}$ and the next-higher-order function $f^{(n+1)}$).

Now, equation 9.27 must of course be modified in the presence of collisions. Since, by definition, the rate of change of $f(\vec{x}, \vec{v}, t) d^3x d^3v$ is equal to the increase in hard-spheres in $d^3x d^3v$ as a result of collisions, we have, in general, that

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla f = \mathcal{G}[f] - \mathcal{L}[f], \quad (9.29)$$

where $\mathcal{G}[f]$ and $\mathcal{L}[f]$ – the *gain* and *loss* terms, respectively – represent the number of collisions at time t in which one of the final and initial hard-spheres is in the phase space element $d^3x d^3v$.

Consider a sphere-sphere collision. Let the incoming and outgoing distributions be given by f_1, f_2 and $\tilde{f}_1, \tilde{f}_2$, respectively. Also, assume that the pre- and post-collision velocity-space regions occupied by hard-spheres 1 and 2 are given by $d^3v_1, d^3\tilde{v}_1$ and $d^3v_2, d^3\tilde{v}_2$, respectively.

Now consider the loss term $\mathcal{L}[f]$ in equation 9.29. The probability of a loss is proportional to four terms: (1) the number of type-1 hard-spheres already in the volume ($= f_1$); (2) the number of type-2 hard-spheres entering the volume ($= f_2 d^3v_2$); (3) the probability, $\mathcal{P}[\{\vec{v}\}] = \mathcal{P}(v_1, v_2; \tilde{v}_1, \tilde{v}_2)$, that two hard-spheres with velocities v_1, v_2 will actually collide and make transitions to states with velocities $\tilde{v}_1, \tilde{v}_2$; (4) the total volume of the allowed outgoing velocity-space ($= d^3\tilde{v}_1 d^3\tilde{v}_2$). Integrating over all possible momenta, we find that the loss term is given by

$$\mathcal{L}[f] = \int \mathcal{P}(v_1, v_2; \tilde{v}_1, \tilde{v}_2) f_1 f_2 d^3v_2 d^3\tilde{v}_1 d^3\tilde{v}_2. \quad (9.30)$$

Similar reasoning gives the *gain* term:

$$\mathcal{G}[f] = \int \mathcal{P}(\tilde{v}_1, \tilde{v}_2; v_1, v_2) \tilde{f}_1 \tilde{f}_2 d^3v_2 d^3\tilde{v}_1 d^3\tilde{v}_2. \quad (9.31)$$

Our final form for the Boltzman equation is then obtained by substituting these last two expressions for the gain and loss terms into equation 9.29 and adding the term $\frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} f(\vec{x}, \vec{v}, t)$ to the LHS for the case where there is an external force $\vec{F}$ ($\nabla_{\vec{v}}$ is the gradient operator with respect to $\vec{v}$ and m is the hard-sphere mass):

$$\frac{\partial f_1}{\partial t} + \vec{v} \cdot \nabla f_1 + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} f_1 = \int \mathcal{P}[\{\vec{v}\}] \left\{ \tilde{f}_1 \tilde{f}_2 - f_1 f_2 \right\} d^3v_2 d^3\tilde{v}_1 d^3\tilde{v}_2, \quad (9.32)$$

where $f_1 = f(\vec{x}, \vec{v}_1, t)$, $\tilde{f}_1 = f(\vec{x}, \tilde{\vec{v}}_1, t)$, etc. As we can see, Boltzman's equation is a rather complicated nonlinear integro-differential equation for f . It is in fact generally intractable. Nonetheless, by a simple line of reasoning, Boltzman was able to show that equation 9.32 leads to equilibrium and that the equilibrium distribution is the *Maxwell-Boltzman distribution*.

9.1.8 Equilibrium Solutions of Boltzman's Equation

By definition, the equilibrium distribution f_0 is one which does not depend on time. For simplicity assume further that the system is uniform in space so that f_0 is not a function of position, and set all external forces $\vec{F} = 0$. The LHS of equation 9.32

then vanishes identically and the problem reduces to solving for the distribution f_0 such that the RHS vanishes:

$$\int \mathcal{P}[\{\vec{v}\}] \left\{ f_0(\vec{v}_1) f_0(\vec{v}_2) - f_0(\vec{v}_1) f_0(\vec{v}_2) \right\} d^3 v_2 d^3 \vec{v}_1 d^3 \vec{v}_2 = 0, \quad (9.33)$$

where $\vec{v}_1$ is a given velocity.

A sufficient condition for f_0 to solve equation 9.33 is that the term in the curly brackets itself vanishes:

$$f_0(\vec{v}_1) f_0(\vec{v}_2) - f_0(\vec{v}_1) f_0(\vec{v}_2) = 0 \implies f_0(\vec{v}_1) f_0(\vec{v}_2) = f_0(\vec{v}_1) f_0(\vec{v}_2), \quad (9.34)$$

where $(\vec{v}_1, \vec{v}_2) \rightarrow (\vec{v}_1, \vec{v}_2)$ represents any valid collision. This is called the condition of *detailed-balance*. (See discussion box below – Boltzman’s *H-Theorem* – for a proof that this condition is also a *necessary* condition for equilibrium).

Taking the logarithm of both sides of the expression on the RHS of this equation, we have

$$\log f_0(\vec{v}_1) + \log f_0(\vec{v}_2) = \log f_0(\vec{v}_1) + \log f_0(\vec{v}_2), \quad (9.35)$$

which should remind the reader of an *additive conservation law*. Since the only conserved quantities for spinless particles (which we are assuming our hard-spheres to be) are momentum and energy, we conclude that $\log f_0$ must be some linear combination of v^2 and the three components of $\vec{v}$, along with some arbitrary constant:

$$\log f_0 = \log c_1 - c_2(\vec{v} - \vec{v}_0)^2 \implies f_0 = c_1 e^{-c_2(\vec{v} - \vec{v}_0)^2}, \quad (9.36)$$

where c_1, c_2 and the three components of $\vec{v}_0$ are arbitrary constants. Apart from the unevaluated constants,[†] we recognize this as having the form of the *Maxwell-Boltzman distribution*.

A gas is not in equilibrium when its distribution function differs from the Maxwell-Boltzman distribution. On the other hand, it can also be shown that if a system possesses a slight spatial nonuniformity and is not in equilibrium, then the distribution function will monotonically relax in velocity space to a *local* Maxwell-Boltzman distribution, or to a distribution where $\rho = N/V$, $\vec{v}$ and temperature T all show a spatial dependence [bal75].

[†]The values of the constants are easy to find. From the fact that the number of hard-spheres $N = \int f(\vec{x}, \vec{v}, t) d^3 x d^3 p$, for example, we find that, in equilibrium, $(N/V) = \int f_0(\vec{v}) d^3 v = c_1 \int \exp\{-c_2(\vec{v} - \vec{v}_0)^2\} d^3 v \rightarrow c_1 = (c_2/\pi)^{3/2} (N/V)$. The average velocity $\langle \vec{v} \rangle = (\int \vec{v} f_0(\vec{v}) d^3 v) / (\int f_0(\vec{v}) d^3 v) = (c_1/V) \int \vec{v} \exp\{-c_2(\vec{v} - \vec{v}_0)^2\} d^3 v = \vec{v}_0$, so that if there is no net translational motion, $\langle \vec{v} \rangle = \vec{v}_0 = 0$. Using this, we find that the average kinetic energy E of a hard-sphere is equal to $E = (\int \frac{1}{2} m \vec{v}^2 f_0(\vec{v}) d^3 v) / (\int f_0(\vec{v}) d^3 v) = 3m/4c_2 \rightarrow c_2 = 3m/4E$. Substituting this into our earlier expression for c_1 , we have that $c_1 = (3m/4\pi E)^{3/2} (N/V)$. Finally, using the *equipartition theorem* [huangk63], we set $E = \frac{3}{2} kT$, where k is Boltzman’s constant and T is the absolute temperature. Putting all of this together gives the familiar Maxwell-Boltzman distribution:

$$f_0(\vec{v}) = \frac{N}{V} \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{m\vec{v}^2}{2kT} \right).$$

Boltzman's H-Theorem: Let us consider a binary elastic collision of two hard-spheres in more detail. Using the same notation as above, so that $\vec{v}_1, \vec{v}_2$ represent the velocities of the incoming spheres and $\vec{\tilde{v}}_1, \vec{\tilde{v}}_2$ represent the velocities of the outgoing spheres, we have from momentum and energy conservation that

$$\begin{cases} \vec{v}_1 + \vec{v}_2 = \vec{\tilde{v}}_1 + \vec{\tilde{v}}_2, \\ |\vec{v}_1|^2 + |\vec{v}_2|^2 = |\vec{\tilde{v}}_1|^2 + |\vec{\tilde{v}}_2|^2. \end{cases} \quad (9.37)$$

From these two conditions we deduce that (1) $d^3\vec{v}_1 d^3\vec{v}_2 = d^3\vec{v}_1 d^3\vec{v}_2$ (i.e. that the transformation $(\vec{v}_1, \vec{v}_2) \rightarrow (\vec{\tilde{v}}_1, \vec{\tilde{v}}_2)$ is orthogonal), and (2) $\vec{\tilde{v}}_1 = \vec{v}_1 + (\vec{\nu} \cdot \hat{n})\hat{n}$ and $\vec{\tilde{v}}_2 = \vec{v}_2 - (\vec{\nu} \cdot \hat{n})\hat{n}$, where $\vec{\nu} \equiv \vec{v}_2 - \vec{v}_1$ and $\hat{n}$ is a unit vector along the line of the two centers of the colliding hard spheres (see figure 9.6).

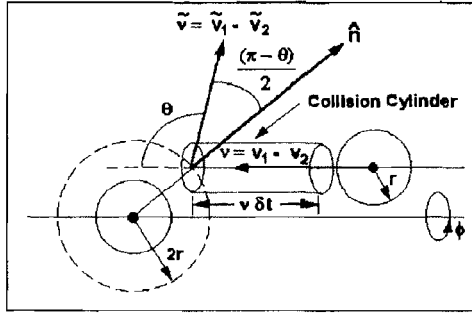


Fig. 9.6 Collision of two hard-spheres shown in a reference frame in which sphere #1 is at rest; $\hat{n}$ is a unit vector along the line of the two centers of the colliding spheres.

In the relative coordinate system in which the first sphere is at rest, a collision can occur only if the center of the second sphere lies within the "collision cylinder" as shown in figure 9.6. Now, the volume of the cylinder is equal to $b d\phi db |\nu| \delta t$. From figure 9.6 it should be clear that

$$b db d\phi = r \cos\left(\frac{\theta}{2}\right) \left| \frac{db}{d\theta} \right| d\theta d\phi = \frac{r^2}{2} \cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) d\theta d\phi = \frac{r^2}{4} d\Omega, \quad (9.38)$$

where $d\Omega = \sin\theta d\theta d\phi$ is the solid angle of the "scattered" sphere.

Using the definition of the gain (equation 9.31) and loss (equation 9.30) terms, we find

$$\mathcal{G}[f] - \mathcal{L}[f] = \frac{r^2}{4} \int d\Omega \int d^3v_2 |\vec{\nu}| (\bar{f}_1 \bar{f}_2 - f_1 f_2). \quad (9.39)$$

For more general interactions - i.e. not necessarily between two hard-spheres - we introduce a differential scattering cross section $\sigma(\nu, \theta)$, defined by $b db d\phi = \sigma(\nu, \theta) d\Omega$. Boltzman's equation (equation 9.32) becomes

$$\frac{\partial f_1}{\partial t} + \vec{v} \cdot \nabla f_1 + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} f_1 = \int d\Omega \int d^3v_2 \sigma(\nu, \theta) |\vec{\nu}| (\bar{f}_1 \bar{f}_2 - f_1 f_2). \quad (9.40)$$

Now, to show the necessity for the condition given in equation 9.34, we define the

function

$$H(t) \equiv \int d^3v f(\vec{v}, t) \log f(\vec{v}, t), \quad (9.41)$$

where f is the distribution function satisfying equation 9.40. Differentiating $H(t)$ with respect to time yields

$$\frac{dH}{dt} = \int d^3v \frac{\partial f}{\partial t} (1 + \log f) \implies \frac{dH}{dt} = 0 \text{ if } \frac{\partial f}{\partial t} = 0. \quad (9.42)$$

The fact that the condition $dH/dt = 0$ is the same as the condition of detailed-balance, and therefore that equation 9.34 is a necessary condition for the solution of equation 9.33, follows from the proof of Boltzman's H-Theorem:

Boltzman's H-Theorem: If $f(\vec{v}, t)$ is a solution of Boltzman's equation (equation 9.40) and $H(t)$ is defined by equation 9.41, then $\frac{dH(t)}{dt} \leq 0$.

Proof: Substituting equation 9.40 into equation 9.42 gives

$$\frac{dH}{dt} = \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\nu, \theta) \mid \vec{\nu} \mid (\tilde{f}_1 \tilde{f}_2 - f_1 f_2)(1 + \log f_1). \quad (9.43)$$

Noting that $\sigma(\nu, \theta) \mid \vec{\nu} \mid$ is invariant under an exchange $\vec{v}_1 \longleftrightarrow \vec{v}_2$, we make this change of variables, add the new expression to equation 9.43 and divide the sum by 2:

$$\frac{dH}{dt} = \frac{1}{2} \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\nu, \theta) \mid \vec{\nu} \mid (\tilde{f}_1 \tilde{f}_2 - f_1 f_2)(2 + \log f_1 f_2). \quad (9.44)$$

Now change variables $(\vec{v}_1, \vec{v}_2) \longrightarrow (\tilde{\vec{v}}_1, \tilde{\vec{v}}_2)$, and recall that $d^3\tilde{v}_1 d^3\tilde{v}_2 = d^3v_1 d^3v_2$ and $\mid \vec{\nu} \mid = \mid \vec{v}_2 - \vec{v}_1 \mid = \mid \tilde{\vec{v}}_2 - \tilde{\vec{v}}_1 \mid$:

$$\frac{dH}{dt} = \frac{1}{2} \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\nu, \theta) \mid \vec{\nu} \mid (f_1 f_2 - \tilde{f}_1 \tilde{f}_2)(2 + \log \tilde{f}_1 \tilde{f}_2). \quad (9.45)$$

Finally, we add equations 9.44 and 9.45 and divide by 2:

$$\frac{dH}{dt} = \frac{1}{4} \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\nu, \theta) \mid \vec{\nu} \mid (\tilde{f}_1 \tilde{f}_2 - f_1 f_2)(\log f_2 f_1 - \log \tilde{f}_1 \tilde{f}_2). \quad (9.46)$$

It remains only to observe that since $(x - y)(\log y - \log x) \leq 0$ for any real numbers x and y (with equality holding only if $x = y$), the integrand of the integral in equation 9.46 is never positive. We conclude that $dH/dt = 0$ if and only if the integrand vanishes identically: $\tilde{f}_1 \tilde{f}_2 = f_1 f_2$, which is the condition of detailed balance. —QED— ■

Notice that since $H(t)$ is monotonically nonincreasing and is bounded below (this is easy to verify), the above proof also shows that, for an arbitrary initial condition, $\lim_{t \rightarrow \infty} f(\vec{v}, t) = f_0(\vec{v})$.

The general problem of finding nonequilibrium solutions to Boltzman's equation is, as already mentioned above, an exceedingly difficult problem. Two tools that have proven invaluable in providing insight into nonequilibrium phenomena,

and that play an important role in the construction of lattice gas models, are the exploitation of conservation laws and the *Chapman-Enskog Expansion*, the latter being a simple but powerful method to solve Boltzman's equation through successive approximation.

9.1.9 Conservation Laws $\rightarrow$ Equations of Hydrodynamics

In this section we show how the fundamental equations of hydrodynamics – namely, the continuity equation (equation 9.3), Euler's equation (equation 9.7) and the Navier-Stokes equation (equation 9.16) – can all be “recovered” from the Boltzman equation by exploiting the fact that in any microscopic collision there are dynamical quantities that are always conserved; namely (for spinless particles), *mass*, *momentum* and *energy*. The derivations in this section follow mostly [huangk63].

Suppose that $\kappa = \kappa(\vec{x}, \vec{v})$ is some quantity associated with a hard-sphere such that in any collision between spheres that takes place at position $\vec{x}$, we have that

$$\kappa_1 + \kappa_2 = \tilde{\kappa}_1 + \tilde{\kappa}_2, \quad (9.47)$$

where $\kappa_i = \kappa(\vec{x}, \vec{v}_i)$, $\tilde{\kappa}_i = \kappa(\vec{x}, \vec{\tilde{v}}_i)$, $i = 1, 2$. The quantity κ is thus a *conserved quantity*. We now prove the following theorem.

General Conservation Theorem: *If $\kappa(\vec{x}, \vec{v})$ is a conserved quantity and $C[f]$ is the collision term in the Boltzman equation (i.e. $C[f]$ is equal to the RHS of either equation 9.32 or equation 9.40), then*

$$\int \kappa(\vec{x}, \vec{v}) C[f] d^3v = 0. \quad (9.48)$$

Proof: We begin by explicitly setting $C[f]$ equal to the RHS of equation 9.40 in equation 9.48:

$$\int \kappa(\vec{x}, \vec{v}) C[f] d^3v = \int d\Omega \int d^3v_2 \int d^3v_1 \sigma(\nu, \theta) |\vec{\nu}| \kappa_1 (\tilde{f}_1 \tilde{f}_2 - f_1 f_2). \quad (9.49)$$

Now transform the RHS of this equation into three new expressions by the following changes of variables: (1) $\vec{v}_1 \longleftrightarrow \vec{v}_2$, (2) $\vec{v}_1 \longleftrightarrow \vec{\tilde{v}}_1$ and $\vec{v}_2 \longleftrightarrow \vec{\tilde{v}}_2$, and (3) $\vec{v}_1 \longleftrightarrow \vec{\tilde{v}}_2$ and $\vec{v}_2 \longleftrightarrow \vec{\tilde{v}}_1$. Since the quantity $\sigma(\nu, \theta) |\vec{\nu}|$ remains invariant under each change of variables, each of the three expressions obtained in this way is equal to the original expression on the RHS of equation 9.49. We can therefore set $\int d^3v \kappa C[f]$ equal to the sum of the three new expressions and the RHS of equation 9.49, divided by 4:

$$\int \kappa(\vec{x}, \vec{v}) C[f] d^3v = \frac{1}{4} \int d\Omega \int d^3v_2 \int d^3v_1 \sigma(\nu, \theta) |\vec{\nu}| \{ \kappa_1 + \kappa_2 - \tilde{\kappa}_1 - \tilde{\kappa}_2 \} (\tilde{f}_1 \tilde{f}_2 - f_1 f_2). \quad (9.50)$$

Since κ is a conserved quantity, equation 9.47 holds, and $\int d^3v \kappa C[f]$ is identically equal to zero. –QED– ■

We can obtain a more immediately useful form of the conservation theorem by directly multiplying Boltzman's equation (equation 9.40) by κ and integrating over $\vec{v}$. Noting that the RHS vanishes identically due to the general conservation theorem we have just proven, we have

$$\int \kappa(\vec{x}, \vec{v}) \left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} \right) f(\vec{x}, \vec{v}, t) = 0. \quad (9.51)$$

Using the definitions $n(\vec{x}, t) \equiv \int f(\vec{x}, \vec{v}, t) d^3v$ and $\langle \alpha \rangle \equiv \frac{1}{n} \int \alpha f(\vec{x}, \vec{v}, t) d^3v$, and the fact that $\lim_{|\vec{v}| \rightarrow \infty} f(\vec{x}, \vec{v}, t) = 0$, we obtain the following conservation theorem for Boltzman's equation:

Conservation Theorem: *If $\kappa(\vec{x}, \vec{v})$ is any conserved quantity and $\langle \alpha \rangle \equiv \frac{1}{n} \int \alpha f(\vec{x}, \vec{v}, t) d^3v$ is an average with respect to the solution f of Boltzman's equation, then, in component form,*

$$\frac{\partial \langle n\kappa \rangle}{\partial t} + \frac{\partial \langle nv_i \kappa \rangle}{\partial x_i} - n \left\langle \sum_i v_i \frac{\partial \kappa}{\partial x_i} \right\rangle - \frac{n}{m} \left\langle \sum_i F_i \frac{\partial \kappa}{\partial v_i} \right\rangle - \frac{n}{m} \left\langle \sum_i \frac{\partial F_i}{\partial v_i} \kappa \right\rangle = 0. \quad (9.52)$$

In the following, we will assume that all forces are velocity-independent and thus set the last term of this expression equal to zero.

9.1.9.1 Continuity Equation

Since the continuity equation (equation 9.3) is essentially a restatement of the principle of conservation of mass, we should not be surprised to learn that it is easily recovered from Boltzman's equation by setting $\kappa = m$ in equation 9.52:

$$\frac{\partial \langle mn \rangle}{\partial t} + \sum_i \frac{\partial \langle mn v_i \rangle}{\partial x_i} = 0 \implies \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0, \quad (9.53)$$

where $\rho \equiv m \cdot n(\vec{x}, t)$ and $\vec{u}(\vec{x}, t) \equiv \langle \vec{v} \rangle$.

9.1.9.2 Euler's Equation

Euler's equation (equation 9.7) may be recovered from Boltzman's equation as a consequence of the conservation of momentum, but only in the *zeroth-order approximation* to the full distribution function. Setting $\kappa = mv_i$ in equation 9.52 gives, in component form,

$$\frac{\partial \langle \rho v_i \rangle}{\partial t} + \sum_j \frac{\partial \langle \rho v_i v_j \rangle}{\partial x_j} - \frac{\rho}{m} F_i = 0, \quad (9.54)$$

or

$$\frac{\partial u_i}{\partial t} + \sum_j u_j \frac{\partial u_i}{\partial x_j} - \frac{1}{m} F_i = -\frac{1}{\rho} \sum_j \frac{\partial P_{ij}}{\partial x_j}, \quad (9.55)$$

where we have again used $\vec{u}(\vec{x}, t) \equiv \langle \vec{v} \rangle$ and set $\langle v_i v_j \rangle = u_i u_j + \langle (v_i - u_i)(v_j - u_j) \rangle$. We have also introduced the pressure tensor $P_{ij} \equiv \rho \langle (v_i - u_i)(v_j - u_j) \rangle$.

In order to get this expression into a more familiar form (equation 9.7), we now consider the zeroth-order approximation to f . We assume that f is locally a Maxwell-Boltzman distribution, and treat the density ρ , temperature $T(\vec{x}, t) \equiv \frac{m}{3k} \langle |\vec{v} - \vec{u}|^2 \rangle$ (where k is Boltzman's constant), and average velocity $\vec{u}$ all as slowly changing variables with respect to $\vec{x}$ and t . We can then write

$$f(\vec{x}, \vec{v}, t) \approx f_0(\vec{x}, \vec{v}, t) = n \left(\frac{m}{2\pi kT} \right)^{3/2} e^{-\frac{m}{2kT} |\vec{v} - \vec{u}|^2}. \quad (9.56)$$

To zeroth-order, P_{ij} is given by

$$\begin{aligned} P_{ij}^{(0)} &= \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int d^3v (v_i - u_i)(v_j - u_j) e^{-\frac{m}{2kT} |\vec{v} - \vec{u}|^2}, \\ &= \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int d^3z z_i z_j e^{-\frac{m}{2kT} z^2}, \\ &= \delta_{ij} P, \end{aligned} \quad (9.57)$$

where $P = \frac{1}{3} \rho \left(\frac{m}{2\pi kT} \right)^{3/2} \int d^3z z^2 e^{-\frac{m}{2kT} z^2} = nkT$. Substituting $P_{ij}^{(0)} = \delta_{ij} P$ back into equation 9.55 for P_{ij} yields Euler's equation (equation 9.7):

$$\frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} - \frac{1}{m} \vec{\nabla} \cdot \vec{P} = -\frac{1}{\rho} \nabla p. \quad (9.58)$$

Euler's equation is thus recovered as a direct consequence of momentum conservation, but only via the zeroth-order approximation to the full solution to the Boltzman-equation.

9.1.9.3 Navier-Stokes Equations

The recovery of the Navier-Stokes also follows from momentum conservation but requires that a *first-order approximation* be made to the full solution to the Boltzman-equation. We sketch the main steps of the "recovery" below (see [huangk63]).

In order to obtain a first-order approximation to the exact solution of the Boltzman equation, we first write

$$f = f_0 + \Delta, \quad (9.59)$$

where f is the exact solution, f_0 is the equilibrium distribution (equation 9.56), and Δ is their difference, and assume that the deviation of f from equilibrium decays simply in time due to collision processes. In particular, we replace the collision term in Boltzman's equation ($C[f] = \mathcal{G}[f] - \mathcal{L}[f]$; see equation 9.29) with

the approximation

$$\mathcal{C}[f] \approx \frac{f - f_0}{\tau}, \quad (9.60)$$

where τ is the characteristic *collision time* (or mean free flight time) and measures the rate of recovery from a non-equilibrium state.[†]

Now, Δ can be calculated to first-order by substituting $f = f_0 + \Delta$ into Boltzmann's equation (equation 9.32), using the approximation introduced in equation 9.60, and assuming that $\Delta \ll f_0$:

$$\left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} \right) (f_0 + \Delta) \approx -\frac{\Delta}{\tau} \implies \Delta = -\tau \left(\frac{\partial}{\partial t} + \vec{v} \cdot \nabla + \frac{\vec{F}}{m} \cdot \nabla_{\vec{v}} \right) f_0. \quad (9.61)$$

It is tedious but straightforward to show that (see [huangk63])

$$\Delta = -\tau \left\{ \frac{1}{kT} \sum_i \frac{\partial(kT)}{\partial x_i} U_i \left(\frac{m}{2kT} U^2 - \frac{5}{2} \right) + \frac{1}{kT} \sum_{ij} \Lambda_{ij} (U_i U_j - \frac{1}{3} \delta_{ij} U^2) \right\} f_0, \quad (9.62)$$

where $\vec{U} \equiv \vec{v} - \vec{u}$ and $\Lambda_{ij} \equiv \frac{1}{2} m \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$.

Using this expression for Δ , we now calculate the first-order approximation to the pressure-tensor P_{ij} :

$$\begin{aligned} P_{ij} &= \frac{\rho}{n} \int d^3v (v_i - u_i)(v_j - u_j)(f_0 + \Delta), \\ &= \delta_{ij} P - \frac{\tau \rho}{nkT} \sum_{kl} \Lambda_{kl} \int d^3U U_i U_j (U_k U_l - \frac{1}{3} \delta_{kl} U^2) f_0, \\ &= \delta_{ij} P - \frac{2\mu}{m} (\Lambda_{ij} - \frac{m}{3} \delta_{ij} \nabla \cdot \vec{u}), \end{aligned} \quad (9.63)$$

where $P = nkT$ and $\mu = \frac{m^2 \tau}{kT} \int d^3U U_1^2 U_2^2 f_0 = \tau nkT$ is the *coefficient of viscosity*.[‡]

[†] Assuming that $\Delta \ll f_0$ and that f_0 varies appreciably only over distances $|\vec{x}| \approx L$, it is easy to show that $\Delta/f_0 \approx -\lambda/L$, where λ is the mean free path length; i.e. f_0 is a good approximation if the characteristic wavelengths of ρ , T and $\vec{u}$ are all much greater than the mean free path. The exact solution f can then be expanded in powers of the factor λ/L . This systematic expansion is called the *Chapman-Enskog expansion*, and is the subject of the next section.

[‡] Huang [huangk63] gives a simple plausibility argument justifying our calling μ the coefficient of viscosity. Consider a fluid with average velocity given by $u_x = \alpha + \beta y$ and $u_y = u_z = 0$, where α and β are some constants; i.e. our fluid undergoes a horizontal flow with, say, linearly increasing velocity with height. Let $\mathcal{F}$ be the frictional force experienced by the fluid above any plane perpendicular to the y -axis, per unit area of the plane. Since $\mathcal{F}$ represents the total flow of the x -component of momentum in the y direction, it is given by $\mathcal{F} = mn \langle (v_x - u_x)(v_y - u_y) \rangle = m \int d^3v (v_x - u_x)(v_y - u_y)(f_0 + \Delta)$. Using equation 9.61 to approximate Δ , we find $\vec{v} \cdot \nabla f_0 = -\Delta/\tau \implies \Delta = -\frac{\tau m}{kT} v_y (v_x - u_x) \beta f_0 = -\frac{\tau m}{kT} U_y U_x \frac{\partial u_x}{\partial y} f_0$, where $\vec{U} \equiv \vec{v} - \vec{u}$. Thus, $\mathcal{F} = -\frac{\partial u_x}{\partial y} \frac{\tau m^2}{kT} \int d^3U U_x^2 U_y^2 f_0$. Since the coefficient of viscosity is defined by the expression $\mathcal{F} = -\mu \frac{\partial u_x}{\partial y}$, where μ is the coefficient of viscosity, we read off immediately from our expression

The Navier-Stokes equations are “recovered” by substituting this first-order expression for the pressure tensor into the conservation theorem with $\kappa = mv_i$ (i.e. into equation 9.55).

9.1.9.4 Heat Conduction Equation

The general heat-conduction equation, along with the familiar diffusion equation, are both consequences of energy conservation and, like we have just seen for the Navier-Stokes equation, require a first-order approximation to the solution of Boltzmann's equation.

Setting $\kappa = \frac{1}{2}m |\vec{v} - \vec{u}|^2$ in equation 9.52, where, as before, $\vec{u} \equiv \langle \vec{v} \rangle$, gives

$$\frac{1}{2} \frac{\partial \langle \rho |\vec{v} - \vec{u}|^2 \rangle}{\partial t} + \sum_i \frac{\partial \langle \rho v_i |\vec{v} - \vec{u}|^2 \rangle}{\partial x_i} - \frac{1}{2} \rho \sum_i \langle v_i \frac{\partial (|\vec{v} - \vec{u}|^2)}{\partial x_i} \rangle = 0. \quad (9.64)$$

Defining the temperature $T \equiv \frac{m}{3k} \langle |\vec{v} - \vec{u}|^2 \rangle$ (where k is Boltzmann's constant) and heat-flux $\vec{Q} \equiv \frac{1}{2}m\rho \langle (\vec{v} - \vec{u}) |\vec{v} - \vec{u}|^2 \rangle$, so that $\frac{1}{2}m\rho \langle v_i |\vec{v} - \vec{u}|^2 \rangle = Q_i + \frac{3}{2}\rho k T u_i$ and $\rho \langle v_i (\vec{v} - \vec{u}) \rangle = P_{ij}$, equation 9.64 may be rewritten as

$$\frac{3}{2} \frac{\partial (\rho k T)}{\partial t} + \sum_i \frac{\partial Q_i}{\partial x_i} + \frac{3}{2} \sum_i \frac{\partial (\rho k T u_i)}{\partial x_i} + \sum_{ij} m P_{ij} \frac{\partial u_j}{\partial x_i} = 0, \quad (9.65)$$

or, using the fact that $P_{ij} = P_{ji}$, as

$$\rho \left[\frac{\partial}{\partial t} + \sum_i u_i \frac{\partial}{\partial x_i} \right] (kT) + \frac{2}{3} \sum_i \frac{\partial Q_i}{\partial x_i} = -\frac{2}{3} \sum_{ij} \Lambda_{ij} P_{ij}, \quad (9.66)$$

where $\Lambda_{ij} \equiv \frac{1}{2}m \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$.

Using the expression for Δ appearing in equation 9.62, we find that, to first-order, the heat-flux $\vec{Q}$ is given by

$$\begin{aligned} \vec{Q} &= \frac{m\rho}{2n} \int d^3v (\vec{v} - \vec{u}) |\vec{v} - \vec{u}|^2 \Delta, \\ &= -\frac{\tau m^2}{2kT} \int d^3U \vec{U} U^2 \left(\frac{m}{2kT} U^2 - \frac{5}{2} \right) \left(\sum_i U_i \frac{\partial (kT)}{\partial x_i} \right) f_0, \\ &= -K \nabla (kT), \end{aligned} \quad (9.67)$$

where $K = \frac{m^2 \tau}{6kT} \int d^3U U^4 \left(\frac{m}{2kT} U^2 - \frac{5}{2} \right) f_0 = \frac{5}{2} \tau n k T$ is the coefficient of thermal conductivity.

Substituting this expression for $\vec{Q}$ and the first-order expression we found earlier for the pressure-tensor (equation 9.63) into equation 9.66 yields the general heat conduction equation:

$$\left(\frac{\partial}{\partial t} + \vec{u} \cdot \nabla \right) (kT) = \frac{1}{c_V} (\nabla \cdot \vec{u}) (kT) + \frac{K}{\rho c_V} \nabla^2 (kT), \quad (9.68)$$

for $\mathcal{F}$ that $\mu = \frac{\tau m^2}{kT} \int d^3U U_x^2 U_y^2 f_0$.

where $c_V = 3/2$. The familiar diffusion equation is “recovered” by setting $\vec{u} = 0$:

$$\rho c_V \frac{\partial(kT)}{\partial t} - K \nabla^2(kT) = 0. \quad (9.69)$$

9.2 Lattice Gas Models

In the previous section we saw that the *Navier-Stokes equations* (equation 9.16), the fundamental equations describing incompressible fluid flow, are in general analytically intractable. Thanks mostly to the enormous advances in parallel computation that have been made in recent years, however, a powerful new CA approach to modeling hydrodynamics called the *lattice gas (LG)* method has emerged. The idea is to reproduce the desired macroscopic behavior of a fluid by modeling, in typically discrete CA fashion, the underlying microscopic dynamics. Unlike more conventional *molecular dynamics* approaches [boon80] or *finite-difference approximations* (FDA) of the Navier-Stokes equations themselves [hack85], LGs offer the advantage of considerably reduced programming requirements, increased efficiency in both computer memory usage and execution efficiency and – compared to even top-of-the-line Cray X-MP supercomputers – an *orders-of-magnitude* increase in execution speed (see section 9.2.5 and Appendix A).

We will shortly see that in order to achieve an emergence of a suitable macrodynamics out of a discrete microscopic substrate, one must have three basic “ingredients” [hass89]: (1) local thermodynamic equilibrium, (2) conservation laws, and (3) a “scale separation” between the levels at which the microscopic dynamics take place (among kinetic variables living on a *micro-lattice*) and the collective motion itself appears (defined by hydrodynamical variables on a *macro-lattice*; see figure 9.7). We shall also see that a critical role is played by the symmetry of the underlying lattice. The main goal of this section is to show how a LG achieves these basic ingredients from (i) a set of identical unit-massed particles, all moving with the same velocity and allowed to exist only at the vertices of a given lattice, (ii) total discretization (space, time and particle velocity), (iii) a simple set of collision rules respecting both particle-number and momentum conservation, and (iv) an *exclusion principle* forbidding more than one particle with the same velocity from occupying a given lattice site.

While many variants of the basic model can be considered (more than one kind of particle, multi-speed particles, different lattice geometries, etc.), we will show that there is a very well defined minimal set of rules which suffice to define a LG system whose macroscopic behavior reproduces that predicted by the Navier-Stokes equations *exactly*. As such, a particular LG system should be considered as being neither some oversimplified version of molecular dynamics nor as a generic CA equivalent of an FDA; rather, it is a *self-contained universe on to itself*. That is to say, while it is certainly not wrong to think of LGs as *nothing* more than useful alternatives to conventional floating point methods for simulating solutions to partial differential equations (PDEs), it is becoming increasingly apparent that

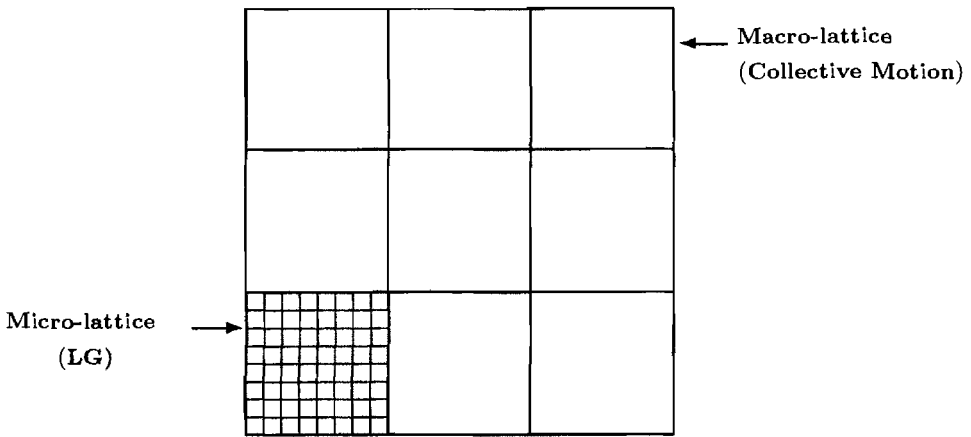


Fig. 9.7 *Micro-lattice* regime of kinetic variables versus the *Macro-lattice* regime of the collective/emergent hydrodynamics.

LGs can also serve as powerful alternatives to PDEs themselves in modeling physical systems. The distinction is an important one. It must be remembered, however, that not all PDEs (and perhaps not all physical systems; see chapter 12) are amenable to a LG simulation. Moreover, even if a candidate PDE is selected for simulation by a LG, there is no currently known “cookbook” recipe allowing a researcher to go from the PDE to a LG description (or vice versa). Nonetheless, by their very nature, LGs lend themselves to modeling any partial differential equation (PDE) for which the underlying physical basis for its construction involves a large number of particles with local interactions [wolf86c].

In addition to being used to build models leading to the Navier-Stokes equations in both two- ([burges87], [roth88]) and three-dimensions ([frisch87], [rem89]), LGs have been successfully applied to studies of buoyancy effects [burges87], combustion phenomena [clav86], the wave equation [chenh88], various linear and non-linear diffusion equations [bog89], seismic P-waves [roth87], magnetohydrodynamics ([chenh87a], [chenh87b], [mont87a], [mont87b]), and Burger’s equation (used to describe weak shock waves) [bog87], among others. It remains an open question whether LG techniques are applicable to other systems such as electromagnetic wave propagation or, more speculatively, quantum field theories [hass89]. The reader is encouraged to consult the many recent surveys and conference proceedings for further details; see, for example, [liv88], [monaco89], [doolen90], and [doolen91].

Aside from providing virtually real-time simulation capability (particularly when run on dedicated parallel-processing hardware such as the Connection machine [hill85], RAP1 [clouq87] or CAM-8 ([marg90a], [toff91])); see Appendix A), perhaps the single greatest virtue of LGs is that once they are properly defined, they can be realized exactly [marg86], with no roundoff error or any need to appeal to sets of simplifying assumptions in order to run. This is in stark contrast to the

usual method of “solution” of nonlinear PDEs such as the Navier-Stokes equations, which, except for a few special cases where the geometry is especially simple or conveniently simplified, amounts to some clever means of approximation (or, in the case of FDA methods, inevitably leads to the appearance of undesirable round-off errors).

9.2.1 A Short History

Historically, LGs date back to the early 1960s. Broadwell [broad64] is usually credited with being the first to come up with a LG-like solution to a rarefied gas “shock problem.” By constraining the motion of a single particle to lie only along the links of a regular lattice, Broadwell managed to obtain an analytic solution to Boltzman’s equation, thus doing away with the need to solve the full set of Navier-Stokes equations. Broadwell’s model amounts to being only a pseudo-discretization, however, because while the velocity set is finite, space and time remain continuous. A similar approach was taken by Kadanoff and Swift in 1968 [kadan68], who introduced a more fully discrete lattice model that displayed sound waves, but in which time was still continuous.

Although these, and other, early attempts were generally successful at modeling special kinds of fluid flow (there was good agreement, for example, between Broadwells’ constrained solutions to Boltzman’s equation and the results of more detailed models of the Navier-Stokes equations), they did not as a group really provide any real insight into the possibilities of microscopic modeling of fluids. A deeper insight had to await Hardy, de Pazzis and Pomeau’s introduction of the first fully discrete LG model – with discrete *space*, *time* and particle *velocities* – in 1973 [hardy73].

Motivated by a desire to explore fundamental questions such as ergodicity, and inspired by the Ising spin model of statistical mechanics, Hardy *et.al.*’s approach – now known as the HPP model (see discussion below) – was to populate a regular two-dimensional four-neighbor Euclidean lattice with a single-species of particle. The particles were allowed to live only at the lattice sites and to undergo binary collisions with their nearest-neighbors. While this simple model displayed a number of interesting properties, including an approach to a local equilibrium and an emergence of a macrodynamics on a scale much larger than the microscopic mean-free-path (see figure 9.9 showing the development of a circular sound-wave), the macrodynamics that did emerge was unfortunately not entirely consistent with the predictions of the Navier-Stokes equations. The difficulty in reproducing the correct behavior lay in the symmetry of the lattice (for a reason that we will get to shortly in our discussion below), a flaw that was subsequently corrected by Frisch, Hasslacher and Pomeau in 1986 [frisch86]. Frisch, *et.al.*’s model, called the FHP model, used a hexagonal neighborhood and led to a global behavior that was consistent with the Navier-Stokes equations in the limit of low viscosity and large lattice size. An appropriate three-dimensional model was introduced in the same year by d’Humi re, Lallemand and Frisch [d’Hum86a].

So what does the list of basic properties of a LG necessary to yield an emergent behavior consistent with the incompressible Navier-Stokes equations look like? Such

a LG must satisfy the following five properties [hass89]:

- A population of identical particles residing on the sites of $\mathcal{L}$, each having unit mass and moving from site to site with the same average speed.
- A discrete regular lattice $\mathcal{L}$ whose local neighborhood symmetry is such that the momentum flux density tensor Π_{ij} is isotropic; the isotropy of Π_{ij} is an important point that will be taken up in the ensuing discussion.
- A minimal set of symmetric binary and triple collision rules conserving both momentum and particle number.
- A completely discrete phase space (i.e. discrete values of lattice-site positions, particle velocities and time, so that particles move from site-to-site and collisions taken within discrete time steps).
- An “exclusion” principle prohibiting more than one particle from occupying a given site or moving in a given direction at a given time.

We begin by describing the HPP model, which satisfies all of the above requirements except for the isotropy of the momentum flux density tensor. As we shall, however, this early model nonetheless has some very interesting and suggestive properties, despite not being able to reproduce Navier-Stokes-like behavior exactly.

9.2.2 HPP Model

Consider the Hardy, de Pazzis and Pomeau (HPP) LG model [hardy73]. In this model, particles of unit mass and unit speed live on sites of a two-dimensional four-neighbor Euclidean lattice and are allowed to move along the lattice links. No more than one particle may occupy a given site or move in a given direction at a given time. The only nontrivial collision rule is shown in figure 9.8: when two particles collide head-on at a site, they scatter into the two orthogonal directions. All other configurations are left unaltered.

In order to write down the microscopic equations of motion more formally, we consider a size $N \times N$ 4-neighbor lattice $\mathcal{L}$ with periodic boundary conditions. At each site (i, j) there are four cells, each of which is associated with one of the four neighbors of site (i, j) . Each cell at time t can be in one of two states defined by a Boolean variable $n_{i,j}^{(\beta)}(t)$ where $\beta = 1, \dots, 4$ labels, respectively, the east, north, west and south neighbors of site (i, j) :

$$n_{i,j}^{(\beta)}(t) = \begin{cases} 1 & \text{if site } (i, j) \text{ is “occupied” by a particle} \\ & \text{moving in direction } k, \\ 0 & \text{if site } (i, j) \text{ is “unoccupied”.} \end{cases} \quad (9.70)$$

Each site of the lattice may thus be represented by a 4-bit word $\vec{n}_{i,j} = (n_{i,j}^{(1)}, \dots, n_{i,j}^{(4)})$,

where a '1'-entry denotes the presence of a particle moving in the direction defined by the bit position within the word.

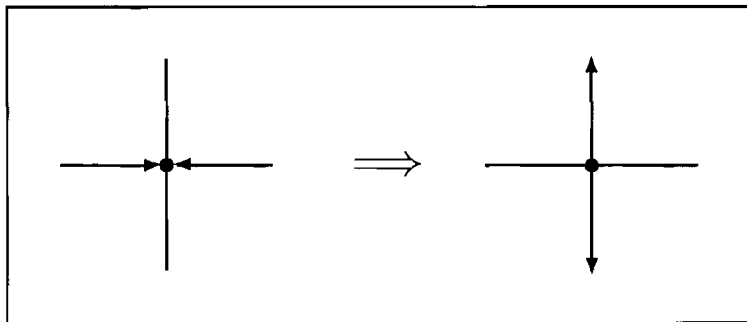


Fig. 9.8 The only nontrivial collision rule in the HPP model.

The equations of motion consist of a set of rules for $n_{ij}^{(\beta)}(t+1)$ in terms of $n_{ij}^{(\beta)}(t)$. Consider first the form of the equations in the absence of collisions. Since, if there were no collisions, particles would simply move from site to site along their respective links, the dynamics would be prescribed simply by $n_{ij}^{(\beta)}(t+1) = n_{i,j}^{(\beta)}(t)$ for $\beta = 1, \dots, 4$. If we now add the possibility of collisions, a *collision operator*, $\mathcal{C}_\beta[n]$, must be added to the RHS of this equation:

$$n_{ij}^{(\beta)}(t+1) = n_{ij}^{(\beta)}(t) + \mathcal{C}_\beta[\vec{n}_{i,j}(t)]. \quad (9.71)$$

Consider site (i, j) 's east neighbor. The corresponding collision operator $\mathcal{C}_1$ consists of two terms: a *source* term ' $(1 - n^{(1)})n^{(2)}(1 - n^{(3)})n^{(4)}$,' which is equal to '1' if and only if there are initially no particles in either the east or west directions to site (i, j) and there are particles to the north and south, and a *sink* term ' $-n^{(1)}(1 - n^{(2)})n^{(3)}(1 - n^{(4)})$,' which is equal to '-1' if and only if there are initially no particles in either the north or south directions to site (i, j) and there are particles to the east and west. Going through the same reasoning for (i, j) 's remaining neighbors yields the following set of four microscopic equations of motion:

$$\begin{cases} n_{ij}^{(1)}(t+1) &= n_{ij}^{(1)}(t) + \mathcal{C}_1[\vec{n}_{i,j}(t)] &= n_{ij}^{(1)}(t) + \bar{n}^{(1)}n^{(2)}\bar{n}^{(3)}n^{(4)} - n^{(1)}\bar{n}^{(2)}n^{(3)}\bar{n}^{(4)}, \\ n_{ij}^{(2)}(t+1) &= n_{ij}^{(2)}(t) + \mathcal{C}_2[\vec{n}_{i,j}(t)] &= n_{ij}^{(2)}(t) + n^{(1)}\bar{n}^{(2)}n^{(3)}\bar{n}^{(4)} - \bar{n}^{(1)}n^{(2)}\bar{n}^{(3)}n^{(4)}, \\ n_{ij}^{(3)}(t+1) &= n_{ij}^{(3)}(t) + \mathcal{C}_3[\vec{n}_{i,j}(t)] &= n_{ij}^{(3)}(t) + \bar{n}^{(1)}n^{(2)}\bar{n}^{(3)}n^{(4)} - n^{(1)}\bar{n}^{(2)}n^{(3)}\bar{n}^{(4)}, \\ n_{ij}^{(4)}(t+1) &= n_{ij}^{(4)}(t) + \mathcal{C}_4[\vec{n}_{i,j}(t)] &= n_{ij}^{(4)}(t) + n^{(1)}\bar{n}^{(2)}n^{(3)}\bar{n}^{(4)} - \bar{n}^{(1)}n^{(2)}\bar{n}^{(3)}n^{(4)}, \end{cases} \quad (9.72)$$

where we have used the shorthand $\bar{n} = 1 - n$.

9.2.2.1 Conservation Laws

Equation 9.72 shows that HPP collisions give rise to three conservation laws: (i) total number of particles ($\sum_{\beta} C_{\beta} = 0$), (ii) momentum in the x -direction ($C_1 - C_3 = 0$), and (iii) momentum in the y -direction ($C_2 - C_4 = 0$).[†]

The dynamics is clearly invariant under all discrete transformations preserving the underlying lattice (discrete translations, rotations by $\theta = \pi/2$ and mirror reflections) and is invariant under a *duality transformation* (i.e. an exchange of occupancy, $0 \longleftrightarrow 1$). Unfortunately, the HPP model also has some *spurious* conservation laws, such as the total momentum in the x -direction along each horizontal line and the total momentum in the y -direction along each vertical line. Such spurious conservation laws – which plague other models as well – obviously have no analog in continuum fluids and must somehow be dealt with if the desired fluid behavior on the macro-scale is to be reproduced. In the HPP LG, the spurious conservation laws induce an anisotropic viscosity on the macroscopic level and thus preclude an exact reproduction of Navier-Stokes behavior; the emergent behavior in this case is thus only *approximately* Navier-Stokes-like.

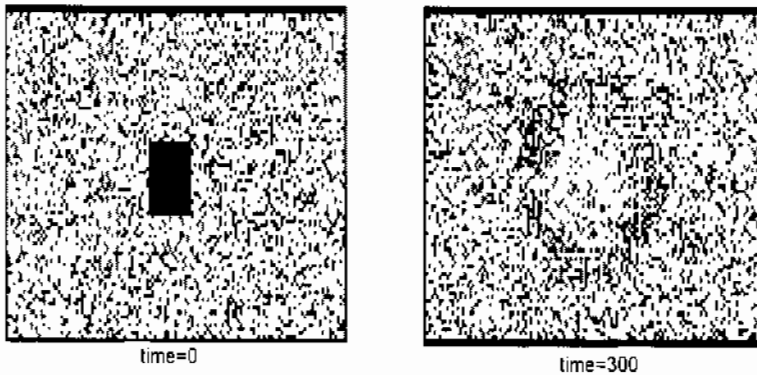


Fig. 9.9 Wave propagation in the HPP lattice gas, starting from a localized “disturbance.” Notice the appearance of a circular wave front on the macro-scale despite the discrete anisotropy at the microscopic (i.e. dynamical) level.

9.2.2.2 Behavior

Despite not being able to exactly reproduce Navier-Stokes behavior, the HPP nonetheless displays some very interesting behavior. Figure 9.9 shows a typical evolution of the HPP model starting from an initial condition in which there is a tightly-packed region of particles at the center of a 256×256 lattice. This central region expands rapidly outward, creating an alternating series of compressions and rarefactions of the surrounding “gas.” The result is an outwardly propagating *sound*

[†]While it is true that if each particle is endowed with a unit of “kinetic-energy,” the total kinetic energy is also conserved, this conservation law is indistinguishable from the particle number conservation.

wave, reminiscent of the effect of dropping a stone into an initially stagnant pool of water. The most striking thing is that the sound wave is *circular*, despite the fact that the microscopic dynamics – defined on a discrete 4-neighbor lattice – is itself strongly anisotropic. The figure thus shows a clear example of an emergence on a macro-scale of a symmetry not present in the microscopic dynamics ([marg86], [toff87]).

We make three additional remarks. First, while ergodicity has not yet been rigorously proven, relaxation to equilibrium has been shown numerically ([hardy73], [hardy76]). Second, on a time scale commensurate with the length-scale of the disturbance, the HPP LG effectively behaves as an elastic medium [toff87]. That is to say, the resulting behavior is *strongly underdamped*. The particles initially contained in the tightly-packed central region do not just slowly diffuse out of that region, they rush out of it! Finally, there is an emergent high-level speed-of-sound c that is considerably less than the microscopic speed of any of the constituent particles.

Using the latter as a unit of speed, one finds that $c = 1/\sqrt{2}$, and is independent of direction and density of the LG [salem86]. The HPP LG thus also furnishes us with our first example of a purely mechanical property that emerges only on the macroscopic level.

9.2.3 FHP Models

The original FHP model [frisch86] and its variants ([d’Hum86b], [d’Hum87c], [rivet86], [wolf86c]), generalizes the four-neighbor HPP model by allowing single-speed particles to move along the links of a two-dimensional hexagonal lattice. Each site is linked to its six nearest neighbors by unit vectors $\hat{c}_\beta$, defined by

$$\hat{c}_\beta = \hat{x}\left(\frac{2\pi k}{6}\right) + \hat{y}\left(\frac{2\pi k}{6}\right), \quad k = 1, \dots, 6. \quad (9.73)$$

The input and output configurations at site (i, j) of the LG are defined by the occupancy of the each of the six links connecting (i, j) to its neighbors. The specification of a local state therefore requires either 6 or 7 bits, depending on whether we also allow rest-particles at the center site. These added bits obviously increase the number of possible local configurations over those in the HPP model. In 6-bit models, for example, there are a total of $2^6 = 64$ possibilities. In choosing a representative set of collision rules we must be careful to conserve both particle number and momentum and to eliminate any spurious conservation laws. As for the HPP model, we must also respect an “exclusion” principle: no more than one particle may occupy a given site or move in a given direction at a given time. Figure 9.10 shows the set of possible initial and final states for collisions in the FHP model.

Consider a “head-on” collision between particles incoming along directions $\hat{c}_\beta$ and $\hat{c}_{k+3}$. There are two possible outcomes such that both particle number and momentum are conserved: the output must consist of two particles emerging either along directions $\hat{c}_{k+1}$ and $\hat{c}_{k+4}$ (figure 9.10-b) or along $\hat{c}_{k-1}$ and $\hat{c}_{k-4}$ (figure 9.10-c). We can either have the system always choose the same output channel, which

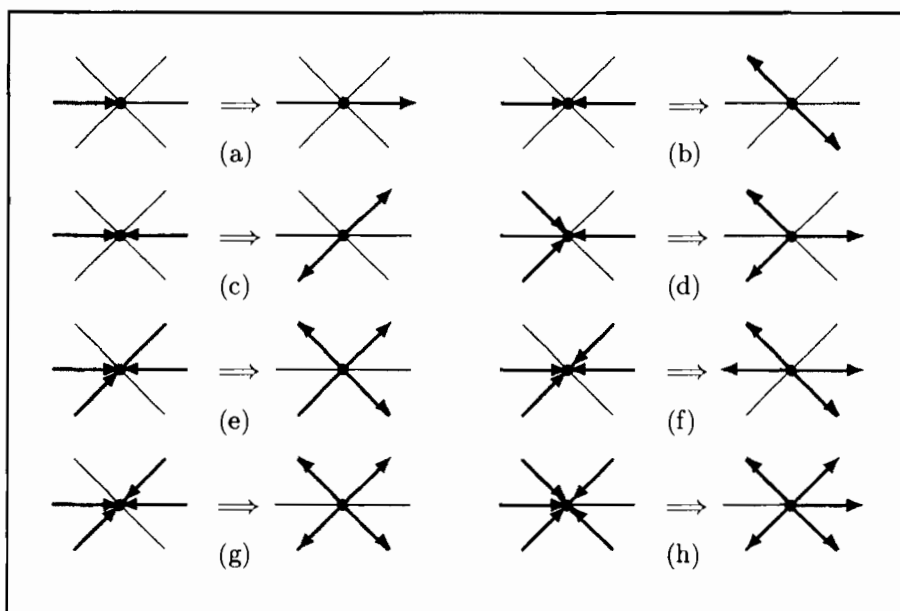


Fig. 9.10 The eight possible collision rules for the FHP model.

keeps the model deterministic but introduces an artificial chirality by breaking the mirror-symmetry, or use a nondeterministic rule that has the system choose either of the two possible outcomes with equal likelihood.

Whatever scheme we choose for treating head-on collisions, however, unless we also have *triple collisions*, spurious conservation laws are inevitable. In addition to the total particle number and momentum, it is easy to see that head-on collisions also conserve the *difference in particle number in opposite directions*; that is, the difference in particle numbers in directions $\hat{c}_\beta$ and $\hat{c}_{k+3}$. A simple way to fix this problem is to introduce a triple-collision of the form $(\hat{c}_\beta, \hat{c}_{k+2}, \hat{c}_{k+4}) \rightarrow (\hat{c}_{k+1}, \hat{c}_{k+3}, \hat{c}_{k+5})$ (figure 9.10-d). The resulting “minimal” LG, consisting only of the collision rules shown in figures 9.19a through 9.10-d, is called the FHP-I model. Notice that while FHP-I, as it stands, is *not invariant* under duality, it can be made so simply by including the duals of the binary collisions (figures 9.10-f,g).

There are other, more complex, variants of this minimal model. FHP-II, for example, is a 7-bit variant of FHP-I, adding a zero-velocity rest particle and a few collision extra rules involving that rest particle [frisch87]. FHP-III is a “collision-saturated” version of FHP-II ([frisch87], [d’Hum87c]). There are also 8-bit variants that include up to three rest particles per site and use particles of different mass ([d’Hum87c], [wolf86c]). For simplicity, we will not consider models with rest particles.

9.2.4 Equations for Macroscopic LG Behavior

The generalized form of equation 9.71,

$$n_\beta(\vec{x}, t+1) = n_\beta(\vec{x}, t) + C_\beta[\vec{n}(\vec{x}, t)]. \quad (9.74)$$

where $n_\beta(\vec{x}, t)$ here refers to the occupancy ($= 0, 1$) of the node at position $\vec{x}$ and time t of a particle moving in direction $\hat{c}_\beta$ (equation 9.73), and C_β a general collision operator, expresses the exact discrete microscopic dynamics of a general LG system. While no approximations are involved at this level, however, the equation as it stands tells us little about the macroscopic properties of the system.

In order to obtain the equations describing macroscopic behavior, we consider an ensemble of LGs, each defined on lattices of equal size and whose initial conditions are sampled from some given distribution. We will assume that starting from an arbitrary initial ensemble, the system evolves to ensembles whose statistical properties depend only on the values of the conserved quantities. While the actual evolution of the LG involves a particular configuration and does not involve statistical ensembles, the resulting statistical analysis may nonetheless still be applicable if the given configuration is representative of the ensemble [wolf86c]. We will in fact use ensemble averages to help construct the kinetic equations describing the average rates for processes in the LG, and deduce various macroscopic hydrodynamic quantities by performing local spatial averages. We follow Wolfram [wolf86c], Hasslacher ([hass88b], [hass89]), Frisch, *et.al.* [frisch87] and Boghosian [bog90]. Although the arguments presented below are quite general and could be applied to a variety of geometries and dimensions, we will, unless otherwise noted, perform all explicit calculations on a two-dimensional hexagonal lattice.

9.2.4.1 Boltzman's Equation

We begin by introducing the one-particle distribution function $f_\beta(\vec{x}, t)$,

$$f_\beta(\vec{x}, t) = \langle n_\beta(\vec{x}, t) \rangle, \quad (9.75)$$

where $\langle \dots \rangle$ denotes an ensemble average; $f_\beta(\vec{x}, t)$ gives the probability of finding a particle moving in direction $\hat{c}_\beta$ at position $\vec{x}$ and time t . Next, as in our derivation of the (continuous) Boltzman's equation (see equations 9.26 – 9.32), we observe that there are two ways in which f_β can change in time: (1) unimpeded particle motion from one site to another, and (2) collisions among particles at a given lattice site.

In the first case (i.e. in the absence of all collisions), we know that all particles at position $\vec{X}$ with velocity $\hat{c}_\beta$ at time T move to the site at position $\vec{X} + \hat{c}_\beta$ at time $T + 1$:

$$f_\beta(\vec{X} + \hat{c}_\beta, t+1) = f_\beta(\vec{X}, t), \quad (9.76)$$

or, in terms of the scaled variables $\vec{X} = \delta_x \vec{x}$ and $t = \delta_t T$ where $\delta_x, \delta_t \ll 1$,

$$f_\beta(\vec{x} + \delta_x \hat{c}_\beta, t + \delta_t) - f_\beta(\vec{x}, t) = 0. \quad (9.77)$$

If we Taylor expand the first term according to $f(x_0 + h, y_0 + k) = \sum_i \frac{1}{i!} (h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y})^i f(x_0, y_0)$, we get

$$\delta_t \frac{\partial f_\beta}{\partial t} + \delta_x \hat{c}_\beta \cdot \nabla f_\beta + \frac{1}{2} \delta_t^2 \frac{\partial^2 f_\beta}{\partial t^2} + \delta_x \delta_t (\hat{c}_\beta \cdot \nabla) \frac{\partial f_\beta}{\partial t} + \frac{1}{2} \delta_x^2 (\hat{c}_\beta \cdot \nabla)^2 f_\beta + O(\delta^3) = 0. \quad (9.78)$$

Taking the lowest order terms δ_x and δ_t , we have the basic collisionless form of the discrete Boltzman equation:

$$\frac{\partial}{\partial t} f_\beta(\vec{x}, t) + \hat{c}_\beta \cdot \nabla f_\beta(\vec{x}, t) = 0. \quad (9.79)$$

Including collisions yields the full Boltzman equation:

$$\frac{\partial}{\partial t} f_\beta(\vec{x}, t) + \hat{c}_\beta \cdot \nabla f_\beta(\vec{x}, t) = C_\beta[\{f\}], \quad (9.80)$$

where $C_\beta[f]$ is the LG collision operator. As was true in the continuous case, the LG collision operator is generally quite complicated, as it can depend on two-particle, three-particle and possibly higher-order distribution functions. Indeed, a simple glance back at the HPP collision operator given in equation 9.72 suggests that we can generally expect its ensemble average analogue to likewise be strongly nonlinear.

Equation 9.80 generally gives the temporal evolution of f_β in terms of two-particle and higher-order distribution functions appearing in $C_\beta[f]$. The temporal evolution of the two-particle distribution function is in turn found from a similar equation involving three-particle and higher-order distribution functions. And so on. Equation 9.80 is but the first in the set of equations making up the so-called BBGKY hierarchy [bal75]. To simplify matters, we will, as before, make Boltzman's "molecular chaos" assumption, thereby effectively truncating the BBGKY hierarchy at its first level. Namely, we assume that, prior to collisions, all sets of particles are statistically completely uncorrelated. This permits us to write all multi-particle distribution functions appearing in $C_\beta[f]$ in terms of the one-particle distribution function f_β . Put another way, the molecular chaos assumption is equivalent to making the approximation

$$\langle C_\beta[\vec{n}] \rangle \approx C_\beta[\langle \vec{n} \rangle] = C_\beta[\{f\}]. \quad (9.81)$$

On a hexagonal lattice, for example, the two-particle distribution function $f_{23}^{(2)}$, is in this approximation written as $f_{23}^{(2)} = (1 - f_1)f_2f_3(1 - f_4)f_5f_6$.

Two and Three Particle Collision Operator for the FHP LG: Let us look more closely at the form of the LG collision operator for a hexagonal lattice. Conceptually, it is constructed in almost the same manner as its continuous counterpart.[†] In particular, we must examine, at each site, the gain and loss of particles along a given direction.

Let $f_\beta(\vec{x}, t)$ be the probability that a particle moving into the direction $\hat{c}_\beta$ is at the site positioned at $\vec{x}$ and time t , and consider, first of all, only two-particle collisions. A particle may scatter into the direction $\hat{c}_\beta$ only if it comes from a binary collision involving

[†]See discussion following equation 9.29.

particles moving in the $\hat{c}_{\beta+1}$ and $\hat{c}_{\beta+4}$ or $\hat{c}_{\beta+2}$ and $\hat{c}_{\beta+5}$ directions (see equation 9.73 and figure 9.10). The probability that a particle will scatter into the $\hat{c}_{\beta}^{\text{th}}$ direction due solely binary collisions is therefore given by

$$p_{\beta}^{\text{gain, (binary)}} = (1 - f_{\beta})f_{\beta+1}(1 - f_{\beta+2})(1 - f_{\beta+3})f_{\beta+4}(1 - n_{\beta+5}) + (1 - f_{\beta})(1 - f_{\beta+1})f_{\beta+2}(1 - f_{\beta+3})f_{\beta+4}n_{\beta+5}. \quad (9.82)$$

Similarly, since a loss of particle from the $\hat{c}_{\beta}^{\text{th}}$ direction can only result from a binary collision of particles incoming from the $\hat{c}_{\beta}^{\text{th}}$ and $\hat{c}_{\beta+3}^{\text{th}}$ directions, and there are two possible output channels (namely ' $\hat{c}_{\beta}, \hat{c}_{\beta+3}$ ' $\rightarrow$ ' $\hat{c}_{\beta-1}, \hat{c}_{\beta+2}$ ' and ' $\hat{c}_{\beta}, \hat{c}_{\beta+3}$ ' $\rightarrow$ ' $\hat{c}_{\beta-2}, \hat{c}_{\beta+1}$ '), the probability of a loss in the $\hat{c}_{\beta}^{\text{th}}$ direction due to binary collisions is given by $p_{\beta}^{\text{loss, (binary)}} = -2f_{\beta}(1 - f_{\beta+1})(1 - f_{\beta+2})f_{\beta+3}(1 - f_{\beta+4})(1 - f_{\beta+5})$.

Handling the triple-collision gain-loss term in the same way, the complete two- and three- particle collision term for the $\hat{c}_{\beta}^{\text{th}}$ direction can be written in the following form [hass88b]:

$$\mathcal{C}_{\beta}^{2,3} = [\hat{n}_{\beta+1}\hat{n}_{\beta+4} + \hat{n}_{\beta+2}\hat{n}_{\beta+5} - 2\hat{n}_{\beta}\hat{n}_{\beta+3} + \hat{n}_{\beta+1}\hat{n}_{\beta+3}\hat{n}_{\beta+5} - \hat{n}_{\beta}\hat{n}_{\beta+2}\hat{n}_{\beta+4}] \prod_{i=0}^5 (1 - f_{\beta+i}), \quad (9.83)$$

where $\hat{n}_{\beta} \equiv f_{\beta}/(1 - f_{\beta})$.

9.2.4.2 Continuity Equation

The one-particle distribution function f_{β} specifies both the total particle density ρ and momentum density $\rho\vec{u}$, where $\vec{u}$ is the average fluid velocity:

$$\begin{cases} \rho &= \sum_{\beta} f_{\beta}, \\ \rho\vec{u} &= \sum_{\beta} \hat{c}_{\beta} f_{\beta}. \end{cases} \quad (9.84)$$

Conservation of these quantities implies that (compare to equation 9.48)

$$\begin{cases} \sum_{\beta} \mathcal{C}_{\beta} &= 0, \\ \sum_{\beta} \hat{c}_{\beta} \mathcal{C}_{\beta} &= 0. \end{cases} \quad (9.85)$$

Using the first condition in Boltzman's equation (equation 9.80), we have

$$\frac{\partial}{\partial t} \sum_{\beta} f_{\beta} + \sum_{\beta} \hat{c}_{\beta} \cdot \nabla f_{\beta} = \sum_{\beta} \mathcal{C}_{\beta}[\{f\}] \implies \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\vec{u}) = 0, \quad (9.86)$$

which we recognize as the continuity equation (see equation 9.3). Here we have our first example of an equation that is constructed out of microscopic primitives but describes the macroscopic average behavior of a LG "fluid."

9.2.4.3 Euler's Equation

Using Boltzman's equation (equation 9.80) and momentum conservation (the second of the two expressions in equation 9.85), yields

$$\frac{\partial}{\partial t} \sum_{\beta} \hat{c}_{\beta} f_{\beta} + \sum_{\beta} \hat{c}_{\beta} (\hat{c}_{\beta} \cdot \nabla f_{\beta}) = 0 \implies \frac{\partial(nu_i)}{\partial t} + \sum_j \frac{\partial}{\partial x_j} \Pi_{ij} = 0, \quad (9.87)$$

where

$$\Pi_{ij} = \sum_{\beta} (\hat{c}_{\beta})_i (\hat{c}_{\beta})_j f_{\beta} \quad (9.88)$$

is the *momentum flux density tensor*. Unlike the previous case, however, no simple macroscopic result can be derived for Π_{ij} [wolf86c].

Recall that equations 9.86 and 9.100 have been both derived using only the *first-order* terms in the Taylor series expansion of our basic kinetic equation (equation 9.77). It is easy to show that if instead all terms through *second-order* in δ_x and δ_t are retained, the continuity equation (9.86) remains invariant but the momentum equation (9.100) requires correction terms [wolf86c]. The LHS of equation 9.100, to second order in $\delta_x \sim \delta_t \sim \delta \ll 1$, is given by

$$\sum_{\beta} \left(\frac{\partial}{\partial t} + \hat{c}_{\beta} \cdot \nabla \right) \hat{c}_{\beta} f_{\beta} + \frac{1}{2} \delta \frac{\partial}{\partial t} \sum_{\beta} \left(\frac{\partial}{\partial t} + \hat{c}_{\beta} \cdot \nabla \right) \hat{c}_{\beta} f_{\beta} + \frac{1}{2} \delta \sum_{\beta} \{ \hat{c}_{\beta} \cdot \nabla \frac{\partial}{\partial t} + (\hat{c}_{\beta} \cdot \nabla)^2 \} \hat{c}_{\beta} f_{\beta} = 0. \quad (9.89)$$

The correction term is thus essentially a geometrical effect, arising from breaking the form of a Galilean covariant derivative [hass88b]. In continuum fluids, as we have seen, the covariant derivative typically has the form $d/dt = \partial/\partial t + \vec{u} \cdot \nabla$, as implied by Galilean invariance. In the discrete case, however, the LG fluid acts as though it were composed of a mixture of different components, each moving with velocities $\hat{c}_{\beta}$; each component thus contributes a different factor to the covariant derivative of various quantities. Notice that in this case the second order correction term vanishes if f_{β} satisfies the first-order equation (9.100).

Chapman-Enskog Expansion: As we have seen above, the momentum flux density tensor Π_{ij} depends on the one-particle distribution function f_{β} , which is itself a solution of the discrete Boltzman's equation (9.80). As in the continuous case, finding the full solution is in general an intractable problem. Nonetheless, we can still obtain a useful approximation through a perturbative Chapman-Enskog expansion.

Assuming that our LG is in a local equilibrium, it is reasonable to expect that the one-particle distribution functions should depend only on the macroscopic parameters $\vec{u}(\vec{x}, t)$ and $\rho(\vec{x}, t)$ and their derivatives [wolf86c]. While there is no reason to believe that this dependence should be a particularly simple one, it is reasonable to expect that both $\vec{u}$ and ρ are slowly varying functions of $\vec{x}$ and t . Moreover, in the subsonic limit, we can assume that $|\vec{u}| \ll 1$.

Expanding f_{β} around the global equilibrium solution f_{eq} at $\vec{u} = 0$ in available scalar products using the vectors $\hat{c}_{\beta}$ and $\vec{u}$, we have, formally, in the homogeneous fluid approximation ($\nabla \vec{u} = 0$),

$$f_{\beta} = f_{\text{eq}} \left\{ 1 + \eta_1 \hat{c}_{\beta} \cdot \vec{u} + \eta_2 [(\hat{c}_{\beta} \cdot \vec{u})^2 + \alpha_2 |\vec{u}|^2] + \eta_3 [(\hat{c}_{\beta} \cdot \vec{u})^3 + \alpha_3 |\vec{u}|^2 (\hat{c}_{\beta} \cdot \vec{u})] + \dots \right\} \quad (9.90)$$

We can fill in some of the unknown quantities almost by inspection. By symmetry, for example, we know that on a two-dimensional hexagonal lattice $f_{\text{eq}} = \rho/6$. Also, the constraints given in equations 9.84 determine the coefficients η_1 , α_2 and α_3 :

$$\begin{cases} \eta_1 &= 2, \\ \alpha_2 &= -\frac{1}{2}, \\ \alpha_3 &= -\frac{3}{4}. \end{cases} \quad (9.91)$$

To proceed any further requires us to make some assumptions about f_{β} . We again take our cue from the continuous case (see section 9.1), where we had used Boltzman's H-theorem to arrive at the general form for the equilibrium distribution function. In that case, we had found that the form was given by the Maxwell-Boltzman distribution. In the discrete case, however, we must be careful to respect an effective "exclusion principle": *no more than one particle moving in a given direction is allowed to occupy a given site at a given time*. The correct discrete analogue of the continuous H-function (equation 9.41) is given by

$$H = \sum_{\beta} \tilde{f}_{\beta} \log \tilde{f}_{\beta}, \quad (9.92)$$

where $\tilde{f}_{\beta} \equiv f_{\beta}/(1 - f_{\beta})$ [wolf86c].

Arguing as before that when the equilibrium condition $dH/dt = 0$ holds, we have *detailed balance* – i.e. that all products $\tilde{f}_{\beta_1} \tilde{f}_{\beta_2} \dots$ must be equal for all sets of initial and final particles $\{\beta_1, \beta_2, \dots\}$ taking part in the collisions – we see that $\log(\tilde{f}_{\beta})$ must be some linear combination of quantities conserved during the collisions, or $\log(\tilde{f}_{\beta}) = -a - b\vec{u} \cdot \hat{c}_{\beta}$, where $a = a(\rho, |\vec{u}|^2)$ and $b = b(\rho, |\vec{u}|^2)$ are functions of the conserved quantities ρ and $|\vec{u}|^2$. Given that we have a system whose particles obey an exclusion-principle, it should therefore come as no surprise that the one-particle distribution functions must therefore have the Fermi-Dirac form

$$f_{\beta} = \frac{1}{1 + \exp[a + b(\vec{u} \cdot \hat{c}_{\beta})]}. \quad (9.93)$$

One can actually prove a stronger result: *all* nondeterministic LG models that satisfy semi-detailed balance and possess no spurious conservation laws have universal equilibrium solutions whose mean populations are given by the Fermi-Dirac distribution (equation 9.93) [frishc87].

As long as we are in the subsonic limit, so that $|\vec{u}| \ll 1$, we can expand the coefficients a and b as follows: $a = a_0 + a_1 |\vec{u}|^2 + \dots$, $b = b_0 + b_1 |\vec{u}|^2 + \dots$. Substituting these subsonic expansions back into equation 9.93, and setting $\vec{u} = 0$

yields $a_0 = \ln(\frac{1-f_{eq}}{f_{eq}})$. The remaining coefficients are obtained in a straightforward fashion from the expansion

$$\frac{1}{1+\gamma e^x} = \frac{1}{1+\gamma} - \frac{\gamma}{(1+\gamma)^2}x - \frac{\gamma(1-\gamma)}{2(1+\gamma)^3}x^2 - \frac{\gamma(1-4\gamma+\gamma^2)}{6(1+\gamma)^4}x^3 + \dots, \quad (9.94)$$

and the constraints appearing in equations 9.91. The complete Chapman-Enskog expansion (equation 9.90) is then given by

$$f_\beta = f_{eq} \left\{ 1 + 2(\hat{c}_\beta \cdot \vec{u}) + \frac{2(1-2f_{eq})}{1-f_{eq}} \left[(\hat{c}_\beta \cdot \vec{u})^2 - \frac{1}{2} |\vec{u}|^2 \right] + \frac{4}{3} \frac{1-6f_{eq}+6f_{eq}^2}{(1-f_{eq})^2} \left[(\hat{c}_\beta \cdot \vec{u})^3 - \frac{3}{4} |\vec{u}|^2 (\hat{c}_\beta \cdot \vec{u}) \right] + \dots \right\}, \quad (9.95)$$

or, using $f_{eq} = \rho/6$,

$$f_\beta = \frac{\rho}{6} \left\{ 1 + 2(\hat{c}_\beta \cdot \vec{u}) + 4 \frac{\rho-3}{\rho-6} \left[(\hat{c}_\beta \cdot \vec{u})^2 - \frac{1}{2} |\vec{u}|^2 \right] + 8 \frac{6-6\rho+\rho^2}{(\rho-6)^2} \left[(\hat{c}_\beta \cdot \vec{u})^3 - \frac{3}{4} |\vec{u}|^2 (\hat{c}_\beta \cdot \vec{u}) \right] + \dots \right\}. \quad (9.96)$$

Using this expansion for f_β , and the easily verified relations

$$\begin{cases} \sum_\beta (\hat{c}_\beta)_i (\hat{c}_\beta)_j &= 3\delta_{ij}, \\ \sum_\beta (\hat{c}_\beta)_i (\hat{c}_\beta)_j (\hat{c}_\beta)_k &= 0, \\ \sum_\beta (\hat{c}_\beta)_i (\hat{c}_\beta)_j (\hat{c}_\beta)_k (\hat{c}_\beta)_l &= \frac{3}{4}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \end{cases} \quad (9.97)$$

where $\hat{c}_\beta$ is given by equation 9.73, we can now explicitly evaluate the momentum flux density tensor Π_{ij} (equation 9.88). We find that

$$\Pi_{ij} = \frac{\rho}{2}(1-g(\rho)u^2)\delta_{ij} + \rho g(\rho)u_i u_j, \quad (9.98)$$

where

$$g(\rho) = \frac{3-\rho}{6-\rho}. \quad (9.99)$$

The LG version of Euler's equation (equation 9.100) thus becomes

$$\frac{\partial(\rho u_i)}{\partial t} + \sum_j \frac{\partial}{\partial x_j} \{ \rho g(\rho) u_i u_j + \dots \} = \frac{\partial p}{\partial x_i}, \quad (9.100)$$

where $p = \frac{\rho}{2}(1-g(\rho)u^2/2)$. Comparing this to the expression we had derived earlier for continuous fluids (equation 9.7), we see that the two are the same provided that

the lattice “correction” term $g(\rho) = 1$.[†] In our discussion of the LG equivalent of the Navier-Stokes equations below, we will show how $g(\rho) \neq 1$ can be absorbed into a set of rescaled variables.

We make two additional comments. First, notice that when $u \sim 0$, the momentum flux density tensor reduces to the diagonal term $p\delta_{ij}$, where the pressure $p = c_s^2\rho$ and c_s is the *speed of sound*. We thus conclude that the speed of sound in the FHP-I LG is given by

$$c_s = \frac{1}{\sqrt{2}}. \quad (9.101)$$

Second, while all of the preceding calculations have been carried out specifically for the two-dimensional hexagonal lattice, all of the quoted results can be generalized to other lattices and dimensions. In the case where the LG is defined on a d -dimensional lattice and there are $\mathcal{V}$ velocity vectors (where $\mathcal{V} = 6$ for FHP-I), for example, we have the more general result that [frisch87]

$$\begin{cases} f_{\text{eq}} &= \frac{\rho}{\mathcal{V}}, \\ g(\rho) &= \frac{d}{d+2} \frac{\mathcal{V} - 2\rho}{\mathcal{V} - \rho}. \end{cases} \quad (9.102)$$

9.2.4.4 Navier-Stokes Equations

Recall that in the continuum case we derived the Navier-Stokes equations (9.16) by allowing for the possibility of having nonzero viscous terms in the form for the momentum tensor appearing in Euler’s equation (9.9). While their LG analogs may be derived in essentially the same manner, however, the lack of Galilean invariance tend to make the calculations more involved. We will outline the procedure below.

We begin by going back to the Chapman-Enskog expansion of f_β around the global equilibrium solution $f_{\text{eq}} = \rho/6$ at $\vec{u} = 0$ (equation 9.90), but this time including *all* possible scalar products constructed out of the vectors $\vec{u}$, $\hat{c}_\beta$ and ∇ . Using the first of the three relations in equation 9.97 to suggest the possible forms of the scalar products (such as $\hat{c}_\beta \cdot \hat{c}_\beta$, $\hat{c}_\beta \cdot \vec{u}$, $(\hat{c}_\beta \cdot \nabla)(\hat{c}_\beta \cdot \vec{u})$, etc.), and making sure that the constraints given in equations 9.84 are satisfied, we have the following general form for f_β [wolf86c]:

$$f_\beta = \frac{\rho}{6} \left\{ 1 + 2\hat{c}_\beta \cdot \vec{u} + \zeta_2 \left[(\hat{c}_\beta \cdot \vec{u})^2 - \frac{1}{2} |\vec{u}|^2 \right] + \zeta_3 \left[(\hat{c}_\beta \cdot \nabla)(\hat{c}_\beta \cdot \vec{u}) - \frac{1}{2} \nabla \cdot \vec{u} \right] + \dots \right\}, \quad (9.103)$$

[†]Note that $g(\rho) = 0$ for $\rho = 3$, or when the *density per cell* (remembering that a *cell* on a hexagonal lattice contains 6 sites) is equal to $1/2$. This is a reflection of the *duality-invariance* of the LG; i.e. the equivalence between particles and “holes”.

where the values of the remaining unknown coefficients ζ_2 and ζ_3 can only be determined from an explicit solution of the full LG Boltzman equation (9.80), including collision terms. After performing such a calculation – one method is to use solve for the eigenvalues and right eigenvectors of a suitably linearized form of the collision operator (see [frisch87] for details) – the generalized form of the LG Navier-Stokes equations can be written in the form ([frisch87], [hass87])

$$\frac{\partial(\rho u_i)}{\partial t} + \sum_j \frac{\partial}{\partial x_j} \Pi_{ij} = \sum_j \frac{\partial}{\partial x_j} S_{ij}, \quad (9.104)$$

where Π_{ij} is the momentum flux density tensor defined in equation 9.98 and S_{ij} is the *viscosity stress tensor*:

$$S_{ij} = \nu(\rho) \left(\frac{\partial(\rho u_j)}{\partial x_i} + \frac{\partial(\rho u_i)}{\partial x_j} - \delta_{ij} \sum_k \frac{\partial(\rho u_k)}{\partial x_k} \right), \quad (9.105)$$

and

$$\nu(\rho) = \frac{1}{12} \frac{1}{\left[\frac{\rho}{6}(1 - \frac{\rho}{6})^3\right]} - \frac{1}{8} \quad (9.106)$$

is the viscosity.

Incompressible Limit: In order to obtain the more familiar form of the Navier-Stokes equations (9.16), we take the low-velocity (i.e. low Mach number $M = |\vec{u}|/c_s$) limit of equation 9.104. We also take a cue from the continuous case, where, if the incompressible Navier-Stokes equations are derived via a Mach-number expansion of the full compressible equations, *density variations become negligible everywhere except in the pressure term* [frisch87]. Thus setting $\rho = \rho_{eq} + \rho'$, and allowing density fluctuations only in the pressure term, the low-velocity limit of equation 9.104 becomes

$$\frac{\partial \vec{u}}{\partial t} + g(\rho_{eq})(\vec{u} \cdot \nabla) \vec{u} = -\frac{1}{\rho_{eq}} \nabla p' + \nu(\rho_{eq}) \nabla^2 \vec{u}. \quad (9.107)$$

Comparing this expression to its counterpart in continuous fluids (the top expression in equation 9.16), which we reproduce here,

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \vec{u}, \quad (9.108)$$

we see that, just as in the comparison between the continuous and LG versions of Euler's equation (equations 9.7 and 9.100), the only difference between the two expressions comes from the lattice correction term $g(\rho_{eq})$, defined in equation 9.99 above.

“Recovery” of Galilean Invariance: There is a simple “trick” that is often used to transform equation 9.107 into the conventional Navier-Stokes equations.

The trick involves using the correction factor $g(\rho_{\text{eq}})$ to rescale *time*, *pressure* and *viscosity*. Specifically, we set

$$t = \frac{1}{g(\rho_{\text{eq}})} \epsilon^{-2} t' T, \quad p' = \frac{\rho_{\text{eq}} g(\rho_{\text{eq}})}{c_s^2} \epsilon^2 P', \quad \nu(\rho_{\text{eq}}) = g(\rho_{\text{eq}}) \nu', \quad (9.109)$$

and rescale the variables $\vec{x} = \epsilon^{-1} \vec{x}'$ and $\vec{u} = \epsilon \vec{u}'$, where ϵ^{-1} is roughly on the order of the macroscopic lattice size. Taking the incompressible limit of equations 9.104 and 9.105, and keeping only leading order terms in ϵ , we get

$$\frac{\partial \vec{u}'}{\partial T} + (\vec{u}' \cdot \nabla') \vec{u}' = -\frac{1}{\rho_{\text{eq}}} \nabla' P' + \nu' \nabla'^2 \vec{u}', \quad (9.110)$$

where $\nabla' = \partial/\partial \vec{x}'$. The rescaling has thus restored Galilean invariance (at least, *formally*) and thereby recovered the conventional Navier-Stokes equations.

Isotropy of the Momentum Flux Density Tensor: If we trace back our derivation of the macroscopic LG Euler's and Navier-Stokes equations, we see that the only place where the geometry of the underlying lattice really enters is through the form for the momentum flux density tensor, $\Pi_{ij} = \sum_{\beta} (\hat{c}_{\beta})_i (\hat{c}_{\beta})_j f_{\beta}$, where $\hat{c}_{\beta} = \hat{x}(\frac{2\pi k}{6}) + \hat{y}(\frac{2\pi k}{6})$, $k = 1, \dots, \mathcal{V}$ are the allowable unit velocity vectors, and f_{β} is our unknown distribution function, to be found from the Chapman-Enskog expansion (equation 9.103).

Consider the general tensor $\mathcal{E}_{i_1 i_2 \dots i_n}^{(n)} = \sum_{\beta} (\hat{c}_{\beta})_{i_1} (\hat{c}_{\beta})_{i_2} \dots (\hat{c}_{\beta})_{i_n}$. Using the Chapman-Enskog expansion for f_{β} and this definition for $\mathcal{E}^{(n)}$, Π_{ij} may be written in the following form [wolf86c]:

$$\begin{aligned} \Pi_{ij} = f_{\text{eq}} \left\{ \mathcal{E}_{ij}^{(2)} + \gamma_1 \sum_k \mathcal{E}_{ijk}^{(3)} u_k + \gamma_2 \left(\sum_{kl} \mathcal{E}_{ijkl}^{(4)} u_k u_l - \sum_k \mathcal{E}_{ijkk}^{(4)} u_k u_k \right) \right. \\ \left. + \gamma_3 \left(\sum_{kl} \mathcal{E}_{ijkl}^{(4)} \frac{\partial u_l}{\partial x_k} - \sum_k \mathcal{E}_{ijkk}^{(4)} \frac{\partial u_k}{\partial x_k} \right) \right\}. \end{aligned} \quad (9.111)$$

Now, in order for us to recover standard hydrodynamical behavior, we require that the momentum flux density tensor be isotropic; i.e. invariant under rotations and reflections. In particular, from the above expansion we see that Π_{ij} must be isotropic up to order $\mathcal{E}^{(4)}$ in order for the leading terms in the momentum equation to be isotropic. Recalling that if a tensor is isotropic then it must be proportional to a scalar, one can derive a set of conditions for the tensors $\mathcal{E}^{(n)}$ to be isotropic. In the case of lattices composed of regular $\mathcal{V}$ -sided polygons, for example, these conditions are given by [wolf86c]

$$(\mathcal{E}^{(2)} \mid \mathcal{V} > 2), \quad (\mathcal{E}^{(3)} \mid \mathcal{V} \geq 2, \mathcal{V} \neq 3), \quad (\mathcal{E}^{(4)} \mid \mathcal{V} > 2, \mathcal{V} \neq 4), \quad (\mathcal{E}^{(5)} \mid \mathcal{V} \geq 2, \mathcal{V} \neq 3, 5), \dots \quad (9.112)$$

These conditions show us immediately that in the case of the four-neighbor HPP lattice ($\mathcal{V} = 4$) $\mathcal{E}^{(4)}$ is nonisotropic, and the macroscopic equations therefore cannot yield a Navier-Stokes equation. For the hexagonal FHP lattice, on the other hand, we have $\mathcal{V} = 6$ and Π_{ij} is isotropic through order $\mathcal{E}^{(4)}$. Wolfram [wolf86c] predicts what models are conducive to Navier-Stokes-like dynamics by using group theory to analyze the symmetry of tensor structures for polygons and polyhedra in d -dimensions.

9.2.5 LG Computers

Now that we have covered the formalism behind the LG approach in some detail, we are in a position to compare this emerging new technique with more conventional and established floating-point methods. Although the difference between LGs and, say, finite difference approximations (FDAs), should be obvious, there is a sense in which FDAs themselves could be considered CA-like simulations. After all, the method entails nothing more than substituting finite differences on a regular grid for derivatives and then using finite floating point truncations of the continuous fields. The difference between the two methods, of course, lies in how they treat the effectively finite set of field values: unlike floating-point methods, in which there is strict hierarchical order between individual bits, LGs treat each bit on a par with every other bit [frisch87].

We begin our discussion of LG computers by considering some of the generic advantages and disadvantages of using LGs to simulate fluid dynamics. Later on in this section we will provide a brief overview of some of the more popular LG computers that are now in use.

9.2.5.1 Dynamic Range

What do we gain by simulating fluids with lattice gases vice using standard techniques like FDAs? Certainly not *dynamic range*. Following Boghosian [bog90], consider a LG with 4 bits per site and $2^4 = 16$ micro-lattice sites per macro-lattice site. Would this LG be a more efficient fluid-dynamics “processor” than a FDA in which 4×16 bits per macro-lattice sites are packed into floating-point numbers? Assuming that the value of the dependent variable for the LG that we are interested in is obtained by adding together all of the corresponding bits in the microlattice, then the number of possible values of the dependent variable is 65 for the LG, but $\sim 2^{64}$ for the FDA (assuming it is run on a 64-bit machine like a Cray X-MP). In other words, we should not expect LGs to have anywhere near the raw dynamic range of floating-point methods.

9.2.5.2 Accuracy

What about intrinsic accuracy? The answer depends on what we mean by “accuracy.” If we are searching for some way to compute various quantities to an arbitrarily large number of decimal places, then LGs are again perhaps not the best way to go. Since the dependent variable is recovered from the microlattice dynamics, the spatial and/or temporal averaging that must be performed to do so results in an unavoidable *noise content*. On the other hand, having a certain amount of noise in the system does have its benefits. For example, an omnipresent background noise assures us that any emerging singularities are probably fairly robust (i.e. *physical*) and are not just artifacts of the underlying analytical formalism [hass89].

Moreover, while averaging precludes our obtaining an arbitrarily fine accuracy, we could paraphrase Toffoli’s description of a basic strength of *all* CA systems (made in another context [toff84]), and point out that the fact that LGs have no analogue

of round-off error, implies that any results that are obtained by using them must therefore have the strength of *theorems*. To be more precise, LGs possess what has come to be known as *bit-democracy*. That is to say, unlike FDAs, where some bits naturally carry more weight (i.e. are more significant) than others, LGs use every bit of memory on an equal footing with every other bit of memory. Finally, it is worth noting that if accuracy is interpreted as meaning a close adherence to conservation laws, LGs of course best any conceivable floating-point method: mass and momentum, for example, are conserved *exactly*.

9.2.5.3 Memory Efficiency

Let us look at memory usage a bit more carefully.[†] Suppose we are using a Cray X-MP computer with a 64-bit word length. Labeling the six directions of a given site on a hexagonal lattice by $A, B, \dots, F$, we can associate each bit in the 6-bit word W_A with a different site of the lattice, say the first 64 sites in the first row. In each case we assign the value ‘1’ or ‘0’ to a given bit depending on whether or not a particle moving in direction A is or is not present at that site. We do the same for the remaining 63 bits of W_A and for the remaining 5 directions. In this way, we have completely encoded all of the information contained in the first 64 sites of the first row into the six words $W_A, W_B, \dots, W_F$. Bit-democracy assures us that each of these bits is treated in exactly the same way as all of the others.

Now, suppose that the CRAY’s memory has a storage capacity of 5×10^8 64-bit words. At $10 - 2/3$ sites per word, this means that the CRAY can effectively store the information content of about 5×10^9 sites, or a number which is several *orders-of-magnitude* greater than that which is typically used by conventional floating point methods. While in some respects this comparison is an unfair one – it being a textbook example of a comparison between “apples” and “oranges,” in that the apparent gain in raw site-number is partially washed away by the inevitable averaging process – there is nonetheless a bona-fide efficiency that arises purely from how the LG computer processes its information.

Since all computer operations are fundamentally bit-oriented, there is a very natural correspondence between LG states and their evolution (via bit-state collision rules) and the bit-by-bit logical operations of the computer tasked with implementing the evolution of those states. In essentially one clock-cycle, for example, a single logical operation like a Boolean AND or NOR can be carried out on two 64-bit words. If the computer is a CRAY X-MP/416, which has eight logical function units, a total of $8 \times 64 = 512$ sites can effectively be processed every clock-cycle. Assuming that each clock-cycle lasts about 10 nanoseconds, a CRAY X-MP/416 should in principle be able to process the information content of about 512×10^8 sites each second. Since a fairly typical two-dimensional hexagonal LG requires about $\sim 30 - 100$ logical operations in order to fully implement the collision rules, a CRAY X-MP/416 should be able to fully process a total of about 5×10^8 sites each second.

[†]We follow [hass89], [desp90] and [shimo90].

9.2.5.4 Programming Efficiency

Another obvious advantage that the LG method typically enjoys over floating-point methods is one of programming efficiency. Because LG “dynamics” are a natural transcription of the kinetic processes taking place on the micro-lattice, the actual program code is generally concise and straightforward, and often amounts to little more than a few dozen lines of FORTRAN.

Boundary conditions, whether the fluid is allowed to flow freely, constrained to move along a cylindrical pipe or must make its way past a series of complex obstacles, are generally much easier to incorporate into the dynamics than for floating-point simulations. We merely *tag* boundary-sites with an extra bit that tells incoming particles that they are to bounce back in the direction from which they came whenever they encounter such sites. To the accuracy that is determined by the inter-site spacing on the underlying lattice, arbitrarily complex geometric shapes can be specified in this manner. Greater care must be taken with specifying boundary conditions for floating-point methods, particularly if they involve any sharp edges or corners, for which some form of adaptive grid techniques must usually be applied.

Finally, we should mention that the stability of a running “program” itself is never really an issue for LG simulations, unlike that for floating-point methods for which certain (sometimes unforeseen) conditions can lead to serious software crashes.

9.2.5.5 Reynold's Number Scaling

Recall from our earlier discussion of Reynold's number (see section 9.1.4) that turbulence and other interesting phenomena appear only for high values of $\mathcal{R}$ (i.e. for $\mathcal{R} \gg 1$). It is therefore important that whatever the method of simulating the fluid, that method must be able to reach these high values. Unfortunately, LG simulation of fluids with high $\mathcal{R}$ exacts a high cost in terms of the required computational resources. While the problem is not an insurmountable, and there are some subtleties involved, LGs generally appear to be less efficient in this regard than direct numerical solutions to the Navier-Stokes equations ([orsz86], [frisch86], [frisch87], [hass89]).

In order to estimate an upper bound for attainable $\mathcal{R}$'s, consider a LG with lattice spacing l_0 , speed-of-sound c_s , kinematic viscosity ν . Reynold's number is then given by

$$\mathcal{R} = \frac{\text{characteristic length} \times \text{characteristic velocity}}{\text{kinematic shear viscosity}} = \frac{vL}{\nu} = \frac{ML}{l_0}, \quad (9.113)$$

where L is the size of the lattice, v is the characteristic flow velocity, $M = v/c_s$ is the Mach number, and we have used the fact that the viscosity ν must be at least of order $c_s l$. The above result follows from the observation that the “microscopic” viscosity must equal the viscosity that determines the dissipation of the hydrodynamical modes on the “macroscopic” level [orsz86]. Now, since for a d -dimensional lattice, the number of lattice sites n is of order $n \sim (L/l_0)^d$, we get the following rough

bound on n in terms of $\mathcal{R}$ and M :

$$n \begin{matrix} > \\ \sim \end{matrix} \left(\frac{\mathcal{R}}{M} \right)^d \quad (9.114)$$

We can also estimate the required computational work. Since the evolution time of the LG is of order L/v and the time required to update a single step on the lattice is of order l_0/c_s , the LG simulation requires roughly $L/(l_0M) = \mathcal{R}/M^2$ time steps. Assuming that the computational work for each site is of order 1, we have that the LG simulation therefore requires a memory storage space of order $S \sim (\mathcal{R}/M)^d$ and a computational work requirement of order $W \sim \mathcal{R}^{d+1}/M^{d+2}$.

These values can be compared to predicted values for numerical solutions of the incompressible Navier-Stokes equations. For $d = 2$, for example, we have the lower bounds $S_{d=2} \sim (\mathcal{R}/M)^2$ and $W_{d=2} \sim \mathcal{R}^3/M^4$ for a LG and the bounds $S_{\text{num}, d=2} \sim \mathcal{R}$ and $W_{\text{num}, d=2} \sim \mathcal{R}^{3/2}$, where the bounds for the numerical solutions are obtained from the Batchelor-Kraichnan theory of two-dimensional equilibrium range dynamics ([kraich67], [bat69], [herr74]). In three-dimensions we have $S_{d=3} \sim (\mathcal{R}/M)^3$ and $W_{d=3} \sim \mathcal{R}^4/M^5$ for a LG and $S_{\text{num}, d=3} \sim \mathcal{R}^{9/4}$ and $W_{\text{num}, d=3} \sim \mathcal{R}^3$ [orsz86].

Chapter 10

Neural Networks

In previous chapters, we have examined a variety of generalized CA models, including reversible CA, coupled-map lattices, reaction-diffusion models, random Boolean networks, structurally dynamic CA and lattice gases. This chapter covers an important field that overlaps with CA: *neural networks*. Beginning with a short historical survey, chapter 10 discusses associative memory and the Hopfield model, stochastic nets, Boltzman machines, and multi-layered perceptrons.

10.1 Introduction

In the last chapter we argued that lattice gases currently represent the most promising *practical* applications of pure CA modeling. Indeed, with the help of fast dedicated hardware such as the CAM-6 and CAM-8 simulators, many heretofore intractable but technologically important hydrodynamical problems such as fluid flow near and around airplane wings are becoming computationally accessible for the first time. There is, however, another burgeoning field that is distinct from but has much in common with CA, itself harbors an immense theoretical importance, and also shows an enormous practical potential: *artificial neural networks* (NNs).

One might facetiously ask, "How can a three year old baby put a CRAY X-MP supercomputer to shame?" The very serious answer is that "She can recognize uncle Seymour's face infinitely faster!" No matter how powerful a computer one has, no matter how powerful an imaging system and image recognition software one is using, it is a fact that a young child will be infinitely better at recognizing certain patterns than the state-of-the-art hardware/software combination. Aside from the obvious fundamental question "Why?," an equally important question is whether or not a child's internal processing is something that can itself be mimicked or even directly simulated.

Part of the answer may lie in the tacit assumption latent in the question itself: how a child processes information is distinctly different from the way traditional

computers process information. One is obviously parallel, the other is serial; one is algorithmic, diligently following a specific set of instructions one instruction at a time, the other is essentially “free form,” organizing information and defining computational “routes” seemingly on-the-fly; etc. The full answer depends on how well we are able to navigate our way on an emerging paradigm shift in the way computation is itself understood.

Neural nets represent a radical new approach to computational problem solving. The methodology they represent can be contrasted with the traditional approach to artificial intelligence (AI). Whereas the origins of AI lay in applying conventional serial processing techniques to high-level cognitive processing like concept-formation, semantics, symbolic processing, etc. – or in a *top-down* approach – neural nets are designed to take the opposite – or *bottom-up* – approach. The idea is to have a human-like reasoning emerge on the macro-scale. The approach itself is inspired by such basic skills of the human brain as its ability to continue functioning with noisy and/or incomplete information, its robustness or fault tolerance, its adaptability to changing environments by learning, etc. Neural nets attempt to mimic and exploit the parallel processing capability of the human brain in order to deal with precisely the kinds of problems that the human brain itself is well adapted for.

10.1.1 *Connection Between Neural Nets and CA*

That there is a connection between CA and NNs, at least conceptually, should come as no surprise. Fundamentally, CA represent a paradigm whereby the conventional emphasis of looking for the origins of complex behaviors in sets of “complex” building blocks is shifted to an entirely different mode-of-thought in which complexity itself is viewed as an emergent phenomenon built upon an assemblage of possibly very “simple” parts. From a purely philosophical point of view, it could also be argued that there is no better known example of a truly emergent phenomenon than that of the emergence of consciousness out of the large network of functionally “simple” (and certainly *unconscious*) neuronal components that make up the human brain. Now, while we have been inexcusably cavalier in our usage of terms like “complex” and “simple” – no respectable neurophysiologist would ever call a neuron simple! – it is safe to say that neural nets arguably represent the prototypical *complex system*.

Reduced to their essentials, CA are dynamical systems consisting of a discrete cellular state space, the nodes of which contain one of a finite number of discrete values, and evolve synchronously in time according to local update rules. Very crudely speaking, a biological neural network likewise consists of a large space of interconnected nodes whose dynamical behavior is a local function of other nodes to which it is connected. Artificial neural nets can be loosely thought of as being nothing more than a set of biologically inspired CA rules. Indeed, as we will see below, the earliest model of a neuron is essentially that of a binary-valued automaton evolving according to a simple threshold rule. Much of the discussion of threshold and multi-threshold CA rules in section 5.5 pertains directly to such neural nets.

There exist many excellent books and collections of papers on this broad and

rapidly growing subject. Two recent books by Caudill and Butler [caud90] and Jubak [jubak92] provide good nontechnical introductions. The collections edited by Anderson and Rosenfeld [anderj88] and Shaw and Palm [shaw88] contain most of the important early landmark papers. Some of the better texts are those by Amit [amit89], Hecht-Nielsen [hecht90], Hertz, Krogh and Palmer [hertz91], and Peretto [peret92]. A more neurophysiological approach is taken by MacGregor [macg87]. The classic book by Minsky and Papert debunking the usefulness of single-layer perceptrons (see discussion below) called *Perceptrons* [minsky69] has recently been re-released in an expanded version [minsky88] and is a must-read. The excellent monograph by Goles and Martinez [goles90] discusses threshold and multi-threshold functions, and contains a particularly lucid discussion of Lyapunov functions. There are also journals that specialize in neural nets such as *Neural Computation*, published by MIT and *Neural Networks*, published by Pergammon.

10.1.2 A Short History

Table 10.1 lists some important developments in neural net research. This list is by no means exhaustive and is intended only to highlight some of the key events.

~ Year	Development	Developers
1943	First Neuron Model	McCulloch-Pitts [mccul43]
1949	Synaptic Learning	Hebb [hebb49]
1958	Simple Perceptron	Rosenblatt [rosenbl58]
1960	LMS/Delta Rule	Widrow and Hoff [widrow60]
1969	<i>Perceptrons</i>	Minsky and Papert [minsky69]
1982	Autoassociation	Hopfield [hopf82]
1982	Parallel Distributed Processing	Feldman, et.al. [feld82]
1983	Boltzman Machine	Hinton [hinton83]
1985	Back Propagation	Rumelhart, et.al. [mcc86a]
1990	i80170NX Chip	Intel Corporation

Table 10.1 A few key historical developments in neural net research.

There are four main points to be taken from table 10.1: (1) The first serious work on neural nets dates back to 1943, so that while neural nets have been getting increasingly more press in recent years, it cannot be said that they are of "recent origin." (2) There is a thirteen year gap between the publication of Minsky and Papert's enormously influential book called *Perceptrons* in 1969 and the publication of a mainstream neural net physics paper by Hopfield in 1982, emphasizing the idea of memories as dynamically stable attractor states. This is not necessarily meant to imply that neural net research had not been going on in the intervening years (see, for example, [kohon74], [mals73], and [grossb76a]), but it is certainly true to say that Minsky and Papert's powerful critique discouraged more than few researchers from entering the (at that time) fledgling field. (3) Long stretches of time sometimes pass between the introduction of a basic design and when that

design gains a more practical utility with a concomitant learning rule. For example, while it was known fairly early on that some of the limitations of Rosenblatt's simple perceptron could be overcome by adding "hidden" neurons, it was not until Rumelhart, *et.al.*'s backpropagation rule was introduced in 1985 that an appropriate learning rule was finally found. (4) Just as for CA studies in general, for which software emulations are nice to have for prototyping and preliminary study but are clearly inadequate for any large-scale simulation – lattice gases, for example, would have remained nothing more than an interesting theoretical exercise had it not been for dedicated simulators like RAP1 and CAM-6 – neural nets do not really come into their own as *problem solvers* unless their designs are hard wired into silicon. The Intel chip listed in table 10.1 is but one example of a growing number of increasingly more powerful and fully programmable chips appearing on the commercial market.

10.2 Biological Origins

The human brain is a neural net consisting of about ten billion interconnected neurons. Figure 10.1-a shows a schematic representation of a single neuron. At the risk of grossly oversimplifying the brain's enormously complex physiology, we will only focus on a relatively few functional parts of a single neuron.

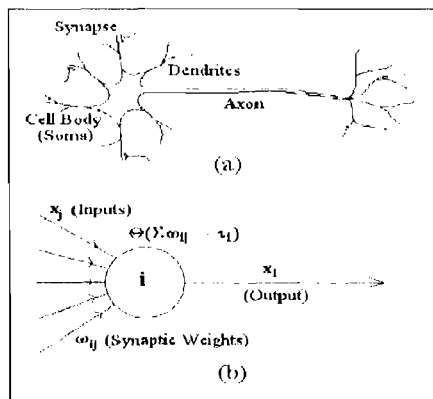


Fig. 10.1 Schematic representations of (a) a biological neuron, and (b) a McCulloch-Pitts artificial neuron.

Tree like networks of nerve fiber called *dendrites* protrude outward from the neuron's cell body, or *soma*. Extending outward from the soma is also a long fiber called the *axon* that itself eventually branches out into a set of strands and sub strands. At the ends of these strands are the transmitting ends of communication junctions between nerve fibers called *synapses*. The receiving ends of these junctions exist both on dendrites and on the somas themselves. Each neuron is typically connected to several thousand other neurons.

The actual transmission of signals across a synaptic junction is a complicated chemical process that depends on a release of a neurotransmitter from the trans-

mitting end of a synapse. The neurotransmitter either raises or lowers the electrical potential inside the soma of the receiving neuron. If the electrical potential exceeds a certain threshold, a signal, or *action potential*, is transmitted down the axon. When this happens, the neuron is said to have “fired.” The action potential then branches out via synapses into the adjoining neurons. After each neuron “fires,” it must wait for a period of time called the *refractory period* (~ 1 msec) before it is able to fire again.

10.3 McCulloch and Pitts

The first simple model of a neuron was proposed by McCulloch and Pitts in 1943 [mccul43]; see figure 10.1-b. Abstracting the complex dynamics of real neurons, their idea was to pattern a neuron after a simple activation process and thus model it as a *binary threshold automaton*. That is to say, as a simple local processor that computes the weighted sum of the inputs from its neighbors and outputs either the value 1 (i.e. when “firing”) or 0 (when “not firing”), depending on whether the sum exceeds a certain threshold:

$$x_i(t+1) = \Theta\left(\sum_j w_{ij}x_j(t) - \tau_i\right), \quad (10.1)$$

where $x_i(t) \in \{0, 1\}$ is the value of the i^{th} neuron at time ‘ t ’, $\{w_{ij}\}$ is the set of synaptic weights, each of which can be either positive or negative depending on whether a given synapse is *excitatory* or *inhibitory* ($w_{ij} = 0$ if no synapse exists between neurons ‘ i ’ and ‘ j ’), τ_i is the threshold value for the i^{th} neuron, and $\Theta(x)$ is the unit step function:

$$\Theta(x) = \begin{cases} 1 & \text{if } x \geq 0, \\ 0 & \text{else.} \end{cases} \quad (10.2)$$

Now, to be sure, McCulloch-Pitts neurons are unrealistically rendered versions of the real thing. For example, the assumption that neuronal “firing” occurs synchronously throughout the net at well defined discrete points in time is simply wrong. The tacit assumption that the structure of a neural net (i.e. its connectivity, as defined by the set of synaptic weights) remains constant over time is known to be false as well. Moreover, while the input-output relationship for real neurons is nonlinear, real neurons are not the simple threshold devices the McCulloch-Pitts model assumes them to be. In fact, the output of a real neuron depends on its weighted input in a nonlinear but *continuous* manner. Despite their conceptual drawbacks, however, McCulloch-Pitts neurons are nontrivial devices. McCulloch-Pitts were able to show that for a suitably chosen set of synaptic weights $\{w_{ij}\}$, a synchronous net of their model neurons is *capable of universal computation*. This means that, in principle, McCulloch-Pitts nets possess the same raw computational power as a conventional computer (see section 6.4).

While nets composed of McCulloch-Pitts neurons are therefore potentially powerful computational devices,[†] one fatal drawback of the basic model is that it does not include any mechanism analogous to *learning*. In McCulloch-Pitts nets, the weights are fixed from the start and the computation itself depends on specifying the initial state of neuronal values and carrying out the dynamics defined in equation 10.2. In contrast, biological brains, as we all know, are not born pre-programmed, but somehow learn over a period of time. The first suggestion of how learning itself might be modeled was made by Hebb in 1949 [hebb49].

10.4 Hebbian Learning Rule

Based upon his studies of real neuronal systems, Hebb [hebb49] proposed the notion that learning takes place via modifications made to the set of synaptic weights. He suggested that a repeated series of activations of one neuron by another through a given synapse gradually increases its conductance and thereby strengthens the neuronal “connection.” In other words, *active connections are reinforced*. Groups of neurons that are synchronously and repeatedly activated therefore tend to form more strongly connected clusters than others whose mutual activation follows only a weakly correlated pattern. While Hebb himself went no further than making this suggestion – he did not go so far as to introduce a formal mathematical model for his learning rule – his proposal nonetheless proved to be enormously influential and spawned considerable subsequent activity to understand and model learning in neural nets. The learning rules for simple Perceptrons and Hopfield nets, discussed below, are both motivated by Hebb’s original suggestion.

10.5 Perceptrons

An important early pioneer in the formal analysis of neural nets (as well as their simulation on digital computers) was Frank Rosenblatt ([rosenbl58], [rosenbl62]). Driven by a desire to “understand the capability of higher organisms for perceptual recognition, generalization, recall and thinking...” [rosenbl58], Rosenblatt introduced a model net composed of McCulloch-Pitts neurons that he called the *Perceptron*. Believing that the synaptic connectivities in real biological nets contain a strong random element, Rosenblatt departed from the McCulloch-Pitts formulation by insisting that a probabilistic description is a more appropriate language to use to describe the behavior of neural nets than symbolic logic.

Consider a particular model of a perceptron called the *photoreceptor*, used to respond to optical patterns, shown schematically in figure 10.2.

The photoreceptor consists of three basic parts: (1) the *retina*, which is made

[†]von Neumann himself showed how to use such nets to reliably carry out conventional arithmetic calculations [vonN63]. He was driven by the problem of how to implement the theoretical design in practice, where one demands that a net continues to function correctly even when one or more of its components malfunction.

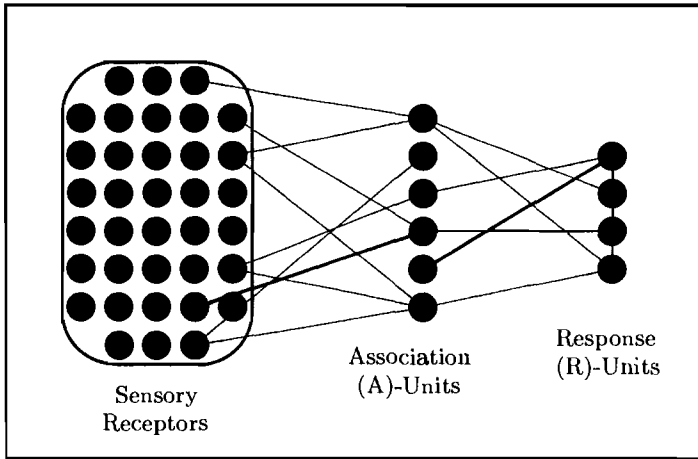


Fig. 10.2 Schematic representation of connections in Rosenblatt's *Photorecptron* [rosenbl58]. The synaptic connections from the S-units to A-units can be either excitatory or inhibitory; connections between A-units and R-units may include inhibitory feedback loops. Response layer units are also linked to other R-units with inhibitory connections.

up of sensory receptors (or S units); (2) a set of *association* (or A) units; and (3) a set of *response* (or R) units. Rosenblatt's idea was to use photorecptrons as devices to *classify patterns* appearing on the retina according to categories defined by the number of excited R-units. Assuming that similar patterns excite roughly the same set of R-units, the response can be taken as a measure of "similarity."

The units of the photorecptron are all McCulloch-Pitts-like threshold logic units. Each S-unit responds to input sensory data in an all-or-nothing manner, transmitting impulses to A-units via connections that are either excitatory or inhibitory. Each A-unit is connected to a random set of S-units called their *origin points*. If the weighted sum of excitatory and inhibitory impulses exceeds a threshold τ of the A-unit, the A-unit fires (in an all-or-nothing manner) an impulse that is sent to the R-unit layer. The R-units, in turn, likewise fire only when a weighted sum of their inputs from a *source set* of A-units exceeds some threshold. Unlike the strictly one-way connectivities between A-units and their set of origin points, however, R-units have two additional feedback links: (1) inhibitory feedback connections with the complement of their A-unit source sets (in order to inhibit activity in any A-units that do not transmit to them), and (2) inhibitory connections with other R-units.

Notice that the only real "dynamics" going on here takes place between the A-units and R-units. The dynamical flow of information proceeds directly from input to output layers with no "hidden" units. We will follow the convention of calling perceptron models that have only input and output layers *simple perceptrons*. As we will shortly see, the absence of a hidden layer dramatically curtails the simple perceptron's problem solving ability.

10.5.1 Learning Rule

To find an appropriate learning rule, we take our cue from Hebb's idea of only reinforcing active connections (see above). Generalizing this notion to include the possibility of both strengthening and weakening connections to inhibit incorrect decisions, one possible learning scheme is to adjust the weights according to:

$$w_i(t+1) = \begin{cases} w_i(t) & \text{if R-unit response is correct,} \\ w_i(t) + \eta x_i & \text{if R-unit response is 0 and should be 1,} \\ w_i(t) - \eta x_i & \text{if R-unit response is 1 and should be 0,} \end{cases} \quad (10.3)$$

where $0 \leq \eta \leq 1$ is a *learning constant* that controls the learning rate. With this rule, the weights remain unchanged either when the perceptron makes a correct decision, or, for a given input i , when the input does not contribute to an incorrect response (since in this case $x_i = 0$).

Other rules are of course possible. One popular choice called the *Delta Rule* was introduced in 1960 by Widrow and Hoff ([widrow60], [widrow62]). Their idea was to adjust the weights in proportion to the "error" ($= \Delta$) between the desired output ($= D(t)$) and the actual output ($= y(t)$) of the perceptron:

$$w_i(t+1) = w_i(t) + \eta \Delta x_i(t), \quad (10.4)$$

where $\Delta \equiv D(t) - y(t)$ and η is the learning constant defined in equation 10.3. Notice that if the actual output is 0 and the desired output is 1, then $\Delta = +1$ and the weights are increased. On the other hand, if the actual output is 1 and the desired output is 0, then $\Delta = -1$ and the weights are decreased. If the perceptron makes the correct decision, the weights remain unchanged. Perceptrons operating with this rule were called ADALINES.[†] We will have more to say about an important variant of this rule called the *least mean square* (LMS) algorithm ([widrow62], [widrow90]) – which attempts to minimize the mean square error between the desired output and the actual output – when we discuss multi-layered perceptrons later on in this chapter.

To summarize, the simple perceptron learning algorithm consists of the following four steps:

Pseudo-Code Implementation of Perceptron Learning Algorithm:

Step 1: Initialize weights $w_i(t=0)$ to be small random values and choose the threshold τ .

Step 2: Present the input values $x_0, x_1, \dots, x_n$.

[†]ADALINE was originally an acronym for *ADaptive LInear Neuron*, but was changed to *ADaptive LInear Element* after interest in neural net research tapered out in the late 1960s. Widrow also introduced the MADALINE (an acronym for *Many ADALINES*), which was essentially a multi-layered net consisting of many connected ADALINES. The MADALINE, in particular, continues to be a useful tool for adaptive nulling of radar jamming and as an adaptive echo canceler in telephone lines.

Step 3: Calculate the perceptron's output

$$y(t) = \Theta\left(\sum_i w_i(t)x_i(t) - \tau\right),$$

where $\Theta(x)$ is defined in equation 10.2.

Step 4: Adjust the synaptic weights according to either of the two learning rules given in equations 10.3 and 10.4.

Being able to define a reasonable looking learning rule, of course, does not guarantee us that we will be able to solve for anything interesting using it. We would like to know the answer to the following question: *given an arbitrary set of input patterns, can we always be assured of finding a perceptron capable of separating out the different pattern classes?*

The partial answer to this question was given by Rosenblatt himself in his *perceptron convergence theorem* [rosenbl58]. The theorem states essentially that if the given pattern classes are separable by the perceptron, then the algorithm outlined above is guaranteed to converge to that separation in a finite number of steps. The full (and, as it turned out, the *fully disappointing*) answer was given years later by Minsky and Papert in their enormously influential book *Perceptrons: An Introduction to Computational Geometry* ([minsky69], [minsky88]). In a series of simple and elegant geometrical arguments, Minsky and Papert demonstrated that perceptrons are in fact fundamentally limited to solving only those sets of problems that are *linearly separable*.

10.5.2 Linear Separability: the XOR Problem

To see what we mean by linear separability, we consider a simple problem that is *not* linearly separable: the so-called XOR problem – to teach a neural net the exclusive-OR function (table 10.2).

x_1	x_2	$x_1 \text{ XOR } x_2$
0	0	0
0	1	1
1	0	1
1	1	0

Table 10.2 The XOR (exclusive-OR) function.

An appropriate perceptron model for this problem is one that has two input neurons (corresponding to inputs x_1 and x_2) and one output neuron, whose value

y given by

$$y = \begin{cases} 1 & \text{if } w_1x_1 + w_2x_2 \geq \tau, \\ 0 & \text{else,} \end{cases} \quad (10.5)$$

where w_1 and w_2 are synaptic weights and τ is some threshold. The problem is to choose values for w_1 and w_2 such that $y = x_1 \text{ XOR } x_2$. As we now show, however, this cannot be done.

Consider the equation $\tau = w_1x_1 + w_2x_2$, which we recognize as being an equation of a straight line in the (x_1, x_2) plane. Figure 10.3 shows this line along with the four points $(0,0)$, $(1,0)$, $(0,1)$, $(1,1)$ corresponding to the four input vectors in table 10.2. If we think of these four points as representing four distinct regions of the plane corresponding to each of four correct outputs for points in those regions, we see that the perceptron is really tasked with the problem of separating these four regions out of the plane. But since a straight line can separate a planar region into only two distinct regions, it clearly does not suffice to perform the required separation. Rosenblatt's perceptron is thus incapable of learning the simple XOR function precisely because this problem is not *linearly separable*. The reader can easily verify that the analogous problem of learning the Boolean AND function (which is separable) is easily handled by a simple perceptron.[†]

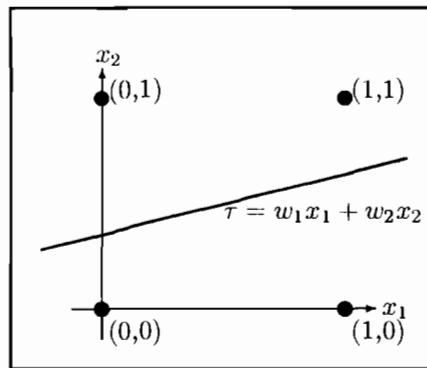


Fig. 10.3 The four points $(0,0)$, $(1,0)$, $(0,1)$, $(1,1)$ corresponding to the input vectors for the XOR problem (see table 10.2). Note how the line $\tau = w_1x_1 + w_2x_2$ divides the plane into only two regions and is thus unable to isolate the points $(0,0)$ and $(1,1)$ from the points $(0,1)$ and $(1,0)$.

In the more general case when there are N input neurons, the space of the x_i 's

[†]It is left as an exercise for the reader to show that the ratio of linearly separable Boolean functions with N arguments ($= N_L$) to the total number of Boolean functions ($= N_B = 2^{2^N}$) is given by $N_L/N_B = (2^{N^2+1}/N!)N_B^{-1} \rightarrow 0$ as $N \rightarrow \infty$. In other words, the set of linearly separable Boolean functions is a set of measure zero.

is divided into two regions defined by the *hyperplanes* determined by the equation

$$\tau = \sum_i w_i x_i. \quad (10.6)$$

Three-dimensional space, for example, would be divided into two regions by a two-dimensional plane.

We emphasize that the simple perceptron's inability to learn the XOR function is *not* just a small shortcoming. Many geometrical recognition problems – such as the recognition of the “connectedness” of figures, as first pointed out by Minsky and Papert [minsky69] – *depend* on the XOR function. The fact that simple perceptrons are not up to the task immediately renders them dysfunctional as far as the general pattern recognition problem is concerned.

A natural question to ask is whether the basic model can be modified in some way that would enable it to correctly learn the XOR function or, more generally, any other non-linearly-separable problem. The answer is a qualified yes: in principle, all that needs to be done is to add more layers between what we have called the A-units and R-units. Doing so effectively generates more “separation lines,” which when combined can successfully separate out the desired regions of the plane. However, while Rosenblatt himself considered such variants, at the time of his original analysis (and for quite a few years after that; see below) no appropriate learning rule was known.

To say that Minsky and Papert's stinging, but not wholly undeserved, criticism of the capabilities of simple perceptrons was taken hard by perceptron researchers, would be an understatement. They were completely correct in their assessment of the limited abilities of simple perceptrons; and they were correct in pointing out that XOR-like problems require perceptrons with more than one decision layer. Where Minsky and Papert erred – and erred strongly – was in their conclusion that since no learning rule for multi-layered nets was then known *and will never be found*, perceptrons represent a dead end field of research.[‡]

Whether it was a direct result of Minsky and Papert's book, or in combination with the unrealistically high hopes for and exaggerated claims about the capabilities of early models, the fact remains that it took fully 17 years following the publication of *Perceptrons* until perceptrons were once again seriously considered viable research tools. During this interval, perceptron research was indeed effectively dead. It was only following the publication of Rumelhart and McClelland's text on parallel distributed processing in 1986 [mcc86a], in which they formally reintroduced the perceptron in a multi-layered configuration and added a powerful new learning rule, that researchers finally came flocking back into the field. Multi-layered nets using back-propagation synaptic weight learning, are today one of the most widely used

[‡]Minsky and Papert also made a second, and more subtly forceful, indictment that probably remains as valid today as it was back in 1969. They cautioned against assuming that “toy” (or small scale) models can always be scaled upwards to deal with larger sized real-world problems. Even if a toy model is “solved” correctly by some appropriate perceptron, there is absolutely no guarantee that there exists another larger perceptron that will be able to solve larger problems. This basic concern remains an issue to this day.

variants of what are broadly classed as neural networks. We will discuss multi-layered perceptrons in a later section.

10.6 The Hopfield Model

While, as mentioned at the close of the last section, it took more than 15 years following Minsky and Papert's criticism of simple perceptrons for a bona-fide multi-layered variant to finally emerge (see *Multi-layered Perceptrons* below), the man most responsible for bringing respectability back to neural net research was the physicist John J. Hopfield, with the publication of his landmark 1982 paper entitled *Neural networks and physical systems with emergent collective computational abilities* [hopf82]. To set the stage for our discussion of Hopfield nets, we first pause to introduce the notion of *associative memory*.

10.6.1 Associative Memory

Consider the basic problem of how information is distributed throughout a system, and the manner in which it is retrieved. We know that in a conventional computer, for example, information is stored in *random-access memory* (RAM). This means that the memory address of where the information actually exists and the information itself are uncorrelated. In order to retrieve the information, one must know its address *exactly*, as even the slightest error renders that information effectively unretrievable. In particular, it is in general impossible to retrieve RAM data if armed only with a partial knowledge of its address. In contrast, *associative memories* (sometimes also called *content-addressable memories*), much like the form of memory believed to be used by human brains,[†] are such that they can be completely retrieved even when searched for with partial information.

Hopfield's neural net model addressed the basic associative memory problem [hopf82]: *Given some set of patterns $\{\mathcal{P}_i\}$, construct a neural net such that when it is presented with an arbitrary pattern $\mathcal{P}^*$, not necessarily an element of the given set, it responds with a pattern from the given set that most closely "resembles" the presented pattern.*

Figure 10.4 shows a schematic representation of how Hopfield's net effectively partitions the phase space into disjoint basins of attraction, the attractor states of which represent some desired set of stored patterns.

While the solution to this problem can be trivially solved by a conventional serial computer program, of course – by say computing the Hamming distance[‡]

[†]This seemingly intuitive notion of having information distributed throughout an assemblage of brain cells vice having it encoded in a localized subset (sometimes called "grandmother cells") was at one time the subject of intense debate. (The "grandmother" part pays homage to the custom followed by proponents of this model to use "grandmother" in an argument of the form, "one recognizes one's grandmother because of a certain set of neurons that fire only when one encounters one's grandmother." The moniker has stuck.)

[‡]Recall that the *Hamming distance* between two bit strings is equal to the number of bits by which

between two test patterns – the challenge is to find a way to solve the problem using McCulloch-Pitts neurons. Specifically, the problem is to find an appropriate synaptic-weight set $\{w_{ij}\}$ such that by first encoding a test pattern $\mathcal{P}^*$ by assigning values to each neuron of a suitably sized McCulloch-Pitts net, the net evolves into the one pattern in the original set of patterns $\{\mathcal{P}\}$ that is closest to it.

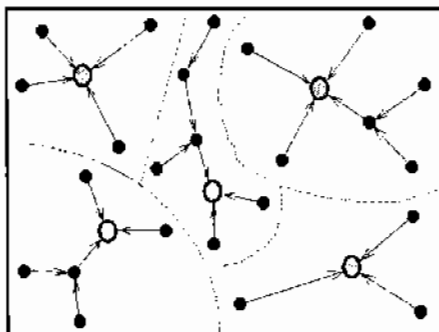


Fig. 10.4 Basins of attraction in the partitioned phase space of a Hopfield neural net.

While the dynamics of Hopfield nets may be simple – we will shortly see, for example, that their attractors consist only of fixed points – they are important for several reasons: (1) Their introduction was in large part responsible for reviving an interest in fundamental neural net research following Minsky and Papert's scathing indictment of the capabilities of simple perceptrons (see above). (2) Hopfield was the first to make the interesting connection between memories and dynamical attractors. (3) By introducing an *energy function* as a primary means of analysis, Hopfield forged a relationship between neural nets and the physics of *spin glasses*.

Recall that spin glasses are magnetic materials in which the interactions among the constituent magnetic moments, or spins, is random ([sherr75]; see section 5.5). Such systems are characterized chiefly by *frustration*, wherein conflicting constraints make it impossible to simultaneously minimize pair-interaction energies.[†] Because the form of the much studied spin glass energy function is essentially the same as that used by Hopfield for his neural net analysis, Hopfield effectively opened up a bridge between two research communities that theretofore had little if anything to say to one another, namely computer scientists and physicists.

they differ.

[†]The relationship between neuronal dynamics and spin magnetic systems actually dates back to 1954 to an idea first proposed by Cragg and Temperley [cragg54]. They compared the “up” and “down” states of a spin on a lattice to either “active” or “inactive” neurons in a neural net. Cragg and Temperley went on to suggest that (1) neural nets should display patches of active or inactive neurons analogous to ferromagnetic domain patterns (i.e. lattice patches of “up” or “down” spins), and (2) as long as neural domain patterns are stable with respect to small random perturbations, they can be used as a form of *memory* [cragg55].

10.6.2 The Model

Hopfield's model consists of a fully-connected, symmetrically-weighted ($w_{ij} = w_{ji}$) McCulloch- Pitts neural net where the value of the i^{th} neuron is updated according to:

$$S_i(t+1) = \text{sgn} \left(\sum_j w_{ij} S_j(t) - \tau_i \right), \quad (10.7)$$

where we have used *bipolar* variables $S_i \in \{+1, -1\}$ instead of binary variables to simplify some of the subsequent equations,[†] τ_i is the required threshold value for the i^{th} neuron, and $\text{sgn}(x)$ is the *sign* function:

$$\text{sgn}(x) = \begin{cases} +1 & \text{if } x \geq 0, \\ -1 & \text{else.} \end{cases} \quad (10.8)$$

It is important to have a symmetric synaptic weight matrix, since even a small deviation away from this symmetry can often make the net *unstable* and therefore unable to settle into a required set of patterns. While it is true that a symmetric weight set $w_{ij} = w_{ji}$ is *neurophysiologically unjustified*, remember that the Hopfield model that we are now discussing is studied more for its historical significance than either its biological realism or practicality.

In equation 10.7, the neuronal site variables $S_i(t)$ can be updated either *synchronously*, where each neuron is simultaneously updated throughout the net, or *asynchronously*, where at each time step only one randomly chosen neuron is updated. While the first choice has the virtue of more closely resembling a conventional CA dynamical updating scheme, the second choice is more physically realistic insofar as the brain does not have an internal clock to synchronize the dynamics of its neurons. In practice, while the two updating schemes produce slightly different behavior, the general behavioral characteristics of the net are the same.

We now need to define the set of symmetric weights, $w_{ij} = w_{ji}$. Given that we want our net to act as a content-associative memory, this set of weights must satisfy two conditions: (1) if the net is presented with a pattern in the stored set, that set of encoded neuronal values representing that stored pattern should remain unchanged – i.e. stored patterns must be stable; (2) if the net is presented with a pattern *not* in the stored set, the net should evolve according to equation 10.7 to the pattern that is closest to it.

[†]One could easily replace the S_i variables by the binary variables $x_i \in \{0,1\}$ by making the substitution $x_i = \frac{1}{2}(S_i + 1)$.

10.6.3 Energy Function

As mentioned above, Hopfield's original approach to this problem was to introduce an *energy function* reminiscent of a spin-glass Hamiltonian:

$$\mathcal{E}[\{S_i(t)\}] = -\frac{1}{2} \sum_{ij} w_{ij} S_i(t) S_j(t) + \sum_i S_i(t) \tau_i. \quad (10.9)$$

In the double sum over indices '*i*' and '*j*,' we assume that $w_{ii} = 0$ for all '*i*.' We could also take $w_{ii} = 1$ but this would simply add a constant term to $\mathcal{E}$.

Figure 10.5 shows what a typical energy "landscape" looks like. It is characterized mainly by the presence of many large and small "hills" and "valleys." The idea will be to exploit this bumpy surface by positioning the desired patterns at the surface's lowest points and evolving to those points from an arbitrary starting configuration by continually decreasing the energy; i.e. *by rolling down the hills*.

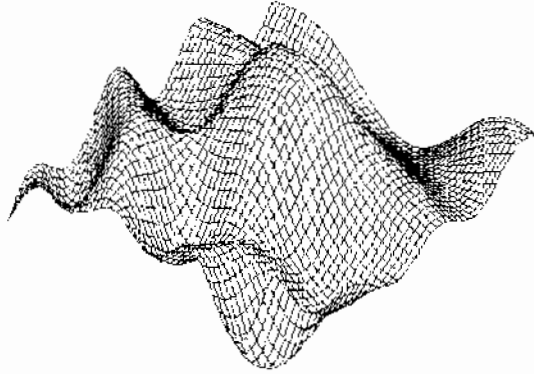


Fig. 10.5. A sample energy landscape.

To see that this is a reasonable approach to take, we look more closely at equation 10.9. It is easy to show that the energy function is in fact a *Lyapunov Function*.[†] In particular, as the neural net evolves according to the dynamics specified by equation 10.7, $\mathcal{E}$ itself either *remains constant* or *decreases*. The attractors of the system therefore reside at the local minima of the energy surface.

To show that $\mathcal{E}$ is a Lyapunov function, we assume that the net evolves asynchronously and calculate the explicit change in $\mathcal{E}$ that is induced by a change in the i^{th} neuron:

$$\begin{aligned} \Delta \mathcal{E}_i &= \mathcal{E}[\{S_i(t+1)\}] - \mathcal{E}[\{S_i(t)\}], \\ &= - \left[\frac{1}{2} \sum_j (w_{ij} + w_{ji}) S_j(t) - \tau_i \right] (S_i(t+1) - S_i(t)), \\ &= -\eta_i S_i(t+1) \left[\frac{1}{2} \sum_j (w_{ij} + w_{ji}) S_j(t) - \tau_i \right], \end{aligned} \quad (10.10)$$

[†]Lyapunov functions are discussed in section 5.5.

where

$$\eta_i = \begin{cases} 0 & \text{if } S_i(t+1) = +S_i(t), \\ 2 & \text{if } S_i(t+1) = -S_i(t), \end{cases} \quad (10.11)$$

and we have used the fact that $S_j(t+1) = S_j(t)$ for all $j \neq i$. We have also purposely left the weight set w_{ij} arbitrary for the moment.

Left in this form, equation 10.10 shows that if the weight set is completely anti-symmetric ($w_{ij} = -w_{ji}$), then $\Delta\mathcal{E}_i \equiv 0$ and the energy function is rendered essentially useless. On the other hand, if we assume weight set is symmetric, then we have that

$$\Delta\mathcal{E}_i = -\eta_i S_i(t+1) \left[\sum_j w_{ij} S_j(t) - \tau_i \right]. \quad (10.12)$$

Since, from equation 10.7 we know that

$$\left(\sum_j w_{ij} S_j(t) - \tau_i \right) S_i(t+1) \geq 0, \quad (10.13)$$

and, from equation 10.11 that η_i is nonnegative, we conclude that $\mathcal{E}$ is a non-increasing function of time:

$$\Delta\mathcal{E}_i \leq 0. \quad (10.14)$$

We thus see that when the energy reaches its lower bound, $\eta_i = 0$ and $S_i(t+1) = S_i(t)$ for all ' i ,' i.e. the asymptotic state of a symmetric, fully connected Hopfield net consists of *fixed points*. The reader may have anticipated this result by recalling our discussion of Lyapunov functions and threshold CA rules in section 5.5. Since Hopfield nets evolve dynamically under a generalized threshold rule, our earlier discussion of the orbits of generalized threshold rules applies. In particular, in section 5.5.1, we showed that generalized threshold rules iterated in *parallel* lead to either fixed points or cycles of period two [goles87a]. Not coincidentally, the tool used in that earlier section was also a Lyapunov function and the argument given there closely parallels the one given above. The excellent book by Goles and Martinez [goles90] discusses many more applications of Lyapunov functions to generalized threshold and multi-threshold functions.

10.6.4 Learning Rule

Having shown that the energy function $\mathcal{E}$ (equation 10.9) is a Lyapunov function, let us go back to the main problem with which we started this section, namely to find an appropriate set of synaptic weights. Using the results of the above discussion, we know that we need to have the desired set of patterns occupy the minimum points on the energy surface. We also need to be careful not to destroy any previously stored patterns when we add new ones to our net. Our task is therefore to find a

set of weights $\{w_{ij}\}$ such that for a given pattern $\mathcal{P}_i$ encoded with a set of neuronal values $\{S_1^{(\mathcal{P}_i)}, S_1^{(\mathcal{P}_i)}, \dots, S_N^{(\mathcal{P}_i)}\}$, the energy function $\mathcal{E}$ is minimized.

We begin again with the energy function:

$$\mathcal{E}[\{S_i\}] = -\frac{1}{2} \sum_{ij} w_{ij} S_i S_j + \sum_i S_i \tau_i. \quad (10.15)$$

We would like each term to be negative. In particular, we would like the second term $\sum_i S_i \tau_i$ to be negative. We could choose a set of thresholds such that the threshold at each site has the opposite sign of the value of that particular neuron. Having done so for pattern $\mathcal{P}_1$, however, does not guarantee that $\sum_i S_i^{(\mathcal{P}_2)} \tau_i$ will be negative for some other pattern $\mathcal{P}_2 \neq \mathcal{P}_1$. A better choice would be to simply set all of the different thresholds to zero. In this case, the threshold term will neither increase nor decrease the energy function for any of the stored patterns, and we can focus our attention on the first term.

Let us now rewrite expression 10.15 by considering separately the contribution made to the weight set by all of the stored patterns except for the k^{th} one ($= w'_{ij}$) and the contribution made by the k^{th} pattern alone ($= w_{ij}^{(k)}$):

$$\begin{aligned} \mathcal{E} &= -\frac{1}{2} \sum_{ij} w'_{ij} S_i S_j - \frac{1}{2} \sum_{ij} w_{ij}^{(k)} S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)}, \\ &= \mathcal{E}' + \mathcal{E}^{(k)}. \end{aligned} \quad (10.16)$$

Since we want to minimize $\mathcal{E}$ for each pattern $\mathcal{P}$ in the set of patterns $\{\mathcal{P}_1, \mathcal{P}_2, \dots, \mathcal{P}_n\}$, for each pattern $\mathcal{P}_k$ we want to make the term

$$\mathcal{E}^{(k)} = -\frac{1}{2} \sum_{ij} w_{ij}^{(k)} S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)} \quad (10.17)$$

as small as possible. Note that whenever we are explicitly considering the k^{th} pattern, the first term, $\mathcal{E}'$, amounts to being essentially a “noise” term with some fixed value.

Now, making $-\frac{1}{2} \sum_{ij} w_{ij}^{(k)} S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)}$ as small as possible amounts to making $\sum_{ij} w_{ij}^{(k)} S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)}$ as large as possible. Since S_i^2 is always positive, we can be assured of having $w_{ij}^{(k)} S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)} > 0$ if we make each term dependent on $|S_i^{(\mathcal{P}_k)}|^2 |S_j^{(\mathcal{P}_k)}|^2$, or by setting

$$\sum_{ij} w_{ij}^{(k)} S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)} = \sum_{ij} [S_i^{(\mathcal{P}_k)}]^2 [S_j^{(\mathcal{P}_k)}]^2 \implies w_{ij}^{(k)} = S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)}. \quad (10.18)$$

Setting $w_{ij}^{(k)} = S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)}$ minimizes the energy function for the k^{th} stored pattern. In order to obtain the set of weights that minimizes $\mathcal{E}$ for the entire set of patterns. Summing over all patterns and adding a normalization factor N^{-1} , where

N is the size of the net, we have:

$$w_{ij} = \frac{1}{N} \sum_{k=1}^n w_{ij}^{(k)} = \frac{1}{N} \sum_{k=1}^n S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)}. \quad (10.19)$$

This is sometimes called the *Hebb Rule*, as a reminder of its similarity to the learning scheme first proposed by Hebb [hebb49] (see above). Strictly speaking, the comparison is not an entirely valid one, of course. For example, while Hebb suggested that only those weights existing between *active* (i.e. “firing”) neurons get strengthened, the expression in equation 10.19 induces a positive weight change between two neurons even when neither of those two neurons is firing. Moreover, as the set of patterns increases, the Hebb rule can even convert an excitatory synaptic connection into an inhibitory one, which is neurophysiologically indefensible.[†]

10.6.5 *Spurious Attractors*

While we have shown that the Hebb rule (equation 10.19) yields the desired dynamical attractors at the local minima of the energy function (equation 10.9), we have not shown that these attractors are in fact the only ones possible in this system. In fact, they are not, and *spurious attractors* are also possible.

It is obvious, for example, that a reversal all of the neuronal values for a given state, $S_i \rightarrow -S_i$, leaves the energy unchanged and therefore also represents a local minimum. There are also stable *mixed states* that are not equal to any of the stored patterns but are linear combinations of an odd number of those patterns [amit85a]. For example, it is easy to show that any symmetric combination of three stored patterns is a stable state:

$$S_i^{(\text{mixed})} \propto \pm S_i^{(\mathcal{P}_1)} \pm S_i^{(\mathcal{P}_2)} \pm S_i^{(\mathcal{P}_3)}. \quad (10.20)$$

Finally, if there are a large number of stored patterns, there may enough mutual interference to give rise to local minima, or *metastable states* – sometimes also called *spin glass states* to emphasize the similarity between the formalisms of Hopfield nets and spin glasses – that are not correlated with any subset of the set of stored patterns [amit85b].

While these spurious states clearly detract from the Hopfield net’s ability to act as a perfect memory, there are ways of dealing with them. Using the metaphor of a ball rolling down the hills of the energy landscape (see figure 10.5), one way of preventing the ball of settling into local (non-optimal) solutions would be to imbue the ball with some amount of intrinsic (thermal) energy that allows it to randomly “jiggle” around in the potential wells and therefore at least have the chance of “jumping” out of local minima. A stochastic version of the Hopfield net and *Boltzman Machines* both take precisely this approach and are discussed briefly below.

[†]We should mention that it is possible to do away with some of the neurophysiological unreasonableness of equation 10.19; see [toul86] for example. We will not discuss these other variants of Hopfield’s basic model.

10.6.6 Memory Storage Capacity

An important practical question is, “How many patterns can a Hopfield net generally store?” Naively, one might think that the number of patterns might be some (possibly sizable) fraction of the 2^N different configuration states available to a size N net. Unfortunately, it turns out that as far as information storage devices go, Hopfield nets are not particularly useful, as it takes a relatively large sized net to hold a relatively small set of patterns. We give a heuristic feel for the magnitudes involved below (see [hertz91]). Rigorous analyses of the capacity of Hopfield nets are given by Abu-Mostafa and Jacques [abu85], McEliece, *et.al.* [mcel87] and Newman [newman88].

In order to make a crude estimate of a Hopfield net’s pattern storage capacity, consider first what it means for a given pattern to be *stable*. From equation 10.7, we see that a pattern $S_i^{(P_l)}$ is stable if

$$\text{sgn}(\mathcal{I}_i^{(P_l)}) = S_i^{(P_l)}, \quad \text{for all } i, \quad (10.21)$$

where $\mathcal{I}_i^{(P_l)}$ is the net input to the i^{th} neuron in the l^{th} pattern:

$$\mathcal{I}_i^{(P_l)} = \sum_j w_{ij} S_j^{(P_l)} = \frac{1}{N} \sum_j \sum_k S_i^{(P_k)} S_j^{(P_k)} S_j^{(P_l)}. \quad (10.22)$$

Let us now rewrite this expression for $\mathcal{I}_i^{(P_l)}$ by taking out of the double sum the term for $k = l$:

$$\mathcal{I}_i^{(P_l)} = S_i^{(P_l)} + \frac{1}{N} \sum_j \sum_{k \neq l} S_i^{(P_k)} S_j^{(P_k)} S_j^{(P_l)}. \quad (10.23)$$

From this we see that the l^{th} pattern is stable if the magnitude of the second term is *less than 1 for all i* , since, if this is so, equation 10.21 shows that the *sign* of $\mathcal{I}_i^{(P_l)}$ remains unchanged.

Now, consider the quantity $C_i^{(P_l)}$ obtained by multiplying this second term by the value $-S_i^{(P_l)}$:

$$C_i^{(P_l)} \equiv -S_i^{(P_l)} \frac{1}{N} \sum_j \sum_{k \neq l} S_i^{(P_k)} S_j^{(P_k)} S_j^{(P_l)}. \quad (10.24)$$

The stability of pattern l depends on the quantity $C_i^{(P_l)}$ in the following way. If $C_i^{(P_l)} < 0$, the second term in the expression for $\mathcal{I}_i^{(P_l)}$ in equation 10.23 has the same sign as $S_i^{(P_l)}$ and thus its stability is unimpaired. On the other hand, if $C_i^{(P_l)} > 1$, $\mathcal{I}_i^{(P_l)}$ changes sign and thus renders the i^{th} site of the l^{th} pattern unstable.

The storage capacity can now be estimated in two steps: (1) First, assume for simplicity that the set of stored patterns is completely random; that is, assume that for each pattern l and neuron i , the probability of having $S_i^{(P_l)} = +1$ is equal to the probability of having $S_i^{(P_l)} = -1$. Now, calculate the probability, P_{unstable} , that a

given site of the l^{th} pattern is unstable:

$$P_{\text{unstable}} = \text{probability } (C_i^{(\mathcal{P}_l)} > 1). \quad (10.25)$$

(2) Define some acceptable threshold probability for stability -- say $P_{\text{unstable}} < 0.01$ -- and solve for the maximum number of patterns, n_{max} , for which this threshold will not be exceeded.

From equation 10.24 we see that $C_i^{(\mathcal{P}_l)}$ is $1/N$ times the sum of $\sim Np$ independent random variables, each of which is equal to either $+1$ or -1 . $C_i^{(\mathcal{P}_l)}$ is thus equal to a binomial distribution with zero mean and variance $\sigma^2 = n/N$ [olkin80]. Assuming that both the size of the net, N , and the number of patterns n is large compared to 1, we can approximate the binomial distribution by a Gaussian distribution having the same mean and variance:

$$P_{\text{unstable}} = \frac{1}{\sqrt{2\pi}\sigma} \int_1^\infty e^{-x^2/(2\sigma^2)} dx = \frac{1}{2} \left[1 - \text{erf} \left(\sqrt{\frac{N}{2n}} \right) \right], \quad (10.26)$$

where $\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x e^{-x^2} dx$ is the *error function*. Solving this equation numerically for a desired stability threshold probability of 0.01, for example, we find that the maximum number of patterns, n_{max} , that can be stored before stability is impaired is $n_{\text{max}} \approx 0.15N$. In general, n_{max} increases linearly [hopf82]:

$$n_{\text{max}} \approx \alpha N, \quad \text{where } \alpha < 1. \quad (10.27)$$

If we are happy with a threshold of $P_{\text{unstable}} = 0.01$, this means that if we want to store a paltry 15 patterns, errors are likely to start appearing unless we use a Hopfield net with at least 100 nodes and $\binom{100}{2} = 9900$ weights. In fact, depending on how one defines the stability criterion, this size requirement can be even more stringent. For example, the above calculation estimates only the *initial stability* of patterns; that is to say, it estimates when the very first signs of instability are likely to appear? A more careful calculation would show that a Hopfield net's recall ability actually deteriorates very rapidly as soon as the maximal pattern capacity is exceeded. One could also require that the net be able to recall *all* of the stored patterns perfectly. In this case, one can show that [weis85]

$$n_{\text{max}} \approx \frac{N}{\log N}. \quad (10.28)$$

the 2^N different configurations can *a priori* be realized on a size N net, taking note of a computational time requirement that itself scales as N^2 , and realizing that even the relatively small number that a Hopfield net can remember is itself heavily constrained (its recall ability deteriorates rapidly as correlations between patterns increases), and it becomes very clear that Hopfield nets are far from being computational powerhouses. Moreover, since Hopfield nets use the same step-function thresholding as simple perceptrons, they suffer from exactly the same limitation

as simple perceptrons: they are no more powerful than *linear classifiers* (see section 10.5).

Pseudo-Code Implementation: The algorithm summarizing the operation of the Hopfield net is given below in pseudo-code.

Step 1: For a given set of patterns $\{\mathcal{P}_1, \mathcal{P}_2, \dots, \mathcal{P}_n\}$, where the i^{th} pattern is encoded by the neuronal values $\{S_1^{(\mathcal{P}_i)}, S_1^{(\mathcal{P}_i)}, \dots, S_N^{(\mathcal{P}_i)}\}$, define the synaptic-weight matrix

$$w_{ij} = w_{ji} = \begin{cases} \sum_{k=0}^n S_i^{(\mathcal{P}_k)} S_j^{(\mathcal{P}_k)} & i \neq j, \\ 0 & i = j, 0 \leq i, j \leq n. \end{cases}$$

Step 2: Initialize the net with the test (or unknown) pattern, $\mathcal{P}^*$:

$$S_i(t=0) = S_i^{\mathcal{P}^*}, \quad 0 \leq i \leq N-1.$$

Step 3: Iterate the update rule until the net converges:

$$S_i(t+1) = \text{sgn} \left(\sum_{j=0}^N w_{ij} S_j(t) \right).$$

Figure 10.6 shows an example of how a Hopfield net that has been trained to store the ten digits 0, 1, ..., 9 (encoded on a 5×9 grid consisting of the 45 neurons making up the net), can be used to retrieve the digit '6' from noisy input.

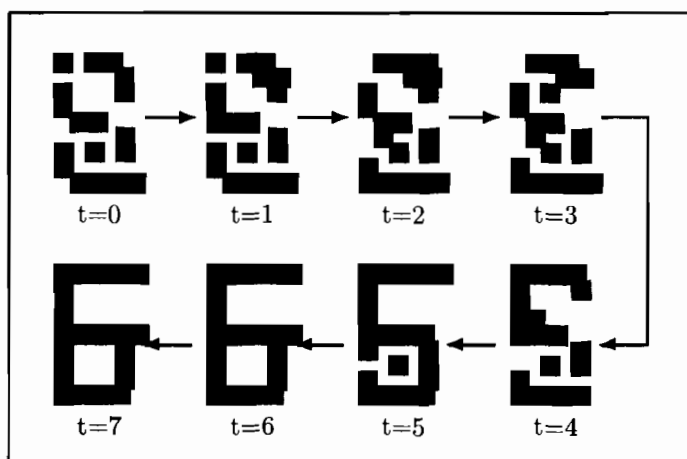


Fig. 10.6 A sample evolution of a noisy digit-6 input by a Hopfield net "trained" to remember the 10 basic digits.

10.6.7 Variants of the Basic Model

There are many variants of Hopfield's basic model, all of which are motivated by a desire to overcome its (sometimes severe) computational limitations. Hopfield himself, for example, was the first to suggest using continuous valued (or analog) vice discrete valued (or binary) neurons [hopf84]. As long as the synaptic weight matrix is symmetric, it can be shown that one can always define a Lyapunov function and the net evolves towards fixed points. It can be argued that, for both neurophysiological and technological reasons, analog neurons represent a more "natural" choice: neurophysiologically, because biological neurons are themselves analog devices; technologically, because real amplifiers have continuous transfer functions.

Hopfield and Tank ([hopf85], [hopf86a], [hopf86b]) showed how to use Hopfield nets to solve general combinatorial optimization problems, and argued that continuous valued variants are actually more useful for this purpose. The main idea is to identify the cost (or objective) function (such as the total path length in a traveling salesman problem) with the energy.

Kinzel ([kinz85a], [kinz85c]) "solved" the spurious state problem (see above) by exploiting the analogy between Hopfield nets and spin glasses. He reduced the number of spurious states by eliminating from the Hebbian learning rule all *frustrated connections*, or all those connections which receive both positive and negative contributions from different patterns). Unfortunately, this modification also reduces the Hopfield net's already poor memory storage capacity. Readers may recall that spin-glass attractor states are arranged in a hierarchical-like manner forming an *ultrametric space* [chowd86]. Parga and Virasoro [parg86] show how ultrametric patterns can be stored in Hopfield nets.

Personnaz, *et.al.* [pers86] modified the Hebbian learning rule so that even non-orthogonal states remain stable, but the modification effectively makes the learning rule a non-local one.

10.7 Stochastic Nets

In the previous section we discussed how a Hopfield net can sometimes converge to a local minimum that *does not* correspond to any of the desired stored patterns. The problem is that while the dynamics embodied by equation 10.7 steadily decreases the net's energy (equation 10.9), because of the general "bumpiness" of the energy landscape (see figure 10.5), whether or not such a steady decrease eventually lands the system at one of the desired minima depends entirely on where the system begins its descent, or on its initial state. There is certainly no general assurance that the system will evolve towards the desired minimum.

Using the metaphor of a ball rolling down the hills of the energy landscape, one way of preventing the ball of settling into metastable solutions is to imbue the ball with some amount of intrinsic, or thermal, energy that would allow it to randomly "jiggle" around in the potential wells and therefore have the chance of "jumping" out of local minima. We can do this formally by introducing a *pseudo-temperature*

T for the Hopfield net and replacing the deterministic threshold dynamics with a stochastic rule [hinton83]:

$$S_i(t+1) = \begin{cases} +1 & \text{with probability } p(e_i), \\ -1 & \text{with probability } 1 - p(e_i), \end{cases} \quad (10.29)$$

where

$$e_i = \sum_j w_{ij} S_j, \quad (10.30)$$

and

$$p(x) = \frac{1}{1 + e^{-2x/T}}. \quad (10.31)$$

We should stress that the temperature T has nothing to do with the real temperature of either a brain or neural circuit. Its sole purpose is to act as a control parameter regulating the amount of “noise” in the stochastic system.

The form of the stochastic transfer function $p(x)$ is shown in figure 10.7. Notice that the steepness of the function near $x = 0$ depends entirely on T . Notice also that this form approaches that of a simple threshold function as $T \rightarrow 0$, so that the deterministic Hopfield net may be recovered by taking the zero temperature limit of the stochastic system. While there are a variety of different forms for $p(x)$ satisfying this desired limiting property, any of which could also have been chosen, this sigmoid function is convenient because it allows us to analyze the system with tools borrowed from statistical mechanics.

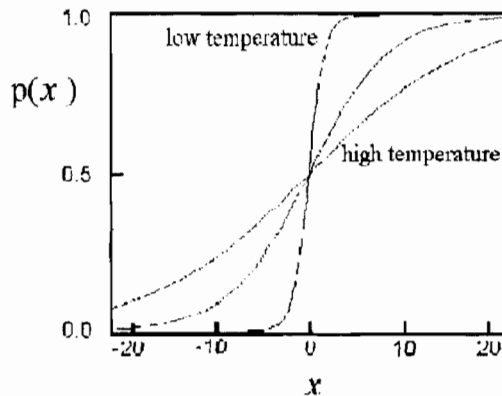


Fig. 10.7 A plot of the transition probability function $p(x) = [1 + \exp(-2x/T)]^{-1}$.

The main difference between looking at stochastic nets rather than their deterministic counterparts is stochastic nets force us to shift our focus of attention: since under a stochastic rule the same initial states generally evolve into different final states, we are in the stochastic case not so much interested in *the* final state of the

system as the average values of stable equilibrium states. It can be shown that any net that has an energy function eventually reaches equilibrium.

Using the fact that we have a well defined energy function (equation 10.9), we know from statistical mechanics that when the system has reached equilibrium, the probability that it is in some state $\vec{S} = (S_1, S_2, \dots, S_N)$ is given by the Boltzman distribution:

$$P(\vec{S}) = \frac{1}{Z} e^{-\mathcal{E}[\vec{S}]/T}, \quad (10.32)$$

where

$$Z = \sum_{\vec{S}} e^{-\mathcal{E}[\vec{S}]/T} \quad (10.33)$$

is a normalization constant called the *partition function* (see section 7.1).

We can then compute the average value ($= \langle \dots \rangle$) of any quantity $f(\vec{S})$ that is a function of the state $\vec{S}$ by computing

$$\langle f \rangle = \sum_{\vec{S}} P(\vec{S}) f(\vec{S}). \quad (10.34)$$

Let us restrict our attention for the moment to the case where the number of patterns $n \ll N$, and look at the system from a *mean-field* point of view (see section 7.1.6).

In the case of spins ($S_i = \pm 1$) on a lattice in statistical mechanics, the Ising Hamiltonian, $\mathcal{H}[\{\vec{S}\}]$, is given by

$$\mathcal{H}[\vec{S}] = - \sum_{(i,j)} J_{ij} S_i S_j, \quad (10.35)$$

where J_{ij} is the inter-spin coupling energy and we have assumed a zero external magnetic field. The total magnetic field acting on site ' i ' is equal to

$$H_i = \sum_j J_{ij} S_j. \quad (10.36)$$

The *mean-field approximation* consists of replacing H_i with its mean-field value H' , obtained by replacing the spins S_j with an average value $\langle S_i \rangle$:

$$H' = Jq \langle S \rangle, \quad (10.37)$$

where we have assumed that $\langle S_i \rangle = \langle S \rangle$ for all i , and $q = |\mathcal{N}|$ is the number of neighbors in each local neighborhood of i .

From equation 10.34 we immediately find that the average magnetization is

given implicitly by the solution to the equation manner:

$$\begin{aligned}
 m \equiv \langle S \rangle &= \frac{1}{Z} \sum_{S=\pm 1} S e^{H'/k_B T} = \frac{e^{H'/k_B T} - e^{-H'/k_B T}}{e^{H'/k_B T} + e^{-H'/k_B T}} \\
 &= \tanh\left(\frac{Jqm}{k_B T}\right),
 \end{aligned} \tag{10.38}$$

where k_B is Boltzman's constant.

Applying exactly the same reasoning to our stochastic net, but using equation 10.9 for the Hopfield energy in place of the Ising Hamiltonian, we obtain the analogous expression

$$\langle S_i \rangle = \tanh\left(\frac{1}{T} \sum_j w_{ij} \langle S_j \rangle\right). \tag{10.39}$$

Inserting the Hebb rule (equation 10.19) and guessing that $\langle S_i \rangle$ is proportional to a stored pattern

$$\langle S_i \rangle = m S_i^{(P)}, \tag{10.40}$$

one can show that [amit85a]

$$m = \tanh\left(\frac{m}{T}\right) \tag{10.41}$$

This tells us immediately that, just as for Ising spins, we have a “spontaneous magnetization” and that there is an effective phase transition for $T = 1$: stored patterns will only be stable for temperatures $T < 1$.[†]

Stochastic nets were first formally studied from this statistical mechanical point of view by Peretto [peret84] and Amit, Gutfreund and Sompolinsky [amit85a, amit85b] (see also [amit89]). Amit *et.al.* were the first to provide the complete phase space properties as a function of T in the more difficult case where the number of stored patterns $n \propto N$ and $N \rightarrow \infty$ limit. In particular, using the load parameter $\alpha \equiv n/N$, Amit *et.al.* found that at $T = 0$ there is a critical value of α , $\alpha_c \approx 0.138$, such that if $\alpha > \alpha_c$ all recall ability is lost. The same is qualitatively true for $T > 0$ but the value of α_c decreases with increasing T . Moreover, it can be shown that maintaining the system at higher temperatures is actually advantageous for doing away with some of the spurious states. For example, mixed states (see equation 10.20) disappear altogether for $0.46 < T < 1$, and only the desired patterns remain stable [hertz91].

[†]The value of T_c depends on the normalization constant for w_{ij} chosen in equation 10.19. What matters here is not the absolute value of T_c but the fact that it has some finite value.

10.8 Boltzman Machines

In the previous section we introduced a simple variant of the basic Hopfield model by replacing Hopfield's deterministic update rule (equation 10.7) with a stochastic one (equation 10.29-10.31). The motivation was to find a way to coax the deterministic system into avoiding getting trapped inside local minima. The stochastic rule was carefully chosen so that when the system reaches equilibrium at a temperature T the states are distributed according to the Boltzman distribution and can therefore be examined with tools borrowed from statistical mechanics. After initializing a system at some relatively high temperature T (high enough so that there is enough "thermal energy" to allow local minima states to be escaped), the remaining step is to find a way to coax the system back to near-zero temperatures. We want to do so because while higher temperatures are in some sense easier to work with (for example, equilibrium is reached relatively quickly at high temperatures), if the temperature is too high, the probability that the desired global minimum states appear is about the same as having undesirable states.

The *Boltzman Machine* generalizes the Hopfield model in two ways: (1) like the simple stochastic variant discussed above, it too substitutes a stochastic update rule for Hopfield's deterministic dynamics, and (2) it separates the neurons in the net into sets of *visible* and *hidden* units. Figure 10.8 shows a Boltzman Machine in which the "visible" neurons have been further subdivided into "input" and "output" sets.

A typical problem for a Boltzman Machine is to obtain a set of weights such that the states of the visible neurons take on some desired probability distribution. Since the Hebb rule (equation 10.19) makes no distinction between "visible" and "hidden" neurons, a new learning rule is needed. Such a rule -- which can be applied to *any* stochastic net that has a symmetric synaptic-weight set -- was first introduced by Hinton, Ackley and Sejnowski ([hinton83], [hinton86], [ackley85]). Conceptually, their new learning scheme combines Hopfield's *energy minimization* with an *entropy maximization* consistent with using the Boltzman distribution to describe state probabilities.

10.8.1 Simulated Annealing

The Boltzman Machine is gradually "cooled" while it is running using a technique called *simulated annealing*. Simulated annealing was first introduced as a computational tool for general combinatorial optimization problems (like the *Traveling Salesman Problem*;[†] see [lawl85]) by Kirkpatrick *et.al.* [kirk83]. It takes its name,

[†]The traveling salesman problem (TSP) is (for a salesman) to find the shortest possible route that takes him from his starting point to each of N cities and back. Since there are $\sim (1/2)(N-1)!$ distinct paths to choose from, it takes on the order $O(N!)$ calculations to find the length of all of these paths. The TSP is known to be an NP-complete problem (see section 12.3.2). Since NP-complete problems are widely conjectured to be intractable, the best "solution" that can be achieved *in principle* is some polynomial-time algorithm that yields close-to-optimal solutions. The Boltzman Machine has been used for this problem with varying degrees of success [aarts89].

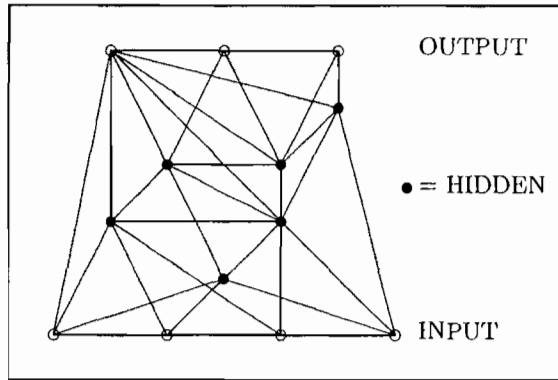


Fig. 10.8 A division of a set of neurons into *input*, *output* and *hidden* units in a Boltzman Machine. (For clarity, not all of the links between neurons are shown; just as for Hopfield nets, in general, $w_{ij} \neq 0$ for all $i \neq j$.)

by analogy, directly from real annealing, where the true (i.e. ground state) properties of a substance are found at low temperatures by a slow careful cooling of that substance. Great care must be taken to assure that the substance (or system) has reached thermal equilibrium as the temperature is progressively lowered. Otherwise, random fluctuations may be permanently “frozen” into the system and the true $T \rightarrow 0$ state will not be attained. If one wants to grow a crystal, for example, but the temperature is lowered too rapidly, the resulting state will be either a crystal with many defects or a glass, which has essentially no crystalline order at all. An excellent reference on simulated annealing and Boltzman Machines is the text by Aarts and Korst [aarts89].

We know that when a system is in equilibrium, its states $\vec{S} = (S_1, S_2, \dots, S_N)$ are distributed according to the Boltzman distribution (see equations 10.32-10.33):

$$P(\vec{S}) \propto e^{-\mathcal{E}[\vec{S}]/T}. \quad (10.42)$$

Now suppose that, regardless of the previous value of site i ($= S_i$), we let $S'_i = +1$ with a probability

$$p_i = \frac{1}{1 + e^{-\Delta E_i/T}}, \quad (10.43)$$

where

$$\Delta E_i \equiv E_{S_i=-1} - E_{S_i=+1} = \sum_j w_{ij} S_j \quad (10.44)$$

is the difference in the energy of the net when $S_i = -1$ and $S_i = +1$.

This prescription, which follows directly from the Boltzman distribution, ensures that any update of the system for $T > 0$ has a finite probability of increasing the energy of the system and thereby of helping the system get out of local minima. The lower the temperature, the less likely are higher energy states: as the temperature

is slowly lowered, the probability that the system will spontaneously jump back into a previously vacated high energy local minimum state steadily decreases. The only difficult part of the process is in deciding exactly how slow is “slow.”

While it is markedly faster to attain an equilibrium at a given temperature T by arriving there from a higher temperature via a simulated annealing than by starting at T initially, the simulated annealing procedure is by no means a fast algorithm. Geman and Geman [gemans84], for example, have shown that in order to be assured of reaching the global minimum state, the temperature at step n must satisfy the bound $T_n \geq c/\log(1+n)$, where c is some constant independent of n . If this theoretical bound is to be satisfied at each step of the cooling schedule, decreasing a system’s temperature from $T = 25$ to $T = 0.1$ would require $n \sim 10^{250}$ steps! Fortunately, one does not in practice have to resort to using such obscenely long cooling schedules in order to obtain reasonable results. The price to be paid, however, is that how one goes about *choosing* an appropriate cooling schedule is very much *ad hoc*.

10.8.2 Learning Rule

We mentioned above that a typical problem for a Boltzman Machine is to obtain a set of weights such that the states of the visible neurons take on some desired probability distribution. For example, the task may be to teach the net to learn that the first component of an N -component input vector has value $+1$ 40% of the time. To accomplish this, a Boltzman Machine uses the familiar gradient-descent technique, but *not* on the energy of the net; instead, it maximizes the *relative entropy* of the system.

To motivate the approach, suppose we had a size $N = 4$ input vector and the problem was as above to teach the net to learn that the first site has value $+1$ 40% of the time. Of the $2^4 = 16$ possible input vectors, 8 have their first component equal to $+1$. The reader should have no difficulty in convincing herself that there are an *infinite* number of ways of assigning probabilities to these 8 vectors such that the 40% probability of occurrence criterion for value $+1$ at the first site is satisfied. Why should we select one particular distribution over any other in this infinite set? Since there is no compelling reason to give any higher weight to any one of the 8 vectors with value $+1$ at the first site, one obvious choice is simply to distribute probabilities *equally*: $P(1, 0, 0, 0) = 5\%$, $P(1, 0, 0, 1) = 5\%$, $\dots$, $P(1, 1, 1, 1) = 5\%$. Recalling elementary information theory (see section 2.1.2), this choice amounts to maximizing the system entropy.

To be a bit more precise, let us use the index α to label the states of the visible neurons, the index β to label the states of the hidden neurons, and the combined index $\alpha\beta$ to label the complete states of the whole system. Then the probability P_α of finding the visible neurons in state α is given by

$$P_\alpha = \sum_\beta P_{\alpha\beta} = \frac{1}{Z} \sum_\beta e^{\mathcal{H}_{\alpha\beta}/T}, \quad (10.45)$$

where

$$\mathcal{H}_{\alpha\beta} = -\frac{1}{2} \sum_{ij} w_{ij} S_i^{\alpha\beta} S_j^{\alpha\beta}, \quad (10.46)$$

and $\mathcal{Z}$ is the partition function (equation 10.33).

On the other hand, we also have a set of *desired probabilities* P_α^* that we want the Boltzman Machine to learn. From elementary information theory, we know that the *relative entropy*

$$\mathcal{S} = \sum_{\alpha} P_{\alpha}^* \log\left(\frac{P_{\alpha}^*}{P_{\alpha}}\right) \quad (10.47)$$

measures the relative difference between the distributions P_{α} and P_{α}^* . Note that $\mathcal{S} \geq 0$ and $\mathcal{S} = 0$ only if $P_{\alpha} = P_{\alpha}^*$ for all α .

We see that our task is none other than to minimize $\mathcal{S}$, which we can do by using gradient descent:

$$\delta w_{ij} = -\eta \frac{\partial \mathcal{S}}{\partial w_{ij}} = \eta \sum_{\alpha} \frac{P_{\alpha}^*}{P_{\alpha}} \frac{\partial P_{\alpha}}{\partial w_{ij}}. \quad (10.48)$$

Using equations 10.45-10.47, we find that δw_{ij} is given by [hertz91]

$$\delta w_{ij} = \frac{\eta}{T} (\langle S_i S_j \rangle_{\text{clamped}} - \langle S_i S_j \rangle_{\text{free}}), \quad (10.49)$$

where $\langle S_i S_j \rangle_{\text{clamped}}$ is the weighted average over the states α (with respect to their probabilities P_{α}^*) of $\langle S_i S_j \rangle$ when the visible neurons are “clamped” in the state α .

Equation 10.49 embodies Hinton, *et.al.*’s Boltzman Machine learning scheme. Notice that it consists of two different parts. The first part, $\langle S_i S_j \rangle_{\text{clamped}}$, is essentially the same as the Hebb rule used in Hopfield’s net (equation 10.19), and reinforces the connections that lead from input to output. The second part, $\langle S_i S_j \rangle_{\text{free}}$, can be likened to a Hebbian *unlearning*, whereby poor associations are effectively unlearned.

Pseudo-Code Implementation: The Boltzman Machine Learning Algorithm proceeds in two phases: (1) a *positive*, or learning, phase and (2) a *negative*, or unlearning, phase. It is summarized below in pseudo-code. It is assumed that the visible neurons are further subdivided into *input* and *output* sets as shown schematically in figure 10.8.

Positive Phase:

- (p1) Clamp the input and output sets of neurons to their correct values.
- (p2) Allow the net to cycle through its states. Compute the energy

$$\Delta E_i = \sum_j w_{ij} S_j,$$

and select the lower energy state with probability

$$p_i = \frac{1}{1 + e^{-\Delta E_i/T}}.$$

(p3) Anneal the net according to the chosen cooling schedule until the system reaches equilibrium at the desired minimum temperature.

(p4) Let the net run through several processing cycles. After each cycle, find all pairs of neurons that are simultaneously in the “firing” state. Average the results.

(p5) Repeat steps (1)-(4) for each of the training vectors. Average the co-firing results to get an estimate for $\langle S_i S_j \rangle_{\text{clamped}}$.

Negative Phase:

(n1) Unclamp the visible neurons and anneal the net until the system reaches equilibrium at the desired minimum temperature.

(n2) Let the net run through several processing cycles. After each cycle, find all pairs of neurons that are simultaneously in the “firing” state. Average the results.

(n3) Repeat steps (n1) and (n2) the same number of times as done in step (p5) and average the co-firing results to get an estimate for $\langle S_i S_j \rangle_{\text{free}}$.

(*) Repeat steps (p1)-(p5) and (n1)-(n3) as many times as are necessary so that $\langle S_i S_j \rangle_{\text{clamped}} - \langle S_i S_j \rangle_{\text{free}}$ is sufficiently small.

10.9 Multi-Layered Perceptrons

We saw in section 10.5 that the simple (i.e. one-layer) perceptrons introduced by Rosenblatt [rosenbl58] are capable of solving only linearly-separable problems. While it was known fairly early on that the addition of one or more “hidden” layers would enable perceptrons to solve a greater range of problems, including *nonlinearly*-separable ones, it took many years from the time the separability problem was first pointed out by Minsky and Papert [minsky69] to the time that a learning rule was finally introduced by Rumelhart and McClelland [mcc86a].[†]

Rumelhart and McClelland’s *Connectionist Approach* (or *Parallel Distributed Processing* (PDP)) was in part a reaction against the high-level symbol manipulation and serial information processing paradigm of artificial intelligence (AI) prevalent in the 1970s. The connectionist approach to problem solving may be loosely thought of as modeling predicated on the brain [feld82]. That is to say, in contrast to traditional *top-down* symbolic AI approaches, connectionism represents a *bottom-up* approach. The interest is not in the explicit modeling of the human brain *per se*, but in the exploitation of the human brain’s parallel processing capability to help

[†]In the interests of historical accuracy, we should point that the learning rule usually credited to Rumelhart and McClelland had actually been introduced independently several times prior to the publication of their book: for example, by Bryson and Ho in 1969 [brys69], Werbos in 1974 [werb74] and Parker in 1985 [parker85]. Nonetheless, Rumelhart and McClelland are rightfully credited with having revived the interest in perceptron research and their book remains a landmark in the field.

solve problems that the human brain is itself well adapted for. A major emphasis is on having a net's "understanding" of a problem or the set of descriptors with which a net learns to describe a solution space be *emergent properties* rather than having them be explicitly embedded as fixed symbolic structures. Rumelhart and McClelland show how connectionist models can have emergent effects that would otherwise be wholly unexpected in the traditional symbolic-processing-AI arena [rumel86a].

10.9.1 The XOR Function Revisited

Consider the Boolean exclusive-OR (or XOR) function that we used as an example of a linearly inseparable problem in our discussion of simple perceptrons. In section 10.5.2 we saw that if a perceptron is limited to having only input and output layers (and no hidden layers), and is composed of binary threshold McCulloch-Pitts neurons, the value y of its lone output neuron is given by

$$y = \begin{cases} 1 & \text{if } w_1x_1 + w_2x_2 \geq \tau, \\ 0 & \text{else.} \end{cases} \quad (10.50)$$

where w_1 and w_2 are synaptic weights and τ is some threshold. This perceptron is unable to learn the XOR function because there is no way to choose values for w_1 and w_2 such that $y = x_1 \text{ XOR } x_2$. If we think of the four possible input states $((0,0), (1,0), (0,1), \text{ and } (1,1))$ as representing four distinct regions of the plane corresponding to the four correct outputs for points in those regions, the perceptron's task is to separate those four regions out of the whole plane (the reader may wish to refer back to figure 10.3). Whatever values we choose for w_1 and w_2 , the equation $w_1x_1 + w_2x_2 = \tau$ remains that of a straight line and is thus able to separate a planar region into only two distinct regions.

As we mentioned above, however, linearly inseparable problems such as the XOR-problem can be solved by adding one or more hidden layers to the perceptron. Figure 10.9, for example, shows a solution to the XOR-problem using a perceptron that has one hidden layer added to it. The numbers appearing by the links are the values of the synaptic weights. The numbers inside the circles (which represent the hidden and output neurons) are the required thresholds τ . Notice that the "hidden" neuron takes no direct input but acts as just another input to the output neuron. Notice also that since the hidden neuron's threshold is set at $\tau = 1.5$, it does not fire unless both inputs are equal to 1. Table 10.3 summarizes the perceptron's output.

x_1	x_2	Hidden Neuron	Output Neuron	$x_1 \text{ XOR } x_2$
0	0	0	0	0
0	1	0	1	1
1	0	0	1	1
1	1	0	0	0

Table 10.3 Output of the one-hidden-layer perceptron shown in figure 10.9.

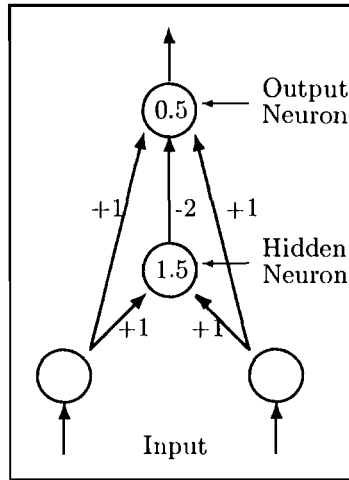


Fig. 10.9 The solution to the XOR problem using a hidden layer of neurons. The numbers appearing by the links are the synaptic weight values; the numbers in the circles (representing the hidden and output neurons) are the required thresholds τ . Note that the solution shown here is *not unique*. Can the reader find another set of synaptic weights and thresholds that give rise to the same answer?

Being able to construct an explicit solution to a nonlinearly separable problem such as the XOR-problem by using a multi-layer variant of the simple perceptron does not, of course, guarantee that a multi-layer perceptron can by itself *learn* the XOR function. We need to find a learning rule that works not just for information that only propagates from an input layer to an output layer, but one that works for information that propagates through an *arbitrary number of hidden layers* as well.

To motivate this new multi-layer learning rule, let us take one step backwards and look more closely at exactly what difference adding hidden layers makes to the problem. If one perceptron is enough to split the plane into two parts, it is reasonable to expect that the XOR problem can be solved by combining the regions separated out by two different perceptrons, as shown schematically in figure 10.10. The idea is to use perceptron $\mathcal{P}_3$ to combine the outputs of $\mathcal{P}_1$ and $\mathcal{P}_2$, which are themselves first used, respectively, to separate out the regions corresponding to the inputs $(x_1 = 0, x_2 = 1)$ and $(x_1 = 1, x_2 = 0)$.

However, while the approach is certainly sound, we see an immediate problem. If we insist on using the strict on-off thresholding of McCulloch-Pitts neurons (equation 10.1), the overall net consisting of perceptrons $\mathcal{P}_1$, $\mathcal{P}_2$ and $\mathcal{P}_3$ will be unable to determine which of the input weights must be increased and which must be decreased. $\mathcal{P}_3$ knows only the output of $\mathcal{P}_1$ and $\mathcal{P}_2$. It does not know which of the real inputs to $\mathcal{P}_1$ and $\mathcal{P}_2$ were on. Since the Hebbian learning rule consists of strengthening the connections between active neurons, it will be impossible to implement in our current configuration because the values of the actual inputs have

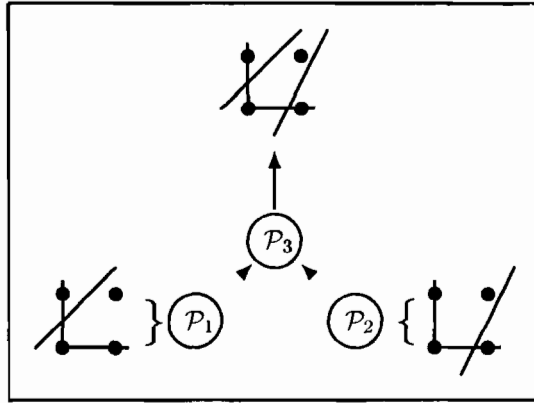


Fig. 10.10 A schematic representation of how perceptrons P_1 and P_2 can be combined to “solve” the Boolean XOR problem; see text.

been effectively erased from memory by the time P_3 has a chance to act.

This “memory erasure” problem is sometimes called the *credit assignment problem* [peret92]. Fortunately, there is an easy way out. We merely generalize the binary (on/off) McCulloch-Pitts neuronal values to *continuous* variables by smoothing out the step-function threshold.

Figure 10.11 shows a smooth sigmoidal threshold function that is often used in practice. It has the same form as the transition probability function used for stochastic nets:

$$y(x) = \frac{1}{1 + e^{-x}}. \quad (10.51)$$

The benefit of using a sigmoidal threshold function (or *any* smooth function that still yields the expected outputs of near-zero and near-one if the weighted sum is, respectively, either much less or much greater than the given threshold)[†] is derived from the additional information that an output value lying between the two extremes of zero and one brings. As we will see below, this additional information about the output of the hidden layer is enough to make appropriate adjustments to the weights on earlier layers.

[†]Note that we are essentially free to choose any continuous function we like, so long as it is *nonlinear*.

As we will discuss a bit later on in this section, adding hidden layers but generalizing the McCulloch-Pitts step-function thresholding to a *linear* function yields a multi-layer perceptron that is fundamentally no more powerful than a simple perceptron that has no hidden layers and uses the McCulloch-Pitts step-function threshold.

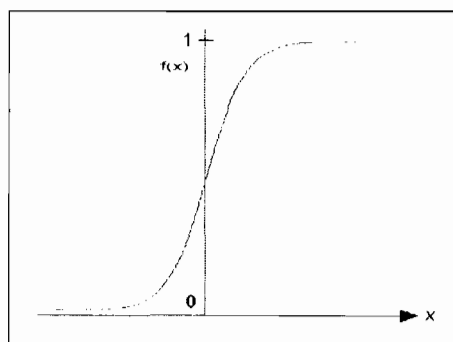


Fig. 10.11 Sigmoidal threshold function: $f(x) = 1/(1 + e^{-x})$.

10.9.2 Backpropagation

We are now ready to introduce the *backpropagation learning rule* (also called the *generalized delta rule*) for multi-layered perceptrons, credited to Rumelhart and McClelland [rumel86a]. Figure 10.12 shows a schematic of the multi-layered perceptron's structure. Notice that the design shown, and the only kind we will consider in this chapter, is strictly *feed-forward*. That is to say, information always flows from the input layer to each hidden layer, in turn, and out into the output layer. There are no feedback loops anywhere in the system.

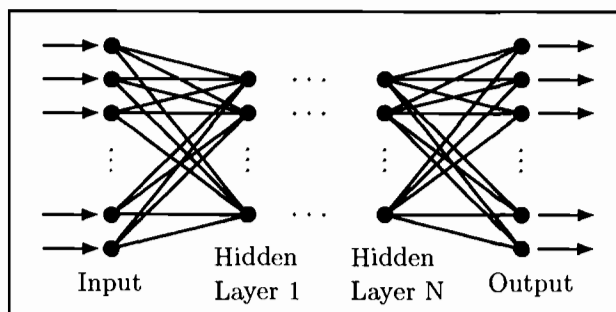


Fig. 10.12 A schematic representation of the multi-layer perceptron model.

Just as was the case with simple perceptrons, the multi-layer perceptron's fundamental problem is to learn to associate given inputs with desired outputs. The input layer consists of as many neurons as are necessary to set up some "natural

correspondence" between the input neurons and the input-fact set that the net is to be trained on. For example, if the problem is to learn the 26 letters of the alphabet, the input fact set might consist of digitized samples of handwritten characters. In this case, a natural choice might be to associate each grid-point of an $N \times M$ sized digitized lattice with one input neuron. Each neuron is assigned a value of either 1 or 0 depending on whether or not a part of an input sample appears on the grid-point with which it is associated.

The output layer likewise consists of as many neurons as are necessary to set up a natural correspondence between the output neurons and the output-fact set. Using the same example of learning the alphabet, the output space might consist of 26 neurons, one for each letter of the alphabet. A perfect association between input and output facts would be to have – *for each input letter* – the value of the output neuron corresponding to the n^{th} letter equal one and all other output neurons equal zero.

One or more hidden layers are sandwiched between the input and output layers and, for the moment, consist of an arbitrary number of neurons. There are unfortunately no theorems dictating what number should be used for a given problem, but useful heuristics do exist. We will comment on some of these heuristics a bit later on.

The backpropagation learning rule gives a prescription for adjusting the initially randomized set of synaptic weights (existing between all pairs of neurons in each successive layer) so as to minimize the difference between the perceptron's output of each input fact and the output with which the given input is known (or desired) to be associated. The backpropagation rule takes its name from the way in which the calculated error at the output layer is propagated backwards from the output layer to the N^{th} hidden layer to the $(N - 1)^{\text{th}}$ hidden layer, and so on. Because this learning process requires us to "know" the correct pairing of input-output facts beforehand, this type of weight adjustment is called *supervised learning*.

10.9.2.1 Derivation

Let us now look at the backpropagation rule in more detail. Consider for concreteness, a net with one hidden layer (see figure 10.13). Let σ_k^p represent the value of the k^{th} input neuron corresponding to the p^{th} training fact; let the values of the hidden neurons be given by h_j ; and let the values of the output neurons be given by $\mathcal{O}_i$. The set $\{w_{jk}\}$ is the set of weights for the links between the input and hidden layers; the set $\{w'_{ij}\}$ is the set of weights for the links between the hidden and output layers. Finally, let Σ_i^p represent the *expected* value of the i^{th} output neuron corresponding to the p^{th} training fact; i.e. the training set consists of input/output pairs $\{\sigma_k^p, \Sigma_i^p\}$.

Given pattern p , the j^{th} hidden neuron receives a weighted input equal to

$$\mu_j^p = \sum_k w_{jk} \sigma_k^p \quad (10.52)$$

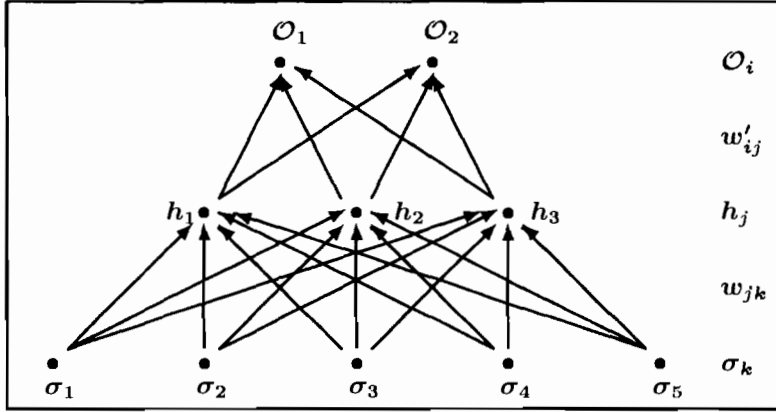


Fig. 10.13 Schematic representation and notation for a three-layer feed-forward multi-layer perceptron; see text.

and yields an output

$$h_j^p = f_\alpha(\mu_j^p) = f_\alpha\left(\sum_k w_{jk}\sigma_k^p\right), \quad (10.53)$$

where $f_\alpha(x)$ is the sigmoidal threshold function shown in figure 10.11 but with a parameter α added to control the steepness of the curve:

$$f_\alpha(x) = \frac{1}{1 + e^{-\alpha x}}, \quad (10.54)$$

Note that the derivative $f'_\alpha(x)$ also takes a rather simple form:

$$f'_\alpha(x) = \alpha f_\alpha(x)(1 - f_\alpha(x)). \quad (10.55)$$

The i^{th} output neuron receives input

$$\mu_i^p = \sum_j w'_{ij} h_j^p = \sum_j w'_{ij} f_\alpha\left(\sum_k w_{jk}\sigma_k^p\right), \quad (10.56)$$

and produces an output

$$O_i^p = f_\alpha\left(\sum_j w'_{ij} h_j^p\right) = f_\alpha\left(\sum_j w'_{ij} f_\alpha\left(\sum_k w_{jk}\sigma_k^p\right)\right). \quad (10.57)$$

Since we want to adjust the weights in such a way that the difference between the network's output ($= O_i^p$) and the actual output ($= \Sigma_i^p$) is minimized, we must

first define a difference measure. Let $D = D(\vec{w}, \vec{w}')$ be equal to

$$\begin{aligned} D &= \frac{1}{2} \sum_{p,i} (\Sigma_i^p - \mathcal{O}_i^p)^2, \\ &= \frac{1}{2} \sum_{p,i} \left\{ \Sigma_i^p - f_\alpha \left(\sum_j w'_{ij} f_\alpha \left(\sum_k w_{jk} \sigma_k^p \right) \right) \right\}^2. \end{aligned} \quad (10.58)$$

The better our choice for the two sets of weights $\{\vec{w}\}$ and $\{\vec{w}'\}$, the closer the net's output $\mathcal{O}_i^p$ comes to the desired output Σ_i^p and the smaller the difference D becomes. An appropriate set of weights can be learned by using the standard *gradient descent algorithm*. Heuristically, the algorithm adjusts each weight w by an amount δw proportional to the gradient of D at a given location (i.e. we seek the minimal “energy state” by “sliding” downhill on the surface defined by $D(\vec{w}, \vec{w}')$).

The calculations are slightly different between the two cases where the weights are between (i) hidden and output layers and (ii) input and hidden layers. For the hidden-to-output connections, the gradient descent algorithm gives

$$\begin{aligned} \delta w'_{ij} &= -\eta \frac{\partial D}{\partial w'_{ij}} = \eta \sum_p (\Sigma_i^p - \mathcal{O}_i^p) f'_\alpha(\mu_i'^p) h_j^p, \\ &= \eta \sum_p \Delta_i^p h_j^p, \end{aligned} \quad (10.59)$$

where we have defined

$$\Delta_i^p \equiv f'_\alpha(\mu_i'^p) (\Sigma_i^p - \mathcal{O}_i^p), \quad (10.60)$$

and η is an adjustable “learning” constant.

For the input-to-hidden connections, we use the chain rule to find that

$$\begin{aligned} \delta w_{jk} &= -\eta \frac{\partial D}{\partial w_{jk}} = -\eta \sum_p \frac{\partial D}{\partial h_j^p} \frac{\partial h_j^p}{\partial w_{jk}}, \\ &= \eta \sum_{p,i} (\Sigma_i^p - \mathcal{O}_i^p) f'_\alpha(\mu_i'^p) w'_{ij} f'_\alpha(\mu_j^p) \sigma_k^p, \\ &= \eta \sum_{p,i} \Delta_i^p w'_{ij} f'_\alpha(\mu_j^p) \sigma_k^p, \\ &= \eta \sum_p \Delta_j^p \sigma_k^p, \end{aligned} \quad (10.61)$$

where

$$\Delta_j^p \equiv f'_\alpha(\mu_j^p) \sum_i w'_{ij} \Delta_i^p. \quad (10.62)$$

Pseudo-Code Implementation: The *Back-propagation* algorithm outlined above may be implemented by following seven steps, to be applied for each pattern ‘ p ’. Assume we have a neural net with L layers ($l = 1, 2, \dots, L$). Let h_i^l represent the output of the i^{th} neuron in the l^{th} layer; h_i^0 is therefore equal to the i^{th} input, σ_i . The weight of the connection between h_j^{l-1} and h_i^l will be labeled by w_{ij}^l .

Step 1: Initialize all weights to small random values.

Step 2: Set the input layer equal to the input values of the first input/output fact pair: i.e. let

$$h_k^0 = \sigma_k^{p=1}, \quad \text{for all } k. \quad (10.63)$$

Step 3: Propagate the input signal forward through the various layers of the net; i.e. calculate

$$h_i^l = f_\alpha \left(\sum_j w_{ij}^l h_j^{l-1} \right) \quad (10.64)$$

for each i and l until the output of the final layer h_i^L has been found.

Step 4: Calculate the Δ ’s for the output layer:

$$\Delta_i^L = f'_\alpha(h_i^L)(\Sigma_i^p - h_i^L). \quad (10.65)$$

Step 5: Obtain the Δ ’s for each of the preceding layers by propagating the errors backwards:

$$\Delta_i^{l-1} = f'_\alpha(h_i^{l-1}) \sum_j w_{ji}^{l-1} \Delta_j^l, \quad l = L, L-1, \dots, 2. \quad (10.66)$$

Step 6: Adjust all weights by $w_{ij} \rightarrow w_{ij} + \delta w_{ij}$, where

$$\delta w_{ij} = \eta \Delta_i^l h_j^{l-1}. \quad (10.67)$$

Step 7: Go back to Step 2 and repeat for the next pattern. Stop when the difference between the computed and desired outputs ($= D$) is less than some pre-assigned threshold.

10.9.2.2 Variations of the Basic Rule

The basic backpropagation algorithm described above is, in practice, often very slow to converge. Moreover, just as Hopfield nets can sometimes get stuck in undesired spurious attractor states (i.e. local minima; see section 10.6.5), so to can multi-layer perceptrons get trapped in some undesired local minimum state. This is an unfortunate artifact that plagues all energy (or cost-function) minimization schemes.

In recent years, a number of alternative formulations to improve convergence have been suggested. Consider the learning constant η , that effectively determines how fast the system moves down a “hill” of the energy surface (see equation 10.59). Although smaller values of η lend stability to the gradient descent method, they also tend to slow it down to impracticably slow rates of convergence. On the other hand, if η is too large, the algorithm tends to oscillate and become unstable. We mention three ways that have suggested to reduce some of this oscillation: (1) using

successively smaller values of the learning constant, (2) continuously adapting the value of the learning constant to how well the converge is doing, and (3) adding a so-called momentum-term. A fourth method is to add a bit of noise at each step of the gradient descent. Using precisely the same argument that we used before for considering a stochastic variant of the Hopfield net (see section 10.7), the idea is to use the noise to knock the system out of local minima.

Use Smaller values of η : In this variant, the gradient descent algorithm is started with a large value of η and thus initially takes relatively big steps towards the solution. As η is lowered at each iteration step, however, smaller and smaller jumps are taken and the system settles into the minimum energy state without overshooting it. The idea is to allow the system to reach that minimum state by bypassing the local minimum using initially large steps. Unfortunately, there are two problems this approach: (1) the optimal lowering rate schedule is unknown and thus becomes another variable, and (2) reduction of the learning constant leads to longer convergence times.

Use an Adaptive η : An alternative method is to continuously *adjust* the learning constant according to how well the algorithm is doing at a given time during its convergence ([cater87], [jacobs88]). One could use the average behavior of the system during its last N steps, for example, to determine whether η ought to be decreased, increased or left unchanged. If the energy change is less than zero on average, η could be increased by some amount ζ_1 . If the energy change is greater than zero, we might try decreasing η by some factor $\zeta_2\eta$. Otherwise, η would be left unchanged. One could also use synaptic-weight-dependent rates [jacobs88] or have different rates for each desired pattern [cater87].

Add Some Inertia: Another way is to add a so-called *momentum term* to our previous expression for calculating the weight-changes (see equations 10.59 and 10.61). That is, instead of using $\delta w_{ij}(t+1) = -\eta \frac{\partial D}{\partial w_{ij}}$, to use instead [rumel86b]

$$\delta w_{ij}(t+1) = -\eta \frac{\partial D}{\partial w_{ij}} + \alpha \delta w_{ij}(t), \quad (10.68)$$

where $0 \leq \alpha \leq 1$ is a constant that determines how much of an influence *past weight changes* have on the current direction of motion in weight space. In practice, it is often set to ≈ 0.9 . The idea is to enhance the net's chances of evolving towards the global minimum by avoiding local minima early on; its *momentum* tending to push the system over local energy increases. The added term also serves to effectively dampen oscillations, particularly along the energy surface's "valleys" or "ravines." Unfortunately, the momentum term can also slow down the convergence rate.

Finally, we mention an approach based on using a different *energy* (or *difference*) *function*. The quadratic form used above (equation 10.58) is simple to use but it is not the only form possible. In fact, we could go through the same derivation steps as above by using any function $f(\mathcal{O}_i^p, \Sigma_i^p)$ of the net's output $\mathcal{O}_i^p$ and actual output

Σ_i^p , as long as it is differentiable and is minimized by $\mathcal{O}_i^p = \Sigma_i^p$. One interesting form that has a natural interpretation in terms of learning the probabilities of a set of hypotheses represented by the output neurons, has recently been suggested by Hopfield [hopf87] and Baum and Wilczek [baum88b]:

$$f = \sum_{p,i} \left\{ \frac{1}{2}(1 + \Sigma_i^p) \log \frac{1 + \Sigma_i^p}{1 + \mathcal{O}_i^p} + \frac{1}{2}(1 - \Sigma_i^p) \log \frac{1 - \Sigma_i^p}{1 - \mathcal{O}_i^p} \right\}. \quad (10.69)$$

In this expression, the term $\frac{1}{2}(1 + \mathcal{O}_i^p)$ is interpreted as the probability that the hypothesis represented by the i^{th} neuron is true (with $\mathcal{O}_i^p = +1$ meaning *true* and $\mathcal{O}_i^p = -1$ meaning *false*), and the term $\frac{1}{2}(1 + \Sigma_i^p)$ is interpreted as the set of desired probabilities. With these, interpretations, f effectively yields the *relative entropy* between these two sets of probability measures.

10.9.3 Model Development: A Short Primer

The previous section introduced the backpropagation rule for multi-layer perceptrons. This section briefly discusses the model development cycle necessary for obtaining a properly functioning net. It also touches upon some of the available heuristics for determining the proper size of hidden layers.

While the details of designing a neural net solution to a problem can be quite involved, the basic strategy is fairly simple. The important point to remember is that designing a net is almost an antithesis of conventional programming. There are no rules or algorithms to write (except for the underlying code defining the learning algorithm, of course). Instead, the effort that is conventionally put into the programming end of a solution is replaced by the effort that must be put into constructing a sample solution set, one that must often be put together without an explicit or *a priori* knowledge of the method of solution. For example, using the example of image recognition ("Uncle Seymour's face"[†]), while most of us are instantly able to recognize the faces of even the most casual of our acquaintances, very few of us are able to describe exactly how we are able to accomplish this task.

Fundamentally, all feed-forward backpropagating nets follow the same five basic steps of a model development cycle:

- *Define the Problem*
- *Define the Input-Output Fact Set*
- *Define the neural net Structure*
- *Train*
- *Test*

It cannot be stressed strongly enough that the first step, *defining the problem*, is far from being a simple task. Great care must be taken to identify precisely what one wishes for the net to "learn."

[†]See the opening paragraphs of this chapter.

There is an telling story about how the Army recently went about teaching a backpropagating net to identify tanks set against a variety of environmental backdrops. The programmers correctly fed their multi-layer net photograph after photograph of tanks in grasslands, tanks in swamps, no tanks on concrete, and so on. After many trials and many thousands of iterations, their net finally learned all of the images in their database. The problem was that when the presumably “trained” net was tested with other images that were not part of the original training set, it failed to do any better than what would be expected by chance. What had happened was that the input/training fact set was statistically corrupt. The database consisted mostly of images that showed a tank only if there were heavy clouds, the tank itself was immersed in shadow or there was no sun at all. The Army’s neural net had indeed identified a latent pattern, but it unfortunately had nothing to do with tanks: *it had effectively learned to identify the time of day!*

The obvious lesson to be taken away from this amusing example is that how well a net “learns” the desired associations depends almost entirely on how well the database of facts is defined. Just as Monte Carlo simulations in statistical mechanics may fall short of intended results if they are forced to rely upon poorly coded random number generators, so do backpropagating nets typically fail to achieve expected results if the facts they are trained on are statistically corrupt.

Once the input-output fact pair database has been put together, the next challenge is to find an appropriate net design; i.e. *how many input and output neurons should be used and how many hidden layers should be placed between them?* Typically, the form of the input-output facts in the database determine the number (and type) of input and output neurons. In the example we used earlier of using a neural net to learn the 26 letters of the alphabet, for example, a natural choice was to use $N \times M$ input neurons to encode an input “image” and 26 output neurons, each of which corresponds to a given letter. If, instead, the problem is to construct a financial predictor, where the input data consists of such facts as the consumer price index, the price of crude oil, the unemployment rate, and so on, and the desired output is an estimate of the Dow-Jones stock average, it is natural to design a net that has as many input neurons as there are available input facts and one output neuron whose value is equal to the predicted Dow-Jones average. Countless other examples could of course also be imagined. The point is that once the problem has been carefully defined and the available information structured in some form, the number of input and output neurons is essentially determined.

The task becomes a little bit more tricky when it comes to selecting an appropriate number of (and size for) the hidden layers.

We have seen that the output neuron in a binary-threshold perceptron without hidden layers can only specify on which side of a particular hyperplane the input lies. Its decision region consists simply of a half-plane bounded by a hyperplane. If one hidden layer is added, however, the neurons in the hidden layer effectively take an intersection (i.e. a Boolean AND operation) of the half-planes formed by the input neurons and can thus form arbitrary (possible unbounded) *convex regions*.[†]

[†]Recall that a *convex region* is a region such that any line joining two points on its boundary only

The number of sides of the convex regions is equal to the number of half-planes whose intersection formed the decision region, and is thus bounded by the number of input neurons.

We thus get our first heuristic insight into the number of required hidden neurons: *the perceptron must contain a sufficient number of hidden neurons to form the decision region required by the problem.* In our one-hidden layer solution of the XOR problem, for example, we saw that a single hidden neuron sufficed (see figures 10.9 and 10.10). What about the more general problem of the realizability of arbitrary Boolean functions? It can be shown that, for a sufficient number of hidden neurons, a multi-layered perceptron with *one hidden layer* can represent any Boolean function ([widrow90], [hertz91]).

Now, what happens if we add a second hidden layer? In fact, two hidden layers are already enough to form *arbitrarily complex decision regions* [lipp87]. We can see why this is so by direct construction. First break up a desired decision region into any number of small hypercubes. Since the hypercubes are convex, the first two layers of the net are by themselves enough to specify whether a given input lies in a particular hypercube. The specification of each hypercube needs $2N$ neurons in the first hidden layer (one for each of its sides) and one neuron in the second hidden layer that performs a Boolean AND of the first hidden layer's outputs. The second hidden layer outputs will have large values only for inputs within each hypercube. By performing a Boolean OR on the inputs representing its own decision regions' hypercubes,[†] the second hidden layer specifies the presence of the input in the decision region it represents if the input lies in any of the hypercubes defined by the first hidden layer. Since we could also have used any other arbitrary convex region instead of hypercubes we thus see that the decision regions generated by perceptrons with two hidden layers can be arbitrarily complex (including regions that are disconnected and/or non-convex), with their complexity being limited only by the number of neurons. At best, if the decision region is connected and convex, the second hidden layer need not contain more than one neuron; at worst, it must contain as many neurons as there disconnected decision regions.

We therefore see that there is no point in designing perceptrons containing more than two hidden layers, since two layers are already enough to generate arbitrarily complex decision regions.

We should mention that while the above discussion assumed strict binary thresholding, the conclusions would not be altered by using sigmoidal nonlinearities. The analysis is in this other case more difficult because the decision regions are formed by smooth curves instead of hyperplanes, but the overall behavior remains qualitatively the same. It is easy to show that in the case of *linear* transfer functions, nothing at all would be gained by adding hidden layers since the output of multiple hidden layers can be reproduced by a single layer.

passes through points that are contained within that region.

[†]A Boolean OR operation will be performed if the synaptic weights between the second hidden layer and the output layer are equal to one and the output neuron's thresholds are set to 0.5 [lipp87].

10.9.3.1 Kolmogorov's Theorem

An interesting theorem that provides some additional insight into the general capabilities of multi-layer perceptrons was proven by Kolmogorov in 1957 [kolmog57]. Its origins actually date back to Hilbert's 13th problem ([hilb00], [lorentz76]) and its relevance to neural nets first pointed out by Hecht-Nielson in 1987 [hecht87].

Hilbert, in a famous address to the International Congress of Mathematicians in 1900, presented a list of 23 problems he thought would guide the further development of mathematics. The 13th problem had to do with solutions of polynomial equations. Specifically, Hilbert asked whether roots of a general algebraic equation could be expressed by sums and compositions of functions of one variable? Hilbert had conjectured that the roots of the equation $x^7 + ax^3 + bx^2 + cx + 1 = 0$, thought of as functions of the three variables a , b and c , could not be represented as sums and superpositions of functions of even two variables. This conjecture was disproved by Arnold in 1957 [arnold57]. In the same issue of the journal that Arnold's proof appeared, Kolmogorov provided his general theorem:

Kolmogorov's Theorem: Any real-valued continuous function f defined on an N -dimensional cube $\mathcal{C}^N$ can be represented as

$$f(x_1, x_2, \dots, x_N) = \sum_{i=1}^{2N+1} \phi_i \left(\sum_{j=1}^N \psi_{ji}(x_j) \right), \quad (10.70)$$

where ϕ_i and ψ_{ji} are continuous functions of one variable and the functions ψ_{ji} are universal for a given dimension N (i.e. are independent of the original function f). The functions ϕ_i are specific to a given f .

While Kolmogorov's original theorem has subsequently been improved upon a number of times, the most interesting formulation for our purposes is due to Hecht-Nielson, who rephrased the theorem in the language of neural nets [hecht87].

Kolmogorov's Theorem (Reformulated by Hecht-Nielson): Any real-valued continuous function f defined on an N -dimensional cube $\mathcal{C}^N$ can be implemented by a three layered neural network consisting of $2N + 1$ neurons in the hidden layer with transfer functions $\alpha^{(ji)}\psi_j$ from the input to the hidden layer and ϕ from all of the hidden neurons to the output. The $\alpha^{(ji)}$ are constants.

Kolmogorov's theorem thus effectively states that a three-layer net with $N(2N + 1)$ neurons using continuously increasing nonlinear transfer functions can compute any continuous function of N variables. Unfortunately, the theorem tells us nothing about how to select the required transfer functions or set the weights in our net.

A related theorem is due to Cybenko [cyb88], who showed that, provided that there are enough neurons in the layer, one hidden layer is enough to compute any continuous function to an arbitrary degree of accuracy.

A detailed discussion of the implications of Kolmogorov's theorem to multi-layered nets is given by Kurkova [kurk92].

10.9.3.2 Capacity

In our discussion of Hopfield nets in section 10.6, we found that the maximal number of patterns that can be stored before their stability is impaired is some linear function of the size of the net: $n_{\max} \propto \alpha N$, where $0 < \alpha < 1$ and N is the number of neurons in the net (see sections 10.6.6 and 10.7). A similar question can of course be asked of perceptrons: *How many input-output fact pairs can a perceptron of given size learn?*

Simple Perceptrons: In the case of simple perceptrons using McCulloch-Pitts thresholding, the answer depends on a careful analysis of linear separability.

Consider a simple perceptron with N continuous-valued inputs and one binary ($= \pm 1$) output value. In section 10.5.2 we saw how, in general, an N -dimensional input space is separated by an $(N - 1)$ -dimensional hyperplane into two distinct regions. All of the points lying on one side of the hyperplane yield the output $+1$; all the points on the other side of the hyperplane yield -1 .

Now let us ask the following question. Given a set of n randomly positioned points in the N -dimensional space, for what fraction of the 2^n possible ± 1 labelings can we find an $(N - 1)$ -dimensional hyperplane that separates them into distinct (like-labeled) sets? We will call an arbitrary labeling a *dichotomy* and a labeling that is linearly separable a *linear dichotomy*. We state, without proof, the result found by Cover ([cover64], [cover65]; see also [duda73]), giving an analytic expression for the fractional number of dichotomies:

$$f(n, N) = \begin{cases} 1 & \text{if } n \leq N + 1 \\ 2^{1-n} \sum_{i=0}^N \binom{n-1}{i} & \text{if } n > N + 1. \end{cases} \quad (10.71)$$

A graph of this function shows that it is not until the number of points n is some sizable fraction of $2(N + 1)$ that an $(N - 1)$ -dimensional hyperplane becomes over constrained by the requirement to correctly separate out $(N + 1)$ or fewer points. It therefore turns out that the capacity of a simple perceptron is given by a rather simple expression: if the number of output neurons is small and independent of N , then, as $N \rightarrow \infty$, the maximum number of input-output fact pairs that can be learned, $n_{\max}$, is given by [cover65]

$$n_{\max} = 2N. \quad (10.72)$$

Multi-layered Perceptrons: As might be expected, additional layers of neurons makes the analysis of the pattern capacity of multi-layered perceptrons more difficult.

The problem was first addressed by Cover ([cover64], [cover65]), who found a lower bound on the minimum number of synaptic weights needed for an ADALINE network (see section 10.5.1) to realize any Boolean function. More recently, Cover's early work has been extended by Baum ([baum88a], [baum89]), who has found a

number of interesting bounds on the ability of multi-layered perceptrons to handle general input-output mappings.

Consider a set $\mathcal{N}$ of n N -dimensional vectors and a function ϕ that assigns a value ± 1 to each element of $\mathcal{N}$ (i.e. ϕ is a dichotomy; see above). Baum [baum88a] showed that if $\mathcal{N}$ consists only of vectors such that no subset of N or fewer of them is linearly dependent, the smallest sized multi-layered perceptron that can realize an arbitrary dichotomy for $\mathcal{N}$ contains one hidden layer consisting of $\lceil (n-1)/N + 1 \rceil$ neurons. The size of this perceptron can only be decreased by putting on a more stringent constraint on the set $\mathcal{N}$.

Baum also showed that, regardless of the number of hidden layers it may possess, unless a multi-layer perceptron has at least on the order of $\mathcal{O}\left(\sqrt{n/\log_2 n}\right)$ neurons, it will be unable to compute an arbitrary function [baum88a].

10.9.3.3 Ability to Generalize

From a practical standpoint, a net designer is just as interested in a net's *generalization ability* as he is about a net's innate pattern capacity. Generalization is the ability to recognize correct relationships in sets of facts that were not part of the original training set. Intuitively, we can expect there to be some kind of trade-off. On the one hand, we obviously do not want a net to be able to store given associations perfectly but completely unable to find similar patterns in new data. A look up table approach would probably make a better choice in this case. On the other hand, we should not expect a net to develop an ability to generalize unless it has seen a sufficient number of patterns that it can learn to generalize from. In this case, we may have to be satisfied with a less than saturated capacity. Indeed, one can show that for good generalization, the training set should be several times larger than the net's expected capacity [baum89].

It is convenient to introduce the *growth function*, $g(n)$, defined as the maximum number of different binary functions realizable by a net on any set $\mathcal{N}$ of n N -dimensional vectors. Since there are 2^n possible dichotomies (see above), we know that $g(n) \leq 2^n$. Vapnik and Chervonenkis [vapnik71] studied the behavior of $g(n)$ and showed that $g(n)$ always starts out equaling 2^n for small n , but that its growth rate slows down at a point $n = d_{VC}$ called the VC-dimension. If $d_{VC} = \infty$, then $g(n) = 2^n$ for all n . If d_{VC} is finite, however, then $g(n) \leq n^{d_{VC}} + 1$ and $g(n)$ does not continue growing exponentially.

Baum and Haussler [baum89] calculated the VC-dimension for the case of a multi-layered net with N threshold neurons and N_w synaptic weights: $d_{VC} \leq 2N_w \log_2(eN)$, where e is the base of the natural logarithm. Using this they found that if the training error is less than $\epsilon/2$ then no more than on an order of $\mathcal{O}\left(\frac{N_w}{\epsilon} \log \frac{N}{\epsilon}\right)$ facts are required for a generalization error $< \epsilon$. In the case of a net with N_i inputs and one fully connected hidden layer with N_h neurons, Baum and Haussler showed that no more than on an order of N_w/ϵ weights are needed for a generalization error $< \epsilon$.

10.9.4 Applications

Since their introduction, feedforward backpropagating neural nets have been used to “solve” a variety of interesting problems. One of the most striking applications has been to speech recognition and synthesis ([peel86],[elman87]). Because of its pedagogical value, we discuss in some detail one such design, called NETtalk, in the following section.

Other applications include playing backgammon [tesauro88], recognizing handwritten zip-codes [lecun89], financial bond rating [duttas88], visual pattern recognition [rumel86c], classification of seismic signals [dowla89], radar signal processing [anderj90], sonar target recognition [gorman88], image compression [cott87], and navigating a car [pomer89].

10.9.4.1 NETtalk

An important and influential application of a multi-layered backpropagating neural net is NETtalk, designed by Sejnowski and Rosenberg in 1987 [sejn87]. NETtalk learns to convert English text into speech and displays many of the characteristics of learning normally ascribed to human learning, including a power-law form for its learning curve and an increase in its ability to generalize as the size of the its training set increases. Moreover, NETtalk is robust and fault tolerant. Its performance degrades gracefully and not catastrophically if its set of synaptic weights is damaged. Once trained, NETtalk is also able to relearn a given fact set much faster after some damage has been done to it than if it had to start from scratch with the original training.

Generating speech from written text is a notoriously difficult problem to solve using conventional programming techniques. Part of the difficulty is due to the fact that words are not always pronounced according to how they are spelled. Although we are all taught the “rules” when we are young, as our experience grows we learn that each rule has its fair share of exceptions. Even a simple sentence like “*This is a sentence,*” shows that spelling can be a poor cue for pronunciation. The first two *s*’s are pronounced differently, but they both appear at the end of word and are both preceded by an *i*. The third *s* is pronounced the same way as the first but instead appears at the beginning of a word. NETtalk deals with this problem by looking at *groups of letters* to provide context sensitivity.

NETtalk’s basic architecture is shown schematically in figure 10.10. NETtalk consists of 203 input neurons, one hidden layer composed of 80 neurons and 26 output neurons. The input consists of a string of 203 letters, with a 7-site long window that slides over the text to provide the necessary context sensitivity for the net to be able learn to pronounce the middle letter. The output consists of 26 elementary speech sounds called *phonemes*. Phonemes are similar to the pronunciation guides found in standard dictionaries. Several sets of phonemes are available. A partial listing of the phonemes used by Sejnowski and Rosenberg, expressed in terms of 21 articulatory features such as *point of articulation*, *voicing* and so on, is shown in table 10.4.

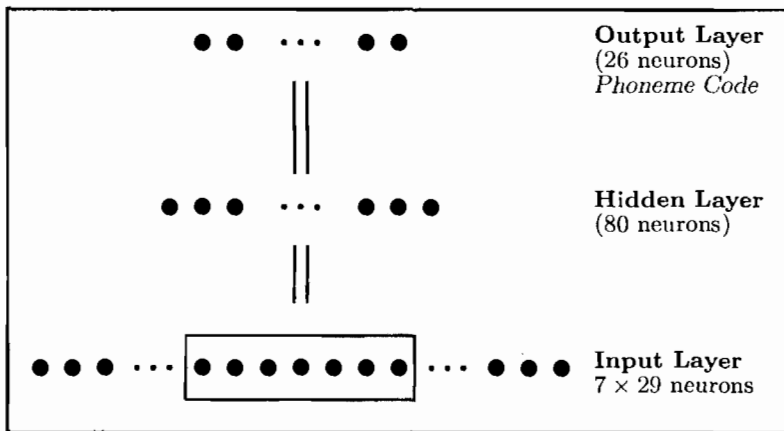


Fig. 10.14 Sejnowski's and Rosenberg's NETtalk architecture.

Phoneme	Sound	Articulatory Features
/a/	father	low, tensed, central2
/b/	bet	voiced, labial, stop
/z/	zoo	voiced, alveolar, fricative
/A/	bite	medium, tensed, front2+central1
/C/	chin	unvoiced, palatal, affricative
/-/	continuation	silent
1	primary stress	strong, weak
<	syllable boundary	right

Table 10.4 A partial listing of phonemes and pronunciations used by NETtalk; after appendix A of [sejn87].

Sejnowski and Rosenberg used two different sets of words for training: (1) 1024 words taken from phonetic transcriptions of informal continuous speech by children and (2) a subset of the 1000 most commonly used words selected from *Miriam Webster's Pocket Dictionary*. NETtalk was trained on a DEC VAX 11/780 mini-computer.

NETtalk managed to learn the informal speech database well enough after only a few training cycles (with each cycle being one complete pass through the database) to utter intelligible speech. Ten passes were sufficient for it to utter fully understandable words, and 50 cycles proved enough for NETtalk to attain a 95% accuracy rate. Initially, NETtalk was able to learn only gross features such as the difference between consonants and vowels. Since it always responded with the same vowel whenever any vowel was input and with the same consonant whenever a consonant was input, in this early phase NETtalk sounded rather like a babbling child. Gradually, NETtalk learned to recognize the boundaries between words and was thus able to begin uttering pseudowords. As its learning was further enhanced,

NETtalk's output steadily improved to the point of intelligibility.

Perhaps the most striking result is an early demonstration of fault tolerance. When Sejnowski and Rosenberg artificially "damaged" the net by adding some amount of random noise to the synaptic weights, they found that NETtalk's ability to "speak" degraded only gradually and not suddenly, as might be expected of a conventional rule based system from which a subset of rules was suddenly deleted.

In the case of the subset of words from *Miriam's Dictionary*, Sejnowski and Rosenberg were more concerned with exploring how the learning rate depended on the number of hidden neurons. The best design was one with 120 hidden neurons, with NETtalk achieving a 98% accuracy rate, which is better than what it was able to achieve with informal speech because of the inherent variability of real-world speech. In comparison, a net *without any hidden neurons* (i.e. a simple perceptron) learned rapidly but was effectively saturated at an 82% accuracy rate. When the 120 hidden neuron version of NETtalk was tested on the full 20,012 words of *Miriam's Dictionary*, NETtalk averaged a 77% accuracy. After subsequent training on the full dictionary, its accuracy rate rose to 85% after the first pass and to 90% after five passes.

Sejnowski and Rosenberg also found that NETtalk's performance improved with an additional hidden layer. Using a design consisting of two hidden layers containing 80 neurons each, NETtalk's performance reached 97% accuracy after 55 passes on the 1000 word database; was 80% on the full set of 20,012 words without additional training and reached 87% accuracy after a single training pass through the full dictionary. However, while the two hidden-layer version of NETtalk was clearly better at generalization than the version with a single hidden layer, the two-hidden layer NETtalk peaked out at about the same accuracy rate as its smaller cousin: its asymptotic performance, reached after 11 passes through the full dictionary, was 91%.

Finally, it is interesting to compare NETtalk's skills with the skills of commercially available text-to-speech systems such as DECTalk. Unlike NETtalk, DECTalk uses both extensive (and labor intensive) look up tables that store the phonetic transcription of common and not so common words and sets of phonological rules for words not in its main look up table. While DECTalk performs undeniably better than NETtalk, the comparison is not really a fair one. DECTalk is a combined result of many years worth of careful linguistic analysis and codification. NETtalk, on the other hand, is a self-contained system that (in the span of a few hours worth of DEC VAX CPU time) can learn enough *on its own* from a set of simple examples to be both intelligible and accurate.

10.10 Further Topics and Suggested Reading

This brief survey has only touched upon some of the more familiar neural net designs, chosen mainly for their pedagogical value. There are of course a large number of other important models, some of which have wide applicability, some of which are optimized for a particular kind of problem.

Adaptive Resonance: One obvious drawback to using a backpropagating net is the need to retrain the net every time a new pattern is added to the training set database. While the net should, in principle, have no problem in learning a new fact, there is the possibility that the newly trained net will “forget” previously stored information. This is sometimes loosely referred to as the *stability-plasticity problem*. One neural net design that addresses this concern head-on is called *Adaptive Resonance*, and is due to Carpenter and Grossberg [carp87]. A critical feature of adaptive resonance is its ability to switch between a learning state in which the net’s internal parameters can be modified (plasticity) and a fixed state wherein previously stored data cannot be damaged (stability).

Supervised Learning: Almost all of our discussion has centered on designs that require some sort of supervision for learning: nets are trained to learn a desired set of input-output relationships, where the output is known *a-priori*. However, we do not always know the output. It is certainly reasonable to expect a net to be able to effectively tell us what latent patterns and similarities exist within a clump of data. For this we need an entirely different neural net design, one that is optimized for finding common features across a range of input patterns in an unsupervised fashion. A well known exemplar of this class is Kohonen’s *Self-Organizing Feature Map* ([kohon84],[kohon90]). A more general approach to unsupervised learning called *competitive learning* is described in [rumel86d]. There are still other schemes, such as Hecht-Nielsen’s *Counterpropagation Networks* [hecht87b], that combine supervised and unsupervised learning in one net.

Tailoring a Design to a Specific Problem: Algorithms such as backpropagation can be viewed as general-purpose designs. By modifying a net’s size, topology, data set, or energy function, such nets can be applied to a wide variety of problems. However, there are problems for which either such a general-purpose design does not suffice or for which a better, optimized, design can be constructed. One such example is Fukushima’s *Cognitron* and larger-scaled *Neocognitron* neural net designs [fuku80], which are specifically tailored to recognize handwritten characters. Both the *Cognitron* and *Neocognitron* can learn with or without a supervisor and represent an approach based on exploiting the anatomy and physiology of the mammalian visual system.

Chapter 11

Artificial-Life

This chapter provides a very brief introduction to what is rapidly becoming one of the central research areas in complex systems theory; namely, *artificial-life* (AL). Owing its origins to von Neumann's early explorations of self-reproducing automata, AL has blossomed in the last decade from being defined by a few toy worlds hardly more sophisticated than Conway's *Life*-rule universe to intricately rendered 3D artificial universes populated with interacting creatures undergoing an open-ended evolution. While even a semi-complete treatment of AL would take us too far afield from the main thread of this book, it is nonetheless important to point out how AL derives, in part, from CA theory. *"Only when we are able to view life-as-we-know-it in the larger context of life-as-it-could-be will we really understand the nature of the beast. Artificial Life is a relatively new field employing a synthetic approach to the study of life-as-it-could-be. It views life as a property of the organization of matter, rather than a property of the matter which is so organized."*—Chris Langton [lang89]

11.1 Introduction

Artificial Life (AL) is an attempt to understand life as it is by examining a larger context of life as it could be. The underlying supposition is that life owes at least as much to its existence to the way in which information is organized as it does to the physical substance (i.e., matter) that embodies that information.

The fundamental concept of AL is emergence, or the appearance of higher-level properties and behaviors of a system that – while obviously originating from the collective dynamics of that system's components – are neither to be found in nor are directly deducible from the lower-level properties of that system. Emergent properties are properties of the "whole" that are not possessed by any of the individual parts making up that whole: an air molecule is not a tornado and a neuron is not conscious.

AL thus studies life by using artificial components (such as computer programs) to capture the behavioral essence of living systems. The supposition is that if the artificial parts are organized correctly, in a way that respects the organization of the living system, then the artificial system will exhibit the same characteristic dynamical behavior as the natural system on higher levels as well. Notice that this bottom-up, synthesist approach stands in marked contrast to more conventional top-down, analytical approaches. AL-based computer simulations are characterized by these five general properties [lang89]:

1. They are defined by populations of simple programs or instructions about how individual parts all interact.
2. There is no single "master oracle" program that directs the action of all other programs.
3. Each program defines how simple entities respond to their environment locally.
4. There are no rules that direct the global behavior.
5. Behaviors on levels higher than individual programs are emergent.

11.2 Local vs. Global

Despite recent progress, AL has not yet matured into a methodology that comes ready-made with IMSL-like algorithms and software routines. At best, it represents a new philosophy; a new way of thinking about some—sometimes very old—problems.

The term *collectivism* has sometimes been used to distinguish this AL philosophy from the more traditional "top down" and "bottom up" philosophies. Collectivism embodies the belief that in order to properly understand complex systems, such systems must be viewed as coherent wholes whose open-ended evolution is continuously fueled by nonlinear feedback between their macroscopic states and microscopic constituents. It is neither completely reductionist (which seeks only to decompose a system into its primitive components), nor completely synthesist (which seeks to synthesize the system out of its constituent parts but neglects the feedback between emerging levels).

As an example of the importance of collectivism, consider a natural ecology. Each species that makes up an ecology composed of a large number of diverse species, co-evolves with other members of the ecology according to a fitness function that is, in part, itself a function of the emerging ecology. Individual members of each species collectively define a (part of the) co-evolving ecology; the ecology, in turn, determines the fitness-function according to which its constituent parts evolve (see figure 11.1).

It is this nonlinear feedback between the information describing individual species (or the system's microscopic level) and the global ecology (or the system's macro-

scopic level) that those species collectively define that determines the temporal evolution – and identity – of the entire system.

Collectivism is thus distinct from both the top-down reductionist approach traditionally favored by most physicists (system as a simple edifice of its microscopic parts), and the more recent neural-net-like bottom-up approach favored by connectionists (system as a synthesis of its constituent parts). The nonlinear inter-level feedback loop that makes up the collective is what makes a traditional linear analysis of such systems difficult, if not impossible.

Analysis proceeds from the assumption that in order to understand a system one must first break it up into its constituent parts. Understanding then comes from the knowledge gained by reconstructing the system. But for systems whose dynamics depend critically on interaction between parts, analysis often misses the essential characteristics of the whole system. *Synthesis* is the complementary act of putting the individual pieces together in order to understand what they do collectively. Understanding complex synthesis requires that both analysis and synthesis be done.

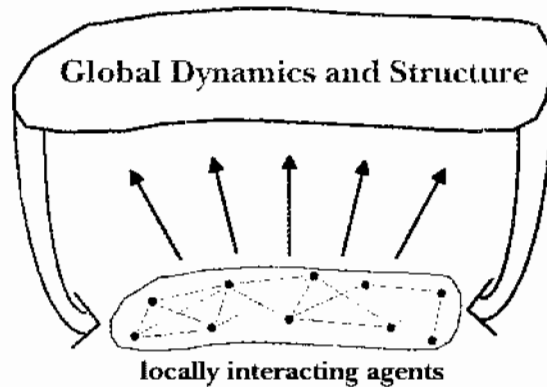


Fig. 11.1 Feedback between local and global levels ($\sim$ Collectivism).

11.3 Self-Organization

Self-organization is a fundamental characteristic of complex systems. It refers to the emergence of macroscopic nonequilibrium organized structures, and is due to the collective interactions of the constituents of a complex system as they react and adapt to their environment. There is no God-like "oracle" dictating what each and every part ought to be doing; parts act locally on local information and global order emerges without any need for external control.

At first sight, self-organization appears to violate the Second Law of Thermodynamics, which asserts that the entropy S of an isolated system never decreases (or, more formally, $\frac{dS}{dt} \geq 0$); see figure 11.2-a. Since entropy is essentially a measure of the degree of disorder in a system, the Second Law is usually interpreted to mean that an isolated system will become increasingly more disordered with time. How, then, can structure emerge after a system has had a chance to evolve?

Upon closer examination, we see that self-organization in complex system does not really violate the Second Law. The reason is that the Second Law requires a system to be isolated; that is, it must not exchange energy or matter with its environment.

For nonisolated systems consisting of noninteracting or only weakly interacting particles (see figure 11.2-b), the entropy S consists of two components: (1) an internal component, S_i , due to the processes taking place within the system itself, and (2) an external component, S_e , due to the exchange of energy and matter between the system and the environment. The rate of change of S with time, dS/dt , now becomes $dS/dt = dS_i/dt + dS_e/dt$. As for an isolated system, . But there are no $dS_i/dt \geq 0$ constraints on dS_e/dt . If dS_e/dt is sufficiently less than zero, the overall entropy of the system can itself decrease. Thus, the entropy of a nonisolated system of noninteracting or only weakly interacting particles can decrease due to the exchange of energy and/or matter between the system and its environment.

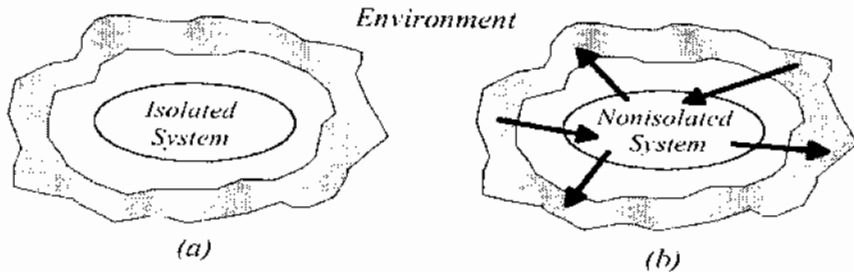


Fig. 11.2 Schematic of Isolated and Nonisolated Systems.

The situation is more complicated for nonisolated systems consisting of strongly interacting particles and when the system is no longer in equilibrium with the environment. Kauffman [kauff93] notes that the “second law really states that any system will tend to the maximum disorder possible, within the constraints due to the dynamics of the system.”

11.4 Emergence

Central to the general science of complexity is the concept of emergence. Emergence refers to the appearance of higher-level properties and behaviors of a system that – while obviously originating from the collective dynamics of that system’s components – are neither to be found in nor are directly deducible from the lower-level properties of that system. Emergent properties are properties of the *whole* that are not possessed by any of the individual parts making up that whole.

One of the simplest, and ubiquitous, examples of emergence is *temperature*, as read by a conventional thermometer. While temperature is a perfectly well-defined physical quantity on the macro-scale, it is a meaningless concept on the

level of a single atom or molecule. At the other extreme, we have one of the most complex (and still controversial) examples of emergence of human consciousness, which mysteriously emerges out of a caldron of interacting neurons. Consciousness cannot be found in any individual neuron, but is the collective property of the whole brain.

11.4.1 *Boids*

One of the most breathtakingly beautiful displays of nature is the synchronous, fluid-like flocking of birds. It is also an excellent example of emergence in complex systems. Large or small, the magic of flocks is the very strong impression they convey of some intentional centralized control directing the overall traffic. Though ornithologists still do not have a complete explanation for this phenomenon, evidence strongly suggests that flocking is a decentralized activity, where each bird acts according to its local perceptions of what nearby birds are doing. Flocking is therefore a group behavior that emerges from collective action.

Craig Reynolds [reyn87] programmed a set of artificial birds—which he called *boids*—to follow three simple local rules:

- *Maintain a minimum distance from other objects (including other boids).*
- *Match the velocity of nearby boids.*
- *Move toward the perceived center of nearby boids.*

Each boid thus "sees" only what its neighbors are doing and acts accordingly. Reynolds found that the collective motion of all the boids was remarkably close to real flocking, despite the fact that there is nothing explicitly describing the flock as a whole. The boids initially move rapidly together to form a flock. The boids at the edges either slow down or speed up to maintain the flock's integrity. If the path bends or zigzags in any way, the boids all make whatever minute adjustments need to be made to maintain the group structure. If the path is strewn with obstacles, the boids flock around whatever is in their way naturally, sometimes temporarily splitting up to pass an obstacle before reassembling beyond it. There is no central command that dictates this action.

Reynolds' Boids is a good example of decentralized order not because the boids' behavior is a perfect replica of the flocking of birds that occurs in nature — although it is a close enough match that Reynold's model has attracted the attention of professional ornithologists — but that much of the boids' collective behavior is entirely unanticipated, and cannot be easily derived from the rules defining what each individual boid does.

11.4.2 *Collective Sorting*

Beckers, et al. [beckers94], have introduced a simple distributed sorting algorithm that is inspired by the self-organized way in which ant colonies sort their brood.

Implemented by robot teams, their algorithm has the robots move about a fenced-in environment that is randomly littered with objects that can be scooped up. These robots (1) move randomly, (2) do not communicate with each other, (3) can perceive only those objects directly in front of them (but can distinguish between two or more types of objects with some degree of error), and (4) do not obey any centralized control. The probability that a robot picks up or puts down an object is a function of the number of the same objects that it has encountered in the past.

Coordinated by the positive feedback these simple rules induce between robots and their environment, the result, over time, is a seemingly intelligent, coordinated sorting activity. Clusters of randomly distributed objects spontaneously and quite naturally emerge out of a simple set of autonomous local actions having nothing at all to do with clustering per se.

The authors suggest that this system's simplicity, flexibility, error tolerance, and reliability compensate for their lower efficiency. While one can argue that this collective sorting algorithm is much less efficient than a hierarchical one, the cost of having a hierarchy is that the sorting would no longer be ant-like but would require a god-like oracle analyzing how many objects of what type are where, deciding how best to communicate strategy to the ants. Furthermore, the ants would require some sort of internal map, a rudimentary intelligence to deal with fluctuations and surprises in the environment (what if an object was not where the oracle said it would be?), and so on. In short, a hierarchy, while potentially more efficient, would of necessity have to be considerably more complex as well. The point Beckers, et al. are making is that a much simpler collective decentralized system can lead to seemingly intelligent behavior while being more flexible, more tolerant of errors, and more reliable than a hierarchical system.

11.5 Edge-of-Chaos

One often hears the phrase edge-of-chaos in discussions of AL, as in "such and such a system appears poised at the edge-of-chaos." As this important concept is still a topic of some debate, we make a few comments regarding it.

Chris Langton [lang92a] opens his *Life at the Edge of Chaos* paper at the Artificial Life II conference with the following intriguing question: "Under what conditions can we expect a dynamics of information to emerge spontaneously and come to dominate the behavior of a physical system?" While his question was, in that paper, motivated chiefly by an understanding that living organisms may be distinguished from inanimate matter by the fact that their behavior is clearly based on a complex dynamics of information, its roots extend considerably deeper.

Langton was able to provide a tentative answer to his question by examining the behavior of the entire rule space of elementary one-dimensional cellular automata rules (see discussion in section 3.2) as parameterized by a single parameter λ . He found that as λ is increased from its minimal to maximal values, a path is effectively traced in the rule space that progresses from fixed point behavior to simple period-

icity to evolutions with longer and longer periods with increasing transients, passes through an intermediate transition region at a critical value λ_c , crosses over into a chaotic regime of steadily diminishing complexity until, eventually, the behavior is again completely predictable at the maximal value of λ and complexity falls back to zero. Because the transition region represents the region of greatest complexity and lies between regions in which the behavior is either ordered or chaotic, Langton christened the transition region as the *edge-of-chaos*.

Langton's tentative answer to the question above is therefore: "We expect that information processing can emerge spontaneously and come to dominate the dynamics of a physical system in the vicinity of a critical phase transition." Langton speculates that the dynamics of phase transitions is fundamentally equivalent to the dynamics of information processing.

Strictly speaking, Langton's edge-of-chaos idea holds true only for the specific system in which it was discovered. Nonetheless, the idea has frequently been used as a general metaphor for the region in "complexity space" toward which complex adaptive systems appear to naturally evolve (see figure 11.3). Kauffman ([kauff91b], [kauff95]), in particular, is a staunch advocate of the idea that systems poised at the edge-of-chaos are optimized, in some sense, to evolve, adapt and process information about their environment.

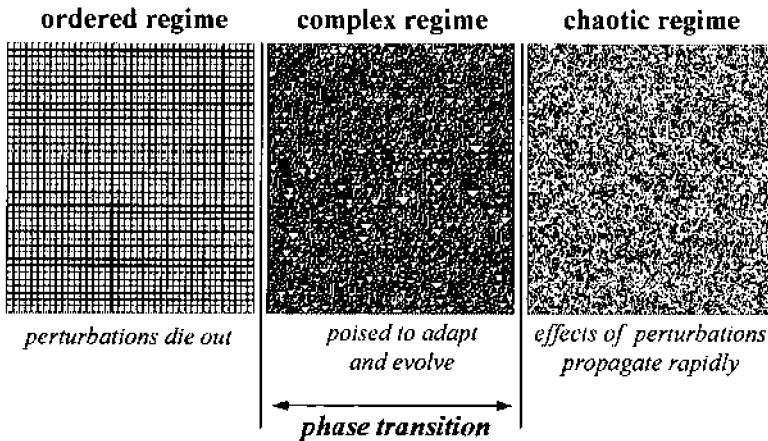


Fig. 11.3 A Schematic illustration of the *Edge-of-Chaos* metaphor.

Effective computation, such as that required by life processes and the maintenance of evolvability and adaptability in complex systems, requires both the storage and transmission of information. If correlations between separated sites (or agents) of a system are too small – as they are in the ordered regime shown in figure 11.3 – the sites evolve essentially independently of one another and little or no transmission takes place. On the other hand, if the correlations are too strong – as they are in the chaotic regime – distant sites may cooperate so strongly so as to effectively mimic each other's behavior, or worse yet, whatever ordered behavior is present may be

overwhelmed by random noise; this, too, is not conducive to effective computation. It is only within the phase transition region – in the complex regime poised at the edge-of-chaos – that information can propagate freely over long distances without appreciable decay. However loosely defined, the behavior of a system in this region is best described as complex; i.e. it neither locks into an ordered pattern nor does it dissolve into an apparent randomness. Systems existing in this region are both stable enough to store information and dynamically amorphous enough to be able to successfully transmit it.

However intuitive the edge-of-chaos idea appears to be, one should be aware that it has received a fair amount of criticism in recent years. It is not clear, for example, how to even define complexity in more complicated systems like coevolutionary systems, much less imagine a phase transition between different complexity regimes. Even Langton's suggestion that effective computation within the limited domain of cellular automata can take place only in the transition region has been challenged.[†]

11.6 Agent-Based Models

Agent-based simulations of complex adaptive systems are becoming an increasingly popular theoretical exploratory tool in the artificial-life community, and are predicated on the basic idea that the (often complicated) global behavior of a real system derives, collectively, from simpler, low-level interactions among its constituent agents. Insights about the real-world system that the agent-based simulation is designed to model can then be gained by looking at the emergent structures induced by the interaction processes taking place within the simulation. Two excellent recent texts on agent-based modeling, as applied to variety of disciplines, are by Ferber [ferb99] and Weiss [weisg99]. Books and collections of papers focusing on applications to social science (and other systems that involve some aspect of "human reasoning") are by Gilbert and Troitzsch [gilb199], Gilbert and Conte [gilb195] and Conte, et al. [cont97].

The purpose behind building an agent-based simulation of real-world system is twofold: it is to learn both the quantitative and qualitative properties of the real system. Agent-based simulations are well suited for testing hypotheses about the origin of observed emergent properties in a system. This is done simply by experimenting with sets of initial conditions at the micro-level necessary to yield a set of desired behaviors at the macro-level. Moreover, agent-based models provide a powerful framework within which to integrate the explanatory power of what – a-priori – may appear to be unrelated disciplines. For example, while basic agent-agent interactions may be described by simple physics and high-level group dynamics, the internal decision-making capability of a single agent may be derived, in part, from a deeper understanding of the psychology of motivation, fear.

The fundamental building block of most models of complex adaptive systems

[†]Mitchell, M., P.T.Hraber and J.P.Crutchfield, "Revisiting the edge of chaos: evolving cellular automata to perform computations," *Complex Systems*, Volume 7, 1993, 89-130.

is the so-called adaptive autonomous agent. Adaptive autonomous agents try to satisfy a set of goals (which may be either fixed or time-dependent) in an unpredictable and changing environment. These agents are "adaptive" in the sense that they can use their experience to continually improve their ability to deal with shifting goals and motivations. They are "autonomous" in that they operate completely autonomously, and do not need to obey instructions issued by a God-like oracle.

Depending on the system being modeled and the environment that an agent populates, an adaptive autonomous agent can take on many different forms. In Beckers et al.'s [beckers94] study of decentralized collective sorting, for example, the agents of the system are simple (nonadaptive) robots that move about their physical environment and make elementary decisions about whether to pick up or drop an object. Examples of adaptive agents populating "cyberspace" are the so-called "software agents" (or "knobots") that are entities that navigate computer networks or cruise the World-Wide-Web searching for relevant bits of data.

In general, an adaptive autonomous agent is characterized by the following properties [maesp90]:

- *Interaction with Environment*: It senses the (often complex and dynamic) environment through its sensors and reacts accordingly.
- *Goal-Driven Motivations*: It is an entity that, by sensing and acting upon its environment, tries to fulfill a set of goals. The goals can take on diverse forms, including satisfying local states and/or end goals, maximizing intermediate rewards, or by keeping the states of internal needs within desired bounds.
- *Intelligence*: It has an internal information processing and decision-making capability by which it uses local information to select actions.
- *Adaptive Dynamics*: Its anticipation of future states and possibilities, based on internal models (which are often incomplete and/or incorrect), often significantly alters the aggregate behavior of the system of which an agent is part.

An agent's goals can take on diverse forms:

- Desired local states.
- Desired end goals.
- Selective rewards to be maximized.
- Internal needs (or motivations) that need to be kept within desired bounds.

Since a major component of an agent's environment consists of other agents, agents generally spend a great deal of their time adapting to the adaptation patterns

of other agents. The adaptive mechanism of an adaptive autonomous agent is typically based on a genetic algorithm (see below).

Insofar as complex adaptive systems can be regarded as being essentially open-ended problem-solvers, their lifeblood consists mostly of novelty. The ability of a complex adaptive system to survive and evolve in a constantly changing environment is determined by its ability to continually find — either by chance, or experience, or more typically both — insightful new strategies to increase its overall “fitness” (which is, of course, a constantly changing function in time).

Some recent examples of agent-based models include ECHO (an agent-based model of natural ecologies [echo]), MOAB (the U.S. Geological Survey’s model of animal behavior [moab]), Sugarscape (a model of the evolution of social systems [epsj96]), TRANSIM (a model of traffic flow [barret97]). The well-known series of *SimCity* and *SimCity*-related commercial games (*SimLife*, *SimAnt*, etc.) all make heavy use of agent-based methodologies [simcity]. A more recent example of a commercial game that is also making original contributions to adaptive-agent modeling methodology is Cyberlife’s *Creatures* (<http://www.cyberlife.co.uk/>). An extensive, annotated web-based listing of agent-based models is maintained by Craig Reynolds at URL address <http://www.red3d.com/cwr/ibm.html>.

Models based on differential equations homogenize the properties of entire populations and ignore the spatial component altogether. Partial differential equations — by introducing a physical space to account for agent movement — fare somewhat better, but still treat the agent population as a continuum. In contrast, agent-based models consist of a discrete heterogeneous set of spatially distributed individual agents, each of which has its own characteristic properties and rules of behavior. These properties can also change (i.e., adapt) as an individual agent evolves in time.

11.6.1 *Agent-Based Simulations vs. Traditional AI*

“It is hard to point at a single component [of an AI program] as the seat of intelligence, there is no homunculus. Rather, intelligence emerges from the interactions of the components of the system. The way in which it emerges, however, is quite different for traditional and behavior-based AI systems.” [steels95]

Agent-based simulations and traditional computer simulations (as well as conventional differential-equation based models) differ in one key respect: while traditional models ignore layers of complexity for the sake of achieving a simplified description of overall behavior of a system, agent-based simulations seek to find the simplest underlying explanation for the observed complexity. Traditional models focus on high-level descriptions because they assume that the behaviors of individual agents must be driven by complicated behavior that itself cannot be modeled. In contrast, agent-based models proceed from the assumption that it is the interaction among agents — all of whom individually behave according to rather simple rules — that leads to the complex behavior that is observed. In general, the conceptual

focus of agent-based models is on finding a set of low-level rules defining the local behavior of individual agents; the collective action of these agents determines the dynamics of the whole system.

Agent-based models take an actively generative (or synthesist) approach to understanding a system, *from the bottom up*.[†] This is in contrast to the purely analytical approach that most traditional models take to the same problem, in which a system is regarded as being "understood" when it has been analyzed, and its essential ingredients distilled, from the top down. Where traditional models ask, effectively, "How can I characterize the system's top-level behavior with a few (equally top-level) variables?," agent-based simulations instead ask, "What low-level rules and what kinds of heterogeneous, autonomous agents do I need to have in order to synthesize the system's observed high-level behavior?"

While a valid and useful answer to the first question can often be found, there is at least one significant drawback to this approach: so many simplifying assumptions must usually be made about the real system, in order to render the top-level problem a soluble one, that other natural, follow-up questions such as "Why do specific behaviors arise?" or "How would the behavior change if the system were defined a bit differently?" cannot be meaningfully addressed without first altering the set of assumptions. An analytical, closed-form "solution" may describe a behavior, however, it does not necessarily provide an explanation for that behavior. Indeed, subsequent questions about the behavior of the system must usually be treated as separate problems.

An important benefit of using an agent-based simulation is that, once the simulation is used to generate the desired behavior, the modeler has immediate and simultaneous access to both the top-level (i.e. generated) behavior of the system and a low-level description of the system's underlying dynamics: i.e. the agent-based simulation thus becomes a powerful methodological tool for not just describing behaviors but explaining why specific behaviors occur. While an analytical solution may provide an accurate description of a phenomenon, it is only with an agent-based simulation that one can fine-tune one's understanding of the precise set of conditions under which certain behaviors emerge.

Any system whose top-level behavior is a consequence of the aggregate behavior of lower-level entities – biological systems, neural systems, social systems, economic systems, among many others – can, in principle, be simulated by an agent-based model.

At first sight, the kinds of problems best suited for agent-based simulations appear to be similar to the kinds of problems for which traditional artificial intelligence (AI) techniques have been developed. How is an agent-based simulation different from a traditional artificial intelligence approach? Maes [maesp94] lists four key points that distinguish traditional AI from the study of adaptive autonomous agents:

[†]Epstein [epsj99] presents a cogent argument for why agent-based models are particularly useful as generative, explanatory, tools in social science.

1. *Target Low-Level Behaviors:* Traditional AI focuses on systems exhibiting isolated "high-level" competencies, such as medical diagnoses, chess playing, and so on; in contrast, agent-based systems target lower-level behaviors, with high-level competencies emerging naturally, and collectively, of their own accord.
2. *Target Open Systems:* Traditional AI has focused on "closed systems" in which the interaction between the problem domain and the external environment is kept to a minimum; in contrast, agent-based systems are "open systems," and agents are directly coupled with their environment.
3. *Target Multi-Objective Goals:* Most traditional AI systems deal with problems in a piecemeal fashion, one at a time; in contrast, the individual agents in an agent-based system must deal with many conflicting goals simultaneously.
4. *Bounded Rationality:* Traditional AI focuses on "knowledge structures" that model aspects of their domain of expertise; in contrast, an agent-based system is more concerned with dynamic "behavior producing" modules. It is less important for an agent to be able to address a specific question within its problem domain (as it is for traditional AI systems) than it is to be flexible enough to adapt to shifting domains.

As agent-based simulation techniques mature, the methodology has the potential to usher in an alternative way to do science; a way that is neither totally deductive nor totally inductive, at least in the conventional sense. While agent-based simulations, like deductive methods, start from a set of primitive rules and assumptions they do not prove theorems; rather, they generate behaviors that must themselves be studied inductively. Unlike traditional induction, however, that uncovers patterns in empirically derived data, agent-based simulations provide the framework for discovering (presumably real-world) high-level patterns that emerge out of the collective interactions of simulated low-level rules.

11.6.2 *Swarm*

Swarm[†] is a multi-agent simulation platform for the study of complex adaptive systems. It is currently under development at the Santa Fe Institute[§]

The goal of the Swarm project is to provide the complex systems theory research community with a fully general-purpose artificial-life simulator. The system comes with a variety of generic artificial worlds populated with generic agents, a large library of design and analysis tools and a "kernel" to drive the actual simulation. These artificial worlds can vary widely, from simple 2D worlds in which elementary agents move back and forth to complex multi-dimensional "graphs" representing

[†]This section is based on the papers "An Overview of the Swarm simulation system," by '94 Swarm Team, Santa Fe Institute and "The Swarm simulation system and individual-based modeling," by D. Hiebler.

[§]World-Wide-Web URL link = <http://www.santafe.edu/projects/swarm/>.

multidimensional telecommunication networks in which agents can trade messages and commodities, to models of real-world ecologies.

Swarm has been intentionally designed to include as few ad-hoc assumptions about the design of a complex system as possible, so as to provide a convenient, reliable and standardized set of software tools that can be tailored by researchers to specific systems.

Though the prototype has been written using the C programming language, it is object-oriented in style. Future versions of Swarm will be implemented using the Objective-C language. Objective-C is an object-oriented extension of the C language that is widely available as part of the GNU C compiler, and is available on the World-Wide-Web.

Everything in Swarm is an object with three main characteristics: Name, Data and Rules. An object's Name consists of an ID that is used to send messages to the object, a type and a module name. An object's Data consists of whatever local data (i.e. internal state variables) the user wants an agent to possess. The Rules are functions to handle any messages that are sent to the object. The basic unit of Swarm is a "swarm": a collection of objects with a schedule of event over those objects. Swarm also supplies the user with an interface and analysis tools.

The most important objects in Swarm, from the standpoint of the user, are agents, which are objects that are written by the user. Agents represent the individual entities making up the model; they may be ants, plants, stock brokers, or combatants on a battlefield. Actions consist of a message to send, an agent or a collection of agents to send the message, and a time to send that message. Upon receiving a message, agents are free to do whatever they wish in response to the message. A typical response will consist of the execution of whatever code the user has written to capture the low-level behavior of the system he is interested in. Agents can also insert other actions into the schedule.

Three other properties of Swarm are noteworthy:

Hierarchical Structure. In order to be better able to simulate the hierarchical nature of many real-world complex systems, in which agent behavior can itself be best described as being the result of the collective behavior of some swarm of constituent agents, Swarm is designed so that agents themselves can be swarms of other agents. Moreover, Swarm is designed around a time hierarchy. Thus, Swarm is both a nested hierarchy of swarms and a nested hierarchy of schedules.

Parallel Dynamics. Swarm has been designed to run efficiently on parallel machine architectures. While messages within one swarm schedule execute sequentially, different swarms can execute their schedules in parallel.

Internal Agent Models. One can argue that agents in a real complex adaptive system (such as the economy) behave and adapt according to some internal model they have constructed for themselves of what they believe their environment is really like. Sometimes, if the environment is simple, such models are fixed and simple; sometimes, if the environment is complex, agents need to actively construct

hypothetical models and testing them against a wide variety of assumptions about initial states and rules and so forth. Swarm allows the user to use nested swarms to allow agents to essentially create and manage entire swarm structures which are themselves simulations of the world in which the agents live. Thus, agents can base their behavior on their simulated picture of the world.

The many kinds of problems that Swarm is well suited for include economic models (with economic agents interacting with each other through a market), the dynamics of social insects, traffic simulation, ecological modeling, simulation games such as SimCity and SimLife, and general studies of complex systems, cellular automata, and artificial life.

11.7 Self-Reproducing Automata

John von Neumann originally conceived of cellular automata as abstract models of “self-reproducing machines”. He was intrigued by the apparent disparity between how, on the one hand, nature handles reproduction – in which the complexity of the offspring is generally at least as great as its parent – and how, on the other hand, mechanical assembly lines appear to inevitably decrease complexity (i.e. the assembly line is generally a more complex “machine” than the machine (or machines) that it is designed to construct). Von Neumann asked the obvious question of whether there was a way to construct a “self-reproducing machine” capable of producing other machines without a concomitant loss of complexity. The following long quote, taken from von Neumann’s seminal work, *The Theory of Automata: Construction, Reproduction, Homogeneity* [vonN66], eloquently summarizes his fundamental motivations (note, in particular, his emphasis on self-reproduction):

We will investigate automata under two important and connected, aspects: those of logics and of construction. We can organize our considerations under the headings of five main questions:

(A) Logical universality. *When is a class of automata logically universal, i.e. able to perform all those logical operations that are all performable with finite (but arbitrarily extensive) means? Also, with what additional – variable, but in the essential respects standard – attachments is a single automaton logically universal?*

(B) Constructibility. *Can an automaton be constructed, i.e. assembled and built from appropriately defined ‘raw materials’, by another automaton? Or, starting from the other end and extending the question, what class of automata can be constructed by one, suitably given, automaton? The variable, but essentially standard attachments to the latter, in the sense of the second question of (A), may here be permitted.*

(C) Construction-universality. *Making the second question of (B) more specific, can any one, suitably given, automaton be construction-universal, i.e. be able to construct in the sense of question (B) (with suitable, but essentially standard, attachments) every other automaton?*

(D) **Self-reproduction.** Narrowing question (C), can any automaton construct other automata that are exactly like it? Can it be made, in addition, to perform further tasks, e.g. also construct certain other prescribed automata?

(E) **Evolution.** Combining questions (C) and (D), can the construction of automata by automata progress from simpler types to increasingly complicated types? Also, assuming some suitable definition of 'efficiency', can this evolution go from less efficient to more efficient automata?

Von Neumann approached the problem with the assurance that since self-reproduction in nature consists of (albeit highly complex) biochemical machines, the actions of a given biological machine should therefore also be describable by an algorithm. Von Neumann then argued that if such an algorithm exists, then there should also be a Universal Turing Machine (UTM) than can perform it; i.e. *there should exist a UTM capable of self-reproduction*. The fundamental conclusion that von Neumann was really after is actually best expressed in reverse order; namely, that fact that such a self-reproducing UTM exists at all, by itself immediately lends credence to the assertion that the processes by which living organisms reproduce themselves (and, arguably, the mechanisms of *Life itself*) are achievable by machines.

Von Neumann was able to construct a self-reproducing UTM embedded within a 29-state/5-cell neighborhood two-dimensional cellular automaton, composed of several tens of thousands of cells. It was, to say the least, an enormously complex "machine". Its set of 29 states consist largely of various logical building blocks (AND and OR gates, for example), several types of transmission lines, data encoders and recorders, clocks, etc. Von Neumann was unfortunately unable to finish the proof that his machine was a UTM before his death, but the proof was later completed and published by Arthur Burks [vonN66].

Von Neumann's machine is actually an example of a *universal constructor*. It must not only carry out logical operations (i.e. act as a universal computer), but must also be able to identify and *manipulate* various components. The universal constructor C must be able to both (1) construct the machine whose "blueprint" appears in symbolic form on its input tape and (2) attach a copy of that same blueprint to the machine once it is constructed. Self-reproduction is the special case where C 's input tape actually contains the blueprint data for C itself. Alas, there are a few subtleties.

Suppose we start with an automaton A that is given a tape with a blueprint B_A on it. The composite machine will then construct a copy of A but it is not, in and of itself, self-reproducing; i.e. the aggregate machine $A + B_A$ creates A , not $A + B_A$. This situation is not remedied by simply adding a description of B_A to B_A , since in this case $A + B_{A+B_A}$ yields $A + B_A$ and not $A + B_{A+B_A}$. Thus, whatever we try seems destined to lead in an infinite regress!

Von Neumann recognized this problem, of course. His solution was to essentially use the cooperative action of several automata to effectively copy a machine's blueprint. He first introduced a 'copier' automaton A' that copies whatever blueprint B it is given. Next, he defined an automaton A'' that inserts a copy of B into the

automaton constructed by $\mathcal{A}$. Let us call the composite structure $\mathcal{A} + \mathcal{A}' + \mathcal{A}''$ by $\tilde{\mathcal{A}}$. Let $B_{\tilde{\mathcal{A}}}$ be the blueprint of $\tilde{\mathcal{A}}$ and let $\hat{\mathcal{A}}$ be $\tilde{\mathcal{A}}$ with $B_{\tilde{\mathcal{A}}}$ inserted as a tape into $\mathcal{A}$. Then $\hat{\mathcal{A}}$ is self-reproducing and, since $\tilde{\mathcal{A}}$ exists before the blueprint $B_{\tilde{\mathcal{A}}}$ is itself defined, no infinite ingress is involved.

11.7.1 Just How Complex Must a Self-Reproducing Automaton Be?

Von Neumann was able to design a self-reproducing automaton using several thousand cells, a five site neighborhood and 29 states per site [vonN66]. A few years later, Thatcher [that70] used the same 29 states but was able to simplify the construction considerably. Codd, in his Doctoral dissertation [codd70], managed to reduce the number of required states to just *eight* states per cell. Codd's model, however, like that of his predecessor's, unfortunately also involved tens of thousands of cells; a simplified proof was later published by Arbib [arbib66].

$\sigma_C \sigma_T \sigma_R \sigma_B \sigma_L$ $\rightarrow \sigma'_C$	$\sigma_C \sigma_T \sigma_R \sigma_B \sigma_L$ $\rightarrow \sigma'_C$	$\sigma_C \sigma_T \sigma_R \sigma_B \sigma_L$ $\rightarrow \sigma'_C$	$\sigma_C \sigma_T \sigma_R \sigma_B \sigma_L$ $\rightarrow \sigma'_C$	$\sigma_C \sigma_T \sigma_R \sigma_B \sigma_L$ $\rightarrow \sigma'_C$
00000 $\rightarrow$ 0	02527 $\rightarrow$ 1	11322 $\rightarrow$ 1	20242 $\rightarrow$ 2	30102 $\rightarrow$ 1
00001 $\rightarrow$ 2	10001 $\rightarrow$ 1	12224 $\rightarrow$ 4	20245 $\rightarrow$ 2	30122 $\rightarrow$ 0
00002 $\rightarrow$ 0	10006 $\rightarrow$ 1	12227 $\rightarrow$ 7	20252 $\rightarrow$ 0	30251 $\rightarrow$ 1
00003 $\rightarrow$ 0	10007 $\rightarrow$ 7	12243 $\rightarrow$ 4	20255 $\rightarrow$ 2	40112 $\rightarrow$ 0
00005 $\rightarrow$ 0	10011 $\rightarrow$ 1	12254 $\rightarrow$ 7	20262 $\rightarrow$ 2	40122 $\rightarrow$ 0
00006 $\rightarrow$ 3	10012 $\rightarrow$ 1	12324 $\rightarrow$ 4	20272 $\rightarrow$ 2	40155 $\rightarrow$ 0
00007 $\rightarrow$ 1	10021 $\rightarrow$ 1	12327 $\rightarrow$ 7	20312 $\rightarrow$ 2	40212 $\rightarrow$ 0
00011 $\rightarrow$ 2	10024 $\rightarrow$ 1	12425 $\rightarrow$ 5	20321 $\rightarrow$ 6	40222 $\rightarrow$ 1
00012 $\rightarrow$ 2	10027 $\rightarrow$ 7	12426 $\rightarrow$ 7	20322 $\rightarrow$ 6	40232 $\rightarrow$ 6
00013 $\rightarrow$ 2	10051 $\rightarrow$ 1	12527 $\rightarrow$ 5	20342 $\rightarrow$ 2	40252 $\rightarrow$ 0
00021 $\rightarrow$ 2	10101 $\rightarrow$ 1	20001 $\rightarrow$ 2	20422 $\rightarrow$ 2	40322 $\rightarrow$ 1
00022 $\rightarrow$ 0	10111 $\rightarrow$ 1	20002 $\rightarrow$ 2	20512 $\rightarrow$ 2	50002 $\rightarrow$ 2
00023 $\rightarrow$ 0	10124 $\rightarrow$ 4	20004 $\rightarrow$ 2	20521 $\rightarrow$ 2	50021 $\rightarrow$ 5
00026 $\rightarrow$ 2	10127 $\rightarrow$ 7	20007 $\rightarrow$ 1	20522 $\rightarrow$ 2	50022 $\rightarrow$ 5
00027 $\rightarrow$ 2	10202 $\rightarrow$ 6	20012 $\rightarrow$ 2	20552 $\rightarrow$ 1	50023 $\rightarrow$ 2
00032 $\rightarrow$ 0	10212 $\rightarrow$ 1	20015 $\rightarrow$ 2	20572 $\rightarrow$ 5	50027 $\rightarrow$ 2
00052 $\rightarrow$ 5	10221 $\rightarrow$ 1	20021 $\rightarrow$ 2	20622 $\rightarrow$ 2	50052 $\rightarrow$ 0
00062 $\rightarrow$ 2	10224 $\rightarrow$ 4	20022 $\rightarrow$ 2	20672 $\rightarrow$ 2	50202 $\rightarrow$ 2
00072 $\rightarrow$ 2	10226 $\rightarrow$ 3	20023 $\rightarrow$ 2	20712 $\rightarrow$ 3	50212 $\rightarrow$ 2
00102 $\rightarrow$ 2	10227 $\rightarrow$ 7	20024 $\rightarrow$ 2	20722 $\rightarrow$ 2	50215 $\rightarrow$ 2
00112 $\rightarrow$ 0	10232 $\rightarrow$ 7	20025 $\rightarrow$ 0	20742 $\rightarrow$ 2	50222 $\rightarrow$ 0
00202 $\rightarrow$ 0	10242 $\rightarrow$ 4	20026 $\rightarrow$ 2	20772 $\rightarrow$ 2	50224 $\rightarrow$ 4
00203 $\rightarrow$ 0	10262 $\rightarrow$ 6	20027 $\rightarrow$ 2	21122 $\rightarrow$ 2	50272 $\rightarrow$ 2
00205 $\rightarrow$ 0	10264 $\rightarrow$ 4	20032 $\rightarrow$ 6	21126 $\rightarrow$ 1	51212 $\rightarrow$ 2
00212 $\rightarrow$ 5	10267 $\rightarrow$ 7	20043 $\rightarrow$ 3	21222 $\rightarrow$ 2	51222 $\rightarrow$ 0
00222 $\rightarrow$ 0	10271 $\rightarrow$ 0	20051 $\rightarrow$ 7	21224 $\rightarrow$ 2	51242 $\rightarrow$ 2
00232 $\rightarrow$ 2	10272 $\rightarrow$ 7	20052 $\rightarrow$ 2	21226 $\rightarrow$ 2	51272 $\rightarrow$ 2
00522 $\rightarrow$ 2	10542 $\rightarrow$ 7	20057 $\rightarrow$ 5	21227 $\rightarrow$ 2	60001 $\rightarrow$ 1
01232 $\rightarrow$ 1	11112 $\rightarrow$ 1	20072 $\rightarrow$ 2	21422 $\rightarrow$ 2	60002 $\rightarrow$ 1
01242 $\rightarrow$ 1	11122 $\rightarrow$ 1	20102 $\rightarrow$ 2	21522 $\rightarrow$ 2	60212 $\rightarrow$ 0
01252 $\rightarrow$ 5	11124 $\rightarrow$ 4	20112 $\rightarrow$ 2	21622 $\rightarrow$ 2	61212 $\rightarrow$ 5
01262 $\rightarrow$ 1	11125 $\rightarrow$ 1	20122 $\rightarrow$ 2	21722 $\rightarrow$ 2	61213 $\rightarrow$ 1
01272 $\rightarrow$ 1	11126 $\rightarrow$ 1	20142 $\rightarrow$ 2	22227 $\rightarrow$ 2	61222 $\rightarrow$ 5
01275 $\rightarrow$ 1	11127 $\rightarrow$ 7	20172 $\rightarrow$ 2	22244 $\rightarrow$ 2	70007 $\rightarrow$ 7
01422 $\rightarrow$ 1	11152 $\rightarrow$ 2	20202 $\rightarrow$ 2	22246 $\rightarrow$ 2	70112 $\rightarrow$ 0
01432 $\rightarrow$ 1	11212 $\rightarrow$ 1	20203 $\rightarrow$ 2	22276 $\rightarrow$ 2	70122 $\rightarrow$ 0
01442 $\rightarrow$ 1	11222 $\rightarrow$ 1	20205 $\rightarrow$ 2	22277 $\rightarrow$ 2	70125 $\rightarrow$ 0
01472 $\rightarrow$ 1	11224 $\rightarrow$ 4	20207 $\rightarrow$ 3	30001 $\rightarrow$ 3	70212 $\rightarrow$ 0
01625 $\rightarrow$ 1	11225 $\rightarrow$ 1	20212 $\rightarrow$ 2	30002 $\rightarrow$ 2	70222 $\rightarrow$ 1
01722 $\rightarrow$ 1	11227 $\rightarrow$ 7	20215 $\rightarrow$ 2	30004 $\rightarrow$ 1	70225 $\rightarrow$ 1
01725 $\rightarrow$ 5	11232 $\rightarrow$ 1	20221 $\rightarrow$ 2	30007 $\rightarrow$ 6	70232 $\rightarrow$ 1
01752 $\rightarrow$ 1	11242 $\rightarrow$ 4	20232 $\rightarrow$ 2	30012 $\rightarrow$ 3	70252 $\rightarrow$ 5
01762 $\rightarrow$ 1	11262 $\rightarrow$ 1	20227 $\rightarrow$ 2	30042 $\rightarrow$ 1	70272 $\rightarrow$ 0
01772 $\rightarrow$ 1	11272 $\rightarrow$ 7	20232 $\rightarrow$ 1	30062 $\rightarrow$ 2	

Table 11.1 Transition function table for Langton's self-reproducing loops (taken from table

1 in [lang86]). Neighborhoods are defined by $\begin{pmatrix} \sigma_T \\ \sigma_L \quad \sigma_C \quad \sigma_R \\ \sigma_B \end{pmatrix} \rightarrow \sigma'_C$.

Langton [lang84], by adopting a somewhat “looser” definition of self-reproduction (see below), managed to construct a self-reproducing structure using the same number of states as Codd’s model but requiring an area of just 10×15 sites! The current lower bound on the minimal complexity necessary for self-reproduction belongs to Byl [byl89], who, using Langton’s own “loose” definition, reduced the system requirements to only *six* states per site and an area of just 4×4 sites.

11.7.2 Langton’s Self-Reproducing Loop

Langton [lang84] had observed that while von Neumann’s, Thatcher’s and Codd’s automata were all clearly *sufficient* for self-reproduction, their enormous complexity did little to settle the question of what is *necessary* for self-reproduction. What might such a set of necessary conditions look like? On the one hand, we know that there are numerous examples of naturally occurring self-reproducing systems none of which, however, are capable of universal construction. It is also highly unlikely that early forms of self-replicating molecules were capable of universal construction [lang84]. On the other hand, calling a simple one-dimensional two state ‘addition modulo 2’ rule “self-reproducing” merely by virtue of its ability to generate replicas of certain local configurations, is silly. In this case, structures are reproduced only as a consequence of the *dynamics* and not by any self-generated (recursive) action taken by the presumably self-reproducing structures themselves. Langton felt that the answer lies somewhere in-between these two extremes, and proceeded by taking a cue from von Neumann’s own construction.

Recall our outline of the von Neumann construction, and the subtlety involved in eliminating what at first sight appears to be an inevitable infinite regress. The subtlety arises essentially because we are forced to think of our blueprint data as both (i) consisting of active instructions that must be executed and (ii) as an assemblage of passive information that is merely a part of the overall structure that must be copied and attached to the offspring machine.

Mindful of this critical dual-naturedness of von Neumann’s machine, Langton adopted the following criteria as necessary for self-reproduction: *the offspring must come into being not through some passive mechanism relying exclusively on the underlying dynamics acting on the original structure (or data contained within the structure) but must be actively determined by the self-reproducing structure itself.* To be sure, reproduction is allowed to take place *in part* because of the particular dynamical rules governing the system; what is required is that the reproduction proceed *mainly* as a result of the actions of the parent structure itself.

Using this looser criterion of self-reproduction – it is looser since, unlike von Neumann’s requirement, it does not force the self-reproducing structure to be capable of universal construction – Langton discovered a relatively simple self-reproducing structure embedded within a two-dimensional CA that we will refer to as Langton’s Loop; figure 11.4 shows a few snapshots of its 151 time-step reproduction cycle.

Consider a two-dimensional array of sites, where each site $\sigma_{i,j} \in \{0, 1, \dots, 7\}$ and evolves according to the four-neighbor von Neumann neighborhood rule defined in table 11.1. Each of the eight states has a specific function to perform. The state

$\sigma = 0$, for example, represents the usual quiescent state; states $\sigma = 1$ and $\sigma = 2$ are used to guide the signal, where $\sigma = 1$ is itself an element of the data path while $\sigma = 2$ forms a protective wall around the signal as it propagates. The remaining five states $3 \leq \sigma \leq 7$ represent the signal, where an individual signal consists of a string of any number of these five states followed by the state $\sigma = 0$.

When a signal reaches a 'T' junction it splits into two copies of itself, one copy traveling along each path. Whenever a '7-0' signal reaches the end of its data path, the path is extended by one site.

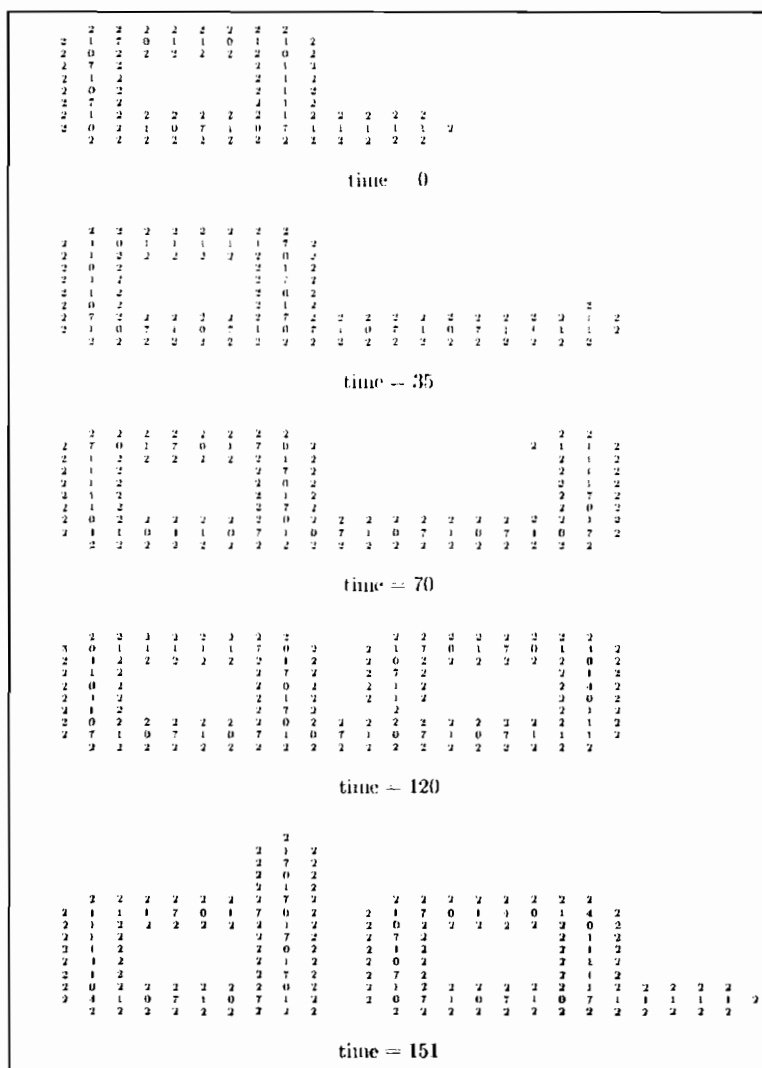


Fig. 11.4 A few snapshot views in the birth of a *Langton-loop offspring*.

Whenever two '4-0' signals reach the end in succession, a *left-hand corner* is created. The state $\sigma = 3$ is used as an intermediate state while a signal is turning a left corner; states $\sigma = 5$ and $\sigma = 6$ separate the offspring loop from its parent.

Applying these rules to the parent loop at time $t = 1$ (see figure 11.4), we find that the parent loop first extends its arm by 6 sites, makes a left turn, adds another 6 sites, turns left again, adds another 6 sites and turns left for third and last time before closing in on itself. At this point states $\sigma = 5$ and $\sigma = 6$ appear and disconnect the two loops, leaving the original parent loop along with the offspring to its right. Since the offspring loop is an exact replica of its parent, it behaves in exactly the same manner and so yields its own offspring (to its right).

Meanwhile, the original parent proceeds to construct a second offspring, this time above itself since its *arm* was rotated by 90 degrees during the original reproduction. This process continues so that, over a period of time, an entire colony expands outward from the original parent. Because a parent always rotates 90 degrees counterclockwise during each reproduction cycle, each parent loop must eventually encounter another loop residing in its potential offspring site. When this happens, the parent loop's arm retracts and that loop eventually *dies*, unable to produce any more offspring. Figure 11.5 shows a snapshot view of the 7th generation colony of *Langton Loops*.

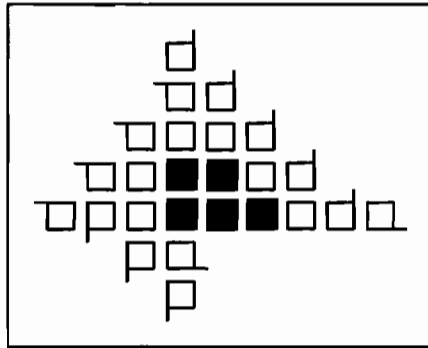


Fig. 11.5 Schematic representation of a 7th-generation *Langton Loop*. Black squares represent "dead" loops; arm-less squares represent "dying" loops.

Byl [byl89] was able to streamline and optimize Langton's construction by, for example, doing away with one of the intermediate states ($\sigma = 3$) and using just one 4-0 signal to make a left turn. Moreover, unlike Langton's model, in which the direction of a signal is determined by an x-0 combination, in Byl's construction it is effectively determined by its *orientation* with respect to the outer wall (the inner wall having also been done away with). By using these modifications, Byl was able to reduce the 8-states per site, 72 sites and 108 transition rules required by Langton's Loop to just 6 states, 12 sites and 57 rules. Byl [byl89] also shows an example of an 8-site configuration that generates an 11-site daughter which in turn

gives rise to an identical 11-site offspring. Byl's structures succeed in both adhering to Langton's set of minimal requirements for self-reproduction and significantly reducing the complexity Langton's own self-reproducing Loop.

11.8 Lindenmeyer Systems

Lindenmeyer systems -- or L-Systems -- were first introduced by Aristid Lindenmeyer in 1968 as a model for the cellular development of filamentous plants [linde68]. We mention them here for three reasons. First, L-systems can be thought of as generalized CA in which the number of sites can increase over time; second, they may be considered as generalized formal languages with interesting similarities and differences with the Chomsky language classes (see chapter 6); third, they are a popular tool among artificial life researchers in modeling (the physical appearance of) real plant forms. This section will briefly introduce the terminology and some of the main ideas behind L-systems. For readers wishing to explore L-systems further, two excellent general surveys are [prus89] and [prus90], the latter of which contains a beautiful collection of L-system-modeled life forms. A more formal mathematical treatment is given in [rozen80] and [rozen86].[†]

In simplest terms, L-systems consist of production rules for rewriting abstract strings of symbols. Unlike Chomsky grammars, however, for which only a single symbol is added to a string at a given "time step" of the string's "evolution," L-systems simultaneously replace each symbol of a string at time 't' by the string to which it is mapped by the production rule. If this sounds familiar, that is because L-system production is essentially a generic CA parallel dynamics in disguise. The only important difference is that, unlike CA systems, which evolve on well-defined underlying geometries (one-dimensional, two-dimensional Euclidean, etc.), L-system evolutions are *independent* of any such intrinsic geometry. The difference in the way L-systems and Chomsky grammars process symbol strings also has some important consequences. For example, there are languages that can be generated by context-free L-systems that cannot be generated by context-free Chomsky grammars.

11.8.1 Context Free L-Systems

Consider the simplest type of L-system; namely, a deterministic context-free L-system, also called a DOL-System. As the name implies, the production rules of such systems are allowed to transform only single symbols; i.e. the dynamics is independent of all "neighboring" symbol values. DOL-Systems are thus generalized CA systems that are allowed to add sites but whose local rule depends only on a given site itself and none of its neighbors.

DOL-Systems are formally defined by the three-tuple $(\mathcal{A}, \mathcal{R}, \alpha(0))$, where $\mathcal{A} = \{a_1, a_2, \dots, a_n\}$ is the *alphabet*; $\mathcal{R} : \mathcal{A} \rightarrow \mathcal{A}^*$, where $\mathcal{A}^*$ is the set of all possible

[†]Readers may also wish to consult an extensive annotated bibliography appearing in [lang89], pp. 625-643.

symbol strings formed from symbols in $\mathcal{A}$, is the *production rule*; and $\alpha(0) \in \mathcal{A}^*$ is the starting point for the production, or *axiom*. We should emphasize that this initial symbol string *does not* live on any lattice; it is a completely abstract quantity (but see below for an example of a kind of “structural” information that may be added to evolving strings). Since the DOL-system must also be *deterministic*, $\mathcal{R}$ must map each $a_i \in \mathcal{A}$ to a unique symbol string $a^* \in \mathcal{A}^*$. If the symbol string at time t , $\tilde{\alpha}(t)$, is given by $\tilde{\alpha}(t) = \alpha_1(t)\alpha_2(t) \cdots \alpha_m(t)$, then the symbol string at time $t+1$, $\tilde{\alpha}(t+1)$, is obtained by replacing each $\alpha_i(t)$, $i = 1, \dots, m$ with the string to which it is mapped by $\mathcal{R}$:

$$\tilde{\alpha}(t+1) = \mathcal{R}[\alpha_1(t)]\mathcal{R}[\alpha_2(t)] \cdots \mathcal{R}[\alpha_m(t)]. \quad (11.1)$$

As a simple example, suppose that $\mathcal{A}$ consists of three elements, $a_1 = 0$, $a_2 = 1$, and $a_3 = 2$ and there are three production rules: $\mathcal{R}[0] \rightarrow 21$, $\mathcal{R}[1] \rightarrow 0$ and $\mathcal{R}[2] \rightarrow 01$. Starting from the axiom $\alpha(0) = 0$, the first few symbol strings are then given by

$$\begin{aligned} \tilde{\alpha}(0) &= & 0 \\ \tilde{\alpha}(1) &= & 21 \\ \tilde{\alpha}(2) &= & 010 \\ \tilde{\alpha}(3) &= & 21021 \\ \tilde{\alpha}(4) &= & 01021010 \\ \tilde{\alpha}(5) &= & 2102101021021 \\ &\vdots & \vdots \end{aligned}$$

From this first example, it is obvious that, apart from a CA-like parallel updating of an ever-increasing number of sites and the set of recursive symbol-strings to which such a dynamics inevitably leads, there is no real internal geometry, as such. Each string at time t remains essentially a static collection of abstract symbols.

11.8.2 Recursive Growth Models

It was mentioned at the outset that L-systems were designed as tools for modeling filamentous plants. Since, as we have just seen, there is no real intrinsic structure or geometry in L-systems, a plant may be given some semblance of physical structure only by an appropriate *graphical* re-interpretation of a somewhat souped-up alphabet.

To be more precise, let us add four *bracketing* symbols “(,” “),” “<,” and “>” to the alphabet $\mathcal{A}$, so that our new alphabet $\mathcal{A}'$ consists of the elements $\{a_1, a_2, \dots, a_n, (,), <, >\}$. We will interpret these new symbols to mean that whenever they appear in a given symbol string – thought of as the n^{th} level branch of a *tree* – the string contained within them will be *drawn* either as an emerging *left* branch, if enclosed by “(” and “),” or as an emerging *right* branch, if enclosed by “<” and “>.” The only constraint we will impose on the set of production rules is that they leave each of the four bracketing symbols fixed: $\mathcal{R}[\beta] \rightarrow \beta$,

where $\beta = (,), < \text{ or } >$. The result, after a suitable graphical rendering, is a rudimentary "tree"-like structure.

For example, suppose our alphabet $\mathcal{A} = \{0, \dots, 4, (,), < , >\}$ and the production rules are given by

$$\begin{cases} \mathcal{R}[0] \rightarrow 2(1)3, & \mathcal{R}[1] \rightarrow 0, & \mathcal{R}[2] \rightarrow 2, \\ \mathcal{R}[3] \rightarrow 2 < 4 > 5, & \mathcal{R}[4] \rightarrow 3. \end{cases} \quad (11.2)$$

The first few iterations are given by:

$$\begin{aligned} \bar{\alpha}(0) &= 0 \\ \bar{\alpha}(1) &= 2(1)3 \\ \bar{\alpha}(2) &= 3(1)1 < 2 > 0 \\ \bar{\alpha}(3) &= 1 < 2 > 0(1)1 < 3 > 2(1)3 \\ &\vdots \end{aligned}$$

This evolution may then be represented graphically as follows (see figure 11.6). The axiom $\bar{\alpha}(0) = 0$ appears as a simple "stem" at time $t = 0$. At time $t = 1$, $\bar{\alpha}(0) \rightarrow 2(1)3$ so that the single stem value '0' is changed to a '2', the stem itself is lengthened by one unit with the value '3' attached at the top and a branch attached on the left-hand side with value '1'. Figure 11.6 traces the evolution of this system for two more time steps.

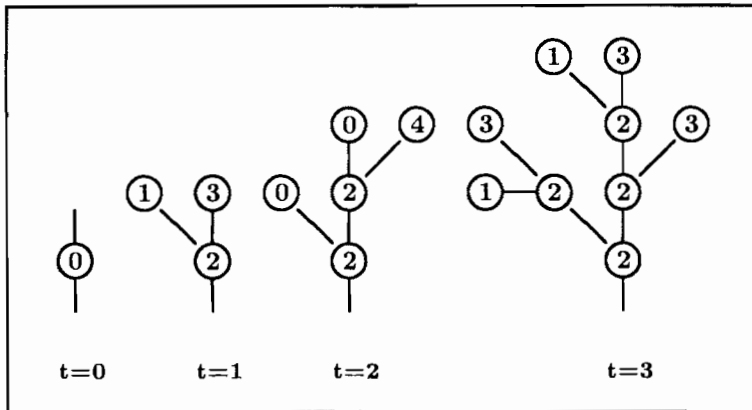


Fig. 11.6 A snapshot of an evolving "tree"-like bracketed DOL-System; see rule defined in equation 11.2.

In figure 11.6, the direction and angle into which the branches sprout has been chosen completely randomly. Admittedly, the figure is (at best) a very crude representation of a real tree. However, by carefully defining how emerging "branches" are to be drawn (as well as perhaps adding a few more bracket symbols to the alphabet), and using more sophisticated graphical rendering tools, these same basic bracketed systems can be used to produce some very complicated and realistic

patterns.[†] One graphical interpretation, for example, based on Seymour Papert's *Turtle Graphics* [pap80], produces a wide variety of fractal curves [piet92, prus90]. Other interpretations have been used to model surfaces and both two and three dimensional cellular structures [prus89, prus90, linde89].

11.8.3 Context Sensitive L-Systems

Deterministic context sensitive L-Systems -- called DIL-Systems [prus89] -- generalize their context-free cousins by allowing productions of the form

$$\mathcal{R}[\alpha_{\text{left}} a_i \alpha_{\text{right}}] \rightarrow \alpha, \quad (11.3)$$

where α_{left} and α_{right} are the *left* and *right* neighboring symbol-strings of symbol $a_i \in \mathcal{A}$, and $\alpha \in \mathcal{A}^*$ is an arbitrary symbol-string to which a_i is mapped by $\mathcal{R}$ in a context-sensitive manner. As for CA rules, there are a variety of special cases: If α_{left} and α_{right} are both single symbols (i.e. if the production rule is analogous to a radius $r = 1$ CA rule), the resulting DIL-System is sometimes called a 2L-System [prus90]. If the production rules have only a one-sided, single-symbol context (i.e. if they are of the form $aa_i \rightarrow \alpha$), the resulting system is called a 1L-System. In general, a (k, l) -System is one whose production rules depend on a length- k left context and a length- l right context. By thus endowing individual symbols a finite neighborhood radius, DIL systems thus represent a more natural generalization of CA systems than their DOL cousins.

The most important conceptual change wrought by context sensitivity is the possibility of information transport and *signal propagation*; indeed, the original idea was to model the interaction between plant parts due to the flow of nutrients or hormones [prus90]. Whereas context free systems furnish an arena in which information can only be transferred from a "parent" string to its "descendent," a context sensitive system allows neighboring sites, or cells, to exchange information.

For example, the following simple 1L-System uses context sensitivity to simulate the propagation of a signal (=1) to the right:

$$\left\{ \begin{array}{lcl} \mathcal{R}[0] & \rightarrow & 0 \\ \mathcal{R}[10] & \rightarrow & 1 \\ \mathcal{R}[1] & \rightarrow & 0 \end{array} \right\} \implies \begin{array}{lcl} \vec{\alpha}(0) = & 1000000 \dots \\ \vec{\alpha}(1) = & 0100000 \dots \\ \vec{\alpha}(2) = & 0010000 \dots \\ \vec{\alpha}(3) = & 0001000 \dots \\ \vec{\alpha}(4) = & 0000100 \dots \\ & \vdots & \vdots \end{array} \quad (11.4)$$

Since, as we have continually been reminded throughout this book, the capacity for some kind of signal propagation is critical for being able to perform arbitrary computational processes, it should come as no surprise that there is a finite intersection between both context-sensitive and unrestricted Chomsky languages -- the latter, of which, we recall require the class of universal computers as their accept-

[†]The reader is particularly encouraged to look at the beautiful color plates in [prus90].

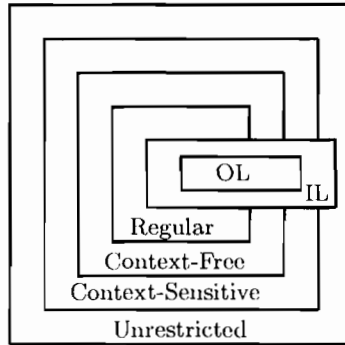


Fig. 11.7 Relationship between the language classes generated by DOL and DIL systems and the four Chomsky languages [prus89].

ing automata (see chapter 6) – and DIL-Systems. A schematic representation of the relation between the language classes generated by L-Systems and Chomsky languages is shown in figure 11.7.

11.9 Vants

Vants represent the one of the simplest – and therefore, most persuasive – examples of *emergence* of high-level structures from low-level dynamics. Discovered by Langton [lang86], vants live on a two-dimensional Euclidean lattice and come in two flavors, *red* and *blue*. Each vant can move in any of four directions (E,W,N,S). Each lattice site is either empty or contains one of two types of food, *green* food or *yellow* food. Vants are fundamentally solitary creatures so that there is a strict conservation of the number of vants.

How a vant moves through the lattice depends on its color. When a red vant enters a site containing green food, for example, it turns to its right, enters the new lattice site, and leaves the previous occupied site colored yellow. When a red vant enters a yellow site, it enters the site on its left and leaves the previously occupied site colored green. A blue vant does exactly the reverse: when it enters a green site it moves into the square on its left and leaves the previously occupied site yellow; when it moves into a yellow site it then moves into the site on its right and leaves the previously occupied site green. If either kind of vant enters an empty site it continues to move straight ahead. If two or more vants enter the same lattice site, they continue with their respective motions – as defined above – as though the site was unoccupied by other vants; i.e. there is no explicit vant-vant interaction at any site.

More formally, let us introduce the “food”-value of lattice site (i, j) at time t , $\zeta_{i,j}(t)$ (= green or yellow); an *occupancy* variable, $\alpha_{i,j}(t)$, which is equal to zero unless the site (i, j) contains at least one vant, in which case $\alpha_{i,j}(t) = 1$; and the vant vector $\vec{\sigma}_n^{(r,b)}(t) = (i, j, d)$, specifying the state of the n^{th} vant at time t , where

the superscript labels the vant's color ($r = \text{red}$ or $b = \text{blue}$), i and j specify the vant's (i, j) lattice position and $d = E, W, N, S$ is its direction.

The food variable at site (i, j) remains unchanged unless the site is occupied, in which case the food type changes from either green $\rightarrow$ yellow, or yellow $\rightarrow$ green:

$$\zeta_{i,j}(t+1) = (\text{green} \cdot \delta_{\zeta_{i,j}(t), \text{yellow}} + \text{yellow} \cdot \delta_{\zeta_{i,j}(t), \text{green}}) \alpha_{i,j}(t) + \zeta_{i,j}(t)[1 - \alpha_{i,j}(t)], \quad (11.5)$$

where $\delta_{x,y}$ is the *Kronecker-Delta* function. Table 11.2 shows the rule table for the $\vec{\sigma}_n^{(r,b)}$ transition.

d	red vants: $\vec{\sigma}_n^{(r)}(t+1)$		blue vants: $\vec{\sigma}_n^{(b)}(t+1)$	
	$\zeta_{i,j}(t) = \text{green}$	$\zeta_{i,j}(t) = \text{yellow}$	$\zeta_{i,j}(t) = \text{green}$	$\zeta_{i,j}(t) = \text{yellow}$
N	(i+1, j, E)	(i-1, j, W)	(i-1, j, W)	(i+1, j, E)
E	(i, j+1, S)	(i, j-1, N)	(i, j-1, N)	(i, j+1, S)
S	(i-1, j, W)	(i+1, j, E)	(i+1, j, E)	(i-1, j, W)
W	(i, j-1, S)	(i, j+1, N)	(i, j+1, N)	(i, j-1, S)

Table 11.2 Vant rules, $\vec{\sigma}_n^{(r)}(t) \rightarrow \vec{\sigma}_n^{(r)}(t+1)$; [lang86].

The single-most intriguing behavior of this simple dynamical system is that despite the “fundamentally solitary” individual vant dynamics – in which each vant effectively moves through the lattice totally oblivious to the motion of any of its cousins – a complex, global, cooperative dynamics nonetheless emerges. This cooperative dynamics results solely from a continual interaction between the sea of vants and an ever-changing collective food pattern. In particular, by coupling two or more vants together – i.e. by allowing each vant to roam freely about, and interact with, a mutual food environment – patterns and structures unattainable by a single vant are able to emerge. Moreover, these patterns and structures are often very obviously *cooperative structures*, requiring the simultaneous cooperative “building efforts” of several vants, working within a localized food area. After watching a typical vant evolution, one is strongly reminded of real ant colonies, in which a global ‘consciousness’ seems to spontaneously emerge out of the mutual interactions among an essentially mindless army of individual ants [levy92]. One is just as strongly inclined to agree with Langton when he speculates that such systems provide evidence that an apparent global ordered collective dynamics *need not* stem from an intrinsically global cooperative dynamics, but may instead be nothing more than an emergent high-level (*phenotype*) construct stemming from an essentially non-cooperative low-level (*genotype*) dynamics: “...such emergent, collective, metastable patterns of dynamical activity must play a role in the distributed dynamics of living and intelligent processes in the real world.”[†]

While a single vant performs little more than a pseudo random-walk, multiple-vant evolutions are ripe with many interesting (Conway *Life*-rule-like) patterns, particularly when the background lattice food color is shown along with the moving

[†]Langton, C., “Self-reproducing loops and virtual ants,” *Artificial Life II Video Proceedings*, Addison-Wesley (1992).

vants. Simply by having two or more vants interact within the same environment, the system is able to give rise to essentially static structures, periodic oscillators, orbiting patterns (in which multiple vants appear to “orbit” around one another while weaving a complex food-trail behind them as they slowly move off to one direction), and particle-like states, in which the combined motions of two or more intertwined vants effectively mimics that of a single but larger vant-organism. Some particles are slow moving, some fast, and “new” particles often emerge out of multi-particle collisions. Perhaps the most startling emergent patterns are those involving *diagonal motion*; recall that, *individually*, vants are incapable of any motion save that of going north, east, south or west.

Although, just as for Conway’s *Life* rule, static displays simply cannot do justice to the dynamical patterns that emerge in the course of a typical vant evolution, figures 11.8 and 11.9 show a few snapshot views. Note that, in both figures, the lattice initially contains only “yellow” food and a site is colored black whenever it contains either green food or a vant of either color.

Figure 11.8 shows the evolution of two red and two blue vants: $\vec{\sigma}_1^{(r)}(0) = (0, 0, E)$, $\vec{\sigma}_2^{(r)}(0) = (1, 1, E)$, $\vec{\sigma}_1^{(b)}(0) = (0, 1, W)$, $\vec{\sigma}_2^{(b)}(0) = (1, 0, W)$. Notice the appearance of food “bridges”, acting as information conduits from one part of a pattern to another; these conduits provide an avenue for vants to make their way quickly across them. Allowed enough “building” time, even a small number of vants are able to construct very complicated conduit networks.

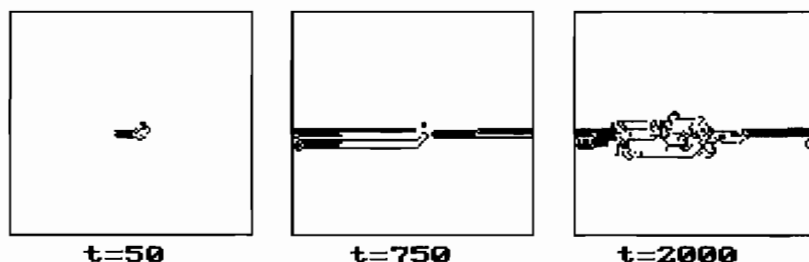


Fig. 11.8 Three snapshots of the evolution of a small colony of vants. The initial condition consisted of $\vec{\sigma}_1^{(r)}(0) = (0, 0, E)$, $\vec{\sigma}_2^{(r)}(0) = (1, 1, E)$, $\vec{\sigma}_1^{(b)}(0) = (0, 1, W)$, $\vec{\sigma}_2^{(b)}(0) = (1, 0, W)$. See text.

Figure 11.9 shows the evolution of a vant system with an initial state consisting of 20 red and 20 blue vants moving in random directions within a 10×10 box at the center of the lattice.

Langton’s vants are but a special case of more generalized “ants” [dewd89b]: let the state of each site of the lattice be labeled 1 through n . As an ant moves through a site with state k , its state changes from k to $k + 1 \bmod n$, and the ant makes either a right or left turn relative to the direction in which it entered the site. In the generalized model, the ant’s direction is determined by a deterministic length- n rule-string. If R_k is the k^{th} bit of the rule-string, and an ant is leaving a site whose previous value was k , then it makes a right turn if $R_k = 1$ and a left turn if $R_k = 0$. In this notation, Langton’s vants are defined by the rule-string $\vec{R} = 10$.

Although, as one might suspect, it is difficult to prove any general theorems about the behavior of generalized “ants,” it is easy to prove the following basic theorem (see [prop94]): *the motion of “ants” moving according to a rule-string that contains at least one ‘0’ and at least one ‘1’ is always unbounded.*

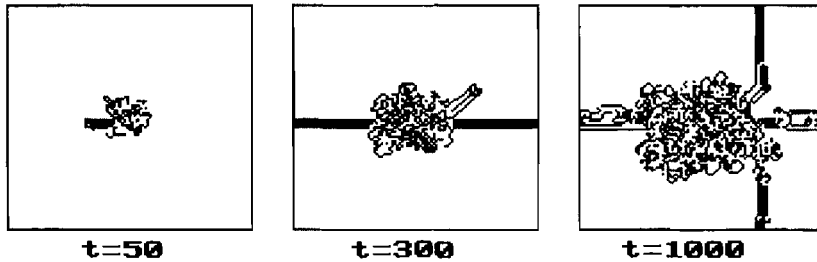


Fig. 11.9 Three snapshots of the evolution of a small colony of vants. The initial condition consisted of 20 red and 20 blue vants moving in random directions within a 10×10 box at the center of the lattice.

11.10 Genetic Algorithms

Genetic algorithms (GAs) are computational models of adaptation and evolution based on natural selection. While their modern form is derived mainly from John Holland’s work in the 1960s (see [holl66], [holl88] and the second edition of Holland’s classic 1975 book, *Adaptation in Natural and Artificial Systems* [holl92]), many key ideas such as using “selection of the fittest”-like population-based selection schemes and using binary strings as computational analogs of biological chromosomes, actually date back to the late 1950s (see, for example, [box57] and [brem62]). More recent work is discussed by Goldberg [goldb89], Davis ([davisl87], [davisl91]) and Michalewicz [mich92]. A comprehensive review of the current state-of-the-art in genetic algorithms, with a particular emphasis on artificial life, is given by Mitchell [mitch93a] and Mitchell and Forrest [mitch94]. The collection of papers appearing in recent conference proceedings ([gref85], [gref87], [schaff89], [belew91], [forr93b]) also makes an excellent source of reference.

The basic idea behind GAs is very simple. Given a “problem” – which can be as well-defined as maximizing a function over some specified interval (see below) or as seemingly ill-defined and open-ended as evolution itself, where there is no *a-priori* discernible or fixed function to either maximize or minimize – GAs provide a mechanism by which the solution space to that problem is searched for “good solutions.” Possible solutions are encoded as *chromosomes* (or, sometimes, as sets of chromosomes), and the GA evolves one population of chromosomes into another according to their *fitness* by using some combination (and/or variation) of the genetic operators of *crossover* and *mutation*. A solution search space together with a fitness function is called a *fitness landscape*. Ultimately, after many generations, the population will, in theory, be composed only of those chromosomes whose fitness values are clustered around the global maximum of the fitness landscape.

Although GA are undeniably powerful computational tools and have been successfully applied to an impressive variety of problems (see below), they certainly do not represent a “cure-all” solution to all types of problems. One finds that, in practice, certain problems are more amenable to this kind of solution scheme than others, and that it is not always obvious why that is so. Much foundational work still remains to be done in developing a complete theory of GA behaviors and capabilities. Figure 11.10 illustrates the basic steps involved in applying a GA.

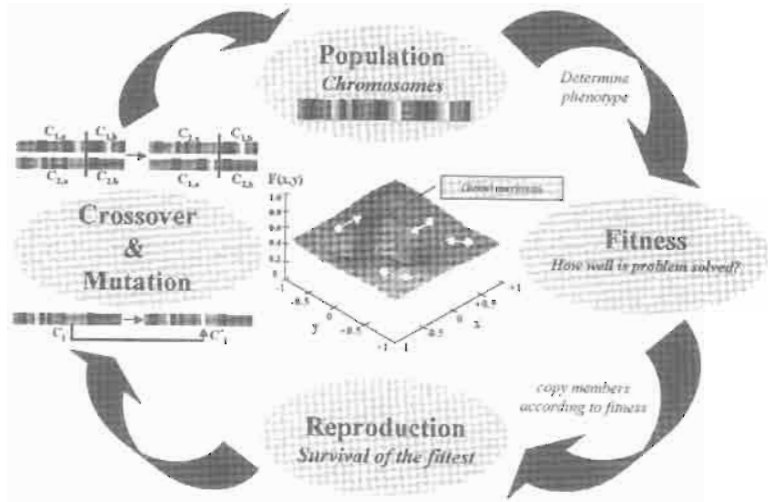


Fig. 11.10 Schematic illustration of the basic steps involved in applying a genetic algorithm.

11.10.1 Genetic Operators

Each chromosome is usually defined to be a bit-string, where each bit position (or “locus”) takes on one of two possible values (or “alleles”), and can be imagined as representing a single point in the “solution-space.” The fitness of a chromosome effectively measures how “good” a solution that chromosome represents to the given problem. Aside from its intentional biological roots and flavoring, GAs can be thought of as parallel equivalents of more conventional serial optimization techniques: rather than testing one possible solution after another, or moving from point to point in the solution phase-space, GAs move from entire populations of points to new populations.

Figure 11.11 shows examples of the three basic genetic operations of *reproduction*, *crossover* and *mutation*, as applied to a population of 8-bit chromosomes. Reproduction makes a set of identical copies of a given chromosome, where the number of copies depends on the chromosome’s fitness (see below). The crossover operator exchanges subparts of two chromosomes, where the position of the crossover is randomly selected, and is thus a crude facsimile of biological sexual recombination between two single-chromosome organisms. The mutation operator randomly flips one or more bits in the chromosome, where the bit positions are randomly chosen.

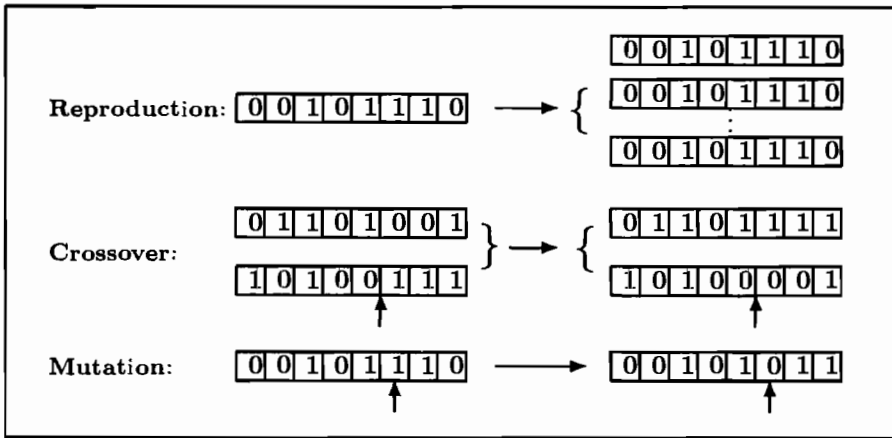


Fig. 11.11 Schematic representation of the basic genetic operations of reproduction, crossover and mutation.

The mutation rate is usually chosen to be small.

While reproduction generally rewards high fitness, and crossover generates new chromosomes whose parts, at least, come from chromosomes with relatively high fitness (this does not guarantee, of course, that the crossover-formed chromosomes will also have high fitness; see below), mutation seems necessary to prevent the loss of diversity at a given bit-position [holl92]. For example, were it not for mutation, a population might evolve to a state where the first bit-position of each chromosome contains the value 1, with there being no chance of reproduction or crossover ever replacing it with a 0.

11.10.2 The Fitness Landscape

As mentioned above, a solution search space, $\vec{x}$, together with a fitness function, $f(\vec{x})$, make up what is called a *fitness landscape*. The term “landscape” comes from visualizing a three-dimensional geographical landscape consisting of heights $h = f(x, y)$ of a two-dimensional location $\vec{x} = (x, y)$. Particular problems, of course, may involve an arbitrary number of dimensions, but it is still helpful to keep this simple image in mind. The term “fitness” comes from Darwinian biology, and refers to the fitness of an individual to survive as a function either of its *phenotype* (or higher-level properties and/or behaviors) or its *genotype* (or lower-level genetic code). Biological fitness is generally very difficult to define since it is usually a complicated (and changing!) function of the interactions between an organism and other organisms and interactions between the organism and its environment. In a biological context and/or biology-based setting (such as in studies of *artificial life*), the fitness landscape is also often referred to as an *adaptive landscape*, paying homage to an idea first introduced by Wright in 1932 [wrights32]. Other “fitness functions,” which, depending on the particular problem, may be considerably easier to define than their biological cousins, include *energy* and *free-energy* landscapes

from physics and chemistry, and *cost* (or *objective*) functions from combinatorial optimization problems in computer science.

As our simple geographical landscape metaphor might suggest, a variety of fitness landscapes are possible, each with their own strengths and weaknesses when it comes to “submitting” to a GA solution: completely flat landscapes, landscapes with a single isolated minimum and/or maximum, landscapes having several minima and/or maxima with equal heights, or landscapes with many unequal and irregularly spaced local minima and/or maxima.

Since GAs, like other combinatorial optimization schemes (such as *Simulated Annealing*[†]), depend essentially on their “hill-climbing” ability to ascend (or descend) towards the desired global maximum (or minimum), how successful the climb – and hence, the approach to the solution – will be, depends on what the landscape looks like. What a given landscape looks like, in turn, depends strongly on its metric; that is, on the function $d = d(\vec{x}, \vec{x}')$ that is used to measure the distance between any two points $\vec{x}$ and $\vec{x}'$. Since GAs tend to keep nearby bits near each other, embedded correlations among subsets of a chromosome’s genes can sometimes be exploited to produce a “natural ordering” for the given landscape [goldb89].

Landscapes with a single smoothly increasing “bump,” such as the one shown in figure 11.12-a, for example, are usually amenable to any systematic climb towards larger values. On the other hand, landscapes with a single isolated maximum that sits on an otherwise even-leveled surface may not be so easy to “solve,” because at no point on the surface is there a clue as to which direction to proceed in to move towards the maximum.

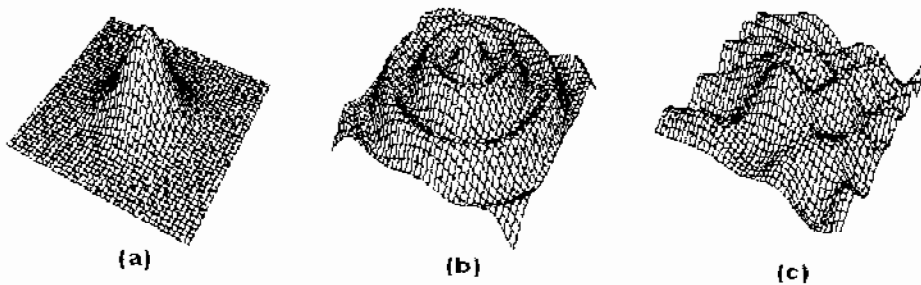


Fig. 11.12 Three sample fitness landscapes: (a) has a single smooth maximum, (b) has many equivalent local maxima and one global maximum, but is circularly symmetric; (c) has many irregularly spaced local maxima, and is a good example of a *rugged landscape*.

More “rugged” landscapes, such as those shown in figures 11.12-b and 11.12-c, with their multiple, and in the case of figure 11.12-c, irregularly spaced and sized, local maxima, may present even greater challenges to “hill-climbing” methods. An excellent review of optimization on rugged landscapes is given by Palmer [palmr91]. Kauffman ([kauff92], [kauff93]) discusses the biological implications of rugged fitness landscapes.

[†]See section 10.8.

11.10.2.1 *NK-Landscapes*

Kauffman ([kauff89], [kauff90a]) has introduced a class of parametrizable fitness landscapes called *NK-landscapes*, that provide a formalism for studying the efficacy of GA evolution as a function of certain statistical properties of the landscape.[†]

Given N binary variables $x_i = \pm 1$, so that $\vec{x} = (x_1, x_2, \dots, x_N)$ represents a vertex of an N -dimensional hypercube, an NK-landscape is defined by a fitness function, $\mathcal{F}$, of the form

$$\mathcal{F}(\vec{x}) = \sum_{i=1}^N f_i(x_i, x_{i1}, x_{i2}, \dots, x_{iK}), \quad (11.6)$$

where the i^{th} contribution, f_i , depends on x_i and K other x_{ij} 's. This functional form for $\mathcal{F}$ represents epistatic interactions between the i^{th} bit and K other bits that are assumed to affect i 's fitness contribution. The K bits associated with each locus can be either the i^{th} bit's immediate neighbors or their positions can be completely random. The functions f_i are usually random functions of their arguments, with values chosen randomly from among the 2^{K+1} possible values. Once all the x_{ij} s and f_i 's are chosen, they remain fixed and the behavior of $\mathcal{F}$ is then explored as a particular instance of a well-defined NK-landscape. The goal is to explore how the statistical properties of NK-landscapes – such as the number of local optima, the average length of an “adaptive walk” from a given point to a global maximum, and so on, and as parametrized by N and K – affect the performance of GAs.

As K increases from 0 (where $\mathcal{F}(\vec{x}) = \sum_i f_i(x_i)$) to $N - 1$ (where $\mathcal{F}$ becomes the sum of N independent random numbers), the NK-landscape goes from having a single maximum to having more and more maxima that become less and less correlated to, finally, being essentially totally random. The parameter K can therefore be used to *tune* the degree of “ruggedness” of the landscape.

Some preliminary suggestions of how NK-landscapes can be used to predict GA performance are discussed by Kauffman [kauff89] and Manderick, de Weger and Spiessens [mand91].

11.10.3 *The Basic Recipe*

Although genetic algorithms come in many different flavors, and are usually fine-tuned in some way to reflect the nuances of a particular problem, they are all more or less variations of the following basic steps:

Step 1: Begin with a randomly generated population, $\mathcal{P}_{K,N}$, of K length- N chromosome-encoded “solutions” to a given problem. Let the n^{th} chromosome C_n be the binary string $C_n = \beta_1\beta_2 \cdots \beta_N$, where $\beta_i \in \{0, 1\}$, $i = 0, 1, \dots, N$.

Step 2: Calculate the fitness, f_n , of each chromosome C_n in the population: $f_n = f(C_n)$.

Step 3: Generate a new size- K population of chromosomes from the old population

[†]NK-landscapes are slightly different representations of Kauffman's *Random Boolean Networks*, discussed in section 8.6.

using *fitness-scaled* genetic reproduction. That is, copy each chromosome C_n a number of times, τ_n , that is proportional to its fitness divided by the average fitness of the entire population: $\tau_n \propto f_n / \sum_i f_i$.

Step 4: Randomly pairing up the chromosomes in the new population, apply the genetic crossover operator to each pair. That is, randomly select a bit-position, say k , for each pair of chromosomes, say C_{n_1} and C_{n_2} , and replace this pair with two new pairs – C'_{n_1} and C'_{n_2} – constructed via genetic crossover: C'_{n_1} consists of the first k bits of C_{n_1} and the last $(N - k)$ bits of C_{n_2} ; and C'_{n_2} consists of the first k bits of C_{n_2} and the last $(N - k)$ bits of C_{n_1} .

Step 5: Loop through each bit of each chromosome in the population and perform genetic mutation; i.e. flip the bit-value ($0 \rightarrow 1$ and $1 \rightarrow 0$) at each locus with some (typically small; see below) probability, p_m . (In practice, this step is combined with step 4.)

Step 6: Goto step 2 and repeat steps 2-6 until desired level of “fitness” is achieved.

11.10.3.1 A Simple Example

As a concrete example, suppose our problem is to maximize the fitness function $f(x) = x^2$, using a size $K = 6$ population of 6-bit chromosomes of the form $C = (\beta_1\beta_2\cdots\beta_6)$, where $\beta_i \in \{0,1\}$, $i = 1, 2, \dots, 6$. C 's fitness is determined by first converting its binary representation into a base-10 equivalent value and squaring: $f(C) = (\sum_{i=1}^6 2^{i-1}\beta_{7-i})^2$.

Init Pop	Initial Fitness	Exp/ Copies	Actual Copies	Mating Pop	Crossover Operation	Mutation Operation	New Fitness
(101101)	2025	1.4	1	(101101)	(<u>1</u> 34) $\rightarrow$ (101001)	(101001)	1681
(010110)	484	0.3	0	(111001)	(22 <u>6</u>) $\rightarrow$ (111101)	(111101)	3481
(111001)	3249	2.2	3	(111001)	(355) $\rightarrow$ (111001)	(111001)	3249
(101011)	1849	1.3	1	(111001)	(4 <u>3</u> 1) $\rightarrow$ (111101)	(1111 <u>1</u> 1)	3969
(010001)	289	0.2	0	(101011)	(553) $\rightarrow$ (101011)	(10101 <u>0</u>)	1764
(011101)	841	0.6	1	(011101)	(622) $\rightarrow$ (011001)	(011001)	625

Table 11.3 One pass (read left to right) through the steps of a basic genetic algorithm scheme to maximize the fitness function $f(x) = x^2$ using a population of six 6-bit chromosomes. The crossover notation $(\alpha_1\underline{n}\alpha_2)$ means that chromosomes C_{α_1} and C_{α_2} exchange bits beyond the n^{th} bit. The underlined bits in the “Mutation Operation” column are the only ones that have undergone random mutation. See text for other details.

Table 11.3 shows the intermediate steps of the first pass through the above six steps of the basic GA recipe. Step 1 is to construct six random bit-strings

representing our original population:

$$\left\{ \begin{array}{l} C_1 = (101101) \\ C_2 = (010110) \\ C_3 = (111001) \\ C_4 = (101011) \\ C_5 = (010001) \\ C_6 = (011101) \end{array} \right. \quad (11.7)$$

These chromosomes have fitness values of 2025, 484, 3249, 1849, 289 and 841, respectively. The average fitness is 1456. By luck of the *fitness-scaled* draw, where the number of copies of a given chromosome is determined according to its fitness, scaled by the average fitness of the entire population, three copies of C_3 are made for the next population (owing to its relatively high fitness), one copy each for chromosomes C_1 , C_4 and C_6 and none for the remaining chromosomes. These copies form the mating population.

Next, we randomly pair up the new chromosomes, and perform the genetic crossover operation at randomly selected bit-positions – chromosomes C_1 and C_4 exchange their last three bits, C_2 and C_6 exchange their last four bits, and C_3 and C_5 exchange their last bit:

$$\left\{ \begin{array}{l} C_1 \times C_4 \text{ at bit 3} = (101^{\downarrow}101) \times (101^{\downarrow}011) \rightarrow (101001) \\ C_2 \times C_6 \text{ at bit 2} = (01^{\downarrow}0110) \times (01^{\downarrow}1101) \rightarrow (111101) \\ C_3 \times C_5 \text{ at bit 5} = (11100^{\downarrow}1) \times (01000^{\downarrow}1) \rightarrow (111001) \\ C_4 \times C_1 \text{ at bit 3} = (101^{\downarrow}011) \times (101^{\downarrow}101) \rightarrow (111101) \\ C_5 \times C_3 \text{ at bit 5} = (01000^{\downarrow}1) \times (11100^{\downarrow}1) \rightarrow (101011) \\ C_6 \times C_2 \text{ at bit 2} = (01^{\downarrow}1101) \times (01^{\downarrow}0110) \rightarrow (011001) \end{array} \right. \quad (11.8)$$

Finally, we mutate each bit of the resulting chromosomes with some small probability – say $p_m = 0.05$. In our example we find that values of the *fifth* bit in C_4 and *sixth* bit in C_5 are flipped. The resulting strings make up our 2nd generation chromosome population. By chance, the first loop through the algorithm has successfully turned up the *most-fit* chromosome – $C_4 = (111111) \rightarrow f(C_4) = 63^2 = 3969$ – but in general the entire procedure would have to be repeated many times to approach the “desired” solution.

11.10.4 How Do GAs Work?

While GAs are very simple to describe and implement on a computer, their behavior can be quite complex: complex in its unpredictability, complex to understand, and often exhibiting a complex-system-like emergent behavior [forr90]. There are a number of fundamental questions concerning how GAs work, not all of which have been completely answered. The first, and obvious, question is how do they manage to work at all? Given the vast number of possible genotypes of a size- N “solution” ($= 2^N$), it is not immediately clear why *any* finite search-strategy – be it serial, parallel, hill-climbing or whatever – should ever consistently come close to the

desired solution in a reasonable time, particularly for large N . Since the efficacy of an optimization scheme depends strongly on the fitness landscape, one would also like to characterize the kinds of fitness landscapes that are most amenable to a GA solution. It is also important to explore ways in which GAs differ from more traditional hill-climbing methods like gradient-ascent. Are all such methods, GAs included, equally adept at “solving” the same sorts of problems? Or are different methods best suited for specific kinds of problems? If so, how are these problems, and presumably their fitness landscapes, different from one another? While it would take us too far afield to explore these and other important questions in any great depth, we will briefly discuss a notion that most formal studies of the theory behind GAs begin with: the *building-block hypothesis*.

11.10.4.1 The Building-Block Hypothesis

An heuristic explanation of why GA work – called the *building-block hypothesis* ([gold89a], [holl92]) – is based on the idea that good solutions tend to be formed out of sets of good building-blocks (or *schemas*). GAs discover these solutions by assigning higher fitness-levels to – and therefore tending to retain, over the course of successive generations – sets of strings containing good schemas.

By schema, we mean templates, or forms for particular kinds of strings. For example, the schema $\mathcal{S} = (1***0)$, where $*$ is a “wildcard” that stands for either bit-value 0 or 1, represents the template for all length-6 chromosomes whose first bit $\beta_1 = 1$ and last bit $\beta_6 = 1$. In this case, since the schema contains one fixed bit and the distance between the outer most fixed bits is 5, $\mathcal{S}$ is said to be an *order-1* schema with *defining length* $\delta = 5$. The above example, in which we used length-6 chromosomes to maximize the function $f(x) = x^2$, illustrates why schema can be thought of as simple building-blocks of “fit” genes. In that example, any chromosome of the form $(1*****)$ is obviously more fit than $(0*****)$, and thus forms a basic building block out of which the best “solutions” must be constructed.

Now, to be sure, not every possible subset of the solution-space can be described as a schema. Simple counting shows that a length- N chromosome can have 2^N possible configurations, and therefore 2^{2^N} possible subsets, but only 3^N different schemas. Nonetheless, it is a central axiom of the building-block hypothesis that it is precisely the set of schemas that are effectively being processed by GAs.

The schema population can be estimated using a simple mean-field-like argument. Let $\mathcal{S}$ represent a schema in a size- K population $\mathcal{P}(t)$ at time t , and $Z(\mathcal{P}, t)$ instances of the schema at time t . Let $f(s)$ be the fitness of the string s , $\bar{f}_{\mathcal{S}}$ be the average fitness of instances of $\mathcal{S}$ at time t , and $\bar{f} = K^{-1} \sum_i f_i$ be the average fitness of the population. Then the expected number of instances of $\mathcal{S}$ at time $t+1$, $Z(\mathcal{P}, t+1)$, is equal to

$$Z(\mathcal{P}, t+1) = \sum_{s \in \mathcal{S}} \frac{f(s)}{\bar{f}} = \frac{\sum_{s \in \mathcal{S}} f(s)}{\bar{f}} = \frac{\bar{f}_{\mathcal{S}}}{\bar{f}} Z(\mathcal{P}, t), \quad (11.9)$$

since, by definition, $\bar{f}_{\mathcal{S}} = \sum_{s \in \mathcal{S}} f(s) / Z(\mathcal{P}, t)$.

This basic difference equation – known as the *Schema Theorem* [holl92] – expresses the fact that the sample representation of schemas whose average fitness remains above average relative to the whole population increases exponentially over time. As it stands, however, this equation addresses only the reproduction operator, and ignores effects of both crossover and mutation.

A lower bound on the overall effect of crossover, which can both create and destroy instances of a given schema, can be estimated by calculating the probability, $p_C(S)$, that crossover leaves a schema S unaltered. Let p_c be the probability that the crossover operation will be applied to a string. Since a schema S will be destroyed by crossover if the operation is applied anywhere within its defining length, the probability that S will be destroyed is equal to $p_c \times \delta(S)/(K-1)$, where $\delta(S)$ is the defining length of S . Hence, the probability of survival $p_S = 1 - p_c \delta(S)/(K-1)$, and equation 11.9 takes the updated form:

$$Z(\mathcal{P}, t+1) \geq \frac{\bar{f}_S}{\bar{f}} \left(1 - p_c \frac{\delta(S)}{K-1} \right) Z(\mathcal{P}, t). \quad (11.10)$$

Finally, in order to also take into account the mutation operator, we note that the probability that a schema S survives under mutation is given by $p_M(S) = (1 - p_m)^{\mathcal{O}(S)}$, where p_m is the single-bit mutation probability and $\mathcal{O}(S)$ is the number of fixed-bits (i.e. the order) of S . With this we can now express the *Schema Theorem* that (partially) respects the operations of reproduction, crossover and mutation:

$$Z(\mathcal{P}, t+1) \geq \frac{\bar{f}_S}{\bar{f}} \left(1 - p_c \frac{\delta(S)}{K-1} \right) \left\{ (1 - p_m)^{\mathcal{O}(S)} \right\} Z(\mathcal{P}, t). \quad (11.11)$$

We conclude from this basic theorem that the sample representation of low-order schemas with above average fitness relative to the fitness of the population increases exponentially over time.[†]

11.10.5 High-Level CA Rule Extraction

Richards, Meyer and Packard [richa90] have suggested a way to extract two-dimensional cellular automaton rules directly from experimental data. The same idea, outlined below, can in principle be used in more general contexts.

Richards, et. al.'s idea is to use a genetic algorithm to search through a space of a certain class of cellular automata rules for a local rule that best reproduces the observed behavior of the data. Their learning algorithm (which was applied specifically to sequential patterns of dendrites formed by NH₄ Br as it solidifies from a supersaturated solution) starts with no a-priori knowledge about the physical system. It, instead, builds increasingly sophisticated “models” that reproduce the observed behavior.

[†]The fact that we have ignored possible crossover and/or mutation induced creations of previously nonexistent instances of schemas means only that the right hand side of the above equation represents a lower bound; the conclusion remains generally valid, as it stands.

Dendritic NH₄ Br data exhibits pattern structure on many different length scales and a dynamics takes place on different time scales. Moreover, there is often very little information available regarding the physical variables describing the dendritic solidification of NH₄ Br. While one can determine whether a given point is solid or liquid, for example, one typically knows nothing about the solute concentration or temperature field in the liquid. Despite this lack of knowledge of what is happening on the micro-level, Richards, et. al.'s algorithm is able to find a rule that qualitatively reproduces the observed data.

Richards, et. al. comment that while the exact relationship between the rule found by their genetic algorithm and the fundamental equations of motion for the solidification remains unknown, it may still be possible to connect certain features of the learned rule to phenomenological models.

"We propose that this type of 'derivability gap' is the rule, rather than the exception for most complex spatial patterns observed in nature. For such phenomena, it may be impossible to derive models which explain observed spatiotemporal complexities directly from fundamental equations and 'first principles.' Though perhaps underivable, the dynamical structure extracted by the learning algorithm is undeniable, and represents a new type of progress, perhaps the primary kind of understanding possible for complex patterns." ([richa90], page 201)

11.11 An Artificial-Life CA Model of Combat

In this section we introduce a mobile CA model of land combat called *EINSTEIN*, developed at the *Center for Naval Analyses*[†] for the US Marine Corps. We include a discussion of this model here because it is an interesting blend of CA-like local dynamics and agent-based modeling techniques.

11.11.1 Background

In 1914, F. W. Lanchester introduced a set of coupled ordinary differential equations—now commonly called the Lanchester Equations¹ (LEs)—as models of attrition in modern warfare. Similar ideas were proposed around that time by [chase88] and [osip95]. These equations are formally equivalent to the Lotka-Volterra equations used for modeling the dynamics of interacting predator-prey populations [hof98]. The LEs have since served as the fundamental mathematical models upon which most modern theories of combat attrition are based, and are to this day embedded in many state-of-the-art military models of combat. [Taylor] provides a thorough mathematical discussion.

LEs are very intuitive and therefore easy to apply. For the simplest case of directed fire, for example, they embody the idea that one side's attrition rate is proportional to the opposing side's size. However, LEs are applicable only under a

[†]The Center for Naval Analyses is a federally funded research and development center. Homepage = <http://www.cna.org>.

strict set of assumptions, such as having homogeneous forces that are continually engaged in combat, firing rates that are independent of opposing force levels and are constant in time, and units that are always aware of the position and condition of all opposing units. LEs also contain a number of significant shortcomings, including modeling combat as a deterministic process and requiring knowledge of "attrition-rate coefficients" (the values of which are, in practice, very difficult to obtain). Moreover, they do not incorporate the human factor in combat; i.e., the psychological and/or decision-making capability of the human combatant.

While the LEs are particularly relevant for the kind of static trench warfare and artillery duels that characterized most of World War I, they are too simple and lack the spatial degrees of freedom to realistically model modern combat. The fundamental problem is that they idealize combat much in the same way as Newton's laws idealize physics.

Models based on differential equations homogenize the properties of entire populations and ignore the spatial component altogether. Partial differential equations—by introducing a physical space to account for troop movement—fare somewhat better, but still treat the agent population as a continuum. In contrast, agent-based models consist of a discrete heterogeneous set of spatially distributed individual agents (i.e., combatants), each of which has its own characteristic properties and rules of behavior. These properties can also change (i.e., adapt) as an individual agent evolves in time.

In agent-based models, the final outcome of a battle—as defined, say, by measuring the surviving force strengths—takes second stage to exploring how two forces might co-evolve during combat. Such models are designed to allow the user to explore the evolving patterns of macroscopic behavior that result from the collective interactions of individual agents, as well as the feedback that these patterns might have on the rules governing the individual agents' behavior.

11.11.1.1 *Land Combat as a Complex Adaptive System?*

Military conflicts, particularly land combat, possess the characteristic features of complex adaptive systems: combat forces are composed of a large number of nonlinearly interacting parts and are organized in a command and control hierarchy; local action, which often appears disordered, induces long-range order (i.e., combat is self-organized); military conflicts, by their nature, proceed far from equilibrium; military forces, in order to survive, must continually adapt to a changing combat environment; there is no master "voice" that dictates the actions of each and every combatant (i.e., decentralized control); and so on. There have also recently appeared a number of papers discussing the fundamental role that nonlinearity plays in combat; see [beyer92], [hedge93], [mill95], [saper95] and [tag96].

EINSTEIN (Enhanced ISAAC[†] Neural Simulation Toolkit), was developed to address the basic question: "To what extent is land combat a self-organized complex

[†]ISAAC = Irreducible Semi-Autonomous Adaptive Combat; ISAAC is an earlier proof-of-concept model originally developed for the US Marines Corps. Both ISAAC and EINSTEIN, which run on PCs running Windows 95/98/NT, can be freely downloaded from <http://www.cna.org/isaac>.

adaptive system?” As such, their intended use is not as full system-level models of combat but as interactive toolboxes (or “conceptual playgrounds”) in which to explore high-level emergent behaviors arising from various low-level (i.e., individual combatant and squad-level) interaction rules.

The idea behind developing these toolboxes is emphatically not to model in detail a specific piece of hardware (M16 rifle, M101 105mm howitzer, etc.). Instead, the idea is to explore the middle ground between—at one extreme—highly realistic models that provide little insight into basic processes and—at the other extreme—ultra-minimalist models that strip away all but the simplest dynamical variables and leave out the most interesting real behavior; i.e. to explore the fundamental behavioral tradeoffs among a large number of notional variables.

The dynamics underlying EINSTEIN is patterned after mobile CA rules, and are somewhat reminiscent of Braitenberg’s Vehicles [brai84]. Specifically, EINSTEIN takes an artificial-life-like bottom-up, synthesist approach to the modeling of combat, rather than the more traditional top-down, or reductionist approach.

11.11.2 *Combat Agents*

The basic element of EINSTEIN is an EINSTEIN Agent (EA) that can represent any primitive combat unit (infantryman, tank, transport vehicle, etc.). Agents are equipped with four main characteristics:

- *Doctrine*: local rules telling an agent how to act in a generic environment.
- *Mission*: goals directing behavior
- *Situational Awareness*: sensors generating an internal map of environment
- *Adaptability*: an internal mechanism to alter behavior and/or rules.

The putative combat battlefield is represented in EINSTEIN by a two-dimensional lattice of discrete sites. Each site of the lattice may be occupied by one of two kinds of agents: red or blue. The initial state consists of either user-specified formations of red and blue agents positioned anywhere on the battlefield. Red and blue “flags” are also usually (but not always) positioned in diagonally opposite corners: a red flag in the red corner and a blue flag in the blue corner. A typical “goal,” for both red and blue agents, is to reach the enemy’s flag in the diagonally opposite corner. EINSTEIN also has the provision of defining a notional terrain.

Each agent exists in one of three states: alive, injured, or killed. Up to ten distinct groups of personalities, of varying sizes, can be defined. Each agent has associated with it a set of ranges (sensor range, fire range, communications range, etc.), within which it senses and assimilates simple forms of local information (see below), and a personality, which determines the general manner in which it responds to its environment.

11.11.3 *Local “Personality” Rules*

Each agent is equipped with a user-specified personality – or internal value system – defined by a six-component personality weight vector, $\vec{w} = (w_1, w_2, \dots, w_6)$,

where $-1 \leq w_i \leq 1$ and $\sum_i |w_i| = 1$. The components of the $\vec{w}$ specify how an individual agent responds to distinct kinds of local information within its sensor and threshold ranges. $\vec{w}$ is also state-dependent: i.e. w_{alive} need not, in general, be equal to w_{injured} . The components of $\vec{w}$ can be negative, in which case they signify a propensity for moving away from, rather than toward, a given entity.

The default personality rule structure is defined as follows. Since there are two kinds of agents (red and blue), and each agent can exist in one of two states (alive and injured), each agent can respond to effectively four different kinds of information appearing within its sensor range r_S : (1) the number of alive friendly (i.e., like-colored) agents; (2) the number of alive enemy (i.e., different colored) agents; (3) the number of injured friendly agents; and (4) the number of injured enemy agents.

Additionally, each agent can respond to how far it is from both its own (like-colored) flag and its enemy's flag. The i th component of $\vec{w}$ represents the relative weight afforded to moving closer to the i th type of information. A personality is defined by assigning a weight to each of the six kinds of information. For example, one agent might give all its attention to like-colored agents, and effectively ignore the enemy.

An example of a fairly aggressive personality is one whose weight vector is given by $\vec{w} = (1/20, 5/20, 0, 9/20, 0, 5/20)$. Such a personality is five times more "interested" in moving toward alive enemies than it is in moving toward alive friendlies (effectively ignoring injured friendlies altogether), and is more interested in moving toward injured enemies than it is even in advancing toward the enemy flag. An agent that has a personality defined by entirely negative weights—say, $\vec{w} = (-1/6, -1/6, -1/6, -1/6, -1/6, -1/6)$ —wants to move away from, rather than toward, every other agent and both flags; i.e. it wants to avoid action of any kind.

An agent's personality weight vector is used to rank each possible move according to a penalty function. The penalty function effectively measures the total distance that the agent will be from other agents (which includes both friendly and enemy agents) and from its own and enemy flags, each weighted according to the appropriate component of $\vec{w}$. An agent moves to the position that incurs the least penalty; i.e., an agent's move is the one that best satisfies its personality-driven desire to "move closer to" or "farther away from" other agent's in given states and either of the two flags.

A "penalty" is computed for each possible move: $Z_1, Z_2, \dots, Z_N$. If the movement range $r_M = 1$, $N = 9$; if $r_M = 2$, $N = 25$. The actual move is the one that incurs the least penalty. If there is a set of moves (consisting of more than one possible move) that incur exactly the same minimum penalty, an agent randomly selects the actual move from among the candidate moves making up that set.

11.11.3.1 Meta-Rules

An agent's default personality may be augmented by a set of meta-rules that tell it how to alter its default personality according to various environmental conditions and contexts. The three simplest meta-rule classes define the local conditions under

which an agent is allowed to advance toward enemy flag (class 1), cluster with friendly forces (class 2), and engage the enemy in combat (class 3).

For example, a class-1 meta-rule prevents an agent from advancing toward the enemy flag unless it is locally surrounded by some threshold number of friendly agents. A class-2 meta-rule can be used to prevent an agent from moving toward friendly agents once it is surrounded by a threshold number. Finally, a class-3 meta-rule can be used to fix the local conditions under which an agent is allowed to move toward or away from possibly engaging an enemy agent in combat. Specifically, an agent is allowed to engage an enemy if and only if the difference between friendly and enemy force strengths -- locally -- exceeds a given threshold.

Other meta-rule classes include retreat, pursuit, support and hold position. A global rule set determines combat attrition, communication, reconstitution, and reinforcement.

11.11.4 *Combat*

Combat is adjudicated in the simplest possible manner. During the combat phase of an iteration step for the whole system, each agent X (on either side) is given an opportunity to fire at all enemy agents Y that are within a fire range r_F of X 's position. If an agent is shot by an enemy, its current state is degraded either from alive to injured or from injured to dead. Once dead, that agent is permanently removed from further play. The probability that a given enemy agent is shot is fixed by user specified single-shot probabilities for red-by-blue and blue-by-red.

This basic combat "logic" may be enhanced by three additional functions: (1) *defense*, which adds a notional ability to agents to be able to withstand a greater number of "hits" before having their state degraded, (2) *reconstitution*, which adds a provision for previously injured agents to be reconstituted to their alive state, and (3) *fratricide* (or *friendly fire*), which adds an element of realism to ISAAC combat by making it possible to inadvertently "hit" friendly forces.

EINSTEIN's combat adjudication engine also includes weapon and ammunition selection, suppression effects, lethality contours, and individual- and squad-based targeting strategies.

11.11.5 *Sample Behavior*

Despite its simple local rule base, EINSTEIN has an impressive repertoire of emergent collective behaviors: forward advance, frontal attack, local clustering, penetration, retreat, attack posturing, containment, flanking maneuvers, Guerrilla-like assaults, among many others.

Moreover, behaviors frequently arise that appear to involve some form of "intelligent" division of red and blue forces to deal with local "firestorms" and skirmishes, particularly those forces whose personalities have been evolved (via a genetic algorithm; see below) to perform a specific mission. It is important to point out that such behaviors are not hard-wired but rather an emergent property of a decentralized and nonlinear local dynamics. A small sampling of behaviors is shown below.

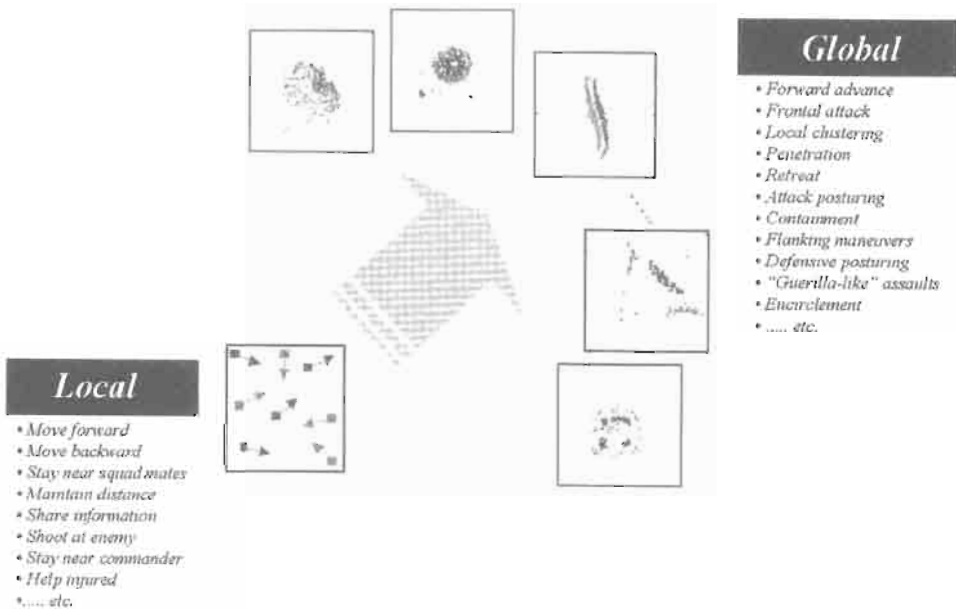


Fig. 11.13 Illustration of how mobile CA (here used to model elementary "combat") can be used to explore the relationship between primitive rules governing behavior on the micro-scale and emergent behavior on the macro-scale; see text.

11.11.5.1 Sample # 1: Fluid-like Collisions

Figure 11.14 shows several frames of a simulated engagement that is reminiscent of a collision between two viscous fluids. The initial state (not shown) consists of 90 red and 90 blue agents occupying random positions within 20-by-20 squares near the lower left and upper right regions of an 80-by-80 lattice; respectively. The blue force has a personality defined by the weight vector $w_{\text{blue}} = (1/15, 4/15, 1/15, 4/15, 0, 1/3)$. Each of the red agents is assigned a random personality (which is constrained only in giving zero weight to moving toward the red flag located in the lower left corner of the battlefield).

Red and blue forces collide head-on but are dispersed and aligned along two narrow columns at time $t=50$. The two sides continue battling each other in this manner, with neither side gaining an advantage or advancing closer to its enemy's. By time $t=75$, several blue agents have found a way to sneak around the bottom of red's column-like formation. This group is able to advance toward red's flag unchallenged because it is unseen by the red agents making up red's central column. By time $t=125$, a cluster of red agents breaks away from what used to be the central column and advances towards blue's flag. Meanwhile, blue forces continue advancing toward red's flag at the bottom of the frame.

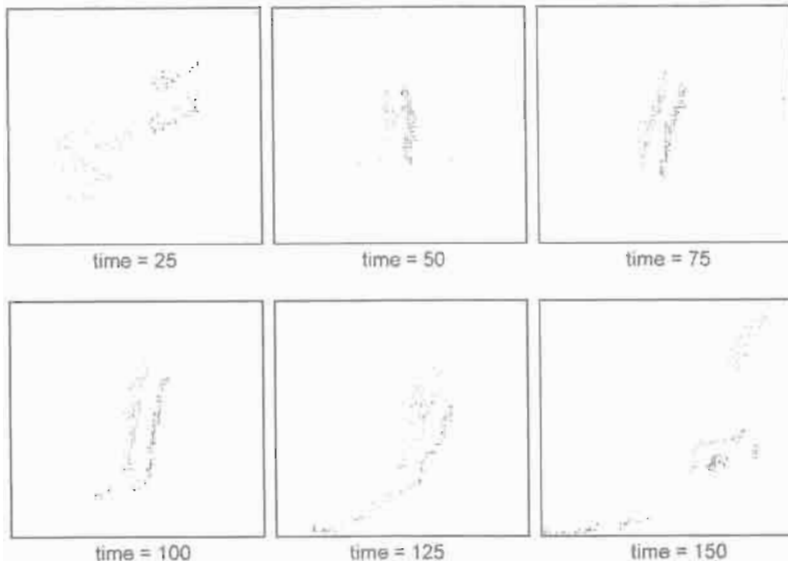


Fig. 11.14 Fluid-like “collision” between red and blue EINSTEIN agent forces.

11.11.5.2 Sample # 2: Non-Monotonic Behavior

Figure 11.15 shows an instructive example of non-monotonic behavior. The three rows contain snapshots of three separate runs in which red’s sensor range is systematically increased in increments of two: $r_{S,red} = 5$ for the top sequence; $r_{S,red} = 7$ for the middle sequence; $r_{S,red} = 9$ for the bottom sequence. Blue’s sensor range, $r_{S,blue}$, remains fixed at $r_{S,blue} = 5$ throughout all three runs. In each of the runs, there are 100 red and 50 blue agents. Red is also the more aggressive force: blue will engage in combat if the number of friendly and enemy agents is locally about even, while red will do so even if outnumbered by four enemy combatants. Both sides are endowed with the same fire range ($r_F = 4$), the same single-shot probability ($p = 0.005$) and can simultaneously engage the same maximum of 3 enemy targets. Note that the flags for this sample run are located near the middle of the left and right edges of the notional battlefield.

The top row of figure 11.15 shows screenshots for when red’s sensor range is equal to blue’s. Here the red force effectively “barrels” its way through the blue defenses into blue’s flag. As red advances toward blue’s flag, a number of agents are stripped away from the central red-flag:blue-flag axis as they respond to the presence of nearby blue agents. The snapshots for the middle row of figure 11.15 show that when red’s sensor range is two units greater than blue’s, red is not only able to mass almost all of its forces on the blue flag (a later snapshot would reveal blue’s flag completely enveloped by red forces by time $t=100$), but to defend its own

flag from all blue forces as well. In this instance, the red force knows enough about, and can respond quickly enough to enemy action such that it is able to march into enemy territory effectively unhindered by enemy forces and “scoop up” blue agents as they are encountered.

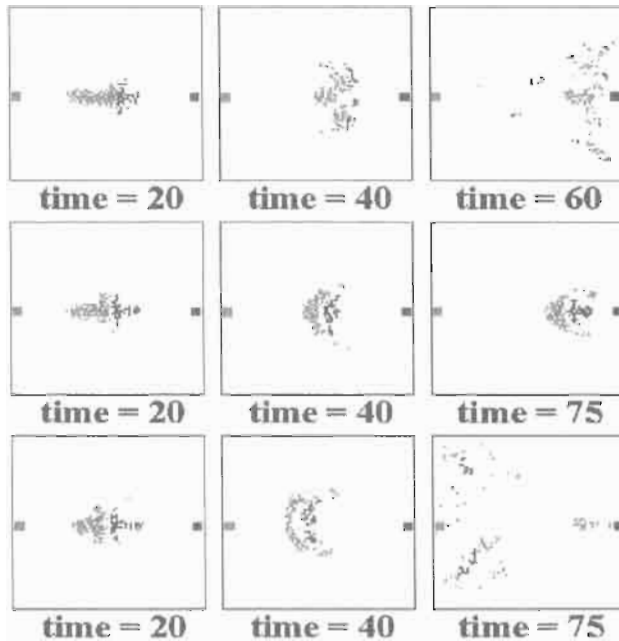


Fig. 11.15 Example of non-monotonic behavior in EINSTEIN.

What happens when red’s sensor range is increased still further? One might intuitively guess that red can only do at least as well; certainly no worse. However, as the snapshots for bottom row of figure 11.15 reveal, when red’s sensor range is increased to $r_{S,red} = 9$, red does objectively worse than it did in any of the preceding runs. “Worse” here means that red is less effective in (a) establishing a presence near the blue flag, and (b) defending blue’s advance toward the red flag.

This example illustrates that when the resources and personalities of both sides remain fixed in a conflict, how “well” side X does over side Y does not necessarily scale monotonically with X’s sensor capability. As one side is forced to assimilate more and more information (with increasing sensor range), there will inevitably come a point where the available resources will be spread too thin and the overall fighting ability will therefore be curtailed. Agent-based models such as EINSTEIN are well suited for providing insights into more operationally significant questions such as, *How must X’s resources and/or tactics (i.e., personality) be altered in order to ensure at least the same level of mission performance?*

11.11.5.3 Sample # 3: GA-Bred Tactics

Figure 11.16 shows an example of a red personality that has been “bred” to perform a specific mission using a GA. The parameters defining the blue side are fixed (except for initial spatial disposition, which is averaged over during the run), and the GA is used to find the “best” red personality that performs the following mission: get as many red forces near blue’s flag as possible while minimizing red casualties.

There are 70 agents on each side and the blue force is stationed in a semi-circle 25 units away from its flag in the upper right corner of the battlefield. Red’s “tactic” – which derives solely from the personality found by the GA to be best suited for this mission – is to exploit a few red agents at the front of the advancing red force, using them to split apart blue’s forces in order to temporarily weaken the center region of blue’s defense.

What is most surprising about many of the runs using GA-derived personalities is that the red force appears to task different agents with different missions, despite the fact that each red agent is endowed with exactly the same personality! Thus, a higher-level tactic – such as use the two forward positioned agents to weaken the enemy’s center – emerges out of the collective interactions of the same low-level decision rules; i.e., an apparently centralized order induced by decentralized local dynamics.

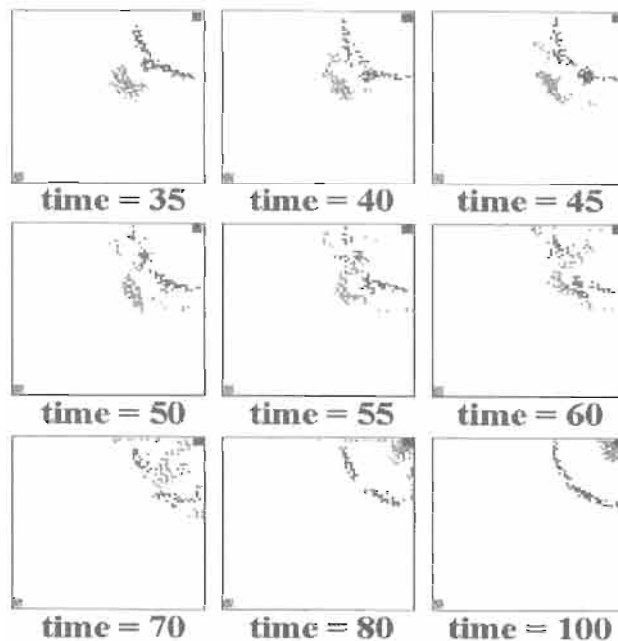


Fig. 11.16 GA-bred red personality to perform mission $M = \text{Get as many forces near blue's flag as possible while minimizing friendly casualties.}$

11.11.6 *Payoffs to Using Agent-Based Models of Combat*

Most traditional models focus on looking for equilibrium “solutions” among some set of (pre-defined) aggregate variables. The LEs are effectively mean-field equations, in which certain variables (i.e. attrition rate) are assumed to represent an entire force, the equilibrium state is explicitly solved for and declared the battle outcome. In contrast, ABMs focus on understanding the kinds of emergent patterns that might arise while the overall system is out of (or far from) equilibrium.

The payoff of an agent-based approach is a radically new way of looking at fundamental issues of land combat. Models such as these are emphatically not to be used for prediction; rather they are best used to enhance understanding. Specifically, agent-based models of combat are designed to help military theorists...

- Understand how all of the different elements of combat fit together in an overall combat phase space: Are there regions that are sensitive to small perturbations, and, if so, might there be a way to exploit this in combat (as in selectively driving an opponent into more sensitive regions of phase space)?
- Assess the value of information: How can I exploit what I know the enemy does not know about me?
- Explore tradeoffs between centralized and decentralized command-and-control (C2) structures: Are some C2 topologies more conducive to information flow and attainment of mission objectives than others? What do emergent forms of a self-organized C2 topology look like?
- Provide a natural arena in which to explore consequences of various qualitative characteristics of combat (unit cohesion, morale, leadership, etc.)
- Explore emergent properties and/or other “novel” behaviors arising from low-level rules (even combat doctrine if it is well encoded): Are there any universal patterns of combat behavior?
- Provide clues about how near-real-time tactical decision aids may eventually be developed using “natural selection” (via genetic algorithms).
- Address questions such as “How do two sides of a conflict co-evolve with one another?” and “Can one side exploit what it knows of this co-evolutionary process to compel the other side to remain out of ‘equilibrium’?”

The strength of agent-based models – not just for military modeling but for modeling in general – lies not just in their providing a potentially powerful new general approach to computer simulation, but also in their infallible ability to prod researchers into asking a host of interesting new questions. This is particularly apparent when EINSTEIN is run interactively, with its provision for making quick “on-the-fly” changes to various dynamical parameters. Observations immediately lead to a series of “What if?” speculations, which in turn lead to further explorations and further questions. Rather than focusing on a single scenario, and estimating the values of simple attrition-based measures of single outcomes (“Who won?”), users of agent-based simulations of combat typically walk away from an interactive session with an enhanced intuition of what the overall combat fitness landscape looks like.

Users are also given an opportunity to construct a context for understanding their own conjectures about dynamical combat behavior. The agent-based simulation is therefore a medium in which questions and insights continually feed off of one another.

What lies at the heart of an artificial-life approach to simulating combat, is the hope of discovering some fundamental relationships between the set of higher-level emergent processes (penetration, flanking maneuvers, containment, etc.) and the set of low-level primitive actions (movement, communication, firing at an enemy, etc.). Recall Wolfram's conjecture that the macro-level emergent behavior of all CA rules falls into one of only four universality classes [wolf83a], despite the huge number of possible local rules. While EINSTEIN's rules are obviously more complicated than those of their elementary CA brethren, it is nonetheless tempting to speculate about whether there exists -- and, if so, what the properties are, of -- a *universal grammar of combat*.

Chapter 12

Is Nature, Underneath it All, a CA?

Build physics, with its false face of continuity, on bits of information!

-- John A. Wheeler

The introductory chapter of this book identified four basic motivations for studying CA. The subsequent chapters have discussed a wide variety of CA models predicated on the first **three** of these four motivations; namely, using CA as... (1) as powerful computational engines, (2) as discrete dynamical system simulators, and (3) as conceptual vehicles for studying **general** pattern formation and complexity. However, we have not yet presented any concrete examples of CA models predicated on the fourth--and arguably the deepest--motivation for studying CA: *as fundamental models of nature*. A discussion of this fourth class of CA models is taken up in earnest in this chapter, whose narrative is woven around a search for an answer to the basic speculative question, "*Is nature, at its core, a CA?*"

Life, Computation, Information Theory and Physics. Do these seemingly disparate subjects have anything deeper in common than the mere fact of their having all been unceremoniously lumped together to start off the concluding chapter of this book?[†] We know that "computation" is something that a computer does, which is really just another name for "information processing," so a connection between computation and information theory does not appear farfetched. We also certainly need to know more than just a bit of physics in order to build and operate

[†]I fondly recall the first day of an introductory graduate statistical mechanics class. As our instructor walked into the class saying something *entirely appropriate* like "So, are we all ready for a lesson in quantum field theory today?", he was of course met with a room-full of blank stares (even a few -- later embarrassed -- behind-the-back giggles). As first-year graduate students we had unfortunately not yet developed the requisite maturity to appreciate the profound link that exists between statistical mechanics and modern field theory. I resolved to never again be as quick to dismiss any "obvious" disparity or seeming disconnectedness between two subjects.

a computer, so maybe lumping physics in with computation and information theory is not so out of place either. *But life?* What does life have to do with anything? The life of the computer operator who took a course in information theory and has a degree in physics ...?

The connection we are after in this chapter, of course, lies much deeper than surface superficiality alone might suggest. The conviction that these seemingly disparate subjects are in fact linked in some very fundamental – albeit, still essentially mysterious – way, is being ever more compellingly argued in mainstream physics journals, conferences and research centers. As the boundaries of what have come to be known as the sciences of *Complexity Theory* and *Artificial Life* are stretched, the disparity among our four otherwise well-defined subjects grows less and less apparent. The irony is that the more we learn about these subjects – or, more precisely, the more we become attuned to the radically new view of the world that these subjects instill in those who study them – the less reliable become our old definitions of the central concepts around which they are built: *life*, *complexity*, *information* and *emergence*. One of the main goals of this chapter is to stimulate the reader into thinking about how these and other important concepts that “we all know the meaning of but never really tried defining before” can be formally and consistently defined within a broader framework.

We issue a mild caution. One must always be mindful of the temptation to see things not as they really are but only how they appear to be at the moment using whatever happens to be the most convenient or “accepted” way of looking at things. This is the dreaded “solution in search of a problem” phenomenon, disguised, in the case of physicists trying to make sense of the world, as the temptation to use whatever is the latest fad or theory simultaneously as a lens and litmus test for reality.

The history of physics teaches us that each generation of physicists develops its own unique style of looking at the world, inevitably leaving behind in its wake not just a laundry list of what it believed was wrong with previous views but a unique imprint on how reality must be *defined* – a definition that is itself destined to be skewed (and sometimes *skewered*) by succeeding generations. Witness the ancient Greek belief that air, fire, earth and water are the only four basic constituents of nature; or Ptolemy’s epicyclical, geocentric model of the solar system; or Newtonian determinism; or Maxwell’s ether and the belief in an absolute reference frame; or ... the list continues. How then may we be sure that the currently fashionable notion of ascribing some deep connection among *life*, *computation*, *information theory* and *physics*, holds any greater truth than the mere happenstance of their increasingly frequent joint appearance in some of the same physics and/or computer science journals?

The honest answer, of course, is that we cannot be sure at all. Time, as the proverbial saying goes, surely will tell. But, after having started off this chapter with an obligatory caution flag against such musings, we will now dive head first in its remaining sections to argue that work done over the last twenty or thirty years, and particularly during the last decade, strongly suggests that the idea that these once truly disparate subjects are in fact fundamentally and deeply linked is not just

a passing fancy but instead points to a profound and heretofore undiscovered basic clue as to how our universe really works. We will also argue that CA, or at least the fundamental concepts that they embody, may well form the backbone of what the next generation of physicists is destined to view – and, we will be so bold as to predict, view *correctly* – as reality.

The vision of fundamental physics in general, and the particular role that complex systems play in shaping that fundamental physics, that this chapter offers can be summarized by the following three visions of the future:

- *The next great strides in science will be founded on the sciences of complexity and artificial life.*
- *Physics, in particular, will expand its horizons and begin exploring the fundamental nature of information, and the role that information plays as a primordial variable shaping the course of development of the universe.*
- *A new world view will emerge in which the universe itself is viewed as a living, evolving, computer.*

Coming as it does at the heels of a rather weighty pedagogical tome, this last chapter is intended to be more of a freewheeling mixture of pedagogy – including discussions of various measures of complexity and recent approaches to reformulating conventional field theory using somewhat less-than-conventional cellular-automata-like premises – and outright fanciful speculation – not all of which is relegated to the last section, entitled, appropriately enough, **Some Final Musings... And a Glimpse of a New Cosmogony**. While we do not expect the reader to necessarily agree, or even be amused, by all of our musings, there should be little doubt but that cellular automata are powerful catalysts for the synthesis of interesting ideas. For cellular automata are nothing if not powerful catalysts...

12.1 CA are Catalysts... But of What?

It is hard to mistake cellular automata for being anything other than what they are: *at best*, discrete approximations of the underlying processes of some (otherwise difficult to analyze) continuous systems, and good enough approximations so that a study of their own behavior actually sheds light on the behavior of those continuous systems; *at worst*, simple “toy” models, which, though not necessarily well grounded in reality and without an explicit agenda to “simulate” anything real, nonetheless lend important insights into the generic properties of self-organizing and/or emergent behavior. We will now argue, however, that cellular automata serve another useful and important purpose: they are wonderful catalysts for forming more speculative theories about how our universe really operates. They do so not by exhibiting particular behaviors, but by embodying a simple set of fundamental concepts and inspiring a particular set of methodologies designed to study their behavior.

Consider, for a moment, what cellular automata represent, fundamentally, as

a conceptual approach to modeling in general. All cellular automata possess, and serve as conceptual prototypes for, three distinctive dynamical and/or general system properties:

- *information is locally finite.*
- *information is communicated and processed locally.*
- *information processing (which might be “locally” very simple) proceeds in a parallel fashion across a large assemblage of interconnected processing sites.*

For the particular class of reversible cellular automata rules, we might also add the fourth property:

- *information is conserved.*

Each of these attributes, if considered within a larger context and reinterpreted as constituting the basic axioms of a more fundamental theory, and not just as attributes of a skeletal toy model of an existing theory, has potentially far reaching consequences. The first attribute, for example, if it is considered within the context of continuum field theories, directly contradicts their axiomatic foundation. All field theories based on the continuum effectively assume that the universe processes an infinite amount of information at each point in space-time (see **Feynman’s Challenge**; section 12.4.3 below). What if a field theory were instead predicated on the idea that the universe processes only a *finite* amount of information? What sort of dynamics would be natural and what kinds of behaviors would emerge? Might such a field theory be CA-like in some fashion? We have only to assume that the universe contains a finite amount of information to be led naturally to the question of whether the real “physics” that is going on owes more of its structure to a primordial “computation” of some sort than “_____” (the reader can fill in the blank with *Grand Unified Field Theory*, or any other continuum-based fundamental theory). A number of serious attempts to formulate finite-information-based field theories have already been made, and we discuss a few of them later in this chapter.

Similarly, the second and third properties hint at a theoretical framework by which the fundamental principles of self-organization and so-called “emergent” phenomena can be themselves explored. Just as the study of chaos has taught us that complex behavior need not always originate in complex dynamics – think of the extraordinarily complicated behavior of the lowly logistic equation (see section 4.1.4.1) – cellular automata teach us that not all phenomena appearing on a given level or scale of observation have explanations that can be derived solely from the dynamics operating on that same level. Cellular automata also teach us that there are behaviors of complex systems that can only be described as “emergent” phenomena; that is, phenomena that, while certainly being made manifest by the interactions of the myriad microscopic components making up the system, cannot be directly deduced from knowing the details of the microscopic dynamics. Link together enough otherwise “simple” parts, allow them to communicate their states locally and let

them evolve in parallel – with a few specks of nonlinearity thrown in – and you will more than likely find something interesting emerge out of that soup that you could not have predicted beforehand merely by looking at the set of dynamical rules that the parts obey. Throw in some Darwinian-like natural-selection of rules, and your soup becomes not only a potent natural problem-solver, but something that comes precipitously close to being called “alive.”

The point of this terse introduction is that cellular automata represent not just a formalism for describing a certain particular class of behaviors (lattice gas simulations of fluid dynamics, models of chemical reactions and diffusion processes, etc.), but a much more general “template” for original and heretofore untapped ways of looking at a large class of unsolved or only poorly understood *fundamental* problems.

Interpreting CA in this much broader light, this chapter addresses the following basic question: “*What general insights does the study of cellular automata give – both on the micro- or macro-scale – into the way our universe works ?*” Unless otherwise stated, whenever we use the phrase “CA-like” in this chapter, we mean any formalism that adheres to the three (or four) basic properties of cellular automata listed above.

12.1.1 Further Reading

For those wishing to pursue the ideas explored in this chapter and related issues in greater depth, there is no better place to begin than with the papers presented at the landmark conference on the Physics of Computation held at MIT in 1982 and collected in volume 21 of the *International Journal of Theoretical Physics* [land82b]. Many of the ideas pertaining to the central topic of this chapter were discussed in this interdisciplinary setting for the first time. Follow on conferences on the same theme were held in Santa Fe, New Mexico in 1988 (with papers collected in *Complexity, Entropy and the Physics of Information* [zurek90]), in Dallas, Texas in 1992 (with papers collected in *Workshop on Physics and Computation: PhysComp '92* [phys93]), and again in Dallas, Texas in 1994 [phys93].

Many landmark papers in the history of the exploration of the connections between entropy, information and computation appear in the excellent collection of reprints edited by Leff and Rex [leff90].

For obtaining more information about the *Science of Complexity*, the reader is urged to consult any of the many recent publications of the *Santa Fe Institute*, particularly the lecture notes series on complexity ([stein89], [jen90a], [nadel91], [nadel92], [nadel93] and [nadel95]). Well written popularized accounts of complexity science are given by Lewin [lewin92], Waldrop [wald93], and Casti [casti94].

Two early discussions of the behavioral complexity of systems are given by Simon [sim62] and Zvonkin and Levin [zvon70]. An early survey of an information-theoretic view of complexity is given by Sahal ([sahal76b]; see also [sahal76a]). Excellent recent reviews of measures of complexity are given by Chaitin [chaitin87], Bennett ([benn87b], [benn90c]), Lindgren and Nordahl [lindg88b] (with particular emphasis on complexity in cellular automata systems), Svozil [svozil93] and Casti ([casti79],

[casti92], [casti94]). The collection of papers edited by Peliti and Vulpiani [peli88] is also a good source of information.

Finally, three excellent (and sophisticated) monographs on the general relationship between “part” and “whole” in physics – a theme which arguably sits at the very heart of complexity theory – are those by Jantsch [jant80], Kafatos and Nadeau [kafa90] and Bohm and Hiley ([bohm93]; see also [bohm80]).

12.2 CA As Embodiments of a Paradigm Shift

Thomas Kuhn, in an influential work on the history of science entitled *The Structure of Scientific Revolutions* [kuhn70], used the phrase “paradigm shift” to describe the essence of what happens when one established way of looking at the world is – either suddenly, or over time – replaced by another.

Putting aside questions of the historical accuracy of Kuhn’s usage of this phrase for this purpose, it is interesting that the word *paradigm* – which is derived from the Greek word *paradeigma*, meaning “pattern” or “structure,” and itself refers to the pattern of beliefs that a society uses to organize itself – can serve well both in the Kuhnian sense of suggesting that cellular automata have become the focus of an important paradigm shift, as well as reminding us of what is basically the essence of that focus, namely the self-organized emergence of “order” (or “patterns” and “structures”) out of an apparent underlying randomness. It is arguable that cellular automata have in fact become the simultaneous focus of not one but two separate paradigm shifts:[†]

Reductionist World-View $\Rightarrow$ Holistic World-View: a shift away from a long held belief that complex self-organized behavior requires a complex underlying dynamics and/or substructure *towards* the new notion that complexity is an emergent/holistic phenomenon that often arises from the interactions among a large assemblage of otherwise simple parts; i.e. the properties of the *parts* must be understood as a dynamics of *whole*.

Physics and Information $\Rightarrow$ Physics of Information: a shift away from the old notion that physics and computation are connected only insofar as computers

[†]Fritjof Capra ([capra86], [capra88]) has been an eloquent spokesman for what he calls an emerging “ecological world view,” arguing that, ultimately, ecological awareness is a deeply religious awareness in which an individual feels connected with the whole (as in the original root meaning of the Latin word *religare*: “to bind strongly”). Capra also believes that the ecological world view represents but a small glimpse of a number of important paradigm shifts now taking place in how we view and understand physical reality: (1) *shift from the part to the whole*; (2) *shift from structure to process*; (3) *shift from objective to “epistemic” science*; i.e. a shift from a view in which descriptions of nature are understood as objective and independent of the human observer to a view in which epistemology, or the understanding of the process of knowledge, must be included explicitly in the description of phenomena; (4) *shift from “building” to “network” as metaphor of knowledge*; and (5) *shift from truth to approximate descriptions*. An excellent related monograph on the relationship between “part” and “whole” in physics is *The Conscious Universe* by Kafatos and Nadeau [kafa90].

are sometimes called upon to solve physics problems towards the new notion that physics and computation are intimately and profoundly interconnected; i.e. towards the notion that computation is rooted in physics and that physics – the *universe* – is essentially a computer.

Evidence of the first paradigm shift is perhaps nowhere stronger than in the emerging new interdisciplinary field of *Artificial Life* (AL) ([lang89], [lang92a], [levy92], [emmec94], [brooksr94]). AL concerns one of the last great frontiers of science: the fundamental principles of life itself. The basic question that AL asks is whether “life” is unique to its biological (and, as yet, only known) form, or is a more general property that is independent of the physical substance in which it is made manifest. Or, as Chris Langton [lang92a] prefers to put it, AL is about life as it *could* be as opposed to life as we *know* it to be.

One of the key motivational principles of AL is that of self-organized *emergent behavior*: the appearance of higher-level properties and behaviors, referred to as an organism’s generalized “phenotype,” that are essentially unpredictable from its generalized “genotype,” or the set of genetic instructions that describes the organism’s DNA. Indeed, artificial life teaches us that the absolutely worst way to tinker with an organism’s phenotype is to tinker with the organism’s phenotype. Perhaps the only way is to manipulate the genotype, then sit back and watch what happens!

The profound nonlinear feedback mechanism between the micro- and macro-scales that appears to be so widespread in living systems is described by the new term – and paradigm – *Collectivism*.[†] Collectivism embodies the idea that higher-level emergent behaviors are best understood via a co-evolutionary, self-organized, micro ↔ macro feedback dynamics. For example, each species that makes up an ecology composed of a large number of diverse species, co-evolves with other members of the ecology according to a fitness function that is, in part, itself a function of the emerging ecology. Individual members of each species collectively define a (part of the)[‡] co-evolving ecology; the ecology, in turn, determines the fitness-function according to which its constituent parts evolve. It is this nonlinear feedback between the information describing individual species (or the microscopic level) and the global ecology (or macroscopic level) that those species collectively define that perpetually drives the evolution of the entire system.

Note that, as a concept, collectivism is really distinct from both the top-down reductionist approach traditionally favored by most physicists (“system” as a simple edifice of its microscopic parts), and the more recent neural-net-like bottom-up approach favored by connectionists (“system” as a synthesis of its constituent parts). Collectivism asserts that a system is more than just a “large-part” synthesized from “smaller-parts,” but is a coherent “whole” whose evolution is continuously redefined

[†]First coined by Chris Langton at the *Artificial Life IV* conference held at MIT [brooksr94].

[‡]An ecology also includes elements of the environment which the species cohabit. A description of the full ecology must therefore encompass not only the co-evolution among its constituent species but the complex interactions between those species and the effects they produce in their local environments.

by a nonlinear feedback mechanism between its macroscopic state and microscopic constituents. A provocative example of collectivism in action is our macro-level (or human phenotype) ability to literally reach down into the micro-scale (or genotype) and manipulate individual bits of our own genetic code. Looked at from the larger perspective of “life,” and the effect that modified DNA can have on the evolution of our species, this is nothing but *life having built a nonlinear feedback mechanism for itself!*

The developmental histories of artificial life and cellular automata have been intertwined ever since von Neumann first showed how to construct a self-reproducing automaton ([vonN66]; see section 11.7). A brief historical overview of artificial life appears in chapter 11.

The second paradigm shift, which is the primary focus of this chapter, concerns both sides of the relationship between physics and computation. It signals an era in which physicists are beginning to recognize that not only does physics have much to say about computation — by helping to understand the fundamental limits of computation, the difficulties in actually building reversible and quantum computers, and so on — but that computation, the abstract principles describing the communication and processing of information, has much to say about fundamental physics. The second, and obviously more provocative, viewpoint grows in importance as the distinction between *simulating* the properties of a physical system and *reproducing* that system’s behavior exactly, becomes blurred.

The role that cellular automata play in shaping and/or helping to elucidate either viewpoint is determined largely by how cellular automata themselves are viewed. On the one hand, cellular automata can be viewed simply as powerful computational tools. While they cannot always be made to exactly duplicate all of the relevant physical processes they are designed to simulate, their dynamics captures enough of a system’s essential properties to faithfully reproduce that system’s most important behaviors. In this view, also, cellular automata are treated as fully discrete dynamical systems providing experimental arenas in which to explore general physical principles. Because cellular automata by definition evolve according to precise, well-defined sets of rules and their states are known exactly at all times, cellular automata can be used to explore symmetries, conservation laws, causality, chaos, long-range correlations, etc., with what Toffoli [toff84a] calls “theorem-like” decisiveness. Recent advances in the use of cellular automata lattice gases as simulators of physical fluids typifies this view (see chapter 9). On the other hand, if it turns out that our universe indeed rests on a foundation of finite, locally communicated and locally processed “information,” cellular automata may also be viewed as prototypes of a fundamental *finite physics*. Cellular automata would in this case emerge as being not just good at *simulating* physics, but as indispensable tools for exactly *recreating* it.

Just as artificial life seeks to answer the question of whether life is really an emergent property of the *organization of matter* and is not just some unique embodiment of its substance, so too it might be said that the goal of finite physics is to see whether physics — what we call “reality” — is fundamentally a property of the *organization of information* rather than a unique embodiment of the interaction

of matter with matter. Lawrence [law93] puts it best when he suggestively refers to matter as a “dense” form of energy (a la $E = mc^2$), and energy as a “dense” form of information. It is perhaps not so crazy to suppose that the next truly great discovery in physics might in some way involve an “Einsteinian”-like link between energy E and information I , a la $I \propto E^2$.

We will argue, in the last section of this chapter, that the time is ripe to begin unifying the two seemingly separate paradigm shifts outlined above – I. *reductionist* world view $\rightarrow$ *Holistic* world view and II. *physics and information* $\rightarrow$ *physics of information* – into one grand, sweeping world view embodying the idea that the same general set of guiding principles responsible for the evolution of life on this planet is in fact responsible for the emergence of the very physics that has made this possible: *physics as emergent phenomenon* and the *universe as living computer*. We begin with a discussion of the physics of complexity.

12.3 Physics of Complexity

Two of the greatest intellectual achievements of 20th century science – *Special Relativity Theory* and *Quantum Mechanics* – were both born of examinations of extremes and both identified fundamental constraints of our universe. In the case of special relativity, of course, it was Einstein’s *gedanken* experiments with the “very fast” that revealed to him the fundamental importance, and limitation, of the speed of the light, c . In the case of quantum mechanics, Heisenberg’s uncertainty relations and Planck’s constant h were both born essentially of an examination of the “very small.” It is tempting to speculate, even at this very early juncture, that before the 20th century takes in its last breath yet another milestone in our understanding of the universe will have been born of another extreme. This time, however, the key insight or insights and whatever fundamental constraints they might reveal, will have been born of an examination of the very *complex*.

12.3.1 What is Complexity?

Just what do we mean when we say that something is “complex?” To make it slightly easier, we should really be ask two separate questions. First, “What is a complex system?”, followed by “What is complex behavior?” While neither of these two questions is particularly easy to answer rigorously, the task is, conceptually at least, made easier if we use cellular automata as paradigms for both: they not only constitute the prototypical complex dynamical system, but their behavior literally spans the spectrum from *null-rule-like* triviality to Conway’s *Life-rule-like* computational universality; the latter of which arguably represents as “complex” a behavior as is likely to be found anywhere. With this image in mind, let us address the above two questions.

12.3.1.1 *First Ask: "What is a Complex System?"*

There are examples of complex systems just about everywhere we look in nature, from the turbulence in fluids to global weather patterns to beautifully intricate galactic structures to the complexity of living organisms. Leaving aside for the moment the problem of quantifying the complexity of the behavior of these systems, or the complex spatio-temporal patterns that their behavior induces, we see that such systems have at least this one fact in common: they all consist of – and their overall behavior stems from – *a large assemblage of interconnected, mutually (and typically nonlinearly) interacting parts.*

A “complex system” must be understood not just in terms of the set of components out of which it is constructed, but the topology of the interconnections and interactions among those components. Any measure of complexity must likewise respect both the *structure* and *dynamics* of a complex system.

Gases, fluids, crystals, and lasers are all examples of complex systems that are familiar to us from physics. Chemical reactions, in which a large number of molecules conspire to produce new molecules, are also good examples. From biology, we have DNA molecules built up from amino acids, cells built from molecules, and organisms built from cells.

Perhaps the quintessential example of a complex system is the human brain, which, consisting of something on the order of 10^{10} neurons with $10^3 - 10^4$ connections per neuron, is arguably the most “complex” complex system on this planet. Somehow, the cooperative dynamics of this vast web of “interconnected and mutually interacting parts” manages to produce a coherent and complex enough structure for the brain to be able to investigate its own behavior.

On a larger scale, the national and global economies and human culture as a whole are also complex systems, exhibiting their own brand of global cooperative behavior. One of the most far-reaching hypotheses of this sort is Lovelock’s controversial “Gaia” hypothesis ([love79], [love88]), which asserts that the entire earth – molten core, ecosystems, atmospheric weather patterns and all – is essentially one huge, complex *organism*, delicately balanced on the proverbial “edge of chaos.”

The emerging new *Science of Complexity* (see [weis88], [lewin92], [wald93], [casti94], [gell94], [wolf94b] and the series of lecture notes from the *Santa Fe Institute*: [stein89], [jen90a], [nadel91], [nadel92], [nadel93]) explores the important question of whether, or to what extent, any or all of the many seemingly disparate complex systems – from the very small to the very large – share a universality of large-scale behavior that stems from a set of basic (and, as yet, largely undiscovered) principles describing the general behavior of complex systems.

Do the complex machinations of the world commodities market, the intricate swirls of the Belousov-Zhabotinski chemical reaction, the firings of the neurons in my brain and the interconnected co-evolving patterns of the earth’s global ecosystem all obey the same core set of underlying universal principles? While no-one yet knows the “deep” answer, evidence strongly suggests that the *qualitative* behavior of systems that emerges on the macro-scale is often very similar for systems that share the same basic structural organization, the same basic set of interactions

among the components out of which they are constructed, the same basic patterns of information flow, etc. It is the goal of the science of complexity to find that core set of universal principles that shape and/or determine a complex system's overall, emergent, behavior. Such a discovery would surely rank alongside *Relativity Theory*, *Quantum Mechanics* and *Chaos Theory* as among the most important elucidations of the workings of this universe in the 20th century.

12.3.1.2 Then Ask: "What is "Complex Behavior?"

It is one thing to describe as we have done informally above, even qualitatively, what a complex system is, and to conjure up myriad examples of complex systems. It is quite another to quantify the notion of complexity itself, to describe the relationship between complexity and information, and/or to understand the role that complexity plays in various physical and/or computational contexts. Each of these difficult problems in fact remains very much open. While we may find it easy enough to distinguish a complex object from a less complex object, it is far from trivial to furnish anything that goes beyond a vague characterization as to how we have done so. Some recent attempts at quantifying the notion of complexity are sketched below.

To set up the problem and in order to appreciate more fully the difficulty in quantifying complexity, consider figure 12.1. The figure shows three patterns: (a) an area of a regular two-dimensional Euclidean lattice, (b) a space-time view of the evolution of the nearest-neighbor one-dimensional cellular automata rule R110, starting from a random initial state,[†] and (c) a completely random collection of dots.

These patterns illustrate the incongruity that exists between mathematically precise notions of entropy (see below), or the amount of disorder in a system, and intuitive notions of complexity.

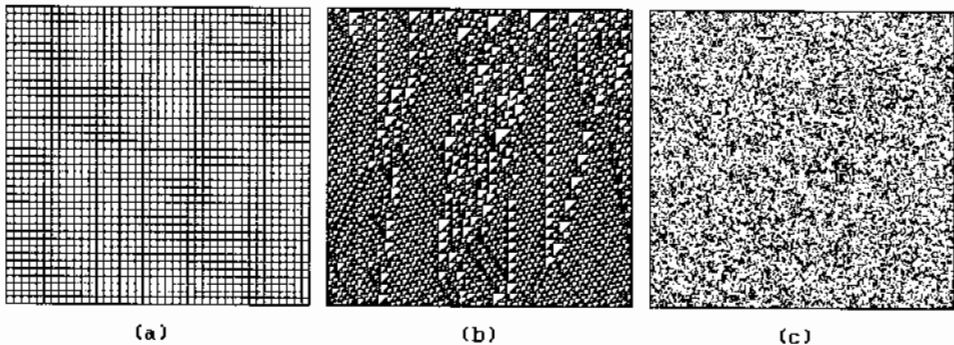


Fig. 12.1 Three patterns illustrating the incongruity between mathematically precise notions of entropy and intuitive notions of complexity. Whereas pattern (b) is intuitively the most complex, it has neither the highest (c) or lowest (a) entropy. See text.

[†]Rule R110 is explicitly defined by $(\sigma_{i-1}\sigma_i\sigma_{i+1}) \rightarrow \sigma'_i$: (000) $\rightarrow$ 0, (001) $\rightarrow$ 1, (010) $\rightarrow$ 1, (011) $\rightarrow$ 1, (100) $\rightarrow$ 0, (101) $\rightarrow$ 1, (110) $\rightarrow$ 1, (111) $\rightarrow$ 0. See chapter 3.

Whereas pattern (b) is intuitively the most complex of the three patterns, it has neither the highest entropy (which belongs to pattern (c)) or the lowest (which belongs to pattern (a)). Indeed, were we to plot our intuitive sense of complexity as a function of the amount of order or disorder in a system, it would probably look something like that shown in figure 12.2. The problem is to find an objective measure of the complexity of a system that matches this intuition.

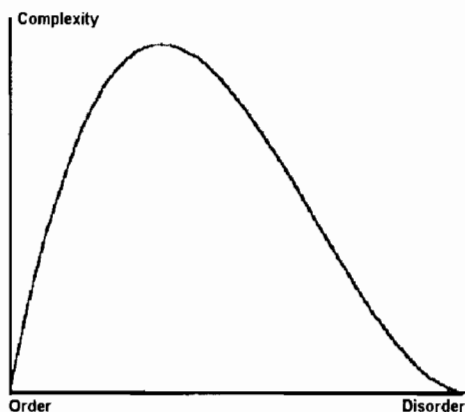


Fig. 12.2. A schematic representation of the “intuitive” relationship between *complexity* and the *degree of disorder* in a system.

12.3.2 Towards a Definition of Complexity

We all have an intuitive feel for complexity. An oil painting by Picasso is obviously more “complex” than the random finger-paint doodles of a three-year-old. The works of Shakespeare are more “complex” than the rambling prose banded out on a typewriter by the proverbial band of monkeys. Our intuition tells us that complexity is usually greatest in systems whose components are arranged in some intricate difficult-to-understand pattern or, in the case of a dynamical system, when the outcome of some process is difficult to predict from its initial state.

The problem is to articulate this intuition formally; to define a *measure* that not only captures our intuitive feel for what distinguishes the complex from the simple but also provides an objective basis for formulating conjectures and theories about complexity. While a universally accepted measure has yet to be defined, a number of interesting proposals have been made in recent years. All such measures of complexity fall into two general classes:

Static Complexity – which addresses the question of how an object or system is put together (i.e. only purely structural informational aspects of an object, or the patterns and/or strengths of interactions among its constituent parts), and is independent of the processes by which information is encoded and decoded.

Dynamic complexity – which addresses the question of how much dynamical or

computational effort is required to describe the information content of an object or state of a system.

Note that while a system's static complexity certainly influences its dynamical complexity, the two measures are clearly not equivalent. A system may be structurally rather simple (i.e. have a low static complexity), but have a complex dynamical behavior. (Think of the chaotic behavior of Feigenbaum's *logistic* equation, for example).

Measure	Type	Virtue	Drawback
<i>Algorithmic Complexity</i>	Dynamic	Measures complexity of given string vice ensemble	Hard to compute; complexity equated with randomness
<i>Computational Complexity</i>	Dynamic	Intuitively equates complexity with difficulty of computation	<i>a priori</i> Unclear how to encode a given "object" as a "function" to compute
<i>Graph Complexity</i>	Static	Captures intuitive "feel" of the complexity of a graph	Not <i>a-priori</i> clear how to extend to more general objects
<i>Hierarchical Complexity</i>	Static	Captures intuitive "feel" of the complexity of a hierarchy	Not <i>a-priori</i> clear how to extend to more general objects
<i>Shannon's Information</i>	Static	Captures only <i>some of the</i> intuitive flavor of complexity	complexity is additive, counter to intuition
<i>Logical Depth</i>	Dynamic	Random strings are "shallow," matching intuition	Hard to apply to physical systems
<i>Simplicial Complexity</i>	Static	Satisfies requirements of a measure of complexity for a simplicial complex	Not <i>a-priori</i> clear how to extend to more general objects
<i>Thermodynamic Depth</i>	Dynamic	Complexity expressed purely as a function of physical quantities	Hard to compute in general

Table 12.1 A quick-and-dirty comparison of some recently suggested measures of complexity.

In the sections below, we outline eight measures of complexity; four of them are static measures, four are dynamic. Table 12.1 summarizes some their main virtues and drawbacks. The fact that we chose to limit our discussion to these eight particular measures should in no way be misunderstood to mean that we believe they are the *only* ones possible, as they represent only a small sampling of recent proposals. Discussions of other measures, and of their respective pros and cons relative to given problems, can be obtained by consulting any of the references listed in the **Further Reading** section above (see section 12.1.1).

12.3.2.1 Complexity as Information?

Given an object composed of N interconnected and interacting “parts,” one might at first be tempted to equate the complexity of an object with its “conventional” information content, as defined by Shannon [sham49]:

$$I = -\sum_{i=1}^N p_i \log_2 p_i, \quad (12.1)$$

where p_i is the probability of the i^{th} event or part of occurring and $\log_2$ is the base-2 logarithm. The logarithm is used because it is the only function consistent with the reasonable demand that information be additive for independent events. That is to say, if there are two independent sets of outcomes, N_1 and N_2 , so that the total number of outcomes is $N = N_1 \cdot N_2$, the information content of N , $\mathcal{I}(N)$, is equal to the sum of the information content of the two independent set of outcomes, $\mathcal{I}(N) = \mathcal{I}(N_1) + \mathcal{I}(N_2)$.

While Shannon’s information does give an indication of how much a given object differs from other “like” objects belonging to the same class, there is a drawback to using it as a measure of complexity. Additivity may be a reasonable requirement to have for a measure of “information,” it is not an *a priori* reasonable demand to make of a measure of “complexity.” The reason is that the complexity of a given system is probably not doubled if two copies of that system are simply merged. If complexity were additive in this way, we could then generate arbitrarily complex objects simply by merging together a desired number of copies of arbitrarily simple objects. This certainly runs counter to our intuition. Thus, while Shannon information captures some of the flavor of complexity – a DNA molecule, for example, has a large (Shannon) complexity because its parts require a great deal of information to describe, while a crystal has little complexity because relatively little information is required to describe its regular structure – it fails to capture enough of the essence of real complexity to be a useful measure. Complexity cannot be additive; at least not in this simple manner (see **Thermodynamic Depth** below).

Another drawback to using Shannon information as a measure of complexity is the fact that it is based on an ensemble of all possible states of a system and therefore cannot describe the information content of a *single state*. Shannon information thus resembles traditional statistical mechanics – which describes the average or aggregate behavior of, say, a gas, rather than the motion of its constituent molecules – more so than it does a “complexity theory” that must address the complexity of individual objects.

Another way of looking at it is that Shannon information is a formal equivalent of thermodynamic entropy, or the degree of disorder in a physical system. As such it essentially measures how much information is missing about the individual constituents of a system. In contrast, a measure of complexity ought to (1) refer to individual states and not ensembles, and (2) reflect how much is known about a system vice what is not. One approach that satisfies both of these requirements is *algorithmic complexity theory*.

12.3.2.2 Complexity of a Graph

One of the simplest ways of modeling a variety of physical structures, from molecules to rigid three-dimensional structures, is the *mathematical graph*.

We begin with a few reminders of basic terminology.[†] A graph G is a finite, nonempty set $\mathcal{V}(G) = \{v_1, v_2, \dots, v_N\}$ of vertices (or nodes), together with (a possibly empty) set of edges $\mathcal{E}(G) = \{e_1, e_2, \dots, e_M\}$. Each edge $e_{ij} \in \mathcal{E}(G)$, connects vertex ' i ' to vertex ' j '. If the edges represent ordered pairs of vertices, then G is a directed graph: each e_{ij} defines an edge directed from ' i ' to ' j ', and is denoted by $e(i, j) = e_{i \rightarrow j}$. If, on the other hand, $e_{ij} = e_{ji}$ for all ' n ', then G is an undirected graph, and all edges are denoted simply by e_{ij} . The size of a G , denoted by $|G|$ is equal to the number of nodes in G .

Perhaps the simplest approach to defining a complexity of graphs is to apply Shannon's information measure to its vertices [dres74]. Let $\mathcal{P}_V = \{V_1^{(\mathcal{P})}, V_2^{(\mathcal{P})}, \dots, V_{h(\mathcal{P})}^{(\mathcal{P})}\}$ be a partition of the vertex set $\mathcal{V}$ of G , so that $\sum_{i=1}^{h(\mathcal{P})} V_i^{(\mathcal{P})} = \mathcal{V}$, where $|\mathcal{P}_V| = h(\mathcal{P})$ depends on the partition. Let $|V_i|$ be the number of nodes in the set V_i . Then the complexity $\mathcal{I}(G)$ of the graph G is given by minimizing Shannon's information over all possible partitions of this vertex set:

$$\mathcal{I}(G) = \min_{\mathcal{P}} \left\{ - \sum_{i=1}^{h(\mathcal{P})} p_i^{(\mathcal{P})} \log_2 p_i^{(\mathcal{P})} \right\}, \quad (12.2)$$

where $p_i^{(\mathcal{P})} = |V_i^{(\mathcal{P})}| / N$, $\log_2 x$ is the base-2 logarithm and the minimum is taken over all possible partitions $\mathcal{P}$ so as to do away with the arbitrariness of the selected partition.

Although this measure is occasionally used, it suffers from a serious drawback. Since it is a function only of the vertex set, it ignores all structural information. For example, all Feynman graphs of a given order are assigned the same "complexity." We can improve upon this measure by including information about a graph's topology.

Topological Complexity: Since a graph is an object that includes both parts (i.e. nodes) and structure (i. e. their interconnectivity pattern), a legitimate measure of complexity of a graph should at least respect sets of topologically equivalent vertices of a graph. One such measure, called *topological complexity* – or *information content*, as it was first called by Rashevsky [rash55], who introduced a version of this measure for dealing with the complexity of organic molecules – is essentially equal to the entropy of the orbits of a graph's automorphism group. To define it we first need to introduce a few more definitions.

Two graphs, G_1 and G_2 are said to be *isomorphic* if there exists a one-to-one mapping $f : \mathcal{V}(G_1) \rightarrow \mathcal{V}(G_2)$ such that $e_{ij} \in \mathcal{E}(G_1)$ if and only if $f(e_{ij}) = e_{f(i)f(j)} \in \mathcal{E}(G_2)$.

An *automorphism* of a graph G is an isomorphism of G onto itself. It is easy to

[†]Basic graph theory is discussed in section 2.1.3.

check that the set of automorphisms of a graph forms a group – the automorphism group, $\mathcal{G}(G)$ – which can also be regarded as a subgroup of $\mathcal{S}_n$, the symmetric group of degree n [boll79]. $\mathcal{S}_n$ consists of all permutations $\pi : \vec{n} \rightarrow \vec{n}$ on the finite set $\vec{n} = \{1, 2, \dots, n\}$.

Now, suppose S is a subgroup of $\mathcal{S}_n$. Then $\mathcal{O}(S) = \{f(i) \mid f \in S\}$, $1 \leq i \leq n$ is called the *orbit* of S . Let $s_1, s_2, \dots, s_h$ be the distinct orbits of S , so that $s_i \cap s_j = \emptyset$ for $i \neq j$ and $\bigcup_{i=1}^h s_i = \{1, 2, \dots, n\}$; that is, the orbits form a partition of the set $\{1, 2, \dots, n\}$.

The *topological complexity*, $\mathcal{C}_T(G)$, of a graph G is then defined by [mowsh68a]:

$$\mathcal{C}_T(G) = -\sum_{i=1}^h p_i \log_2 p_i, \quad (12.3)$$

where $p_i = |s_i|/N$, $1 \leq i \leq h$, and s_i are the orbits of $\mathcal{G}(G)$. Notice that while the topological complexity is formally equivalent to our first attempt at a definition for complexity (see equation 12.2 above) – both are essentially derived from Shannon’s information measure – unlike that first attempt, the topological complexity focuses its attention on a particular partition of G ; namely, the partition that preserves the graph’s topological structure. Despite its being based on Shannon’s information, $\mathcal{C}_T$ does not depend on an “ensemble of graphs.” Rather, $\mathcal{C}_T$ measures the information content of a particular graph relative to a set of transformations under which the graph’s topological structure is invariant.

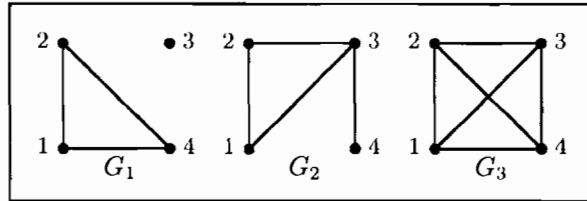


Fig. 12.3 Three sample size-4 graphs for calculating the *topological complexity*, $\mathcal{C}_T$: (a) $\mathcal{C}_T = 0$, (b) $\mathcal{C}_T = 3/2$ and (c) $\mathcal{C}_T = 2 - \frac{3}{4} \log_2 3 \sim 0.811$; see text.

For an example of calculating the topological complexity, consider the three sample size-4 graphs shown in figure 12.3. The automorphism group $\mathcal{G}(G_1)$, for example, is easily found to be $\{\phi, (12), (34), (12)(34), (13)(24), (1423), (1324)\}$, so that $|\mathcal{G}(G_1)|$ and the orbit $\mathcal{O}(G)$ consists of $\{1, 2, 4\}$ and $\{3\}$. Thus $p_1 = 3/4$, $p_2 = 1$ and $\mathcal{C}_T(G_1) = 2 - \frac{3}{4} \log_2 3 \sim 0.811$. The complexity of the remaining two graphs may be found in the same manner.

Mowshowitz ([mowsh68a], [mowsh68b], [mowsh68c], [mowsh68d]) develops this concept of a complexity of graphs considerably further in his four papers, which include discussions of its behavior as a function of various graph operations (complement, sum, Cartesian product, etc.), its extension to directed graphs and infinite graphs and the introduction of a graph entropy based on a chromatic decomposition.

We conclude this section by mentioning two older definitions of complexity, each of which also depends on both the size and vertex structure of a graph G : (1) the number of spanning trees in G ,[†] and (2) the average number of independent paths between vertices in G .

If $B = [b_{ij}]$ is an $N \times N$ matrix in which b_{ii} equals the degree of vertex i , $b_{ij} = -1$ if vertices i and j are adjacent and $b_{ij} = 0$ otherwise, then the number of spanning tree of G is equal to the determinant of any principal minor of B [harary69]. The extremes occur for totally disconnected graphs that have no spanning trees and thus a complexity of zero, and for complete graphs of order N that contain the maximum possible number of distinct trees on N vertices.[‡]

The second measure can be obtained directly from the adjacency matrix $A = [a_{ij}]$ of G . Recalling that $a_{ij} = 1$ if vertices i and j are adjacent and 0 otherwise, it is not hard to show (essentially by using induction on the power k), that $A^k = [a_{ij}^k]$ is equal to the number of paths from i to j containing k edges. Since there are $\binom{N}{2} = \frac{1}{2}N(N-1)$ possible links among N vertices, and the maximal length of a path between two of N vertices is $N-1$, the average number of independent paths between vertices in G is given by $\binom{N}{2}^{-1} \sum_{i,j} \sum_{k < N} [a_{ij}^k]$.

12.3.2.3 Complexity of a Simplicial “Complex”

One way of encoding the geometrical structure of a system is to describe it as a *simplicial complex*. That is to say, to piece it together – or form a “complex” – out of a set of elementary building blocks called simplices. The system could be either a physical object, such as a rock, in which case a simplicial decomposition is one way of digitizing the object’s physical structure[§] or it could be a complicated set of interrelationships among a set of variables describing the dynamical behavior of the system, in which case a simplicial decomposition gives some geometrical information concerning the dynamics.

An n -simplex, $S^{(n)}$, is an n -dimensional generalization of a line. If $x_0, x_2, \dots, x_n$ are points (not all on the same hyperplane), then $S^{(n)}$ is given by the set of all points X such that $x_0 + \dots + x_n = 1$, $x_i \geq 0$ for all i . A simplex is therefore a convex polyhedron formed by the intersection of $n+1$ half planes. A 0-simplex is simply a point, a 1-simplex is a line, a 2-simplex a triangle, a 3-simplex a tetrahedron, and so on. A set $\mathcal{S}$ of simplices is a *simplicial complex*, denoted by $\mathcal{C}$, if (1) every face of a simplex in $\mathcal{S}$ is also an element of $\mathcal{S}$, (2) the intersection of any two simplices in $\mathcal{S}$ is either empty or a face of each of them, and (3) each point of a simplex in $\mathcal{S}$ has a neighborhood in the n -dimensional Euclidean space that intersects only a finite number of simplices in $\mathcal{S}$.

Casti [casti92] introduces a (static) measure of complexity, $K(\mathcal{C})$, for a complex $\mathcal{C}$ satisfying the following three complexity axioms: (i) the complexity of a complex

[†]A spanning tree is any tree subgraph of G that connects all the vertices of G .

[‡] $= N^{N-2}$, a celebrated result due to Cayley [cayley57].

[§]Regge [regge61], Sorkin [sorkin87] and T.D.Lee [tdlee85a], among others, have used a related idea to perform calculations on a discretize space-time; see section 12.5.3.

consisting of a single simplex is equal to 1, (ii) the complexity of a subcomplex (or subsystem) cannot be greater than the complexity of the entire complex (or system), and (iii) the complexity of the complex formed by combining two complexes cannot be greater than the sum of the complexities of the component complexes.

Casti's complexity measure depends on a quantity called the *structure vector* $\vec{Q}$, which encodes multidimensional information about $\mathcal{C}$. Let the dimension of the highest dimensional simplex in $\mathcal{C}$ be equal to D . Then, for each $0 \leq q \leq D$, two simplices $S_i, S_j \in \mathcal{C}$ are said to be q -connected if there exists a sequence of simplices $\{y_{\alpha_i}\} \in \mathcal{C}, i = 1, 2, \dots, r$ such that (1) S_i shares a face of dimension m with y_{α_1} , (2) S_j shares a face of dimension n with y_{α_r} , (3) y_{α_k} and $y_{\alpha_{k+1}}$ share a face of dimension β_k , and (4) $\min\{m, \beta_1, \dots, \beta_{r-1}, n\}$. In other words, q is the smallest-dimensional link in the chain connecting S_i and S_j . Note that if two simplices are q -connected for some $q > 0$, then they must also be p -connected for all $p < q$.

It is easy to show that the q -connection forms an *equivalence relation* on the complex $\mathcal{C}$; it effectively partitions $\mathcal{C}$ into a set of equivalence classes consisting of simplices that are q -connected to one another. The *structure vector* $\vec{Q} = (Q_D, Q_{D-1}, \dots, Q_0)$ is defined to be the vector whose Q_q component is equal to the number of q -connected equivalence classes in $\mathcal{C}$. A simple geometrical way of understanding this ([casti92]) is to imagine that you are looking at a D -dimensional complex through special glasses that permit you to see only those dimensions greater than or equal to q . You would in fact see the complex $\mathcal{C}$ broken apart into $\vec{Q}_q$ disjoint pieces.

In terms of the structure vector $\vec{Q}$, Casti [casti92] shows that the following measure satisfies the three complexity axioms given above:

$$K(\mathcal{C}) = \frac{2}{(D+1)(D+2)} \sum_{i=0}^D (i+1)Q_i, \quad (12.4)$$

where D is the dimension of $\mathcal{C}$, Q_i is the i^{th} component of the structure vector $\vec{Q}$ and the constant before the summation is a normalization constant that is inserted to satisfy the first complexity axiom.

For a further discussion of K and some interesting applications of this measure, see [casti88] and [casti92]. Related material also appears in an earlier book by Casti [casti79].

12.3.2.4 Complexity of Hierarchical Systems

A very natural structure for describing the different "levels" of a complex system, if not the dynamics of their origin, is the *hierarchy*, as first pointed out by Simon [sim62][†] (see figure 12.4). The idea is to cluster the components of a system according to the strength of their mutual interactions by associating the most strongly interacting elements with the topmost of the hierarchy and associating successively weakly interacting components with progressively lower levels. For example, a chunk

[†]"My central theme is that complexity frequently takes the form of hierarchy...and hierarchy, I shall argue, is one of the central structural schemes the architect of complexity uses."

of condensed matter can be hierarchically parameterized by associating the nodes of the top level of the hierarchy with the atoms that make up the chunk of matter, associating the nodes of the next level of the hierarchy with the molecules that are formed out of atoms, the nodes of the next lower level with the crystals formed out of the molecules, and so on. We have also seen that hierarchies can be used to represent the (conjectured) ultrametric distribution of spin-glass equilibrium states (see section 5.5.7.4). Hierarchies have the virtue of both repressing typically rapid low-level fluctuations and imposing global quasi-static constraints by associating large scale structures and/or processes with the highest levels [cecat88].

Ceccato, Hogg and Huberman ([huber85b], [huber86], [cecat88]) have defined a measure of complexity of hierarchies that is (1) entirely objective, being based on the structure of the hierarchy, and (2) is consistent with the intuitive relationship between the complexity and degree of disorder in a system (see figure 12.2) – namely, it is maximal for systems that are *between* those that are completely ordered or completely disordered. Ceccato, *et.al.*'s measure is determined by examining the diversity of a system, as given by the number of different interactions among the different parts and levels of the hierarchy.

Consider, for definiteness, a set of otherwise identical lowest-level components of a system, so that the hierarchy is a *tree* of constant depth. Since we assume that the components are all identical, the only distinction among the various nodes of the hierarchy consists of the structure of the subtrees. Now suppose we have a tree T that consists of β subtrees branching out from the root at the top level. We need to determine the number of different interactions that can occur on each level, independent of the structure of each subtree; i.e. isomorphic copies of trees do not contribute to our count. We therefore need to find the number of nonisomorphic subtrees. We can do this recursively.

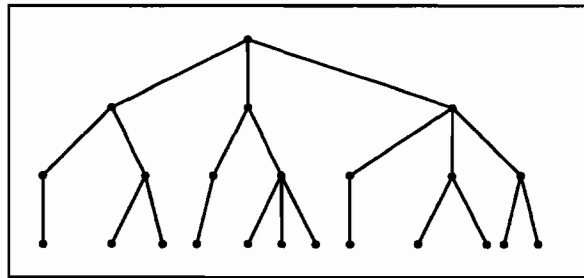


Fig. 12.4 An example of a *hierarchy* composed of three interaction levels and 12 elementary components.

The diversity of the tree T , denoted by $\mathcal{D}(T)$, counts the total number of interactions *between* and *within* all subtrees. We therefore proceed in two steps. First count the number of distinct interactions within the clusters represented by the subtrees; i.e. multiply the diversity of all nonisomorphic subtrees. Second, multiply this result by the number of ways, N_k , that k different clusters

can themselves interact. Since the total number of possible n -ary interactions among k distinct objects is simply the binomial coefficient $\binom{n}{k}$, N_k is thus given by $N_k = k + \binom{k}{2} + \binom{k}{3} + \cdots + \binom{k}{k} = 2^k - 1$. Combining these two steps, Cecatto's *et.al.*'s suggested measure of complexity of a tree, $\mathcal{C}(T)$ may be expressed as follows:

$$\mathcal{C}(T) = \log_2 \mathcal{D}(T) = \log_2 \left\{ f(k_T) \prod_{j=1}^k \mathcal{D}(T_j) \right\}, \quad (12.5)$$

where $\mathcal{D}(T_j)$ is the diversity of the j^{th} subtree, k_T is the number of nonisomorphic subtrees of T and the form factor $f(k_T) = N_k = 2^{k_T} - 1$.[†] Note that $\mathcal{C}(T)$ gives an absolute measure of complexity, that, in general, grows with the size of the tree. A more convenient relative measure, $c(T)$, that allows one to compare the complexities of different sized hierarchies is defined by $c(T) = \mathcal{C}(T)/\mathcal{C}_{\max}^{(S)}$, where $\mathcal{C}_{\max}$ is the maximum value of $\mathcal{C}(T)$ for trees T of size S . In the case of a forest, $\mathcal{F} = \bigcup_i \mathcal{T}_i$, composed of n nonisomorphic trees $\mathcal{T}_i$, the complexity is given by

$$\mathcal{C}(\mathcal{F}) = \sum_{i=1}^n \mathcal{C}(\mathcal{T}_i) + \log_2 f(\bigcup_i \mathcal{T}_i). \quad (12.6)$$

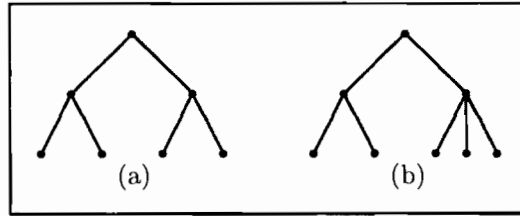


Fig. 12.5 Examples of trees whose subtrees are all identical (a) and different (b).

For example, consider the two trees shown in figure 12.4. The tree in figure 12.4-a has equal (binary) subtrees, so that its diversity $\mathcal{D} = 1$ and complexity $\mathcal{C} = 0$. The same is true for any tree all of whose nodes have a constant branching ratio. On the other hand, the tree shown in figure 12.4-b has two distinct subtrees, each of which has a diversity of $\mathcal{D} = 1$. The diversity of the entire tree is therefore $\mathcal{D} = 2^2 - 1 = 3$.

Huberman and Hogg ([huber85b], [huber86]) extend this measure to metric trees (where the height of the roots of sub trees from their leaves is an added parameter)

[†]The form factor f clearly depends on the number of lower levels that must be considered in order to determine whether two subtrees are isomorphic. More generally, it should contain information about the relative importance of a given subtree in T 's overall clustered structure – a node that gives birth to a large, diverse subtree should be given greater weight than a node that is at the same level but spawns only a thin subtree. In other words, f is really a function of all of the pertinent gross structural features of the tree at a given level: $f = f(k_T, M_T, N_T, \beta_T)$, where M_T is the total number of levels below the given level; N_T is the number of leaves of the given node, and β_T is the number of subtrees emanating from the root.

and random trees, apply it to adaptation in complex systems and give an illustration of a possible connection between this purely static value and a dynamics of the structure. For other points of view of the role hierarchies play in complex system see Pattee [pattee73], Haken [haken83], Salthe [salt85], Nicolis [nicolj86], and Caianiello ([caian87b], [caian87c]).

12.3.2.5 Computational Complexity

Computational complexity measures the time and memory resources that a computer requires in order to solve a problem. For example, given the “problem” of calculating x^{16} for some real x , one might either choose the most straightforward

way to calculate it: $x^{16} = \overbrace{x \times x \times \cdots \times x}^{16}$; or save a little time and instead compute, in turn, $\alpha = x \times x$, $\beta = \alpha \times \alpha$, $\gamma = \beta \times \beta \times \beta$ and $x^{16} = \gamma \times \beta$; or, one might stumble onto a scheme that is easier still in terms of both time and space complexities: $x^{16} = (((x^2)^2)^2)^2$. In general, if we let $\mathcal{N}_{\mathcal{A}}(f)$ represent the number of elementary operations $(+, -, \times, \div)$ required for evaluating the function f , using algorithm $\mathcal{A}$, then we could define a time complexity $\mathcal{C}$ for the evaluation of f as follows:

$$\mathcal{C} = \min_{\mathcal{A} \in \mathcal{A}} \mathcal{N}_{\mathcal{A}}(f). \quad (12.7)$$

Of course, the use of such a measure to find the complexity of an *object*, as opposed to the complexity of a *function*, as defined above, presupposes that there exists some natural encoding of that object as a “formula.” This is far from obvious.

A somewhat more robust measure may be defined by invoking the universal Turing machine. Let $\Sigma_N^{(i)}$ be the initial state of a computation that is designed to solve a size- N problem. If the problem is to find a solution to the Traveling-Salesman problem, for example, N would correspond to the number of cities that the salesman must visit.

Let $\Sigma_N^{(f)}$ represent the final state solution of the computation. Then the computational complexity, $H_C[\Sigma_N^{(f)}]$, is defined to be *the time it takes for the fastest program running on a universal computer U (as measured in number of computing steps, or cycles) to compute $\Sigma_N^{(f)}$* :

$$H_C[\Sigma_N^{(f)}] = \min_{U(\mathcal{P})=\Sigma_N^{(f)}} \tau_U(\mathcal{P}), \quad (12.8)$$

where $\tau_U(\mathcal{P})$ is the time it takes program $\mathcal{P}$ to run on the universal computer U .

The complexity of an object, thought of as a final state of a formal computational process, is then classified according to how fast H_C grows as a function of the problem size. The first nontrivial class of problems – class **P** – for example, consists of problems for which the computation time increases as some polynomial function of N : $H_C[\Sigma_N^{(f)}] \leq \mathcal{O}(N^\alpha)$ for some $\alpha < \infty$. Problems that can be solved with polynomial-time algorithms are called *tractable*; if they are solvable but are not in the class **P**, they are called *intractable*. For example, the problem of determining the

successor state of a size- N linear cellular automata can take a time that is at most linear in N and is therefore in class **P**. Note that if we compare the computation times for the same problem on two different universal computers U_1 and U_2 , we might very well find that their respective polynomial-degree growth factors α_1 (for U_1) and α_2 (for U_2) are different; but, because of the ability of universal computers to simulate each other, it will never be the case that we will find another U_i that has a *faster than polynomial-time* growth function. The set of problems in class **P** is therefore effectively independent of the universal computer used in classifying them.

There is another class of problems, known as *nondeterministic polynomial time* – or class **NP** – problems, which may not necessarily be solvable in polynomial time, but the actual solutions to which may be tested for correctness in polynomial time. The problem of finding a size- N preimage for a linear CA, for example, is a class **NP** problem. While it is obvious that $\mathbf{P} \subseteq \mathbf{NP}$, whether $\mathbf{P} \neq \mathbf{NP}$ remains an open question.

Problem classes that are characterized by their *spatial*, rather than *temporal*, growth requirements may also be defined. Class **PSPACE** problems, for example, require a memory storage space that grows as a polynomial function of the size of the problem size N (but may also require an arbitrary length of time to solve). While there is considerable evidence that $\mathbf{P} \subset \mathbf{PSPACE}$, it too remains an open problem.

Just as there exist universal computers that, given a particular input, can simulate any other computer, there are **NP-complete** (and **PSPACE-complete**) problems that, with that the appropriate input, are effectively equivalent to any **NP** (or **PSPACE**) problem of given size [garey79]. For example, Boolean “satisfiability” – i.e. the problem of determining the truth values of the variable’s of a Boolean expression so that the expression is true – is known to be an **NP-complete** problem [garey79]. If, indeed, $\mathbf{P} \neq \mathbf{NP}$, then the time to solve **NP-complete** problems must grow faster than any polynomial in N . In the case of Boolean satisfiability, or, as we have seen in earlier chapters, the problem of determining the preimages in certain CA, there may be no faster method than one that simply examines each of the exponentially many possible solutions; i.e. $H_C[\Sigma_N^{(f)}] \leq \mathcal{O}(\alpha^N)$ for some $\alpha < \infty$.

We have only given a cursory look at computational complexity.[†] More detailed discussions appear in the texts by Garey and Johnson [garey79], Hopcroft and Ullman [hopc79] and Davis and Weynker [davism83].

12.3.2.6 Algorithmic Complexity

Algorithmic complexity (sometimes also called “algorithmic randomness,” “algorithmic information content,” or “Solomonov-Kolmogorov-Chaitin complexity”) was first introduced by Solomonov [solo64], Kolmogorov [kolmog65] and Chaitin ([chaitin75], [chaitin77], [chaitin79], [chaitin88]) and has recently been extended by Zurek ([zurek89a], [zurek89b], [zurek90b]). The algorithmic complexity of a state

[†]We elaborate a bit more on the notion of “computability” in section 12.8.

s , denoted by $K_U(s)$, is defined as *the length of the shortest computer program $\mathcal{P}_U^*$ (measured in “bits”) such that, when executed on a universal computer U , yields the state s :*

$$K_U(s) \equiv |\mathcal{P}_U^*|. \quad (12.9)$$

Its virtue is its ability to assign a measure of complexity to an individual string, without having to resort to ensembles or probabilities. Its main drawback is that it is typically very hard to calculate exactly. Nonetheless it can be estimated for most systems relatively easily.

Suppose a state s is encoded as a binary string of 10^6 0's and 10^6 1's: $s = 10101010\dots$. While the number of raw bits defining s is huge, its algorithmic complexity is actually very small because it can be reproduced exactly by the following short program: `<print '10'  $10^6$  times>`. On the other hand, a completely random string of 0's and 1's – say $s_{\text{rand}} = 01101000110111101\dots$ – cannot be reproduced by a program that is significantly shorter than the one that simply lists each bit of the string, and therefore cannot be similarly compressed. In this case $K(s_{\text{rand}}) \sim |s_{\text{rand}}|$. Such incompressible strings are called, for obvious reasons, *algorithmically incompressible*. Just as one can show that almost all Hamiltonian dynamical systems are nonintegrable (see section 4.1.5.1), so too it can be shown that almost all numbers (and therefore their corresponding bit-strings) are algorithmically incompressible [chaitin88].

We make three additional comments concerning algorithmic complexity, as defined by equation 12.9. First, while $K_U(s)$ clearly depends on the universal computer U that is chosen to run the program $\mathcal{P}^*$, *because of the ability of universal computers to simulate one another*, the difference between algorithmic complexities computed for universal computers U_1 and U_2 will be bounded by the $\mathcal{O}(1)$ size of the prefix code $\tau_{U_1 U_2}$ allowing any program $\mathcal{P}$ that is executed on U_1 to be executed on U_2 [zurek89b]:

$$|K_{U_1}(s) - K_{U_2}(s)| \leq |\tau_{U_1 U_2}|. \quad (12.10)$$

This finite difference obviously becomes increasingly less important in the limit of very long strings. For purposes of mathematical analysis, $K_U(s)$ can be treated as being effectively independent of U .

The second comment is that while $K(s)$ can always be estimated for finite strings, it is in general impossible to tell whether a string of arbitrary length is random; a difficulty that is due to Godel's incompleteness theorem and first pointed out by Chaitin [chaitin88]. For example, while the binary representations of the decimal parts of π (001001000011111101101...), e (1011011111100001010...) or $\sqrt{2}$ (0110101000010011 11...) may all appear to be random – so that their Shannon complexity is large – each string can in fact be represented considerably more compactly using any number of simple (i.e. short) algorithms; i.e. their algorithmic complexity is essentially zero.

The final comment is that algorithmic complexity is really a better measure of the degree of randomness in a system rather than its complexity. For example,

while we intuitively expect the complexity of a completely random string to vanish (look back at figure 12.1-(c)), its algorithmic complexity is maximal. Gell-Mann [gell88] has suggested that the problem is that algorithmic complexity tells us only how much information is required to encode a state; it tells us nothing about how difficult it is to reproduce that state from, say, its bit-string encoding. What is needed is therefore a measure of how much effort is required to deduce a state from its encoded form; i.e. we need a dynamic measure of complexity.

Zurek ([zurek89b], [zurek90b]) has recently extended the notion of algorithmic complexity to bring it more in line with thermodynamics and conventional statistical mechanics. He proposes that *physical entropy* consists of the sum of (1) the information missing from available measurements of a system (as determined by Shannon's information), and (2) the information that is already contained in the available data (as measured by the system's algorithmic complexity). In this way, the usual Boltzmann-Shannon missing information is generalized to include information about the cost storing information about the system. A detailed discussion of the insights this new notion of physical entropy gives into the whole process of measurement (from a *Maxwell's Demon* perspective; see section 6.4) appears in [zurek89a].

12.3.2.7 Logical Depth

Bennett ([benn86], [benn88b], [benn87b], [benn90c]) has recently introduced a measure of dynamic complexity he calls *logical depth*. The logical depth of an object $\mathcal{O}$, denoted by $\mathcal{D}_U^L(\mathcal{O})$, is defined to be the execution time required by a universal computer U to generate $\mathcal{O}$, while running the minimal-sized program $\mathcal{P}^*$ that does so:

$$\mathcal{D}_U^L(\mathcal{O}) = \tau_U(\mathcal{P}^*), \quad \text{where } U(\mathcal{P}^*) = \mathcal{S}(\mathcal{O}), \quad (12.11)$$

where $\mathcal{S}(\mathcal{O})$ is the bit-string representation of object $\mathcal{O}$ and $\tau_U(\mathcal{P}^*)$ is the time it takes the minimal-sized program $\mathcal{P}^*$ to execute on U . As in the case of algorithmic complexity $K_U(s)$ (equation 12.9), because of the ability of universal computers to simulate one another, $\mathcal{D}_U^L(\mathcal{O})$ is roughly independent of the universal computer U used to measure it.

According to equation 12.11, both highly ordered strings (Ex: figure 12.1-(a)) and completely random ones (Ex: figure 12.1-(c)) are "shallow" since they can both be computed with "short" programs of the form `<print x>`. On the other hand, a number like π , which we previously saw has a minimal algorithmic complexity, by virtue of the computational effort required to generate N digits even from a simple algorithm, is relatively "deep" when compared to most other length- N numbers. Moreover, logical depth obeys what Bennett calls the "slow-growth law," which suggests that deep objects cannot be produced quickly from shallow ones.

Logical depth is thus consistent with our intuitive understanding of complexity. A "complex" biological organism is deep precisely because it requires a long and complex computation to describe. On the other hand, a regularly arranged crystal is

shallow because it can be described by a short algorithm. Likewise, a random state of a physical gas can be reproduced with the simple statement **print** S_G , where S_G represents the state of the gas, so that it too, like the crystal, is logically shallow. This last result is also consistent with our intuition: while a gas is certainly a complex system, it lacks organization and therefore contains little innate complexity.

Perhaps the only drawback to using Bennett's logical depth in practice is that it is hard to apply to physical systems. One might try to substitute the computational effort required to simulate the evolution of a physical system for execution time to generate a given number, but doing so brings into play another variable: the efficiency and realism with which a mathematical model simulates the actual evolution of the physical system. There are countless examples of relatively "simple" physical processes that computers nonetheless have a very hard time simulating (think of your favorite low-dimensional chaotic system). Would we, in such cases, be measuring the complexity of the physical system or the mathematical model used to describe that system?

12.3.2.8 Thermodynamic Depth

Most of the preceding measures of complexity tacitly assume that a state of whatever physical system whose complexity is being measured is amenable to a bit-string representation. Although there are good reasons to make this assumption (see, for example, our discussion of the Church-Turing hypothesis below), it is also not so crazy to suppose that complexity ought to be some function solely of the physical properties of the system in question. Lloyd and Pagels [lloyd88] have recently proposed just such a measure, called *thermodynamic depth*.

Related to Bennett's *logical depth* (see above), the thermodynamic depth, $\mathcal{D}_U^T(S)$ of a system S in state S measures how much information must be processed in order for S to evolve to S .

Lloyd and Pagels deduced this measure as the only one that is consistent with the following three properties (that they postulated must be satisfied by any general measure of complexity $\mathcal{C}$): (1) $\mathcal{C}$ must be a continuous function of the probabilities of the experimentally defined trajectories that can result in the S 's given state; (2) If each of N trajectories leading to the given state are equally weighted (i.e. all probabilities $p_i = 1/N$) then $\mathcal{C}$ must be a monotonically increasing function of N (this guarantees that a more accurate experimental determination of the trajectories leading to the given state cannot decrease the state's complexity); and (3) $\mathcal{C}$ must be additive with respect to intermediate processes – i.e., if a process proceeds from state $S_1 \rightarrow S_M$ via intermediate states $S_1 \rightarrow S_2 \rightarrow S_3 \rightarrow \dots \rightarrow S_M$, then $\mathcal{C}(S_1 \rightarrow S_M) = \sum_{i=1}^{M-1} \mathcal{C}(S_i \rightarrow S_{i+1})$.

Lloyd and Pagels show that these three requirements lead uniquely to an average complexity of a state proportional to the Shannon entropy of the set of (experimentally determined) trajectories leading to the given state ($= \sum_i p_i \log_2 p_i$). The thermodynamic depth of a state S to which the system S has evolved via the i^{th} possible trajectory is equal to the amount of information required to specify that trajectory, or $\mathcal{D}_U^T(S) \propto \log_2 p_i$. In the case of Hamiltonian systems, Lloyd and

Pagels show that thermodynamic depth is proportional to the difference between the state's thermodynamic entropy (i.e. its coarse grained entropy) and its fine-grained entropy, given by $k_B \times \text{volume of points in phase space corresponding to the system's trajectory}$, where k_B is Boltzman's constant.

To be more precise, define a trajectory of macroscopic states of a system S to be an ordered set of macroscopic states $\{S_{i_1}, S_{i_2}, \dots, S_{i_n}\}$, such that S was in state S_{i_1} at time t_1 , in state S_{i_2} at time $t_2 \geq t_1$, and so on. Let $p(S_{i_1}, S_{i_2}, \dots, S_{i_n}, S)$ be the experimentally obtained probability for the trajectory $S_{i_1} \rightarrow S_{i_2} \rightarrow \dots \rightarrow S_{i_n} \rightarrow S$ ending with the final state S . The probability that S evolved to S via the trajectory $S_{i_1} \rightarrow S_{i_2} \rightarrow \dots \rightarrow S_{i_n} \rightarrow S$ is $p(S_{i_1}, S_{i_2}, \dots, S_{i_n} | S) = p(S_{i_1}, S_{i_2}, \dots, S_{i_n}, S)/p(S)$. Lloyd and Pagels [lloyd88] prove that the only function that is consistent with their requirements (1)-(3), given above, is

$$f[\{p(S_{i_1}, S_{i_2}, \dots, S_{i_n} | S)\}] = \tag{12.12}$$

$$-k \sum_{\substack{m_1, m_2, \dots, m_n \\ i_1, i_2, \dots, i_n=1}} p(S_{i_1}, S_{i_2}, \dots, S_{i_n} | S) \log_2 p(S_{i_1}, S_{i_2}, \dots, S_{i_n} | S),$$

where m_j , $j = i_1, i_2, \dots, i_n$ is the number of different possible states S_j , and k is an arbitrary constant.

Thermodynamic depth satisfies several welcome properties: (1) it is a purely objective measure in the sense that a different set of measurements using the same experimental data always yield the same depth; (2) it vanishes for both completely ordered and disordered systems; (3) the complexity of merged copies of a given system increases only by the depth of the copying process (which is, by comparison, typically small), and (4) the slightly subtle, but intuitive, property of "revealed probing." By this we mean that it provides the "prober" the ability to tailor depth of the probe to a desired degree of resolution. As finer and finer details of the microscopic state of a gas are revealed by probing the state of the gas to great accuracy, what may initially appear to be shallow may, which successive probing, be discovered to be deep; on the other hand, the fact that successively finer probes of, say, a crystal yield effectively the same (shallow) depth at all levels reveals that the thermodynamic depth of a crystal is indeed shallow.

Zurek [zurek89b] points out the following connection between algorithmic complexity and thermodynamic depth: if Lloyd's and Pagels' notion of thermodynamic depth is used to define a minimal depth – defined by the size of the smallest program that yields a final state $\Sigma^{(f)}$ from initial state $\Sigma^{(i)}$ – then it is closely approximated by the difference in the algorithmic complexities of the two states. Lloyd and Pagels [lloyd88] also note that while the *absolute depth* of a state – which is proportional to the minimum amount of information necessary to identify a trajectory that the system could have followed to reach the desired state – is the obvious analogue of logical depth (see **Logical Depth** above), the two measures are not the same: absolute depth is measured with respect to the most likely trajectory whereas logical depth is measured with respect to the *algorithmically* most likely trajectory. The two measures are the same only if all one-ended input programs have the same probability.

12.3.3 Emergence

Central to the general science of complexity, and to the study of artificial life in particular, is the notion of *emergence*. Emergence refers to the appearance of higher-level properties and behaviors of a system that – while obviously *originating* from the collective dynamics of that system's components – cannot be directly *deduced* from the lower-level properties or behaviors of that system.

One of the simplest, and ubiquitous, examples of emergence is “temperature,” as read by a conventional thermometer. While temperature is a perfectly well-defined physical quantity on the macro-scale, it is a meaningless concept on the level of a single atom or molecule. At the other extreme, we have one of the most complex (and still controversial) examples of emergence in human consciousness, which mysteriously emerges out of a caldron of interacting neurons. Think also of your favorite chaotic system. There is no more vivid an image of emergence to be had than that of an unexpectedly beautiful strange attractor emerging “out of” a set of otherwise difficult to solve equations.

Indeed, in those rare cases where a nonlinear system can be solved *exactly* – consider, for example, Feigenbaum's logistic equation when $\lambda = 4$ ($x_{n+1} = 4x_n(1 - x_n)$; see chapter 4) which is solved by $x_n = \frac{1}{2}\{1 - \cos(2\pi 2^n y_0)\}$, where $y_0 = (2\pi)^{-1} \cos^{-1}(1 - 2x_0)$ – one might reasonably ask about what real insight into the behavior of the overall system has been gained by simply writing down its “solution”? The real depth, and beauty, of the system resides in its emerging properties. Might this suggest a connection between measures of complexity like *logical depth* and what we intuitively call “emergence”?

The Ugly-Duckling Theorem. The problem of articulating what is meant by *simple*, *complex* and/or *emergent* is perhaps even harder than it appears at first sight. Why this is so can be appreciated by using a basic result – called the *Ugly-Duckling* theorem – proved by Watanabe ([wat85], wat86]). Suppose that the number of predicates that are simultaneously satisfied by two nonidentical objects $\mathcal{O}_A$ and $\mathcal{O}_B$ is a fixed constant, P . The rigorous form of the theorem asserts that the number of predicates that are simultaneously satisfied by neither $\mathcal{O}_A$ nor $\mathcal{O}_B$ and the number of predicates that are satisfied by $\mathcal{O}_A$ but not by $\mathcal{O}_B$ are both also equal to P . While this simple assertion is easy enough to prove directly, and may appear innocuous at first, it has rather important consequences.

Imagine that there are only three objects in the world, labeled by some arbitrary convention, $(\circ, \circ, \bullet)$. One may at first be tempted to assert that there are two “kinds” of objects: two $\circ$'s and one $\bullet$. But there are other ways of partitioning this set. For example, line them up explicitly this way: $\circ \circ \bullet$. An implicit new organizing property seems to emerge: the leftmost $\circ$ and the rightmost $\bullet$ share the property that they are NOT in the middle. Let's label that property “ $\circ$ ” too, and the property of being in the middle “ $\bullet$ ”. Now, substituting the new property for each of the original objects, we have $\circ \circ \bullet \rightarrow \circ \bullet \circ$.

Had one sorted these three objects according to the new property (that discriminates according to spatial position), one would again have two kinds of objects, but in this case they would have been different ones.

But we can play this game repeatedly, since there are endless possible properties that can *arbitrarily* be called $\circ$ and $\bullet$. Unless there is a well-defined measure of *specialness*, by

which one set of properties can be identified as better, or different, from any of the others, there is no objective way to assert that some objects are more similar than others. (By the way, the $\circ$ is the ugly duckling, which turns out to be just as similar to the two swans – $\bullet$ and $\bullet$ – as the two swans are similar to one another!)

The Ugly-Duckling theorem thus loosely states that *there can never be an internally objective way to ascribe a measure of similarity (or dissimilarity) between any two randomly chosen subsets of a given set*. In other words, an asymmetry can be induced only via some necessarily external sense of “esthetics.”

Watanabe points out that “logical atomism is based on a non-logical criterion.” [wat85] That is to say, any discussion of cognitive processes that introduces a set of atomic predicates and then draws distinctions between syntactical and semantic properties is flawed because no set of atomic predicates can be defined without assuming an ad-hoc semantics: “...if we consider y_1 and y_2 as atomic propositions (in the philosopher’s sense of the word), z_1 and z_2 become molecular propositions. But if we consider z_1 and z_2 as atomic, y_1 and y_2 become molecular. The distinction between these two views is purely accidental and arbitrary from the logical point of view. To claim that one set is directly given empirically while the other set is not amounts to claiming that one mode of observation is more fundamental than another mode of observation (which can be reduced from the former by a simple additional circuitry in the apparatus), which has no logical significance.”

What does all of this have to with measures of complexity? In light of Watanabe’s result, one must now ask, “What is the external esthetic that identifies one system as being objectively more, or less, complex (or interesting) than another?”

Other examples of emergence include (i) the characteristic spirals of the Belousov-Zhabotinsky chemical reaction [tyson76], (ii) the Navier-Stokes-like macroscopic behavior of a lattice gas that consists, on the micro-scale, of simple unit-bit billiards moving back and forth between discrete nodes along discrete links [hass88a], and, more recently, (iii) the seemingly “purposeful” task of forming clusters of randomly distributed objects – a behavior common in, say, ant colonies “organizing” the carcasses of their dead companions – that spontaneously and quite naturally emerges out a simple set of autonomous actions having nothing to do with clustering *per se* (as recently demonstrated by Beckers, Holland and Deneubourg [beckers94], in the context of exploring collective robotics). The macroscopic behavior in each of these examples is unexpected *despite* the fact that the details of the microscopic dynamics is well-defined.

A schematic representation of emergence is given in figure 12.6, which depicts the first three levels of a dynamical hierarchy and the “rules” or “laws” describing their behavior. The first, or lowest, level might be thought of as the level on which a CA system is usually defined. It consists of the lattice sites and values that define the microscopic dynamics.

Any elementary 2-state one-dimensional rule would be a good example of the lowest order $\Psi^{(1)}$. As we have seen repeatedly in the preceding chapters, however, knowing *only* the microscopic rules (typically) does little to further one’s understanding of the overall behavior of the system. In fact, what often occurs, is that there appears an entire hierarchy of behaviors, each existing on different levels, where the description of the n^{th} level – here simplistically represented by a single

n^{th} order “rule” $\Psi^{(n)}$ – need not bear any simple or obvious relation to “lower” order rules.

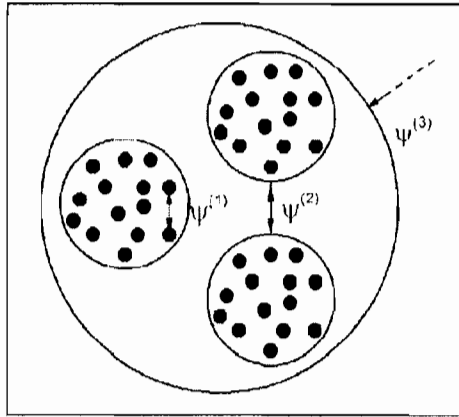


Fig. 12.6. Schematic representation of the first three levels of a “dynamical hierarchy,” or, to use Baas’ term ([baas94]; see below), *hyperstructure*. Level-1 is described by microscopic rules $\Psi^{(1)}$; level-2 by second-order rules $\Psi^{(2)}$, and so on.

Think of the unexpected emergence of “gliders,” “shuttles” and “spaceships” in Conway’s *Life* rule (section 3.4.4) as a second-order phenomenon built upon the formal, or first-order, specification of the two-dimensional binary *Life* rule. A third-level might consist of a part of a quantum gravity computation that is built upon an appropriate configuration of second-level glider-like primitives (which we know can be done, at least for large enough spaces, from the fact that *Life* is universal; see section 3.4.5).

While emergence, as a concept, is central to the study of complexity, the reader would be sadly mistaken in assuming that it is anything close to being well-defined. As we have seen already with the idea of complexity itself, and as we will shortly see again with the concept of information, when it comes to defining exactly what we mean by “emergence,” the only thing we can honestly assert is that we *know it when we see it* (and even then some of us might choose to call it something else anyway!). Nonetheless, there have been a few recent attempts to erect a more formal framework.

Cariani [cariani91], for example, identifies three major conceptions of emergence: *computational emergence*, *thermodynamic emergence*, and what he calls *emergence relative to a model*. Computational emergence is essentially the view advocated above; namely, that complex global behaviors arise out of a large assemblage of local computational interactions. Cariani criticizes this view on semantic grounds: if an outside observer observes a program whose function he does not know, how can that observer objectively tell if the computations are emergent? Thermodynamic emergence – which is the physical analogue of computational emergence, describing certain behaviors of reaction-diffusion systems, attractor states in dynamics systems and so on – may be said to suffer from the same drawback.

Cariani advocates the view of emergence relative to a model, where the model is introduced to embody the set of an observer's expectations as to how the system in question will behave in the future. If the system behaves in an unexpected way – i.e. in such a way that the model no longer faithfully describes the behavior of the system – the system's behavior can then be formally called “emergent.” The modeling framework itself consists of *measurements*, or the semantic operations that relate the formal symbols of the model to the state of an actual system, and *computations*, or the syntactic operations that relate the formal symbols of the model to other symbols. Pragmatic, or intentional, operations, are those that determine an appropriate set of measurements and computations for satisfying the purposes of the observer. The point of these definitions, is that once having set up an epistemological framework for describing operations of modeling relations, the same formal framework can then be used to “describe the operations of the modeling relations as they appear in organisms, devices, and other observers.”[†]

Another approach, based on tying together the notions of emergence and hierarchy via the generalized *hyperstructure* (figure 12.6), is suggested by ([baas93], [baas94]). Baas also distinguishes between two types of emergence: *deducible* and *observational*. Deducible emergence refers to higher-level processes that can be determined in theory from lower-order structures (ex: phase-transitions in the thermodynamic limit). Observational emergence refers to higher-order processes that cannot be deduced from lower-order structures (ex: Godel's theorem, which asserts that any consistent, finite logical system contains statements that are true but are unprovable within the system [godel31]; here, observation is the truth function). Baas [baas94] ends one of his sections with the provocative question, “Does emergence in some cases... take the rank among the ‘laws of nature’?”[‡]

12.4 Physics of Information

Campbell [campj82], in his *Grammatical Man: Information, Entropy, Language and Life*, was one of the first to assert the importance of adding *information* to our short list of fundamental descriptors of nature:

“Evidently nature can no longer be seen as matter and energy alone. Nor can all her secrets be unlocked with the keys of chemistry and physics, brilliantly successful as these two branches of science have been in our century. A third component is needed for any explanation of the world that claims to be complete. To the powerful theories and physics must be added a late arrival: a theory of information. Nature must be interpreted as matter, energy and information.”

[†]For a discussion of emergence in Tom Ray's *Tierra* system ala Cariani's emergence-relative-to-a-model, see [ray92].

[‡]An affirmative answer to which resonates strongly with some of our own views outlined in the last section of this chapter; see section 12.10.

12.4.1 *Just What is Information?*

“Information” is one of those widely used but strangely elusive words that can plausibly be made to refer to almost anything and at the same time remain stubbornly difficult to define precisely. Complicating matters is the fact that the word “information” takes on a myriad of related but subtly different meanings depending on whether it is used by an electrical engineer, a physicist, a biologist, or one’s aunt Irene.

According to the CD-ROM version of the Second Edition of the Random House Unabridged Dictionary [rand93], information “applies to facts told, read, or communicated that may be unorganized and even unrelated,” and is defined to be “knowledge communicated or received concerning a particular fact or circumstance,” or “data at any stage of processing (input, output, storage, transmission, etc.).” The word itself comes from a Latin derived Middle English word *informen* (c1275), which means “to form,” or “shape.” To this we might add Shannon’s [shann49] more technical communications-theory definition that the number of *bits* of information contained in a given outcome of a set of N possible outcomes, is given by $\log_2 N$, where $\log_2 x$ is the base-2 logarithm of x . The logarithm is the only function consistent with the reasonable demand that information must be *additive for independent events*. That is to say, if there are two independent sets of outcomes, N_1 and N_2 , so that the total number of outcomes is $N = N_1 \cdot N_2$, we demand that the information content of N , $\mathcal{I}(N)$, is equal to the sum of the information content of the two independent set of outcomes, $\mathcal{I}(N) = \mathcal{I}(N_1) + \mathcal{I}(N_2)$. Notice that Shannon’s information is purely syntactic, and is devoid of any semantic meaning. In order to attach a meaning to information, that information must be first interpreted within a given context.

It is this last point that we wish to stress: *information is something that is distinct from whatever system might be used to process it*. The words on this page, for example, contain information whether or not the reader happens to be processing them at this particular instant. Their information content therefore neither depends on, nor consists of, the meaning that the reader might extract or derive from them, but is defined solely in terms of whatever is encoded in the English language by the authors.[†] Now, that is not to say that a greater, or different, information content cannot be ascribed to the same words via a semantic reinterpretation – readers well versed in complex systems theory or general physics, for example, are likely to derive a considerably deeper meaning from this text than a below-average high-school student – only that there is a primitive core information content that is independent of any interpretation. Stonier’s ([ston90], [ston93]) two monographs on “Information Physics” (see below), begin by pointing out this dichotomy between (1) the information that is intrinsically contained within a system, and (2) the information that is conveyed by a system to some receptor.

Tying these notions more closely to the world of computers and computation, we all know that information is the elemental “stuff” of computers. It forms the

[†]Or, more precisely, whatever is encoded in the document typesetting language LaTeX.

elemental language that computers speak and it constitutes the sole substance of what computers process. We also know that there is no one unique way of describing information. It is not something that has heretofore lent itself to the same kind of experimental scrutiny as, say, the measurement of the mass or charge of an object. While a measurement of mass clearly gives us some information about an object, the word “information” in this context is typically used only to convey a sense of what knowledge has been gained about that object, and does not imply that it is anything physical itself. The fundamental question is whether, and in what sense, information is a *physical* quantity, on a par with conventional primitives like matter and energy. That is to say, whether information is something that does not just describe our state of knowledge or ignorance about an object or system, but is itself a tangible, physical element of that object or system. The resolution of the paradox of *Maxwell’s Demon* (see below) can be used to argue that the information content of a physical system contributes to its entropy and can therefore be thought of as a physical quantity in its own right.

Information Physics is a catch-all phrase that refers to attempts to found a physics on a notion of primordial information. Such attempts are based on two basic premises: (1) that information exists independently of any semantics that must be used to ascribe a meaning to it, and (2) all observables found in nature are essentially “data structures” that the universe uses to encode information with. An “electron” in this view, for example, is interpreted as a data structure encoding the eight (currently known) properties of what we call an electron (mass, charge, spin, etc.). The aim of information physics is to find the appropriate language, or dynamics, for whatever makes up this primordial information.

12.4.2 *A Few Hints to Get us Started*

12.4.2.1 *Thermodynamics and Information Theory*

Any computation, whether performed by a slide rule, computer work station or brain, is inherently a physical process, and as such is therefore subject to whatever laws and limitations apply to physical systems in general. It is a natural question to ask, then, whether there exists a fundamental thermodynamic limit to computation; i.e. whether there is a minimum amount of energy that is required to perform a given logical operation?

There are three important milestones in the history of thermodynamics and computation:

- The recognition that the information content of a physical system contributes to its entropy.
- The recognition that entropy increase (and energy dissipation) is not, fundamentally, a consequence of inefficient electrical circuit design and functioning, but is a direct consequence of irreversible logical computation.

- The recognition that there is no fundamental thermodynamic limitation to constructing fully reversible, energy dissipationless, computers; both classical and quantum.

The earliest hint that physics and information might be more than just casually related actually dates back at least as far as 1871 and the publication of James Clerk Maxwell's *Theory of Heat*, in which Maxwell introduced what has become known as the paradox of *Maxwell's Demon*. Maxwell postulated the existence of a hypothetical "demon" that positions himself by a hole separating two vessels, say A and B. While the vessels start out being at the same temperature, the demon selectively opens the hole only to either pass faster molecules from A to B or to pass slower molecules from B to A. Since this results in a systematic increase in B's temperature and a lowering of A's, it appears as though Maxwell's demon's actions violate the second law of thermodynamics: *the total entropy of any physical system can only increase, or, for totally reversible processes, remain the same; it can never decrease*. Maxwell was thus the first to recognize a connection between the thermodynamical properties of a gas (temperature, entropy, etc.) and the statistical properties of its constituent molecules.

Succeeding years saw a number of important contributions to issues relating to Maxwell's Demon, and to the growing understanding of the connection between the information content of a physical system and its entropy: Szilard [szil29], who provided a detailed analysis of the thermodynamics of Maxwell's Demon, arguing that the demon's observation, which constitutes a measurement and therefore an entropy increase, compensates completely for the entropy decrease resulting from the demon's action; Turing [turing36], who laid the groundwork for formal computation theory; Shannon [shan48], who developed the mathematical formalism appropriate for discussing the fundamental limitations to information transmission through noisy channels; and von Neumann, who, in a 1949 lecture [vonN66], was the first to assert that any computer operating at temperature T must dissipate at least $kT \ln 2$ units of energy ($\sim 3 \cdot 10^{-21}$ joules at room temperature) "per elementary act of information, that is per elementary decision of a two-way alternative and per elementary transmittal of one unit of information."

The relationships between thermodynamic entropy and Shannon's information-theoretic entropy and between physics and computation have been explored and hotly debated ever since. It is now well known, for example, that computers can, in principle, provide an arbitrary amount of reliable computation per kT of dissipated energy ([benn73], [fredkin82]; see also the discussion in section 6.4). Whether a dissipationless computer can be built in practice, remains an open problem. We must also remember that computers are themselves physical (and therefore, ultimately, quantum) devices, so that any exploration of the limitations of computation will be inextricably linked with the fundamental limitations imposed by the laws of physics.

12.4.2.2 *The Quantum Measurement Problem*

A second hint of a more intimate connection between physics and information comes from quantum mechanics. One of the most persistent fundamental problems of quantum mechanics is the so-called *measurement problem* [wheel83a]: the reconciliation of the deterministic evolution of a system's state vector with the apparently random projection of that state vector onto a measured eigenvalue. The problem is made even more complex when we realize that if quantum mechanics supplies a correct and complete description of the world – so that, in particular, any measuring apparatus we may care to use is itself a quantum mechanical system – there must be a single state vector Ψ that describes the combined state of *system + measuring device*. However, Ψ must then be “collapsed” by a “measurement” of the measuring device by another measuring device. We can, of course, combine this second measuring device with our already combined system to form a larger system of *system + measuring device 1 + measuring device 2*, but at some point we will be forced to ask, “where is the ultimate observer?” If it was not the first measuring device, or the second, is it the physicist's optic nerve? His brain? Perhaps, as von Neumann [vonN55] and Wigner [wigner67] have suggested, the collapse of the state vector ultimately depends on an observer's consciousness? Whatever the answer – the quantum measurement problem remains an active and controversial subject for speculation – at its core the problem has to do with how information is transferred from system to system and how it interacts within a system (or systems). Paired down even more, it might be said that the measurement problem owes at least a part of its existence to the fact that a quantum universe is effectively observing itself, an observation that will take on more weight as we discuss Godel's and Turing's theorems.

12.4.2.3 *Black Holes*

A third hint of a connection between physics and information theory comes from the thermodynamics of *Black Holes*, which is still a deep mystery that embodies principles from quantum mechanics, statistical mechanics and general relativity.

The connection in this context owes its origin to the existence of *singularities*, or regions of space-time in which known laws of physics presumably break down [schiff93]. That singularities must be a part of space-time is a celebrated result due to Hawking and Penrose, who proved this result assuming only that space-time is a smooth manifold.

Singularities pose a fundamental problem for several reasons, not the least of which is the possibility of a breakdown of predictability. If we think of a singularity as a line that perforates a family of surfaces, each one of which represents an instant of time, and then attach corresponding light cones to the world line of a singularity, we see that the future evolution of any point inside these light cones is rendered effectively unpredictable because of our inability to specify the boundary condition at the singularity [schiff93]. While Penrose's *cosmic censorship* hypothesis [penrose69] – which asserts that singularities are effectively concealed or “clothed”

by an event horizon – seemed to rid the universe of naked singularities, there was also Wheeler’s problem (*Wheeler’s Demon*) of black holes’ violation of the second law of thermodynamics:[†] it cannot be known whether a system with finite entropy has been thrown into a black hole.

Our most important insight into the connection between thermodynamics and black holes comes from a celebrated result obtained by Bardeen, Carter and Hawking [bard73], that the four laws of black hole physics can be obtained by replacing, in the first and second laws of thermodynamics, the entropy and temperature of a thermodynamical system by the black hole event horizon (or “boundary” of the black hole) and surface gravity (which measures the strength of the gravitational field at the black hole’s surface).

The surface area of the event horizon, for example, always increases when more radiation or matter falls into a black hole. Moreover, if two black holes merge together, the surface area of the combined black hole is greater than the sum of the surfaces of the two original black holes. This suggests that the surface area is analogous to thermodynamic entropy; with the increase in surface area being analogous to the second law of thermodynamics. The relationship between the entropy of a black hole and the surface area of its event horizon, $\mathcal{A}$, is given by the Bekenstein-Hawking formula, :

$$S_{\text{Black Hole}} = \frac{kc^3\mathcal{A}}{4G\hbar}, \quad (12.13)$$

where k is Boltzman’s constant and G is the gravitational constant.

The first law of thermodynamics states, essentially, that a small change in the entropy of a system is proportional to a change in the energy, with the constant of proportionality being the temperature, T . Bardeen, *et.al.* showed that a similar relation holds between the change in mass of a black hole and the area of its event horizon, with the constant of proportionality being equal to the surface gravity. If we assume that the area of the event horizon is analogous to entropy, this suggests that surface gravity must be analogous to temperature.[‡]

While Bardeen, *et.al.*’s analogy between thermodynamic entropy and a black hole’s area was certainly suggestive, a further insight was needed to establish a physical connection between them. Bekenstein ([beken72], [beken80], [beken81]) – building on Hawking’s proof that black holes are not, in fact, black, but emit particles with the same thermal spectrum as a black body radiator [hawk75] – showed that the second law of thermodynamics can be generalized to include black holes if the entropy, S , of the system to be “thrown into” a black hole satisfies the

[†]The second law of thermodynamics essentially states that the entropy of a thermodynamic system always increases with time.

[‡]The Hawking-Bekenstein relation between the temperature T and surface gravity κ is given by $T = \frac{1}{2\pi} \frac{\hbar}{kc} \kappa$, where k is Boltzman’s constant and c is the speed of light. The analogy is strengthened somewhat by the further observation that, just as the temperature is the same everywhere within a system that is in equilibrium, so too the surface gravity is the same everywhere on the black hole’s event horizon.

bound:

$$S \leq \frac{2\pi RE}{\hbar c}, \quad (12.14)$$

where R is the proper size of the system and E is the energy.

12.4.2.4 Discrete Physics

Finally, though the idea certainly has not yet entered the mainstream physics “consciousness,” researchers are taking an increasingly interested look into what a finite-information – i.e. what a *CA-like* – formulation of field theory might look like. Lest there be any misunderstanding, when we use the phrase “CA-like formulations of field theory” we are *not* referring to lattice gauge field theories, whose discretization exists solely as a computational convenience, but to (often) radically new approaches to fundamental physics that take as their basic axiom the supposition that, locally, the universe processes a finite amount of information. Some proponents of this view, most notably Fredkin [fredkin82], have even argued that the universe is *literally* a CA.

A discussion of reversible computation, as well as some speculations concerning the fundamental limitations of computation, have already been given in section 6.4; we will not repeat that discussion here. In the remaining sections of this chapter we instead wish to focus our attention on somewhat more speculative connections between physics and computation and in what way the universe itself might be thought of as a computer.

12.4.3 Feynman’s Challenge

What better place to begin our discussion of physics and information than with a quote from Richard Feynman, who, towards the latter part of his life, became increasingly interested in the nature of computing in general and the fundamental limits of computation in particular.[†]

Richard Feynman was universally admired for his penchant for intuitively (and seemingly effortlessly) being able to sift through clouds of largely irrelevant verbiage and somehow immediately focusing directly on the critical question or problem that that verbiage often so poorly conveys. This is nowhere more evident than in Feynman’s “hypothesis” that when it comes right down to it, fundamentally, the universe cannot possibly be processing an infinite amount of information at each space-time point [feyn65a]:

“It bothers me that, according to the laws as we understand them today, it takes a computing machine an infinite number of logical operations to figure out what goes on in no matter how tiny a region of space, and no matter how tiny a region of time. *How can*

[†]Interested readers should read Jagdish Mehra’s superb recent scientific biography of Richard Feynman [mehra94]. Chapter 24 of Mehra’s book discusses Feynman’s ideas about the fundamental limits of computation.

all that be going on in that tiny space? Why should it take an infinite amount of logic to figure out what a tiny piece of space-time is going to do? So I have often made the hypothesis that ultimately physics will not require a mathematical statement, that in the end the machinery will be revealed and the laws will turn out to be simple, like the checker board with all its apparent complexities.”

While it cannot be said that Feynman was an advocate of CA-like field theories – Mehra reports, in fact, that Feynman was often at odds with Fredkin in their discussions about Fredkin’s *Digital Mechanics* [mehra94] – just the fact that someone of Feynman’s stature would take an active interest in such problems and be willing to stress the fundamental inadequacies of existing approaches to fundamental physics, was enough to “emphasize that this is an interesting subject.”[†]

12.4.4 *Pregeometry?*

John Archibald Wheeler has been an eloquent spokesman for the need to search for what he calls a *pregeometry*, or a set of basic elements out of which what we normally think of geometry is built, but which are themselves devoid of a specific dimensionality (see [wheel62]-[wheel90]). “Space-time...often considered to be the ultimate continuum of physics, evidences nowhere more clearly than at big bang and at collapse that it cannot be a continuum. Obliterated in those events is not only matter, but the space and time that envelope that matter....if cloth is built out of thread and nothing more, we are led to ask out of what ‘pregeometry’ the geometry of space and spacetime are built.” [wheel80b][‡]

Wheeler has, over the years, introduced a number of tentative but nonetheless intriguing suggestions as to what form this pregeometry might take. It is not important that none of these ideas have been, or are likely to be, developed in anything that approaches a complete form; Wheeler seemingly abandons particular approaches almost as quickly as he creates them. What is of importance here is just the suggestion that our conventional continuum theories have only limited applicability; that there is something more fundamental than spacetime itself.

12.4.4.1 *Pregeometry as a “Bucket of Dust”*

One of Wheeler’s earliest attempts at formulating a pregeometry started with a so-called *Borel set*, which we can think of as being just a pristine set of points – or a “*Bucket of Dust*” – that has not yet been assembled into a manifold of a particular

[†]The quote is attributed to Rolf Landauer by Mehra ([mehra94], page 540) as part of a remark Landauer made about Feynman’s participation at the 1981 MIT Conference. Landauer was referring to Feynman’s interest in ferreting out the connections between quantum mechanics and computation, but his sentiment could equally well be extended to encompass Feynman’s deep interest in fundamental physics.

[‡]Readers interested in exploring the full range of Wheeler’s philosophical speculations concerning fundamental physics should consult the excellent collection of Wheeler’s essays, *At Home in the Universe* [wheel94].

dimensionality [wheel64]. Wheeler conceived of a space-time structure somehow naturally emerging out of such a Borel set via a Feynman path-integral-like sum over configurations. He had hoped that, for some appropriate weighting scheme, our familiar four dimensions would be given special preference. On the other hand, he recognized immediately that in order to even define a Feynman “path,” one must start with at least a rudimentary notion of what is meant by “distance” between two otherwise pristine points [wheel80b]. One might also object that we would be using a calculational tool borrowed from a mechanics operating on the “manifold” that we are trying to somehow build from scratch – namely Feynman’s path integral approach[†] – to provide a pregeometric synthesis for that same manifold. This would be rather like using a logical rule of inference to “prove” the validity of the same logical rule of inference. The “bucket of dust” idea was soon abandoned by Wheeler.

12.4.4.2 *Pregeometry as the “Calculus of Propositions”*

Another one of Wheeler’s early novel approaches was to imagine pregeometry as the *Calculus of Propositions* (see section 44.5 of [misner73]). Just as concepts like “temperature” and “entropy” emerge only out of the statistical mechanics of a system composed of a large number of interacting molecules – and have no definable meaning for a given molecule – so too, Wheeler suggested, conventional physics might emerge out of the statistical analysis of a propositional calculus in the limit where both the number and size of elementary propositions is very large. The idea is not as preposterous as it might first sound. For example, a calculus of propositions has been shown to provide a very viable formalism with which to describe the basis of quantum mechanics [jammer74].

12.4.4.3 *Pregeometry as “It from Bit”*

Wheeler opens a recent speculative paper exploring the links between physics and information in the following impassioned style [wheel90]:

“No escape is evident from four conclusions: (1) The world cannot be a giant machine, ruled by any pre-established continuum physical law. (2) There is no such thing at the microscopic level as space or time or spacetime continuum, (3) The familiar probability function or functional, and wave equation or functional wave equation, of standard quantum theory provide mere continuum idealizations and by reason of this circumstance conceal the information-theoretic source from which they derive. (4) No element in the description of physics shows itself as closer to primordial than the elementary quantum phenomenon, that is, the elementary device intermediated act of posing a yes-no physical question and eliciting an answer or, in brief, the elementary act of observer participancy. Otherwise stated, every physical quantity, every it, derives its ultimate significance from bits, binary yes-or-no indications, a conclusion which we epitomize in the phrase, *it from bit*.”

[†]A deep tool, to be sure, but nonetheless a calculational tool conceived of and operating very much on the geometric and not pregeometric level.

“It-from-bit” embodies the central notion that every *it* – that is, every aspect of reality: electrons, protons, photons, fields of force, or even the what we call space-time itself – is in the deepest sense a derivative of experimentally deduced answers to “yes/no” questions; that is, to *bits*. If we allow ourselves for a moment to go back to the roots of what it is that we by convention call “reality,” we see that it is something that is literally defined by a particular sequence of “yes/no” responses elicited from either a mechanical or (our own biological) sensory apparatus; in other words, reality’s origin is fundamentally information-theoretic.

12.4.4.4 The Combinatorial Hierarchy

Wheeler’s “it-from-bit” idea remains an original and highly speculative vision. A program that comes closest to matching the spirit of this vision has been followed for a number of years by Bastin, Noyes, *et.al.* ([bastin79], [noyes84], [noyes86], [noyes87]). Their ambitious “it-from-bit”-like program is called the *Combinatorial Hierarchy* (CH), and has the eventual aim of effectively describing all of physics as a growing universe of *bit strings* generated by a simple recursive algorithm. Bastin, *et.al.* start with the premises of finiteness, discreteness, finite computability and absolute non-uniqueness.

The CH is built upon the binary symbols 0 and 1 and uses addition *modulo 2* ($= \oplus_2$) as its basic mathematical operation. The symbols are grouped as ordered bit strings of length n ($n = 1, 2, \dots$): $S_i = (\dots, x_i, \dots)_n$ where $x_i \in \{0, 1\}$ and $i = 1, 2, \dots, n$. A comparison between two such strings is called a “discrimination:” $\mathcal{D}(S_i S_j) = (\dots, x_i \oplus_2 x_j, \dots)_n$. Discrimination is patterned after a general (quantum mechanical) “scattering” process, in which the result of a scattering between two different systems is a third system that differs from either. The goal is to use discrimination as a mathematical model describing atomic processes.

Starting from strings of a given length, new strings are formed by concatenating a sequence of them. A newly generated string is said to constitute a new level in the CH when it represents all combinatorially possible concatenations of strings on the previous level. That this makes some sense is due to closure under discrimination. That is to say, the comparison operator $\mathcal{D}$ effectively creates sets that are closed under discrimination. For example, if α and β are equal to 1, the set $\{\alpha, \beta, \alpha + \beta\}$ is closed under $\mathcal{D}$ since the discrimination between any two elements of this set is equal to the third element from the same set. A *discriminately closed subset* (DCSS) is defined to be a set of one or more nonnull strings, such that a discrimination between any two distinct strings results in a string contained in the same set.

Suppose we start from a basis set consisting of m linearly independent strings (that is, strings for which no sum of two or more different strings is null). In general, the number of DCSS’s is given by the number of ways of choosing m objects $1, 2, \dots$ up to n at a time ($= 2^m - 1$). Bastin, *et.al.* define their CH by starting from length-2 strings ($m = 2$), from which they obtain the first level consisting of $2^2 - 1 = 3$ DCSSs: $\{(10)\}, \{(01)\}, \{(10), (01), (11)\}$. To obtain the next level, these three DCSSs must be represented by a set of linearly independent quantities containing the same information about discriminate closure as the sets themselves.

Bastin, *et.al.* look for a set of invertible, linearly independent 2×2 matrices that have only the members of these sets as eigenvectors as maps that preserve discrimination (invertibility is required since only null strings can be mapped to null strings). Defining the mapping by $(ABCD)(xy) = (Ax + Cy, Dx + By)$, where $A, B, C, D, x, y \in \{0, 1\}$ and writing the resulting strings as $(ABCD)$, the three strings mapping the discriminate closure at level 1 are given by (1110), (1101) and (1100). Using this new set as our set of linearly independent basic strings, we can form $2^3 - 1 = 7$ DCSSs. Mapping these 7 DCSSs by 4×4 matrices we get 7 16-bit strings which form the basis for $2^7 - 1 = 127$ DCSSs. Finally, we go one more step to obtain $2^{127} - 1 \approx 10^{38}$ DCSSs composed of 256-bit strings. At this stage we must stop because there are too few linearly independent matrices left to map them.[†]

What is interesting about this simple construction is the particular sequence of cumulative sizes of the different hierarchical levels that it generates: $3, 3 + 7 = 10, 10 + 127 = 137 (\approx \hbar c/e^2), 137 + 2^{127} - 1 \approx 10^{38} (\approx \hbar c/Gm_{\text{proton}}^2 = (M_{\text{Planck}}/m_{\text{proton}})^2)$.[‡] Bastin, *et.al.* [bastin79] interpret these numbers as the inverse of the superstrong, strong, electromagnetic, and gravitational coupling constants and suppose that “the cumulative levels refer to systems of bosons with increasingly refined definitions of their possible interactions.” A physical interpretation of the CH is supplied by (1) identifying various quantum numbers with configurations of the hierarchy, and (2) defining an extended space for the particles to exist in.

Starting from this discrete, self-generating recursive bit-string model, the authors – in a series of papers ([bastin79], [noyes84], [noyes86], [noyes87] and references therein) – outline constructions for much of what might be called fundamental physics: $3 + 1$ Minkowski space with a discrete metric, the Einstein-deBroglie relation, quantized action, conventional quantum mechanical commutation relations for both linear and angular momentum, etc. In this ambitious ongoing program, Bastin, *et.al.*’s ultimate goal is no less than to provide a strictly finitist conceptual framework for fundamental physics.

12.4.4.5 Other Attempts at Pregeometry

Wheeler and Bastin, *et.al.* are certainly not alone in their search for an underlying pregeometry. Lehto, Nielson and Ninomiya [lehto86], for example, introduce an idea that is actually fairly close to Wheeler’s original “Bucket-of-sand” conception. Motivated by a desire to find at least one pregeometric model that gives rise to Einstein’s general relativity in the continuum limit, they essentially “build” spacetime out of an underlying abstract and dynamical simplicial complex. They quantize their pregeometric model using the Euclidean path-integral formalism so that the correct continuum theory emerges. They “...emphasize...that spacetime continuum

[†]The mathematical structure of the CH is discussed in detail in [bastin79].

[‡] M_{Planck} is the so-called Planck-mass $l_{\text{Planck}}c^2/G \approx 2.2 \times 10^{-5}$ g, and represents but one of several important fundamental scales, all based on the Planck-length $l_{\text{Planck}} = (G\hbar/c^3)^{1/2} \approx 1.6 \times 10^{-33}$ cm; Planck-time $t_{\text{Planck}} = l_{\text{Planck}}/c \approx 5.4 \times 10^{-44}$ sec; Planck-energy $E_{\text{Planck}} = l_{\text{Planck}}c^4/G \approx 1.3 \times 10^{19}$ GeV; Planck-temperature $T_{\text{Planck}} = E_{\text{Planck}}/k \approx 1.4 \times 10^{32}$ K.

may not exist at the fundamental level, but instead there exists some kind of lattice structure (not only as a technical tool). There is no a priori manifold and no Riemannian metric, only discrete ‘spacetime’!” [lehto86]

Other notable attempts at defining a pregeometry include those of Finkelstein [finkel89], by using what he calls *Quantum Set Theory*, Penrose [penrose87], by using spin networks, Sorkin [sorkin87] and Chew and Stapp ([chew87a], [chew87b]) by using causal graph theory and “gentle” quantum events as building blocks of space-time, Hemion [hemion80], by treating space-time as a partially ordered set, and Akama [akama78], by deriving the space-time metric from lepton-antilepton and quark-antiquark pairs.

12.4.5 Kantor’s “Information Mechanics”

Frederick Kantor, in his *Information Mechanics* ([kant77], [kant82]) distills the essence of information physics into the following three postulates:

- *Information is conserved*
- *Information is communicable*
- *Information is finitely accessible*

Seeking to define what are conventionally treated as primitive concepts like “space,” “time,” “mass,” “charge,” “spin,” and so on in terms of more primitive, or primordial, information, Kantor argues that if one assumes his three fundamental postulates, no more than four independent constants are required [kant77]: (1) the linear size of the universe U (for calibrating units of length), $\mathcal{R}_U$; (2) accessibility of information (in bits), $\mathcal{I}$; (3) coefficient of local propagative communication (for calibrating units of time in terms of units of length), c ; and (4) the energy per information bit (strictly for convenience in using instruments already calibrated in terms of mass and/or energy), $E_{\mathcal{I}}$. Kantor uses his axiomatization of information mechanics to derive a “relativistic quantum mechanics,” with which he is able to find an approximate relationship among the fundamental constants α , h , c , m_e and G and to provide alternative formulations of the cosmological red shift and gravity. The conceptual picture of nature that emerges from Kantor’s theory is a universe consisting of “coupled-wave entities” that have “the properties which would warrant calling them objects, able to represent information, and able ... to interact with each other without necessarily being destroyed in doing so.”

12.4.6 Stonier’s “Information Physics”

Where Kantor uses “information” more as a conceptual vehicle for reorganizing conventional physics than as some fundamental constituent of the measurables of physics, Stonier, in a series of papers and monographs ([ston86a], [ston86b], [ston90] and [ston93]), takes the idea of an information physics to its logical extreme by postulating that information is a basic property of the universe and that “matter

and energy comprise merely the surface" [ston90]. Information, for Stonier, is not just a whimsical, or incorporeal, mental construct with which we try to make sense of the world, but is an intrinsic property of the universe. To the two basic ingredients of the structure of the universe – *matter* and *energy* – we must therefore add a third fundamental component: *information*. "Information and energy must not be viewed as opposites of a bipolar system, rather, they must be considered as the two angles of a triangle, with matter comprising the third." ([ston90], see figure 12.7). The three sides of this triangle represent the extremes, or boundaries, of our universe: (i) a mixture of pure energy and matter, without information, constitutes a plasma of fundamental particles; (ii) a mixture of pure information and matter, lacking energy, is exemplified by a crystal at 0 deg K; and (iii) a mixture of pure information and pure energy, without matter, consists of massless particles such as photons propagating through space devoid of matter. Assuming Stonier's axiom that information is as "real" as energy and matter, the important question now becomes, "How does this assumption alter our perception of the universe, and the physics that describes its dynamics?"

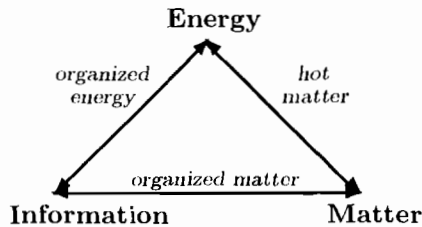


Fig. 12.7 Stonier's Fundamental Triad of matter, energy and information [ston90].

While information is an "implicit component of virtually every single equation governing the laws of physics,"[†] physics has never really addressed information itself as a physical quantity, particularly its manifest form in the *organization* of various structures. Stonier's first axiom of information physics is that the *information content and organization of a system are intimately interrelated, information being a function of the linkages binding simpler into more complex units*, from which he derives three theorems: (1) all organized structures contain information (and, as a corollary, there can be no organized structures that do not contain some form of information); (2) any information that is added to a system manifests itself by causing the system to become more organized, or reorganized; (3) any organized system has the capacity to release or convey information. Information is something that organizes space and time: what mass is to the manifestation of matter, and heat to energy, organization is to information. Just as "energy" is normally defined as the capacity to perform work, "information" is defined as the capacity to organize

[†]See [ston90], page 28.

a system (or to maintain a system's current organization). Similarly, just as "heat" is essentially a product of the interaction between matter and energy, "structure" represents the product of the interaction between matter and information.

It would take us too far afield to discuss all of Stonier's ideas and arguments. We therefore conclude this section with a just a short summary of the basic propositions of information physics [ston90]:

- The structure of the universe consists of three basic components: matter, energy, and information.
- Physical information is a function of (1) structural organization, (2) thermodynamic entropy, and/or (3) the amount of "useful" work required to create it.
- The universe is organized into a hierarchy of information levels.
- The absence of structure within a structure may carry information as real as the structure itself; i.e. holes and spaces within an otherwise organized structure may actually carry a significant part of that structure's organization, and hence, information.[†]
- Physical information is made manifest in a variety of forms: time, distance, direction, information properties of fundamental particles, information properties of various forms of energy, etc. all represent different forms of information.
- Energy and information are interconvertible.
- Heat is a form of energy lacking information. The term "heat," as used in this context, is equivalent to, say, uncorrelated photons in a crystal, or the random motion of molecules in a gas. It represents vibrational energy which tends to disorganize, rather than organize, systems.
- Physical constants reflect nature's algorithms. They reflect an ordering of physical systems or events. The human perception of that natural order is reflected in how much constants are expressed mathematically.

If information is really a basic property of the universe, why has it been apparently overlooked as such by physicists for so long? Stonier thinks this is due largely to the confluence of two factors: (1) It is very easy to overlook something that is, by its very nature, ubiquitous and obvious. Given that nature is well described by other "givens" such as time and distance, and that energy itself is interconvertible with information (see above), there was never a compelling need to explore other "fundamental" descriptors or constituents of nature. (2) Until the emergence of communications theory and the concepts and technology behind information processing systems, there was also no incentive for defining and studying information as an entity onto itself. Stonier [ston90] concludes his earlier monograph with

[†]Stonier uses the example of a hole left behind in an atomic shell after it loses an electron. This hole constitutes a particulate form of information that Stonier calls an *infor*, which he adds as a particulate manifestation of information to the two classes of particulate manifestations of matter and energy, namely fermions and bosons. See appendixes A and B in [ston90].

a prescient plea for incorporating information into a more global phenomenology of nature:

"Any general theory of information must begin by studying the physical properties of information as they manifest themselves in the universe. This must be done before attempting to understand the various, and much more complex forms of human information. The next step must involve an examination of the evolution of information systems beyond physical systems – first in the biological, then in the human, cultural sphere. As information physics develops, hopefully, there will emerge new insights which will advance our understanding of information... At this point in history, information physics needs a Clerk Maxwell."[†]

12.4.7 *Frieden's Extreme Physical Information Principle*

Roy Frieden, a researcher at the Optical Sciences Center of the University of Arizona, has recently introduced what he believes is the fundamental principle underpinning physics itself ([frieden98]; see also [matth99]). His idea is that all of the basic laws of physics (Newton's equation, Maxwell's equations, Schroedinger's equation, etc.) stem directly from the same fundamental source: *the information gap between what nature knows and what nature allows us to perceive*.

It is intriguing that Frieden does not use Shannon's information measure; rather he uses a less well-known measure predicated on classical measurement theory called *Fisher Information*. Fisher information ($= \mathcal{I}_F$), first introduced by R. A. Fisher in the mid-1920s, effectively measures how much information can be obtained from a physical system [fish59]. Suppose you want to know where a molecule of gas is. However you go about measuring it, the resulting measurement will inevitably have a certain amount of error associated with it. In particular, there will always be intrinsic errors in the system itself; i.e. randomness associated with the temperature of the gas and the perturbation caused by observing the gas. It is well known how to describe such random errors with simple statistical distribution functions. Fisher information effectively measures how much information you can extract from a physical system, given all the errors.

The Fisher information $\mathcal{I}_F$ in a single measurement of a physical system is given by

$$\mathcal{I}_F = 4 \int \left(\frac{dq(x)}{dx} \right)^2 dx, \quad (12.15)$$

where x is a fluctuation in the measurement and $q(x)$ is the (real) probability amplitude for x . It can be shown that, under certain conditions, $\mathcal{I}_F$ obeys an inequality identical to Boltzman's H -theorem (see chapter 8):

$$\frac{d\mathcal{I}_F}{dt} \leq 0. \quad (12.16)$$

[†]See [ston90], pages 112-113.

In other words, $\mathcal{I}_F$ is a monotonic measure of the system's disorder.

It is the gradient-squared term that caught Frieden's attention. Frieden noticed that it almost always appears in the Lagrangians for various physical phenomena. The Lagrangian for classical mechanics, for example, is $\frac{1}{2}(\partial q/\partial t)^2 - V$. The Lagrangian for the Schrodinger equation contains the term $\nabla\psi \cdot \nabla\psi^*$. The reader can perhaps recall at least a half-dozen other simple examples from basic physics (see Table 1.1 in [frieden98]).

Where does this gradient-squared term come from? Frieden's answer is that this gradient-squared term represents information. Specifically, the amount of Fisher information contained in intrinsic data. The others terms of a given Lagrangian represent information residing in the phenomenon being measured. Thus, Frieden asserts that all Lagrangians consist solely of two forms of Fisher information: *data information* ($\equiv I$) and *phenomenological information* ($\equiv J$).

Frieden's theory is that any physical measurement induces a transformation of Fisher information $J \rightarrow I$ connecting the phenomenon being measured to intrinsic data. What we call physics – i.e. our objective description of phenomenologically observed behavior – thus derives from the *Extreme Physical Information* (EPI) principle, which is a variational principle. EPI asserts that, if we define $K \equiv I - J$ as the net physical information, K is an *extremum*. If one accepts this EPI principle as the foundation, the status of a Lagrangian is immediately elevated from that of a largely *ad-hoc* “construction” that yields a desired differential equation to a measure of physical information density that has a definite prior significance.

While the EPI principle is intuitive – and, arguably goes far in establishing an interesting connection between information and physics – Frieden's discussions thus far lack a certain coherence. For example, many of his derivations of Lagrangians using EPI themselves seem a bit *ad-hoc* and not rigorous. Nevertheless, the basic idea is admittedly very appealing, at least on esthetic grounds. It will be interesting to see how it is developed.

12.5 Lattices and Field Theories

The use of discrete lattices as conceptual vehicles for doing away with divergences in field theory dates back to Heisenberg in 1930 [heis30], who is arguably the first to both propose and reject the idea. Since then, the idea has been proposed many times: by Snyder [snyd47], who introduced a set of relativistic commutation relations between space and time coordinates in 1947; by Regge [regge61], who used polyhedral approximations of Riemannian manifolds to provide an algorithm for calculating the temporal evolution of geometry in Einstein's General Relativity; and by Wilson [wilk74] and Kogut [kogut75], who introduced the lattice to modern gauge field theories; to name only a few.

All of these approaches, however, have at least this one basic point in common: the only reason that a lattice structure is introduced is to formally prevent the appearance of ultraviolet divergences and thus “simplify” the otherwise difficult calculations that must be made on the continuum. In other words, *it is the*

continuum – and not the approximating skeletonized lattice – that is the physical object.

In this section we explore three attempts at discretizing space-time with a radically unconventional view: each assumes that it is the continuum that is an approximation to a fundamentally discrete underlying substructure. The question is, “What effect does this assumption have on our understanding of fundamental physics?”

12.5.1 Field Theory Reformulated as a CA: I

Svozil attacks the question of whether quantum fields are cellular automata directly [svozil87]. Taking a more limited view than either Fredkin [fredkin93] or Lee [tdlee85a] (we will explain in what way shortly), Svozil asks whether it is possible to make conventional field theory emerge on the macroscopic level by discretizing the states and coordinates of a continuous field $\phi(\vec{x}, t)$. The macroscopic time evolution would be defined, on the more fundamental level, by some local microscopic cellular automaton rule Γ , so that

$$\tilde{\phi}(t+1, \vec{n}) = \Gamma[\{\tilde{\phi}(t, \vec{n} \in \mathcal{N})\}], \quad (12.17)$$

where $\tilde{\phi}$ is the discretized version of the continuous field ϕ , and $\mathcal{N}$ represents the neighborhood of the site symbolized by $\vec{n}$. The discrete field function $\tilde{\phi}$ (we will from this point on drop the *tilde*) is assumed to take on a finite (or possibly countably infinite) number of values. Svozil retains a connection between the discretized field theory and cellular automata by noting that, from a topological point of view, the dual lattice formed by contracting the n -dimensional cells to singular points while retaining their connectivities (i.e. their topologies) is equivalent to a cellular automaton (see figure 12.8).

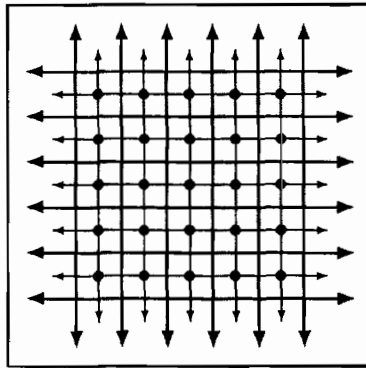


Fig. 12.8 Schematic showing the equivalence between n -dimensional cells (outlined by dark lines) and the dual lattice formed by contracting them to nodes (solid circles) which retaining their connectivity (outlined by light lines).

Having thus established at least a formal equivalency between a discretized field theory on a lattice and CA, Svozil invokes the so-called *no-go* theorem to show that field theory cannot be discretized in this simple fashion. The *no-go* theorem (see [karst81] and [niel81]) states essentially that under a set of only “mild assumptions” it is *impossible to formulate a local, unitary, charge conserving lattice field theory without effectively doubling the size of the predicted fermion population* (i.e. “species doubling”; see discussion box).

The no-go theorem makes two important assumptions: (1) that the field theory is constructed using a locally homogeneous Hermitian Hamiltonian that is bilinear in the fermion fields, and (2) that the charges are bilinear in the fermion fields and are locally defined, conserved and quantized. Svozil thus considers two immediately obvious alternatives to a CA-like formulation that circumvents the no-go theorem: (a) *give up locality of the transition rule*, an idea which would at least be consistent with the nonlocality imposed by the EPR paradox[†], and (b) *give up the idea of local charges*, and replace them with a “smeared out” charge. This second idea is equivalent to treating a particle as some kind of “composite” state consisting of several nearby cells (recall Minsky’s discussion in [minsky82]).

Svozil also suggests a third possibility, whereby a discretized field theory is strictly local in a higher dimensional space $d > 4$ but *appears to be nonlocal* in $d = 4$. While the physical reasons for a such a dimensional reduction remain unclear, such a “dimensional shadowing” clearly circumvents the no-go theorem by postulating a local dynamics in a higher dimension (see figure 12.9).

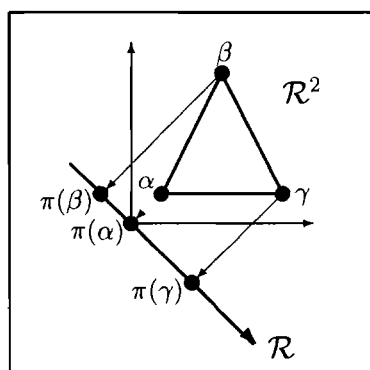


Fig. 12.9 *Dimensional Shadowing*: the points α, β and γ are all nearest neighbors in $\mathcal{R}^2$ but the connections between projections $\pi(\beta)$ and $\pi(\gamma)$ appear to be nonlocal in $\mathcal{R}$.

While Svozil certainly does a credible job in questioning how a local fermion field theory on a tessellated space might still be made able to circumvent the species doubling problem and thereby be converted (at least formally) into a CA-like theory, one could also argue that Svozil does not take his argument as far as it could be

[†]Section 12.8 discusses the EPR paradox, Bell’s theorem and Aspect *et.al.*’s epistemological measurements.

taken. Unlike some of the more speculative approaches taken by, say, Fredkin [fredkin93], Lee [tdlee85a] or Nielson [niel83], Svozil does not attempt to find a more fundamental theory out of which a conventional field theory somehow “naturally emerges.” Rather, Svozil asks the more reserved question of what underlying assumptions of our *current field theories* must be changed in order to make their discretizations appear more CA-like.

Scalars and Fermions on a Lattice: Field theories are usually discretized in one of two ways: (1) by discretizing both space and time (which is the so-called Euclidean formulation introduced by Wilson [wilk74]), and (2) by discretizing only the spatial dimensions (which is the Hamiltonian lattice formulation introduced by Kogut and Susskind [kogut75]). For our discussion, we will use the Euclidean formulation with a space-time lattice spacing ‘ a ’. Using the four-vector n to label the lattice sites, four-dimensional integrations will be replaced by a discrete sum: $\int dx^4 \rightarrow a^4 \sum_n$.

Scalar Fields: Consider a continuous field theory in Euclidean space with action

$$S(\phi) = \int d^4x \left\{ \frac{1}{2} (\partial_\mu \phi)^2 + V(\phi) \right\}, \quad (12.18)$$

where

$$V(\phi) = \frac{1}{2} m^2 \phi^2 + \frac{\lambda}{2} \phi^4, \quad (12.19)$$

ϕ is a scalar field, m is the mass and λ is a constant.

To discretize this theory, we attach the field to every lattice site n and make the substitution for its derivative:

$$\phi(x) \rightarrow \phi_n, \quad \partial_\mu \phi \rightarrow \frac{1}{a} (\phi_{n+\vec{\mu}} - \phi_n), \quad (12.20)$$

where $\vec{\mu}$ is the four-vector of length a in the direction of μ .

With these substitutions, the scalar action becomes

$$S(\phi) = \sum_n \left\{ \frac{a^2}{2} \sum_{\mu=1}^4 (\phi_{n+\vec{\mu}} - \phi_n)^2 + a^4 \left(\frac{m^2}{2} \phi_n^2 + \frac{\lambda}{4!} \phi_n^4 \right) \right\}. \quad (12.21)$$

To obtain the spectrum for the free-field theory (i.e. for $\lambda = 0$), it is useful to replace the ϕ_n with its Fourier transform $\phi(k)$:

$$\phi_n = \int \frac{d^4k}{(2\pi)^4} e^{ik \cdot n} \phi(k). \quad (12.22)$$

Since wavelengths smaller than twice the size of the lattice spacing are meaningless, we take the above integral over one *Brillouin zone* of the reciprocal lattice; i.e. we take $-\pi/a \leq k_\mu \leq \pi/a$, where $k_\mu = k \cdot \mu$.

Substituting equation 12.22 into 12.21 yields the free field action

$$S = \frac{1}{2} \int \frac{d^4k}{(2\pi)^4} \left\{ \sum_\mu \frac{4}{a^2} \sin^2 \left(\frac{ak_\mu}{2} \right) + m^2 \right\} \phi(-k) \phi(k). \quad (12.23)$$

In particular, we see that each mode in momentum space contributes the quantity

$$S(k) = m^2 + \sum_{\mu} \frac{4}{a^2} \sin^2\left(\frac{ak_{\mu}}{2}\right). \quad (12.24)$$

While this differs from the standard $m^2 + k^2$, the two expressions are equal in the continuum limit as $a \rightarrow 0$. A discretization of a continuous scalar field theory thus presents no particular difficulties. As we see immediately below, however, the same is not true of fermion fields.

Fermion Fields: Consider now a fermion field ψ and make the same sort of substitution as above $\partial_{\mu}\psi \rightarrow \frac{1}{a}(\psi_{n+\bar{\mu}} - \psi_n)$. The fermionic action becomes

$$S = \sum_n \left\{ \frac{a^3}{2} \sum_{\mu} \bar{\psi}_n \gamma^{\mu} (\psi_{n+\bar{\mu}} - \psi_{n-\bar{\mu}}) + ma^4 \bar{\psi}_n \psi_n \right\}, \quad (12.25)$$

where the γ matrices are Euclidean so that $\{\gamma_{\mu}, \gamma_{\nu}\} = \gamma_{\mu}\gamma_{\nu} + \gamma_{\nu}\gamma_{\mu} = 2\delta_{\mu\nu}$ and $\delta_{\mu\nu}$ is the Kronecker-delta function, and $\bar{\psi} \equiv \psi^{\dagger}\gamma_0$, where $\psi^{\dagger}$ is the Hermitian conjugate of ψ .

If, as before, we take the Fourier transform of ψ_n , we get

$$S = \int \frac{d^4k}{(2\pi)^4} \bar{\psi}(-k) \left\{ i \sum_{\mu} \gamma_{\mu} \frac{\sin(ak_{\mu})}{a} + m \right\} \psi(k), \quad (12.26)$$

from which we see that the discretized fermionic dispersion relation is given by

$$S(k) = \frac{\sin^2(ak_{\mu})}{a^2} + m^2. \quad (12.27)$$

It is easy to see that this expression has two *minima* within the Brillouin zone. One minimum is at $k = 0$ and gives the correct continuum limit. The other, however, is at $k = \pm\pi/a$ and carries an infinite momentum as the lattice spacing $a \rightarrow 0$. In other words, discretizing the fermion field leads to the unphysical problem of *species doubling*. (In fact, since there is a doubling for each space-time dimension, this scheme actually results in $2^4 = 16$ times the expected number of fermions.)

12.5.2 Field Theory Reformulated as a CA: II

Gerald 't Hooft, in a speculative 1988 paper [thooft88], suggests that a suitably defined deterministic, local reversible cellular automata might provide a viable formalism for constructing field theories at the Planck scale.

In this paper, 't Hooft introduces several "toy models" that hint that typically nondeterministic quantum mechanical behavior can be achieved using local deterministic laws, in the sense that a basis can be found in terms of which the wave function does not "spread." He shows how a CA-like formalism can be used to

construct a Hilbert space and a Hamiltonian so that, at long distance scales, they effectively behave as quantum field theories.

On a slightly more conceptual level, 't Hooft's toy models hint that it may be possible to define a set of *mutually commuting observables that algebraically generate a desired Hilbert space*. It is important to understand that 't Hooft is not referring to conventional *macroscopic* variables, such as pointers on a detection device, but rather to a set of what he calls "primordial" variables, that lurk beneath the surface, so to speak, and form the basis of the usual observables. Conventional variables, like mass, energy, and so on, are viewed as *nonprimordial* observables that mix different primordial states. 't Hooft's proposal is that... [thooft88]

"...for describing the real world, a complete set of such primordial observables can be found, and that the nonprimordial observables are not essential. They are needed *only* to enable physicists to make statistically significant predictions of the future at large distance scales, where the microscopic primordial observables are by far too complicated and change much too rapidly (chaotically?) to be directly observed. It is quite conceivable that the microscopic primordial observables are only relevant at the Planck scale... perhaps a cellular automaton can be found that has QCD as its thermodynamic limit."

Consider a deterministic local reversible CA; i.e. start with an infinite array of sites, $\vec{x}$, arranged in some regular fashion, and assume each site can be any of N states labeled by $0 \leq \sigma(\vec{x}) < N$. If the number of sites is $\mathcal{N}$, the Hilbert space spanned by the states $\{\sigma(\vec{x})\}$ is $N^{\mathcal{N}}$ dimensional. The state at time $t + 1$, $\sigma_{t+1}(\vec{x})$ depends only on the values $\sigma_t(\vec{x}')$ that are in the immediate neighborhood of $\vec{x}$. Because the cellular automata is reversible, the mapping $\sigma_t(\vec{x}) \rightarrow \sigma_{t+1}(\vec{x}')$ is assumed to have a unique inverse and the evolution operator $U(t, t + 1)$ in this Hilbert space is unitary.

't Hooft offers as an example the following construction. Since at every link connecting the neighboring sites $\vec{x}$ and $\vec{x}'$, the states $(\vec{x}, \vec{x}')$ can be in any of N^2 possible states, let the evolution operator $U_{\vec{x}, \vec{x}'}$ be an element of the permutation group $P^{(N^2)}$, where the links $(\vec{x}, \vec{x}')$ links are ordered in some way. The cellular automaton is then defined by the operation

$$U(t + 1, t) \equiv \prod_{\vec{x}, \vec{x}'} U_{\vec{x}, \vec{x}'}. \quad (12.28)$$

The problem now is to find the corresponding Hamiltonian. 't Hooft shows that the most "obvious" construction, obtained by rewriting $U(t + 1, t)$ as a product of cyclic elements, unfortunately does not work because at the end of the calculation there is no way to uniquely define the "vacuum" state. Given a cellular automaton with a "local" unitary evolution operator $U = \prod_{\vec{x}} U_{\vec{x}}$ and the commutator $[U_{\vec{x}}, U_{\vec{x}'}] = 0$ if $|\vec{x} - \vec{x}'| > d$ for some $d > 0$, the real problem is therefore to find a Hamiltonian

H such that the following three properties are satisfied:

$$\left\{ \begin{array}{l} U(t+1, t) = e^{-iH}, \\ H = \sum_{\vec{x}} \mathcal{H}(\vec{x}), \text{ i.e. } H \text{ is extensive,} \\ [\mathcal{H}(\vec{x}), \mathcal{H}(\vec{x}')] = 0 \text{ if } |\vec{x} - \vec{x}'| > d', \text{ i.e. } \mathcal{H}(\vec{x}) \text{ is local} \end{array} \right. \quad (12.29)$$

Since it may be possible to satisfy these conditions with a finite d' , it may be easier to instead consider the less stringent final condition $|\mathcal{H}(\vec{x}), \mathcal{H}(\vec{x}')| < f(|\vec{x} - \vec{x}'|)$, where $\lim_{x \rightarrow \infty} f(x) = 0$. 't Hooft offers one possible construction for a Hamiltonian satisfying these conditions.

Write $U_{\vec{x}} = e^{-iA(\vec{x})}$. If V is the set of all sites, we can also write $V = V_1 \cup V_2 \cup \dots \cup V_n$, where we have assumed that there are only a finite number of non overlapping subsets V_i . For example, in one dimension, $n = 2$ and V_1 and V_2 could represent the sets of even and odd valued sites, respectively. Now divide the set of operators $U_{\vec{x}}$ into "commuting classes," defined by $[U_{\vec{x}_1}, U_{\vec{x}_2}] = 0$ whenever $\vec{x}_1$ and $\vec{x}_2$ are both elements of the same subset V_i . We can then write (perhaps after some additional transformations are performed): $U = U_1 \cdot U_2 \cdot \dots$, where $U_j = \exp\{-i \sum_{\vec{x} \in V_j} A(\vec{x})\} \equiv e^{-iA_j}$. The full product can be conveniently expressed in terms only of commutators by using the Baker-Campbell-Hausdorff expansion:

$$e^A e^B =; \exp\left\{A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A, [A, B]] + \frac{1}{12}[[A, B], B] + \dots\right\}. \quad (12.30)$$

While each term in the resulting series has the form required by equation 12.29, the caveat is that as each commutator connects sites $\vec{x}$ and $\vec{x}'$ that are a distance d apart, the terms of order n in A_i and A_j yield contributions to $\mathcal{H}(\vec{x})$ that obey the third condition in equation 12.29 only for $d' = nd$. In other words, we also need to require that the Baker-Campbell-Hausdorff series has a sufficient degree of convergence.[†]

't Hooft concludes his paper by writing down a Hamiltonian that directly reproduces the automaton described by equation 12.28, in the case where the sites populate a one-dimensional lattice and the local neighborhood is defined only by nearest sites. The toy system is essentially a one-dimensional massless fermion gas, consisting of right- and left- propagating particles, constrained to stay farther apart than some limiting distance, d .

It is worth pointing out that 't Hooft [thooft80] had speculated about using a discrete space-time as an alternative to the continuum for solving the divergence problems in quantum gravity even before becoming acquainted with CA. Starting from the desire to maintain an invariance under an interchange between two lattice points,[‡] 't Hooft provides some order on the resulting lattice by defining a suitable

[†]'t Hooft addresses the convergence of the Baker-Campbell-Hausdorff series in appendix A of his paper [thooft88].

[‡]So that if there is an interaction between any two given points, there must be an interaction between *all* other points of the lattice as well; we can expect a fundamentally discrete theory of

metric tensor. While his metric establishes a basis for temporal ordering and at least a crude formalism for describing spacelike and timelike distances, 't Hooft acknowledges that these early ideas are no more than suggestive speculations on a possible conceptual approach to the problems plaguing quantum gravity. His main message is that "it will not be sufficient to just improve our mathematical formalism of fields in a continuous Riemann space but that some more radical ideas are necessary and that totally new physics is to be expected in the region of the Planck length."

12.5.3 *Field Theory Reformulated as a CA: III*

T.D. Lee, in a series of papers ([tdlee83a] -- [tdlee86]), outlined a theory in which (i) *time is treated as a discrete dynamical variable*, (ii) *field theory is discretized on a random lattice* and (iii) *difference equations are taken as the basis of fundamental physics*. These papers carefully trace the structure of the theory through all the different phases of mechanics: from classical mechanics to nonrelativistic quantum mechanics (developed with Friedberg [fried83]) and to relativistic quantum field theory (developed in collaboration with Christ, Friedberg and Ren [christ82]).

The use of a random lattice to restore both rotational and translational symmetry to a theory is in itself not new (see, for example, [christ82] and [itzyk86]). But all other random lattice discretizations invariably treat the lattice itself as only an approximation of the continuum theory, assuming that it is only the limit of zero lattice spacing that has any real physical meaning. Lee, in the series of papers referred to above, takes the exact opposite view: *a finite lattice spacing is considered fundamental and it is the continuum theory that is thought of as approximate*. At worst, random lattices restore some cherished continuous symmetries, maintain unitarity, and remove divergences by providing a covariant cutoff parameter. At best, random lattice theory "may change our concept of space-time in a fundamental way." [tdlee85a]

Now, to be sure, Lee nowhere talks about, nor does he advocate, cellular automata or CA-like modeling of field theory. His formalism is well grounded on conventional field theoretic concepts and, except for a fundamental limit on the number of allowable field measurements in a given space-time volume, neither the values of any space-time coordinates nor the values of the fields themselves are constrained in any other way. What he is suggesting, and what makes his ideas resonate (at least a bit) with CA-inspired field theories, is that we should give a critical look at using difference equations -- and not differential equations -- as the fundamental equations of physics. For this reason, we think it important to give at least a rudimentary sketch of Lee's approach.

gravity to be extremely nonlocal in character.

12.5.3.1 Locality

Lee's point of departure is to question the veracity of the concept of locality. Consider two points, A and B, separated by some spatial distance δx and time difference δt so that $c\delta t < \delta x < l_P \sim 10^{-33}$ cm, where c is the speed of light and $l_P = (\hbar G/c^3)^{1/2}$ is the Planck length. Since $c\delta t < \delta x$, A and B are outside of each other's light cone and local field theory assures us that these two experiments can be performed completely independently of one another. Heisenberg's uncertainty principle, however, asserts that these two measurements will also yield an energy fluctuation on the order of $\Delta E \sim \delta t^{-1} > l_P^{-1}$. We know that the gravitational field associated with such an energy fluctuation is very strong at these very small distances. Its Schwarzschild radius is in fact on the order of $R \sim G\Delta E > G/l_P$, where $G = l_P^2$ is Newton's gravitational constant. Since this implies that $R > \delta x$, the assumption that A and B are independent is rendered highly suspect. It is therefore likely that the concept of locality itself breaks down at the Planck length and that the correct fundamental physical theory is nonlocal in character. Lee explores one candidate for a nonlocal theory, but one which at the same time retains all of the desired features of conventional field theories (Lorentz invariance, gauge symmetries, unitarity, etc.).

12.5.3.2 Classical Mechanics

Lee begins by postulating that within a time interval τ , a particle can assume only N possible space-time positions, $(\vec{x}_n, t_n)$, $n = 1, 2, \dots, N$. The ratio

$$\rho \equiv \frac{N}{\tau} \quad (12.31)$$

is a fundamental constant of the theory.

The "classical" continuous action

$$S_c = \int_0^\tau \left\{ \frac{1}{2} \left(\frac{d\vec{x}}{dt} \right)^2 - V \right\} dt, \quad (12.32)$$

where V is the potential and only the spatial variable $\vec{x}(t)$ is a dynamical variable,[†] is replaced by the "discrete" action S_d given by [tdlee85a]

$$S_d = \sum_n \left\{ \frac{1}{2} \vec{v}_n^2 - \frac{1}{2} [V(\vec{x}_n) + V(\vec{x}_{n-1})] \right\} (t_n - t_{n-1}), \quad (12.33)$$

where $\vec{x}_n = (\vec{x}_n - \vec{x}_{n-1})/(t_n - t_{n-1})$.

Fixing the end-points at $\vec{x}(t=0) = \vec{x}_i$ and $\vec{x}(t=\tau) = \vec{x}_f$, we recall that the classical equations of motion are obtained by setting the variation of the action with

[†]We have also set the mass $m = 1$.

respect to spatial changes to zero:[†]

$$\frac{\delta S_c}{\delta \vec{x}(t)} = 0 \implies \frac{d^2 \vec{x}}{dt^2} = -\nabla V. \quad (12.34)$$

In the case of the discrete theory, there are two set of equations, since both $\vec{x}_n$ and t_n are considered dynamical variables:

$$\begin{cases} \frac{\delta S_d}{\delta \vec{x}_n} = 0 \implies \frac{\vec{x}_{n+1} - \vec{x}_n}{\frac{1}{2}(t_{n+1} - t_{n-1})} = -\nabla V(\vec{x}_n), \\ \frac{\delta S_d}{\delta t_n} = 0 \implies E_n \equiv \frac{1}{2}v_n^2 + \frac{1}{2}[V(\vec{x}_n) + V(\vec{x}_{n-1})] = E_n. \end{cases} \quad (12.35)$$

The first equation gives the discrete version of Newton's equation; the second equation gives energy conservation. We make two comments: (1) Notice that while energy conservation is a natural consequence of Newton's equation in continuum mechanics, it becomes an independent property of the system in Lee's discrete mechanics; (2) If time is treated as a conventional parameter and not as a dynamical variable, the discretized system is not time-translationally invariant and energy is not conserved. Making both $\vec{x}_n$ and t_n dynamical variables is therefore one way to sidestep this problem.

It is left to reader to verify that, under Lee's discrete mechanics, both free particles and particles subjected to a constant force behave in essentially the same way as they do under continuous equations of motion. Moreover, the time intervals $\Delta t = t_{i+1} - t_i$ are all equal. While the spatial behavior for non-constant forces (ex: particles in a harmonic oscillator $V \sim \frac{1}{2}\omega x^2$ potential) also remains essentially the same as would be predicted by continuous mechanics, the time intervals Δt are nonuniformly spaced.

12.5.3.3 Nonrelativistic Quantum Mechanics

Lee's discretization of nonrelativistic quantum mechanics is almost as "straightforward" as the discretization of classical mechanics discussed above; he uses Feynman's path integral formalism [feyn65b].

Recall that in the usual continuum theory, the amplitude $K(\alpha, \beta)$ for going from point α to β is an integral over all paths from α to β with each path weighted by a factor $\exp\{iS_c\}$, where $S_c = S_c[\vec{x}(t)]$ is the classical action integral (equation 12.32):[‡]

$$K(\alpha, \beta) = \int_{\alpha}^{\beta} e^{-iS_c} [\mathcal{D}_c x(t)], \quad (12.36)$$

where $[\mathcal{D}_c x(t)] \equiv \lim_{N \rightarrow \infty} \lim_{\epsilon \rightarrow 0} \mathcal{J} \prod_n d^3 x_n$ and $\mathcal{J} \equiv (2i\pi\epsilon)^{-3/2}$. The limits are necessary

[†]See, for example, the text by Goldstein [goldh80].

[‡]We set $m = \hbar = 1$.

because the path integral is actually evaluated by approximating a path $\vec{x}(t)$ by $N - 1$ numbers $\vec{x}(t_1), \dots, \vec{x}(t_{N-1})$, where $t_n = t_0 + n\epsilon$, and first integrating each x_i from $-\infty$ to $+\infty$. After these integrations are carried out, we take the limit $N \rightarrow \infty$.

In Lee's discrete quantum mechanics, the classical action S_c is again replaced by the discrete action S_d (equation 12.33), and, because both $\vec{x}$ and t are variables, the "continuous path" $[\mathcal{D}_c x(t)]$ is replaced by the "discrete path" $[\mathcal{D}_d x(t)] = \mathcal{J} \prod_n d^3 x_n dt_n$, where $\mathcal{J}$ is the same as for the continuous case. The parameter n varies from 1 to N with $N/\tau = \rho \equiv 1/l$ a fundamental constant.

The discreteness in this new theory refers to the discrete nature of all measurements. Each measurement fixes a particle's position $\vec{x}_n$ and time t_n . Both $\vec{x}_n$ and t_n are allowed to take on any value in the spectrum of continuous eigenvalues of the operators $(\vec{x}_n)_{\text{op}}$ and $(t_n)_{\text{op}}$. Notice also that in this discrete theory there is no Hamiltonian and no Lagrangian; only Action.

Lee derives several immediate consequences from his theory [tdlee85a]. For example, he shows that, for $\tau \gg l$, the discrete amplitude, $K_d(\alpha, \beta) \sim \exp\{-i\mathcal{H}\tau\}$, where

$$\mathcal{H} = H_{\text{op}} + \frac{1}{8}l^2[\nabla^2 - V, [\nabla^2, V]] + \mathcal{O}(l^3), \quad (12.37)$$

$H_{\text{op}} = -\frac{1}{2}\nabla^2 + V$ is the Hamiltonian of the continuum theory and $[x, y] = xy - yx$ is the commutator of x and y (the proof appears in [fried83]). Applying this result to the particular example of an electron trapped in a Coulomb potential due to a nuclear charge Z distributed uniformly over a sphere of radius R , Lee estimates the additional energy shift $\Delta E = E_{\text{continuous}} - E_{\text{discrete}}$ that is predicted by his discrete theory. Setting the agreement between experimental measurements and theoretical QED calculations of the Lamb shift to an accuracy $\epsilon \sim 10^{-11}$ rydberg, Lee obtains an upper bound on l : $l < 1.6 \times 10^{-14}$ cm.[†]

12.5.3.4 Scalar Fields on a Random Lattice

Lee next generalizes discrete quantum mechanics to the case of a massless scalar field ϕ interacting with an arbitrary external current J ([tdlee85a], [tdlee85b]).

In continuum field theory, the field $\phi(\vec{x}, t)$ is a dynamical variable and the coordinates $\vec{x}$ and t are only parameters. With the conjugate momentum $\Pi(\vec{x}, t)$, and Hamiltonian operator

$$H = \frac{1}{2} \int \{ \Pi^2 + (\frac{\partial \phi}{\partial \vec{x}})^2 \} d^{n-1}x, \quad (12.38)$$

where $\partial/\partial \vec{x}$ is the $(n-1)$ -dimensional gradient operator, the matrix element of $e^{-\tau H}$ between the initial configuration $\phi_i(\vec{x})$ and final configuration $\phi_f(\vec{x})$ is given

[†]Better bounds ($l < 10^{-15}$ cm) can be obtained using measurements for hyperfine splitting and e^+e^- collisions [fried83].

by the Feynman path integral

$$\langle \phi_f(\vec{x}) | e^{-\tau H} | \phi_i(\vec{x}) \rangle = \int e^{-S_c[\phi]} \mathcal{D}[\phi], \quad (12.39)$$

where

$$S_c = \int_{\Omega} \left\{ \frac{1}{2} \left(\frac{\partial \phi}{\partial x^\mu} \right)^2 - J\phi \right\} d^n x \quad (12.40)$$

is the continuum action, $x^\mu = (\vec{x}, t)$ is the component of a n -dimensional Euclidean vector and the repeated index μ must be summed over $1, \dots, n$. The classical equation of motion is given by Laplace's equation:

$$-\frac{\partial^2 \phi}{\partial x_\mu^2} = J(x). \quad (12.41)$$

To discretize this theory, Lee assumes that in any n -dimensional volume $\Omega = L^{n-1}\tau$, there can be at most N measurements that determine the space-time position x_i of the observation and the value of the field ϕ_i at x_i . The ratio $\rho = N/\Omega \equiv l^{-4}$ is therefore a fundamental constant of the theory.

A discrete action, S_d , may be defined by assuming that only neighboring pairs of sites (say, i and j) are coupled. Each pair contributes to the action a term $(\phi_i - \phi_j)^2$, weighted by a factor λ_{ij} . Since different links l_{ij} can have different lengths and orientations, it is reasonable to assume that they should also contribute with different weights. The integral $\frac{1}{2} \int (\frac{\partial \phi}{\partial x^\mu})^2 d^n x$, in the continuum theory, is in the discrete theory replaced by a sum over all links, $\frac{1}{2} \sum_{l_{ij}} \lambda_{ij} (\phi_i - \phi_j)^2$, and the discrete action thus becomes

$$S_d = \frac{1}{2} \sum_{l_{ij}} \lambda_{ij} (\phi_i - \phi_j)^2 - \sum_i J_i \phi_i. \quad (12.42)$$

The discrete equation of motion is given by the equation:[†]

$$\sum_{j \text{ linked to } i} \lambda_{ij} (\phi_i - \phi_j) = J_i. \quad (12.43)$$

What is the weight set λ_{ij} ? For starters, we know it cannot be simply a constant. Consider N randomly distributed sites $x_1 < x_2 < \dots < x_N$ in one-dimension. Attach a field ϕ_n at each x_n . Then the discrete approximation $d^2\phi/dx^2 \approx (\phi_{n+1} - \phi_n)/(x_{n+1} - x_n) - (\phi_n - \phi_{n-1})/(x_n - x_{n-1})$ is certainly better than $d^2\phi/dx^2 \approx \lambda(\phi_{n+1} - 2\phi_n + \phi_{n-1})$, where λ is a constant. This is so because if ϕ_n is a linear function of x_n then both $d^2\phi/dx^2$ and the first expression are equal to zero but the second expression is not. The idea is then to define λ_{ij} in such a way that the

[†]Note this equation has the simple form of one of *Kirkoff's Laws* for electrical circuits. If we think of ϕ as the electric potential at i and λ_{ij}^{-1} as the resistance of the link l_{ij} , then the current $\mathcal{I}$ flowing from site j to site i along link l_{ij} is given by $\mathcal{I} = \lambda_{ij}(\phi_j - \phi_i)$. Compare to equation 12.43.

discrete analog of Laplace's equation is satisfied for when ϕ_i is a linear function of $\vec{x}_i$.

We know that if $\phi(\vec{x})$ is a linear function of $\vec{x}$, Laplace's equation $\partial^2 \phi / \partial x_\mu^2 = 0$. Thus, when $\phi_i = \alpha + \vec{\beta} \cdot \vec{x}_i$ (where α and $\vec{\beta}$ are constants), we require the weights λ_{ij} to satisfy the analogous equation $\sum_j \text{linked to } i \lambda_{ij}(\phi_i - \phi_j) = 0$ for all i for a random distribution of site $\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N$. To this end, it is useful to introduce the notion of a *dual lattice*.

Simplicial Decomposition and the Dual Lattice: We first define more carefully what we mean by an N -site random lattice $\mathcal{L}_N$. Consider a finite volume Ω in an n -dimensional Euclidean space; for simplicity, we may assume that Ω is an n -dimensional rectangular volume with periodic boundary conditions. Given a random distribution of N sites in Ω , partition that volume into a set of non overlapping *simplices* whose vertices are the sites. For $n=2$, the simplices are triangles; for $n=4$ the simplices take the form of tetrahedra. In general, an n -dimensional simplex consists of $(n+1)$ sites. Details on the simplicial construction, including the calculation of various kinematic properties of the random lattice, are discussed in [christ82] and [tdlee83b].

Using this simplicial decomposition, we may now define a dual lattice constructively as follows [tdlee83b]. Let i be an arbitrary site in $\mathcal{L}$. We say that a point $p \in \Omega$ belongs to i if i is the nearest site to p in $\mathcal{L}$. The *dual to site i* is the volume $\omega_i \equiv \{p \mid p \text{ belongs to } i\}$. We call ω_i an n -dimensional *cell*.[†] The *dual lattice* of the random lattice $\mathcal{L}$ consists of the cells into which $\mathcal{L}$'s volume Ω is divided using the above construction.

The surface of each cell consists of a number of $(n-1)$ -dimensional faces, which are formed by points belonging to two or more sites. Similarly, $(n-2)$ -dimensional faces, consisting of points belonging to three or more sites, are formed by the intersections of these $(n-1)$ -dimensional faces; and so on. In this way, each link in the random lattice is perpendicular to (but does not necessarily intersect) an $(n-1)$ -dimensional face in its dual; each triangle is perpendicular to a $(n-2)$ -dimensional face; and so on.

Figure 12.10 shows a small section of a two-dimensional lattice and its dual; l_{ij} is the length of the link between sites i and j , while $\tilde{l}_{ij}$ is the border length of their dual cells. More generally, in n -dimensions, $\tilde{l}_{ij}$ is the "volume" of the $(n-1)$ -dimensional surface in the dual lattice. In terms of these variables, Lee defines the weights λ_{ij} to be equal to

$$\lambda_{ij} = \begin{cases} \tilde{l}_{ij}/l_{ij} & \text{if } i \text{ and } j \text{ are linked} \\ 0 & \text{otherwise.} \end{cases} \quad (12.44)$$

This choice for λ_{ij} has the following two desirable properties [tdlee85a]: (1) it satisfies the requirement that $\sum_j \text{linked to } i \lambda_{ij}(\phi_i - \phi_j) = 0$ for all i , so that it is a good discrete version of the Laplace operator, and (2) if the external current is

[†]Such cells are called *Voronoi cells* in the literature (see, for example, [ziman79]).

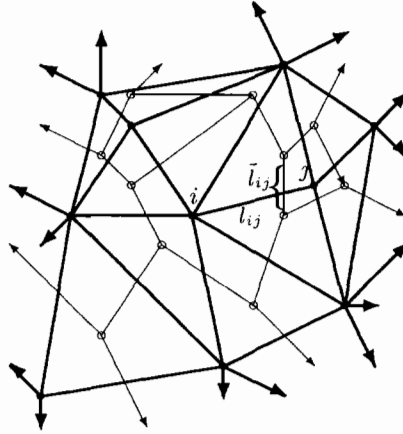


Fig. 12.10 An example of a two dimensional random lattice (dark lines and solid circles) and its dual lattice (lighter lines and open circles).

nonzero only at site 0 (i.e. $J_i = \delta_{i0}$), then, for sites very far from 0, the solution ϕ_i is given by the continuum solution. For $n = 3$ dimensions, for example, $\phi_i \rightarrow (4\pi x_i)^{-1}$ as $x_i \rightarrow \infty$, which agrees with the solution to the continuum equation $-\partial^2 \phi / \partial x_\mu^2 = \delta^3(\vec{x})$, given by $\phi = (4\pi x)^{-1}$.

While we end our discussion of Lee's ideas with scalar fields, interested readers may wish to consult his papers extending this discrete time theory to spin-1/2 fields, gauge fields and quantum gravity ([tdlee83b], [tdlee85a], [tdlee85b]). We quote from the last line of Friedberg's and Lee's seminal 1983 paper [fried83]: "While the analysis...is exploratory in spirit, it suggests the possibility that underneath the present continuum edifice, there may lie an entirely different layer, hitherto unexplored but more fundamental in concept and equally rich in structure."

12.6 Is the Universe a CA?

In many ways, the title of this section is the central question that those with a predilection for toying with fundamental issues eventually find themselves asking. It is also a question that (not unlike the problem of formulating a legitimate – or even an *allowable* – question about "what is really going on" in quantum mechanics), must be asked correctly. It is not enough merely to ask the question in its simplest form. We must first of all be sure of what we are asking.

What do we really mean to ask? Or hope to find? Perhaps that underneath it all, if we could somehow manage to probe deeply enough into the Planck-length scale dimensions of the universe, that there we would find an orderly lattice populated with some analogs of Conway's *Life*-like "gliders?" Or perhaps we expect to find some perfectly simple local "rule" that accounts, on a large enough scale, for all the wonderful complexity that we are still grappling with our field theories to help explain. Neither view, of course, nor others possessed of their rather blatant naivete,

is (at least at present) “physically defensible,” but they will serve as a useful starting point.

We begin with a suggestive, if not impassioned, parable.

12.6.1 A Teasingly Suggestive “Parable”

Consider the evolution of the nearest-neighbor one-dimensional cellular automata rule R110, starting from a random initial state.[†] A few early steps of a sample evolution are shown in figure 12.11.

Forget for a moment that you know that figure 12.11 shows the space-time pattern due to a well defined local deterministic rule, and that the underlying “universe” really consists of nothing but “bits.” Suppose you are told only that this figure represents some sort of “alien physics,” and that you may see as many different samples of this alien world’s behavior as you wish. How are you to make any sense of what is really going on?

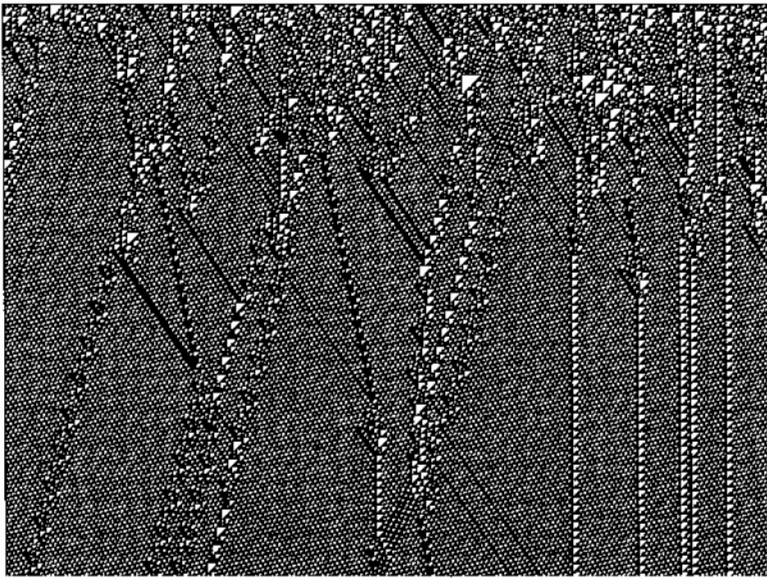


Fig. 12.11. Evolution of elementary one-dimensional rule R110.

Noticing that the figure consists of certain particle-like objects sprinkled on a more-or-less static background, the simplest (most natural?) thing for you to do – and your physics training certainly comes in very handy here – is to begin cataloging the various “particles” and their “interactions.” You begin by methodically writing in your journal observations of the form “There are N particles of size s moving to

[†]Rule R110 is explicitly defined by $(\sigma_{i-1}\sigma_i\sigma_{i+1}) \rightarrow \sigma'_i$: (000) $\rightarrow$ 0, (001) $\rightarrow$ 1, (010) $\rightarrow$ 1, (011) $\rightarrow$ 1, (100) $\rightarrow$ 0, (101) $\rightarrow$ 1, (110) $\rightarrow$ 1, (111) $\rightarrow$ 0. See section 3.1.4.4.

the left with speed v ,” “When a particle p_1 of type $\mathcal{P}$ collides with p_2 of the same type, the result is the set of particles $\{q_1, \dots, q_n\}$,” and so on.

Depending on how many different samples of behavior you have the patience to analyze (and other factors, some of which, such as how representative the initial states in these samples are of the set of all possible initial states, may be beyond your control), you may or may not get a fairly complete picture of what kinds of objects exist and what sorts of interactions are allowed in this one-dimensional alien universe. At worst, you will grow tired long before you have had the chance to record even a small fraction of the total number of possible states in this world.

At best, you will have a long (and likely still incomplete) list of particles and their interactions. What you almost assuredly will *not* have, is any idea that the underlying physics really consists of a single – very simple – local deterministic rule that acts on the real particles that are the fixed sites of a lattice taking on the values 0 or 1. *How different is this alien two-dimensional world from our own?*

While our impassioned parable is admittedly naive, it is also the most straightforward depiction of the heartfelt idea that maybe – just maybe – there is something much, much simpler than what we normally think of as fundamental physics lurking on tinier, Planck-length, scales.[†] The question is whether this much simpler “something” owes anything to CA-like formalisms.

12.6.2 Speculations I: Minsky

In a contribution to the first conference on physics and computation held at MIT in 1982 [land82b], Minsky considered whether a universe satisfying the following two conditions could exist [minsky82]: (1) *each volume of space contains a finite amount of information*, and (2) *over a suitable range of size and speed, the mechanics of the universe are approximately classical*.

Envisioning space-time as a four-dimensional CA lattice, wherein sites take on one of a finite number of values and interact via a local dynamics, Minsky explored various elementary properties of this universe: particle (or “packet”) size and speed, time contraction, symmetry, and how the notion of “field” might be made palatable within such a framework.

The idea that localized particle-like propagating structures can be defined on a lattice was nothing new. For example, Minsky was well aware of the existence of “gliders” in Conway’s *Life* rule. Minsky’s own pedagogical example was effectively a four-state one-dimensional CA with states $\sigma \in \{0, 1, \alpha, \beta\}$ and rules $\phi : (\sigma_{i-1}, \sigma_i, \sigma_{i+1}) \rightarrow \sigma'_i$ given by:

$$\begin{cases} \phi(0, 1, \alpha) \rightarrow 0, & \phi(0, \alpha, \alpha) \rightarrow \beta, & \phi(1, 1, \alpha) \rightarrow \alpha, \\ \phi(\beta, 0, 0) \rightarrow \alpha, & \phi(\beta, \alpha, *) \rightarrow \beta, & \phi(*, \beta, *) \rightarrow 1, \end{cases} \quad (12.45)$$

where ‘*’ is a wild card representing any of the four states.

[†]The allegory is certainly not meant to convey the impression that real high energy physicists are, as a group, little more than tired “bookkeepers.”

Using these rules, it is easy to show that value sequences of the form $\underbrace{11 \dots 11}_n \alpha$, surrounded on either side by an infinite string of 0's, are particle-like propagating "packets." In the case when $n = 4$, for example, the packet moves forward one spatial position every $t = 9$ iteration steps:

$$\begin{array}{ll}
 t = 0 : & 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 1 \ \alpha \ 0 \ 0 \ 0 \\
 t = 1 : & 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ \alpha \ \alpha \ 0 \ 0 \ 0 \\
 t = 2 : & 0 \ 0 \ 0 \ 1 \ 1 \ \alpha \ \alpha \ \alpha \ 0 \ 0 \ 0 \\
 t = 3 : & 0 \ 0 \ 0 \ 1 \ \alpha \ \alpha \ \alpha \ \alpha \ 0 \ 0 \ 0 \\
 t = 4 : & 0 \ 0 \ 0 \ 0 \ \alpha \ \alpha \ \alpha \ \alpha \ 0 \ 0 \ 0 \\
 t = 5 : & 0 \ 0 \ 0 \ 0 \ \beta \ \alpha \ \alpha \ \alpha \ 0 \ 0 \ 0 \\
 t = 6 : & 0 \ 0 \ 0 \ 0 \ 1 \ \beta \ \alpha \ \alpha \ 0 \ 0 \ 0 \\
 t = 7 : & 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ \beta \ \alpha \ 0 \ 0 \ 0 \\
 t = 8 : & 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ \beta \ 0 \ 0 \ 0 \\
 t = 9 : & 0 \ 0 \ 0 \ 0 \ 1 \ 1 \ 1 \ 1 \ \alpha \ 0 \ 0
 \end{array} \tag{12.46}$$

Notice that in this example, the speed of the packet is inversely proportional to the packet's spatial size. While there is certainly nothing unique about this particular representation, it is interesting to speculate, along with Minsky, whether it may be true that, just as the simultaneous "information" about position and momentum is fundamentally constrained by Heisenberg's uncertainty relation in the physical universe, so too, in a discrete CA universe, there might be a fundamental constraint between the volume of a given packet and the amount of information that can be encoded within it.

12.6.2.1 Particle Interactions

How might the interaction between two discrete particles be described by a finite-information based physics? Unlike classical mechanics, in which a collision redistributes the particles' momentum, or quantum mechanics, which effectively distributes their probability amplitudes, finite physics presumably distributes the two particles' *information content*. How can we make sense of the process "*A* scatters *B*," if *B*'s momentum information is dispersed "halfway across the galaxy?" [minsky82]. Minsky's answer is that the universe must do some careful "bookkeeping."

If a particle *A* must know *B*'s total information content before colliding, the collision process must be delayed until *A* has full access to that information. However, such a delay is consistent neither with classical nor quantum mechanics. Minsky instead suggests that the collision proceeds immediately, but with the particles' both working with less than all the information that is classically required; i.e. *the incoming particles' momenta are "estimated."* Outgoing momenta are determined via conventional classical rules, but, because of the estimation errors, each scattered particle leaves behind a "receipt" recording how much momentum was really taken away in the process. Receipts not only mark prospective "event-locations" at which future collisions might take place, but harbor information that can be used to estimate new "real" momenta.

"If we combine mechanics in this way with unobservable receipts, deterministic systems show some qualitative features that resemble quantum, mixed-state systems. Thus one can always measure the "real" momentum in event 1 by the location of event 2. But one cannot yet "observe" the "receipt" momentum of event 1, because it is not until event 2 that it first combines with any "real" momentum - which cannot be "observed" until some subsequent event 3 - by which time it is already mixed with another estimate! And so on. One can never simultaneously measure both estimate and receipts, though all adds up eventually. And all this involves no probabilities at all, just temporary inaccessibility of information!" [minsky82]

It is interesting to note that this primordial bookkeeping scheme also allows for the quantum mechanical phenomenon of *tunneling*. In particular, interactions requiring more momentum than is currently available are permitted, so long as all receipts eventually return their information in new estimates. Moreover, we see that even some qualitative features of quantum *interference* may also arise: two particles could feign a "coherence" of sorts by sharing the same receipt information. Minsky is quick to point out, however, that his scheme almost surely does not yield a correct quantum mechanics; if for no other reason than it would effectively "solve" the hidden-variable problem.

We will not go any further into the interesting speculations Minsky offers in his 1982 paper [minsky82]. The point of these speculations was not to propose a serious alternative model of fundamental physics, *per se*, but to stimulate thinking along the lines of "What if physics were, fundamentally, discrete? How would we describe the processes we now think we understand with our continuous models?" Two questions that we will repeatedly come back to in this concluding chapter.

12.6.3 Speculations II: Zuse

At the same 1982 MIT conference at which Minsky presented his ideas, Konrad Zuse [zuse82] also speculated on what it would take for a CA-like universe to sustain propagating patterns on a cellular lattice (what he called "digital particles"). Echoing Feynman's "challenge" (section 12.4.3), Zuse suggests that "not sufficient criticism has been applied yet to see the consequences which result from" the basic assumption under "which today's physics is operating," namely, that each point in space effectively contains an infinite amount of information. Summarizing ideas that he had been developing for several decades,[†] Zuse focuses on two main questions: (1) *How do we resolve the problem of the universe being demonstrably isotropic with a CA's (Euclidean, hexagonal, etc.) anisotropy?* (2) *What is the information content of a physical particle?*

The answer that Zuse offers to the first question is to use irregularly organized lattices (recall T.D. Lee's random lattice field theory ([tdlee85a]; section 12.5.3) and Ilachinski's speculative reasons for developing his SDCA model ([ilach87]; see section 8.8):

[†]See the translation of Zuse's 1969 paper [zuse80].

"This leads us to the theory of variable and growing automata. Irregularities of the grid structure are a function of moving patterns, which is represented by digital particles. Now, not only certain values are assigned to the single crosspoints of the grid in the concept of the cellular automaton which are interrelated and sequencing each other, but also the irregularities of the grid are itself functions of these values of the just existing interlinking network. One can imagine rather easily that in such a way the interdependence of mass, energy, and curvature of space may logically result from the behavior of the grid structure."

In this scheme, digital particles are still wandering localized clusters of information[†] but (conventional) variables such as space, time, velocity and so on become statistical quantities. Given that no experimental measurement to date has yet detected any statistical dispersion in the velocity of light, the sites of a hypothetical discrete underlying lattice can be no further apart than about 10^{-16} cm.

Though there was of course no way for Zuse to answer his second question (nor is there any way today), the fact that it is being asked at all underscores the essence of the second of the two paradigm shifts listed earlier in this chapter: the notion that *information* is more fundamental than what have traditionally been used as fundamental variables (mass, energy, etc.) . Zuse suggests that if only we could find an appropriate language or formalism with which to describe this primordial information, we would find, for example, that the information content of two or more interacting particles is conserved.

12.6.4 Speculations III: Fredkin

A strong proponent of the view that the universe is *literally* a CA is Edward Fredkin (see [fredkin82], [fredkin90] and [fredkin93]).[‡] In two of his most recent papers, "Digital Mechanics" [fredkin90] and "A New Cosmogony" [fredkin93], Fredkin explores some of the consequences of making what he calls the *finite nature hypothesis*:

"Finite Nature is a hypothesis that ultimately every quantity of physics, including space and time, will turn out to be discrete and finite; that the amount of information in any small volume of space-time will be finite and equal to one of a small number of possibilities. We call models of physics that assume Finite Nature 'Digital Mechanics.' ...we take the position that Finite Nature implies that the basic substrate of physics operates in a manner similar to the workings of certain specialized computers called cellular automata."

Fredkin's finite nature hypothesis makes no assumptions about the actual scale of space-time's discretization. It might be as large as current estimates of the

[†]Zuse does not consider the complicated question of how the integrity of such clusters can be maintained by a rule, or set of rules, operating on a random lattice. Minsky [minsky82] also considers using a random lattice but wonders how to build "particles" into such a universe that would necessarily have to be insensitive to local cell-connection fluctuations.

[‡]The interested reader is encouraged to also look at Parts I and II of the book by Wright [wright88], which is written for a lay audience but contains an engaging discussion of Fredkin's ideas.

upper bound on the possible discontinuity of space ($\sim 10^{-17}$ cm) or as small as the Planck length ($\sim 10^{-30}$ cm). The problem is simply to explore the consequences of assuming there is a definite scale at all, whatever that scale may turn out to be. “Finite nature does not just hint that the informational aspects of physics are important, it insists that the informational aspects are all there is to physics at the most microscopic level.” [fredkin90]

12.6.4.1 *Digital Mechanics*

The formalism with which Fredkin chooses to describe his *digital mechanics* (DM) is a sufficiently large, but finite, reversible universal CA (RUCA). He is careful to distinguish the RUCA from DM itself, which we are to think of as the informational process that is running in the RUCA, likening the need to do so to the obvious distinction between, say, the objects of a chess game (its board, pieces, and rules) and the actual process of playing a game of chess. Whereas RUCA may share certain physically “intuitive” characteristics of our macroscopic world, such as universality, a locally Euclidean structure, determinism, and so on, DM actually describes the correct deeper physics, including asymptotic isotropy, an apparent nondeterminism, Lorentz invariance and so on.

Finiteness is the basic assumption: a finite total volume of space-time and a finite amount of information in a finite volume of space-time. We require universality, of course, since we know that without it nothing much of interest can happen. We can also take a strong cue from our own universe, which allows us to build universal computers. If the underlying micro-physics was not universal we would not be able to do this. Reversibility is desirable because it ensures a strict conservation of information and can be used to create systems that conserve various quantities such as energy and angular momentum despite underlying anisotropies.

For concreteness, let us suppose that the universe has a temporal depth of two to accommodate a Fredkin-type reversibility; i.e. the present and immediate past are used to determine the future, and from which the past can be recovered uniquely. The RUCA itself is deterministic, is applied synchronously at each site in the lattice, and is characterized by three basic dimensional units: (1) *digit transition*, D , which represents the minimal informational change at a given site; (2) the *length*, L , which is the shortest distance between neighboring sites; and (3) an integer *time*, T , which, while locally similar to the time in physics, is not Lorentz invariant and is not to be confused with a “macroscopic” (or observed) time t . While there are no a priori constraints on any of these units – for example, they may be real or complex – because of the basic assumption of finite nature, they must all have finite representations. All other units of physics in DM are derived from D , L and T .

Each site is assumed to harbor a single “digit” of information: a *bit* in the case of two states, a *trit* in the case of three, and so on. A *digit-transition* refers to any digit change, whether temporal, such as when a digit changes from a 0 to a 1, or spatial, such as when a site has a digit 1 while its neighbor has a 0. Other properties emerge as consequences of digit changes. For example, the frequency of temporal digit transitions is related to energy, while the frequency of spatial digit changes is

related to momentum. Fredkin reinterprets the principle of “least action” in his DM as referring to the minimal amount of information in a process. Table 12.2[†] shows a few correspondences conjectured by Fredkin to hold between digital mechanics and physics; it is meant only to convey the flavor of how DM might use its basic units to construct “real” physics.

Continuous Physics	Digital Mechanics
continuity	discreteness
infinitesimals	the digit, units of length and time
digit-transition	D
length	L = cell-to-cell distance
time	T = one clock cycle
mass	DT/L^2
action	D
conservation laws	conservation of information
group theory properties	consequence of RUCA properties
particles	digital machine whose properties (spin, momentum, energy, etc.) is represented by information or an information process

Table 12.2 A few correspondences between elements of continuous physics and Fredkin’s discrete mechanics; from table 1 in [fredkin93].

12.6.4.2 DM Processes

One immediate general consequence of Fredkin’s view of finite nature is that “there can be no information without a means of its representation.” [fredkin90] This means, in particular, that DM allows no processes for which there is no means of interpreting and transforming the information representing the elements of that process. However, there is nothing prohibiting that information from being spread over a large volume or being superimposed over other information representing other unrelated processes. A particle being accelerated by a field, for example, is interpreted as being an interaction between the information representing the motion of the particle and the information representing the state of the field, transforming the information that represents the velocity of the particle.

12.6.4.3 Causality

Because of the assumed (temporal depth of *two*) nature of the reversibility of the underlying universal CA, causality takes on a decidedly non intuitive character: the state of a given site is completely determined by the states of its nearest neighbors in space-time. Letting $\sigma_{\vec{x},t}$ represent the state of the site at $\vec{x}$ and time t ,

[†]Taken from table 1 in [fredkin90].

we know that $\sigma_{\bar{x},t} = \phi_1(\sigma_{\bar{x}-\bar{1},t}, \sigma_{\bar{x}+\bar{1},t}, \sigma_{\bar{x},t-1}, \sigma_{\bar{x},t+1})$. But, we could also compute the *future*: $\sigma_{\bar{x},t+1} = \phi_1(\sigma_{\bar{x}-\bar{1},t}, \sigma_{\bar{x}+\bar{1},t}, \sigma_{\bar{x},t-1}, \sigma_{\bar{x},t+1})$; or *past*: $\sigma_{\bar{x},t-1} = \phi_1(\sigma_{\bar{x}-\bar{1},t}, \sigma_{\bar{x}+\bar{1},t}, \sigma_{\bar{x},t-1}, \sigma_{\bar{x},t+1})$; or a *neighbor*: $\sigma_{\bar{x}\pm\bar{1},t} = \phi_1(\sigma_{\bar{x}-\bar{1},t}, \sigma_{\bar{x}+\bar{1},t}, \sigma_{\bar{x},t-1}, \sigma_{\bar{x},t+1})$.

The result is that while there is, in DM, something that might be called an *information cone* centered at each site, it is not really what we usually think of as a relativistic *light cone*, for which we can point to interior points and definitely say they are causally related and know for sure that points outside of each other's light cones are completely independent. In DM it is simply false to say that only those events inside the information cone of *the past* can influence a present event; the information cone can well consist of lights cones stretching into all directions, forward and back in time.

While this above state of affairs is decidedly counterintuitive, it has the virtue of simply and easily – at least in principle – accounting for one of the deep mysteries of quantum mechanics; namely, an apparent nonlocality as expressed by the Einstein-Podolsky-Rosen gedanken experiment [ein35] and Bell's theorem [bell64] (see discussion box). Finite nature implies that any system that is allowed to evolve from some distant initial state possesses causality in all space-time directions. This implies, in particular, that no part of space can be considered to be causally separated from another, and that therefore the DM universe will always harbor effects that cannot be attenuated by distance.

12.6.4.4 Putting DM to the Test

While the ideas sketched above, as well as their amplifications and many other of Fredkin's musings on DM, are far from being a complete theory, Fredkin nonetheless offers a few suggestions as to how the basic assumption of finite nature might be put to the test. The most important assumption, of course, is that DM harbors what effectively amounts to being a privileged, fixed, anisotropic inertial reference frame; an assumption that is clearly at odds with relativity. This underlying anisotropy might be detectable in certain microscopic events. If the basic units of length, L , and time, T , are large enough, Fredkin suggests that crystals (such as used in very accurate oscillators) might be observed to change their electrical impedance if the combination of their own lattice spacing, spatial orientation, absolute velocity through the DM lattice and driven frequency are in phase with DM's own lattice spacing, orientation and natural frequency [fredkin90]. Finally, a quantization of energy levels in particles might be detectable at very high energies.

Fredkin points out that even if a preferred frame, or underlying lattice, is found, its implications are in one sense only philosophical: the integrity of the theory of relativity remains intact, it is only our philosophical perspective that changes. Similarly, if a deterministic RUCA-like rule is the basis of the real physics, it does not mean that we should all throw away our quantum mechanics texts. On the other, if the finite nature hypothesis is correct and a RUCA-like rule exists and can be found, it should in principle be able to supply us with values of all of the fundamental constants of physics.

Lorentz-Invariance on a Lattice? One of the most obvious shortcomings of a CA-based microphysics has to do with the lack of conventional symmetries. A lattice, by definition, has preferred directions and so is structurally anisotropic. How can we hope to generate symmetries where none fundamentally exist? A strong hint comes from our discussion of lattice gases in chapter 9, where we saw that symmetries that do not exist on the microscopic lattice level often emerge on the macroscopic dynamical level. For example, an appropriate set of microscopic LG rules can spawn circular wavefronts on anisotropic lattices.

Another simple example is the traditional two-dimensional “random-walk” on a four-neighbor Euclidean lattice [toff89]. Despite the fact that the underlying lattice is symmetric only with respect to rotations that are multiples of 90 deg, the probability distribution $p(x, y)$ for a particle that begins its random walk at the origin becomes circularly symmetric in the limit as time $t \rightarrow \infty$: $p(x, y; t) \rightarrow (2\pi t)^{-1} e^{-\frac{1}{2}(x^2+y^2)/t}$ (see figure 12.12).

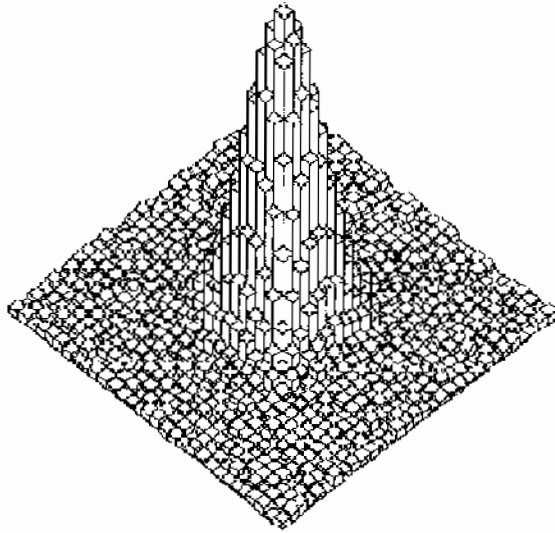


Fig. 12.12. A circularly symmetric Gaussian probability distribution $p(x, y) \sim e^{-x^2-y^2}$ describing a two-dimensional random walk emerges for large times on the macroscopic level, *despite* the fact that the underlying Euclidean lattice is anisotropic.

It is easy to invent rules that conserve particle number, energy, momentum and so on, and to smooth out the apparent lack of structural symmetry (although we have cheated a little in our example of a random walk because the circular symmetry in this case is really a “statistical” phenomenon and not a reflection of the individual particle motion). The more interesting question is whether relativistically correct (i.e. Lorentz invariant) behavior can also be made to “emerge” on a Cartesian lattice. Toffoli ([toff89], [toff90b]) showed that this is possible.

Before outlining Toffoli’s “model” of a deterministic relativistic diffusion CA model, we motivate the discussion by recalling a simple formal analogy that holds between a circular rotation by an angle θ in the (x, y) plane and a Lorentz transformation with velocity

$\beta (\equiv v/c)$ in the (x, t) plane. The Lorentz transformation can be written as

$$\begin{pmatrix} t' \\ x' \end{pmatrix} = \begin{pmatrix} \cosh \theta & \sinh \theta \\ \sinh \theta & \cosh \theta \end{pmatrix} \begin{pmatrix} t \\ x \end{pmatrix}, \quad (12.47)$$

where $\theta = \tanh^{-1} \beta$ is the *rapidity*. Might we exploit this analogy to find a microscopic dynamics on the (x, t) plane for which a Lorentz invariance emerges in the same way as does a circularly symmetric probability distribution for a random walk in the (x, y) plane?

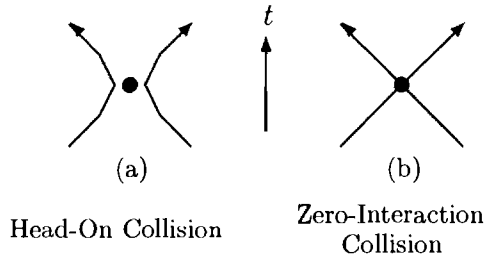


Fig. 12.13 Particle “collisions” in Toffoli’s deterministic diffusion model ([toff89],[toff90b]); see text.

Consider a one-dimensional random walk, with a probability p of moving to the right and probability $q = 1 - p$ of moving to the left. If $p = q = 1/2$, the distribution has mean $\mu = 0$ and spreads in time with a standard deviation $\sigma = \sqrt{t/4}$. In general, though, $\mu = (p - q)t$ and $\sigma = \sqrt{pqt}$. In particular, as p moves away from the center value $1/2$, the center of mass of the system itself moves with velocity $\beta = p - q$.

Suppose we offset this motion by applying a Galilean transformation ($x = x' + \beta t'$). In the new reference frame, the system will move just as it did in the old reference frame but, because $\sigma = \sqrt{pqt} = \sqrt{(1 - \beta^2)t/4}$, its diffusion is slowed down by a Lorentz-Fitzgerald-like time factor $1 - \beta^2$.[†] “Intuitively, as some of the resources of the ‘random walk computer’ are shifted toward producing coherent macroscopic motion (uniform motion of the center of mass), fewer resources will remain available for the task of producing incoherent motion (diffusion).” [toff89]

We now sketch a simple deterministic lattice gas model of diffusion that becomes exactly Lorentz invariant in the continuum limit. We follow Toffoli ([toff89], [toff90b]) and Smith [smithm90].

Consider a one-dimensional lattice populated by particles moving either to the left or right with unit velocity. When two particles collide “head-on” at a site, they reverse direction (figure 12.13-a). If the particles are all identical, head-on collisions are indistinguishable from there being no interactions at all (figure 12.13-b).

Now consider an ensemble of systems in which each system contains a single “marked” particle that is in some way distinguished from a background “sea” of identical particles: we are interested in finding the probability densities $\rho^+(x, t)$ and $\rho^-(x, t)$ for finding this marked particle moving to the right and left, respectively. A typical marked particles’ space-time trajectory is shown in figure 12.14. The background sea of particles gives

[†]Though different from the relativistically correct factor of $\sqrt{1 - \beta^2}$.

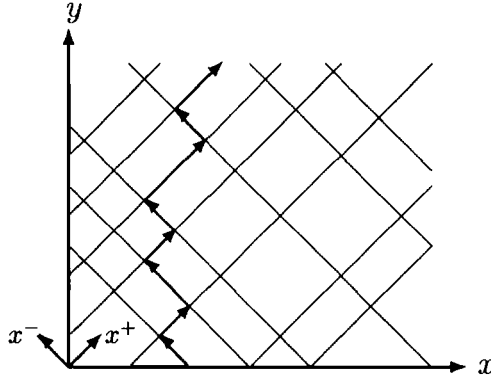


Fig. 12.14 A space-time view of trajectories of particles in Toffoli-Smith's relativistic diffusion model ([toff89], [smith90]). The path drawn with heavy lines shows a typical trajectory for a "marked" particle.

rise to well-defined mean-free-paths $\lambda_+(x^+)$ and $\lambda_-(x^-)$ for a marked particle to reverse direction; $x^\pm \equiv (t \pm x)/\sqrt{2}$ are the light-cone coordinates.

Now define a conserved two-current, $J^\mu = (\rho, j)$, where $\rho \equiv \rho^+ + \rho^-$ and $j \equiv \rho^+ - \rho^-$. The transport equations for ρ^+ and ρ^- are given by

$$\begin{cases} \frac{\partial \rho^+}{\partial t} + \frac{\partial \rho^+}{\partial x} = -\frac{\rho^+}{\lambda_+} + \frac{\rho^-}{\lambda_-}, \\ \frac{\partial \rho^-}{\partial t} - \frac{\partial \rho^-}{\partial x} = -\frac{\rho^-}{\lambda_-} + \frac{\rho^+}{\lambda_+}. \end{cases} \quad (12.48)$$

Adding and subtracting these two equations, gives, respectively

$$\begin{cases} \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x} = 0, \\ \frac{\partial j}{\partial t} + \frac{\partial j}{\partial x} = -j\left(\frac{1}{\lambda_+} + \frac{1}{\lambda_-}\right) + \rho\left(\frac{1}{\lambda_-} - \frac{1}{\lambda_+}\right). \end{cases} \quad (12.49)$$

The background particles are constrained to move with unit speed by the equations

$$\begin{cases} \frac{\partial}{\partial x^+}\left(\frac{1}{\lambda_-}\right) = 0 \\ \frac{\partial}{\partial x^-}\left(\frac{1}{\lambda_+}\right) = 0. \end{cases} \quad (12.50)$$

Defining the two quantities $\sigma^t = 1/\lambda_+ + 1/\lambda_-$ and $\sigma^x = 1/\lambda_- - 1/\lambda_+$ – so that $\sigma^\mu = (\sigma^x, \sigma^t)$ is essentially the two-momentum density of the background particles

– equations 12.49 and 12.50 can be written in the manifestly covariant form

$$\begin{cases} \partial_\mu J^\mu &= 0, \\ (\partial_\mu + \sigma_\mu) \varepsilon^{\mu\nu} J_\nu &= 0 \\ \partial_\mu \sigma^\mu &= 0 \\ \partial_\mu \varepsilon^{\mu\nu} \sigma_\nu &= 0, \end{cases} \quad (12.51)$$

where repeated indices are summed and $\varepsilon^{\mu\nu}$ is antisymmetric in μ and ν . This proves that the model is Lorentz invariant.

Notice that, unlike the earlier random-walk example in which a macroscopic circular symmetry emerged only in a statistical sense, in the relativistic diffusion model just described, Lorentz-invariance is due to individual particle motion. Toffoli proves that Lorentz invariance actually emerges in a similar way for a more general class of rules on a lattice [toff89]. The rules must satisfy only these three properties: (1) the spacetime lattice group (as generated by the particles' allowed motion; see figure 12.13) is free Abelian; (2) the dynamics is invertible; and (3) the only possible interactions are collisions (isolated particles cannot change state). Toffoli observes that qualitatively "relativistic" properties appear to emerge whenever "fixed computational resources have to be apportioned between producing the inertial motion of a macroscopic object as whole and producing the internal evolution of the object itself," and conjectures that "special relativity may ultimately be derived from a simpler and more fundamental principle of *conservation of computational resources*." [toff90b]

12.7 Reversible Computers

Although a completely dissipationless computer has yet to be built, that the prospect of doing so is no longer hindered by principle but is only a question of time is due principally to the combined insights of Landauer [land61] and Bennett [benn73].

Landauer pointed out that a computation causes entropy to increase not because of the information processing *per se*, but because the irreversible logical operations underlying that processing effectively throw out information. Landauer showed that whenever one bit of information is either erased or overwritten, that operation generates an entropy of at least $k \ln 2$, where k is Boltzman's constant.[†] The only way to avoid this entropic increase, according to Landauer, is to use a huge "scratchpad" to store all intermediate results; in this way, all erasures and overwritings would be postponed until after the entire computation was completed, and would be completed, with the concomitant entropy increase, as part of a reset routine for a next computation.

[†]It is interesting to note that modern electronic computers are very far from being energy efficient, as they typically dissipate something on the order of $10^8 kT \ln 2 - 10^{10} kT \ln 2$ joules of energy at temperature T per elementary logical operation. It has been speculated that even Mother Nature's DNA copying machine, dissipates no less than about $100 kT$ per every bit copied.

information is destroyed in an elementary logical operation. Bennett [benn73] questioned the prevalent belief that only irreversible logic gates can be used for computation and introduced a three-tape reversible Turing machine explicitly showing that reversible computers could be built, at least in principle. By thus doing away with a need for Landauer's scratchpad, Bennett showed that the minimal entropy increase (or minimal heat dissipation) was essentially independent of the complexity or number of steps of a computation, and was a function only of the input and output.

Fredkin was the first to construct a reversible logic gate, called the *Fredkin Gate* (see section 6.4.2.1). By showing how arbitrary logic gates – whether reversible or not – could all be built out of his reversible gate, Fredkin thus paved the way towards building real reversible circuits.

The first model for a “reversible computer,” called the *Billiard-Ball Model* (BBM), was introduced by Fredkin and Toffoli in 1982 [fredkin82].[†] The BBM is a classical mechanical *ballistic* model of digital computation based on an idealization of a gas. It consists of an arbitrary number of hard spheres (or balls) of finite diameter that collide elastically both among themselves and with any solid ‘walls’ (or mirrors) that they may encounter during their motion. One can appreciate how the BBM dynamics can be thought of as effectively carrying out computations by making two observations: (1) the presence or absence of a ball at a site can be interpreted as a binary variable taking on either the value 1 or 0, and (2) all lattice neighborhoods in which collisions might occur can be interpreted as Boolean logic gates.

It can be shown that the BBM is capable of universal computation ([fredkin82, marg84, marg88]). Unfortunately, as shown by Zurek [zurek84], the model is also unlikely to ever be realized in practice. Because BBM “computations” all depend so critically on initial ball and mirror placement, the fact that any errors in the initial placement grow exponentially in time effectively renders their results either suspect or meaningless.

Other early designs of classical reversible computers included Landauer's *Bag and Pipes Model* [land82a] (in which pipes are used as classical mechanical conduits of information carried by balls), Brownian motion reversible computers ([benn88], [keyes70]) and Likharev's model based on the Josephson junction [lik82]. One crucial drawback to these models (aside from their impracticality), however, is that they are all decidedly *macroscopic*. If we are to probe the microscopic limits of computation, we must inevitably deal with quantum phenomena and look for a quantum mechanical reversible computer.

12.7.1 Quantum Mechanical Computers

The first to consider quantum mechanical computation was Benioff ([beni81], [beni82a], [beni82b] and [beni84]). His point of departure was to suppose that since

[†]See section 6.4.3 for a discussion of the BBM. Section 6.4.3.2 describes Margolus' ([marg84], [marg88]) transcription of the BBM into a CA.

quantum mechanics is essentially a computational tool used to calculate expectation values for results of a series of repeated physical measurements, the combined system of *computer + computational process* could itself be thought of as a quantum mechanical system evolving according to the equations of quantum mechanics.[†]

Benioff introduced a series of Hamiltonians describing the evolution of a system consisting of spin-1/2 particles (spins up/down corresponding to binary logical states 0/1) occupying the sites of a lattice. The initial state of the system $\Psi(t=0)$ corresponds to the input state of a computation. Benioff's systems evolve, under the action of a Hamiltonian, in such a way that the quantum states $\Psi(0)$, $\Psi(\tau)$, ..., $\Psi(n\tau)$ at times $0, \tau, \dots, n\tau$, correspond to the intermediate steps of a computation. While pointing the way towards a form that quantum mechanical computers might one day take, Benioff's construction had some drawbacks. The Hamiltonians, for example, all include nonlocal many-particle interactions.

A more elegant model of quantum mechanical computers was introduced by Feynman ([feyn85], [feyn86]). Although the formalism is similar to Benioff's – both approaches seek to define an appropriate quantum mechanical Hamiltonian H whose time evolution $e^{-iHt/\hbar}$ effectively represents the execution of a desired computation – Feynman's approach is more powerful because it gives an explicit construction for this Hamiltonian. Feynman's motivation for constructing his model was his belief that certain quantum phenomena fundamentally cannot be simulated by purely classical computers ([feyn82], [feyn87]).

As discussed elsewhere (see section 3.4), in order to construct a computer – classical or quantum – we need a complete set of primitive logic gates. For his set of primitive reversible logic gates, Feynman chose an unconventional set consisting of a **NOT** gate (which is trivially reversible, since **NOT**(0)=1 and **NOT**(1)=0), a two-input/two-output **CONTROLLED NOT** gate and a three-input/three-output **CONTROLLED CONTROLLED NOT** gate. The schematic representations and truth tables for the latter two gates are shown in figure 12.15.

Figure 12.15 shows that the **CONTROLLED NOT** gate has two inputs, x and y , and two outputs, x' and y' . One of the input lines, say x , is a control line and the value of that line remains unchanged: $x' = x$. The other line, y , is the data line. If the control line value is set to 0, the data line value remains unchanged; if the control line value is set to 1, the data line output value is the negated input value. The **CONTROLLED NOT** gate can thus be used to construct both **FAN OUT** (by copying one input into two output data streams) and **EXCHANGE** (by exchanging the values of the inputs). The latter circuit element can be built up by using three **CONTROLLED NOT** gates in succession, using alternating lines for the control line.

Since two input/output lines do not suffice to construct an arbitrary reversible logical function (see discussion in section 6.4.2), Feynman also introduces the three-

[†]Penrose [penrose89] has speculated that human consciousness derives largely from the inherently nonclassical – i.e. quantum – processing that takes place in the human brain; a processing that cannot be described using the traditional Turing Machine model. If this is so, one can hope to understand human consciousness only by developing a fundamental theory of quantum computation.

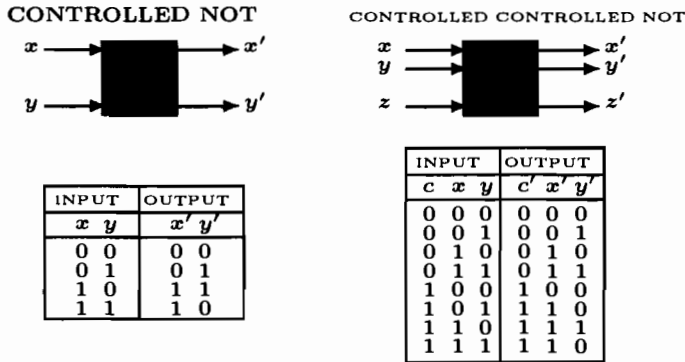


Fig. 12.15 Schematic representations and truth tables for reversible primitives **CONTROLLED NOT** and **CONTROLLED CONTROLLED NOT**, used by Feynman in his construction of a reversible quantum computer [feyn85].

input/ three-output **CONTROLLED CONTROLLED NOT** gate. This gate has two control lines (x and y), whose output is the same as their input and which change the input value of the data line z (i.e. induce the operation $\text{NOT}(z)$) only when they are both equal to 1. If the value of the data line is 0, its output becomes a 1 only when $x = y = 1$, thus effectively yielding an **AND** gate.

When used together, the three gates **NOT**, **CONTROLLED NOT** and **CONTROLLED CONTROLLED NOT** constitute a universal reversible set, and can thus be used to construct an arbitrary logical circuit.

Feynman next explicitly constructs a Hamiltonian that, when applied to a system consisting of interacting parts, effectively performs a set of computations. To do so, Feynman imagines that his quantum mechanical computer consists of appropriately small building blocks he calls “atoms” that can only be in one of two possible states: $|0\rangle$ and $|1\rangle$. Each “atom” represents a single bit of information. The problem is to find a set of operators such that when applied to “atoms,” converts their state in exactly the way that would be expected if their values were passed along input wires of a conventional logic gate. Feynman stresses that in this operator approach, it is the *states* that are changing at each site, and no data is actually being physically passed from one position to another.

Feynman introduces two elementary operators: (1) an *annihilation operator*, a , which changes $|1\rangle$ to $|0\rangle$ but leaves $|0\rangle$ alone; and (2) a *creation operator*, a^* that changes $|0\rangle$ to $|1\rangle$ and leaves $|1\rangle$ alone. Using these two operators, Feynman’s set of primitive gates can be rewritten in operator form according to $A_{\text{NOT}} = a + a^*$, $A_{\text{CONTROLLED NOT}} = aa^*(b + b^*) + aa^*$, and $A_{\text{CONTROLLED CONTROLLED NOT}} = 1 + a^*ab^*b(c + c^* - 1)$.

The remaining step is to write down a general expression consisting of these elementary operators that reproduces an arbitrary computation, such as a summa-

tion of inputs. In general, we would have k operations $A_1, A_2, \dots, A_k$ operating on n input lines. Feynman adds to these n “register” atoms, an additional set of $k + 1$ “program counter” sites. The Hamiltonian can then be expressed as

$$\begin{aligned}
 H &= \sum_{i=0}^{k-1} \{a_{i+1}^* a_i A_{i+1} + A_{i+1}^* a_i^* a_{i+1}\} \\
 &= a_1^* a_0 A_1 + a_2^* a_1 A_2 + \dots + a_0^* a_1 A_1^* + a_1^* a_2 A_2^* + \dots
 \end{aligned} \tag{12.52}$$

It is clear that if all the program counters are unoccupied (i.e. are in the state $|0\rangle$), nothing at all happens: all terms in the Hamiltonian start out with an annihilation operator, and all states thus remain in the state $|0\rangle$ for all time. If we assume that only *one* of the sites $0, 1, \dots, k$ sites is occupied, however, we see that only one site will always be occupied, though not necessarily the same site at different times. If we think of the occupied site, say the first site 0 , as a “cursor,” the Hamiltonian effectively moves the cursor along the program counter sites while the operators A_i operate on the register n . Feynman shows how, by the time the cursor arrives at the final site k , the n register has been multiplied by the entire set of desired operators $A_1, A_2, \dots, A_k$.

The computation could also be made into a ballistic action by adding sites to the left and right of the sites to be used for the actual computation (with appropriate a_i ’s but with no corresponding A_i). Instead of starting the computations by putting a cursor at site 0 , the computation can be initialized with an incoming packet of some specified momentum (i.e. a spin wave) by putting the cursor with different amplitudes at different sites.

Two properties, in particular, make Feynman’s approach superior to Benioff’s: (1) it is time independent, and (2) interactions between all logical variables are strictly local. It is also interesting to note that in Feynman’s approach, quantum uncertainty (in the computation) resides not in the correctness of the final answer, but, effectively, in the time it takes for the computation to be completed. Peres [peres85] points out that quantum computers may be susceptible to a new kind of error: since, in order to actually obtain the result of a computation, there must at some point be a macroscopic measurement of the quantum mechanical system to convert the data stored in the wave function into useful information, any imperfection in the measurement process would lead to an imperfect data readout. Peres overcomes this difficulty by constructing an error-correcting variant of Feynman’s model. He also estimates the minimum amount of entropy that must be dissipated at a given noise level and tolerated error rate.

Margolus [marg90b] generalizes Feynman’s formalism – which applies to strictly *serial* computation – to describe deterministic *parallel* quantum computation in one dimension. Each row in Margolus’ model is a tape of a Turing Machine, and adjacent Turing Machines can communicate when their tapes are located at the same coordinate. Extension of the formalism to more than one dimension remains an open problem.

Bell's Theorem: In a celebrated 1935 paper, Einstein, Podolsky and Rosen (EPR) [ein35] argued that quantum mechanics provides an essentially incomplete description of reality unless hidden variables exist.

Suppose a quantum system consists of a pair of spin- $\frac{1}{2}$ particles, and that the system is prepared in such a way that (1) the total spin angular momentum is zero (i.e. the spins are in the singlet state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)$), and (2) the spins are moving in opposite directions away from each other. Measurements of any component of the spins can be performed on either of the two particles with, say a Stern-Gerlach device. According to quantum mechanics, if a measurement of some component of spin of the first particle results in spin " $\uparrow$," a measurement of the same component of the spin of the other particle must result in " $\downarrow$," and vice versa. So far, so good. But now let us try to interpret this result using the three premises of EPR:

- At the time of a spin measurement on either of the two particles, the two particles are no longer interacting with one another and therefore neither particle "knows" of anything that is being done to the other.
- If, without in any way disturbing a system, we can know with certainty the value of a physical quantity of that system, then there exists an element of physical reality corresponding to that physical quantity.
- If a physical theory is "complete" then every element of physical reality must have a counterpart in that physical theory.

Since quantum mechanics allows us to predict, with certainty, the component of the second spin by measuring the same spin component of the first (and remotely positioned) particle – and to do so without in any way disturbing that second particle – EPR's first two assumptions attribute an element of physical reality to the value of any spin component of either particle; i.e. the spin components must be determinate. On the other hand, assuming that the particles cannot "communicate" information any faster than at the speed of light, the only way to stay consistent with EPR's third postulate is to assume the existence of hidden variables.

In a famous paper, Bell [bell64] showed that locality and the notion that the components of the particles' spins are determinate are *fundamentally incompatible with the spin correlations as predicted by quantum mechanics*. Bell's result, in effect, rules out the possibility of having a local, deterministic theory.

Consider the same pair of spin- $\frac{1}{2}$ particles as above. We can choose to measure say the $\hat{\alpha}$ component of the spin of particle #1 and the $\hat{\beta}$ component of the spin of particle #2. If $\hat{\alpha}$ and $\hat{\beta}$ are not perfectly parallel, then there are four possible results of two measurements: " $\uparrow_1\uparrow_2$," " $\uparrow_1\downarrow_2$," " $\downarrow_1\uparrow_2$," " $\downarrow_1\downarrow_2$." Quantum mechanics predicts the probability for each of these results: $P_{\uparrow_1\uparrow_2}(\hat{\alpha}, \hat{\beta})$, $P_{\uparrow_1\downarrow_2}(\hat{\alpha}, \hat{\beta})$, $P_{\downarrow_1\uparrow_2}(\hat{\alpha}, \hat{\beta})$, $P_{\downarrow_1\downarrow_2}(\hat{\alpha}, \hat{\beta})$, where the probabilities depend, of course, on the unit vectors α and β .

Now consider the expectation value of the product of the two components $\vec{\sigma}_1 \cdot \hat{\alpha}$ and $\vec{\sigma}_2 \cdot \hat{\beta}$:

$$\langle (\vec{\sigma}_1 \cdot \hat{\alpha}) (\vec{\sigma}_2 \cdot \hat{\beta}) \rangle = P_{\uparrow_1\uparrow_2}(\hat{\alpha}, \hat{\beta}) - P_{\uparrow_1\downarrow_2}(\hat{\alpha}, \hat{\beta}) - P_{\downarrow_1\uparrow_2}(\hat{\alpha}, \hat{\beta}) + P_{\downarrow_1\downarrow_2}(\hat{\alpha}, \hat{\beta}). \quad (12.53)$$

According to quantum mechanics,

$$\langle (\vec{\sigma}_1 \cdot \hat{\alpha}) (\vec{\sigma}_2 \cdot \hat{\beta}) \rangle = -\alpha \cdot \beta. \quad (12.54)$$

Bell shows that for any local hidden variable theory, this expectation value must satisfy the following inequality:

$$| \langle (\vec{\sigma}_1 \cdot \hat{\alpha}) (\vec{\sigma}_2 \cdot \hat{\beta}) \rangle - \langle (\vec{\sigma}_1 \cdot \hat{\alpha}) (\vec{\sigma}_2 \cdot \hat{\gamma}) \rangle | - \langle (\vec{\sigma}_1 \cdot \hat{\beta}) (\vec{\sigma}_2 \cdot \hat{\gamma}) \rangle - 1 \leq 0, \quad (12.55)$$

where α, β and γ are unit vectors in three arbitrary directions.

A simple example suffices to show that the quantum mechanical prediction does not, in general, satisfy Bell's inequality. Say, for example, that all three unit vectors lie on the same plane, $\angle(\alpha, \beta) = 60^\circ$, $\angle(\beta, \gamma) = 60^\circ$, and $\angle(\alpha, \gamma) = 120^\circ$. Substituting these values into Bell's inequality yields the nonsensical result that $\frac{1}{2} \leq 0$.

Bell's result, made all the more remarkable for the very few assumptions he makes to derive it, rather dramatically asserts that *either* EPR's three premises are wrong or quantum mechanics is incorrect. However, recent experiments by Aspect, *et.al.* ([aspect82a], [aspect82b]), Ou and Mandel [ou88], and others have shown, virtually conclusively, that nature satisfies the quantum mechanical prediction (equation 12.54) and not Bell's inequality (equation 12.55), thus strongly denying the possibility of local hidden variables. We are thus left with what is arguably one of the deepest mysteries in the foundations of physics: the existence of a profoundly nonclassical correlation between spatially-far separated systems, or *nonseparability*.

All of Bell's papers on the conceptual and philosophical problems of quantum mechanics, including his landmark EPR paper in which he derives his famous inequality, are collected in [bell87]. An excellent collection of papers exploring the philosophical consequences of Bell's theorem appears in a volume edited by Cushing and McMullin [cush89].

12.8 Computability and Physics

Much of modern theoretical physics rests on two fundamental assumptions: (1) that the laws of nature can be understood and "captured" in some appropriate (typically mathematical) form, and (2) that there exist processes in nature that can be "short-cutted;" or processes whose final state may be determined directly, without a need to exhaustively trace through each step of the evolution. Every time a freshman physics student is asked to compute the trajectory of an imagined artillery shell, the legitimacy of the question depends on our ability to effectively "know" where the shell will strike the ground even before the shell itself gets there. But such short-cuts are possible only if the calculation being performed is more sophisticated than the "calculation" carried out by the universe itself. Moreover, since all computations must be carried out on a computer, and the computer is itself a physical system, any physical system that can act as a computer therefore suffers from the same fundamental limitation on the predictability of its behavior as does any general-purpose computer. In particular, Turing's Theorem (see below) tells us that the outcome of a computer's processing can, in general, be determined only by explicitly carrying out each step of the evolution; no shortcut is possible, even in principle. While such *computational irreducibility* is fairly common in mathematics and computation theory, Wolfram [wolf85e] suggests that it is also common in

theoretical physics: “computational reducibility may well be the exception rather than the rule.”

It is important to contrast computational irreducibility with deterministic chaos.[†] Chaotic systems are unpredictable because they display sensitivity to initial conditions. Any ignorance of the details of the initial condition are amplified exponentially in time as trajectories that are initially close by diverge exponentially. But there is nothing preventing our acquiring a perfect knowledge of the system’s long time behavior, provided that we have access to an arbitrary number of “bits” defining the initial state. Even we did not have such a fine-grained knowledge of the initial state, however, a chaotic system’s long-term behavior – such as its basins of attraction and attractors – can still be easy to predict. Not so for computationally irreducible systems. The dynamics of computationally irreducible systems is such that their long-time behavior is effectively undecidable. Even with a perfect knowledge of the initial state, the essential aspects of its long-time behavior – such as whether the trajectory enters a given part of the system’s phase space – remains unpredictable.

12.8.1 *Turing’s Halting Theorem*

There are three important, and related, “decidability” theorems in formal logic and mathematics: (1) *Godel’s Incompleteness Theorem*, which limits what is provable within a formal system by asserting that any consistent, finite logical system harbors more “truths” than are provable within the system [godel31] – thus, one can never program a computer to output an exhaustive list of all true statements about the natural numbers; (2) *Church’s Theorem*, which limits the decidability of provability by asserting that there is in general no way to predict in advance whether a given proposition in a formal system is provable – the best one can do is sit back and start proving things in the system, hoping (but not being able to know in advance) that a given proposition shows up in the list of provable statements; (3) *Turing’s Theorem*, which is closely related to Church’s theorem, and limits what we are able to know about the running of a program by asserting that there is in general no way to know in advance if an arbitrary program will ever stop running.

Consider a universal Turing machine, or computer, $\mathcal{C}$, a set of instructions, or program, $\mathcal{P}$ and input data $\mathcal{D}$. Let $\mathcal{P}(\mathcal{D})$ be the computation performed by $\mathcal{P}$ given $\mathcal{D}$. The *Halting Problem* is to find a general program $\mathcal{P}_H$ that processes any other program $\mathcal{P}$ and a set of input data $\mathcal{D}$, outputting a “yes” if the program $\mathcal{P}$ halts when processing $\mathcal{D}$ and “no” if it does not:

$$\begin{cases} \mathcal{P}_H(\mathcal{P}, \mathcal{D}) = \text{yes} & \iff \mathcal{P}(\mathcal{D}) \text{ halts} \\ \mathcal{P}_H(\mathcal{P}, \mathcal{D}) = \text{no} & \iff \mathcal{P}(\mathcal{D}) \text{ never halts.} \end{cases} \quad (12.56)$$

The halting problem thus asks whether it is possible to tell in advance if a general program will halt its execution; or, put another way, whether an arbitrary program’s

[†]Deterministic chaotic systems are discussed in chapter 4.

processing can, in general, be “shortcutted.”

In a landmark 1936 paper, Turing proved that no such program $\mathcal{P}_H$ exists [turing36]: given an arbitrary program $\mathcal{P}$ and input data $\mathcal{D}$, it is in general impossible to predict before-hand whether, or when, $\mathcal{P}$ will ever finish processing $\mathcal{D}$.

We give a brief sketch of Turing’s proof below. It is essentially a proof-by-contradiction, showing that if an infallible halting-checker program $\mathcal{P}_H$ is assumed to exist, a computation can always be found such that it runs forever if $\mathcal{P}_H$ says it halts, and halts if $\mathcal{P}_H$ says it does not.

Assuming that such a halting-checker program $\mathcal{P}_H$ in fact exists, we can use it to construct another program, $\tilde{\mathcal{P}}$, that uses programs as data inputs, and reverses the roles of its “yes”/“no” responses:

$$\begin{cases} \mathcal{P}_H(\mathcal{P}, \mathcal{P}) = \text{yes} \implies \tilde{\mathcal{P}}(\mathcal{P}) \text{ never halts} \\ \mathcal{P}_H(\mathcal{P}, \mathcal{P}) = \text{no} \implies \tilde{\mathcal{P}}(\mathcal{P}) \text{ halts.} \end{cases} \quad (12.57)$$

Now define a computation $\mathcal{Z} \equiv \tilde{\mathcal{P}}(\tilde{\mathcal{P}})$; that is, the computation resulting from running the program $\tilde{\mathcal{P}}$, initialized with data consisting of its own code, $\tilde{\mathcal{P}}$. What does our supposedly infallible halting-checker program $\mathcal{P}_H$ predict about $\mathcal{Z}$ ’s behavior? On the one hand, $\mathcal{P}_H$ predicts that $\tilde{\mathcal{P}}$ halts when $\mathcal{P}_H(\tilde{\mathcal{P}}, \tilde{\mathcal{P}}) = \text{yes}$, or when $\tilde{\mathcal{P}}(\tilde{\mathcal{P}})$ never halts, meaning that $\mathcal{Z}$ never halts. On the other hand, $\mathcal{P}_H$ predicts that $\tilde{\mathcal{P}}$ never halts when $\mathcal{P}_H(\tilde{\mathcal{P}}, \tilde{\mathcal{P}}) = \text{no}$, or when $\tilde{\mathcal{P}}(\tilde{\mathcal{P}})$ halts, meaning that $\mathcal{Z}$ halts. We thus arrive at a contradiction and conclude that an infallible halting-checker program cannot exist.

An important corollary to Turing’s theorem is that there can also be no general program to predict how long an arbitrary program needs to run. If we had such a running-time-predictor program $\mathcal{R}$, we could use it to compute the amount of time (or number of program steps), $\tau = \mathcal{R}(\mathcal{P}, \mathcal{D})$, for which a program $\mathcal{P}$ starting with data $\mathcal{D}$ will run before halting and then use that information to construct a halting-checker: we could simply define $\mathcal{P}_H(\mathcal{P}, \mathcal{D}) = \text{yes}$ if and only if $\mathcal{P}(\mathcal{D})$ halts within τ steps.

12.8.2 Computational Irreducibility

Turing’s theorem is an example of *computational irreducibility*. It shows that there is, in general, no quick-and-dirty short-cut way of predicting an arbitrary program’s outcome. Since this result applies generally to any universal computer, it must also apply in particular to any physical system that can act as a universal computer. This, in turn, means that if a physical system can behave like a universal computer, there can be no simple way of predicting what the system will do, short of, literally, sitting-back and watching it evolve. Wolfram ([wolf84a], [wolf85e]) has suggested that this kind of computational irreducibility is a common property of physical systems.

We have already seen at least one example of a physical system capable of acting as a universal computer in our discussion of Fredkin and Toffoli’s [fredkin82]

deterministic *Billiard-Ball Model* (BBM) in section 6.4.3. While the BBM has a rather natural continuous dynamics, it is also somewhat contrived, insofar as its “computation” ability depends critically on initial ball and mirror placement. Any errors in the initial placement grow exponentially in time and thus effectively render all results either suspect or meaningless. Its main drawback is that it has infinitely many degrees of freedom. Recently, Moore [moorec90] has shown how a very simple physical system – a classical particle trapped in a three-dimensional box with a finite number of plane and parabolic mirrors – can simulate a universal Turing machine. His construction exploits the generic ability of chaotic systems to split, deform and recombine a bundle of trajectories so that they are continuously pulled apart in one direction and squeezed together in the other. Moore’s dynamics results in the points of the underlying fractal Cantor set of initial conditions being continuously and deterministically “shuffled.” This, together with some strategically positioned mirrors, is enough to implement a full set of Turing-machine actions required for universality. While Moore’s model is also “unnaturally” contrived, it does lend credence to the possibility of building simple real dynamical systems whose behavior is computationally irreducible.

12.8.3 Noncomputability

A real number x is said to be *computable* if there exists a computer program $\mathcal{P}$ such that when a positive rational number ϵ is inputted, $\mathcal{P}$ outputs a rational number r with $|x - r| < \epsilon$ and halts [geroch86]. Thus, 2, π , $\exp(1)$, $\sqrt{\pi^e}$, etc. are all computable numbers.

Are there any noncomputable numbers? They are certain to exist since the cardinality of the set of all possible programs (which is equal to that of the integers) is less than the cardinality of the set of reals. It is, in fact, easy to “construct” a noncomputable number, ζ , using Turing’s *Halting Theorem*: number, in some arbitrary manner, all possible programs that run with, say, a single input instruction: $p_1 \leftrightarrow 1, p_2 \leftrightarrow 2, \dots, p_n \leftrightarrow n, \dots$, and set $\zeta = \sum_{n=1}^{\infty} \alpha_n 2^n$, where $\alpha_n = 1$ if the n^{th} program halts and $\alpha_n = 0$ otherwise. Since the sum definitely converges, we know that $0 \leq \zeta \leq 1$ has a definite value. Unfortunately, the *Halting Theorem* prohibits us from knowing in general, if, or when, an arbitrary program halts. Thus, there is no way to compute the sum; i.e. ζ is a noncomputable number. Other well-known examples of noncomputable numbers are *Chaitin’s number* Ω , which is, roughly speaking, the probability that a given infinite binary string input to a Turing machine eventually halts ([chaitin87]; see also [gardner92]); and the so-called *Busy-Beaver* function ([brady88], [dewd93]).[†] We leave the tantalizing question of

[†]Define an n -state *Busy Beaver* as an n -state Turing machine with a two symbol alphabet $\{0, 1\}$ that is initialized with an input tape consisting entirely of 0’s and outputs the maximal number of 1’s before halting. The number of 1’s is clearly a function only of the number of internal states, n , that the Turing machine’s scanning head can enter. The rather innocent seeming number $B(n)$, equal to the number of 1’s that is written by this n -state Busy Beaver program can be shown, for large enough n , to grow faster than any computable function; i.e. $B(n)$ is noncomputable. The first few values are easy to compute. Since the maximum number of 1’s that can be printed

whether, and in what sense, fundamental physical constants like the speed of light in vacuo, c , or the fine-structure constant $\alpha = e^2/\hbar c$, are computable, to the reader.

12.8.3.1 Church-Turing Thesis

The *Church-Turing Thesis* asserts that every effectively computable mathematical operation corresponds to a suitable program running on a universal Turing Machine. While no one would today dispute the “universal” computational power of a modern personal computer – which takes away somewhat from this original formulation of the C-T Thesis some of its original novelty – an important open question is the validity of what might be called the generalized, or strong, form of C-T Thesis: the proposition that not just any effectively computable process but real *physical* systems correspond to a suitable Universal Turing Machine.

Deutsch [deut85] was the first to point out a possible connection between the C-T Thesis and physics:

“The reason why we find it possible to construct, say, electronic calculators, and indeed why we can perform mental arithmetic, cannot be found in mathematics or logic. The reason is that the laws of physics ‘happen to’ permit the existence of physical models for the operations of arithmetic such as addition, subtraction and multiplication. If they did not, these familiar operations would be non-computable functions.”

The strong form of the Church-Turing thesis thus asserts that no noncomputable physical systems exist: any mathematical function or number that can be determined by a physical process must be computable by a universal Turing machine. It is in this spirit that Geroch and Hartle [geroch86] suggest that the veracity of a physical theory ought to be judged, in part, on whether or not its measurables are computable; and where a “measurable” is to be understood as being any number whose “value” can be determined to a specified degree of tolerance by a precisely defined experimental procedure. While it is not particularly hard to cook up “theories” that include noncomputable numbers – see, for example, Pour-El and Richards’ [pour82] example of a wave equation with noncomputable solutions and Geroch and Hartle’s example of a formally noncomputable observable in a particular version of quantum gravity [geroch86] – a common fatal flaw that prevents most such theories from violating the strong form of the C-T thesis is that they make no provision for *experimentally* measuring the noncomputable number. If it turns out that the universe itself is indeed a “computer” in the Fredkin sense (see section 12.6.4), then it must also be true that the very form of physical laws are themselves constrained by what can be computed.

is 1, for example, $B(1) = 1$. Similarly, we find that $B(2) = 4$ and $B(3) = 6$. While it may be tempting to predict from this that $B(12)$, say, is probably large but not unmanageably so, it can be shown that $B(12) \geq 6 \cdot 4096^{4096^{4096^{\dots 4096^4}}}$, where the dotted region consists of 166 4096’s!. See [dewn93].

12.8.3.2 Computation and Phase Transitions

Langton [lang92] opens his “Life at the Edge of Chaos” paper at the Artificial Life II conference with the following intriguing question: “*Under what conditions can we expect a dynamics of information to emerge spontaneously and come to dominate the behavior of a physical system?*” While his question was, in that paper, motivated chiefly by an understanding that living organisms may be distinguished from inanimate matter by the fact that their behavior is clearly based on a complex dynamics of information, its roots extend considerably deeper. Indeed, our motivation for recalling Langton’s question in this section is the understanding that true “physics” (reality?) may be distinguished from “false physics” by the fact that the real universe is clearly based on a complex dynamics of information.

Langton was able to provide a tentative answer to his question – at least within the somewhat more limited realm of the complex dynamics of CA – by examining the behavior of the entire rule space of elementary one-dimensional CA rules as parameterized by a single parameter λ (see section 3.2.1). Given a rule ϕ , λ is defined to be the fraction of entries in the rule table for ϕ that get mapped to a non-zero value [lang90].

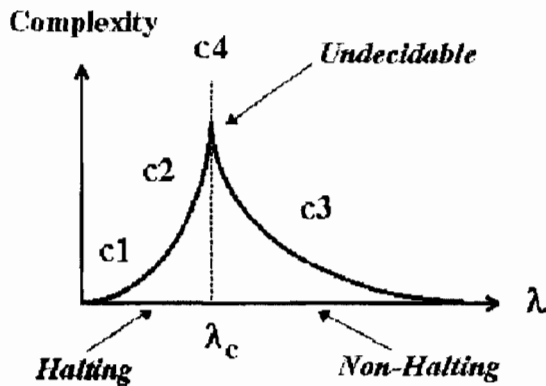


Fig. 12.16. Wolfram’s behavioral classes c1, c2, c3 and c4 overlayed on top of a plot of *Complexity* versus Langton’s λ -parameter; see text. Patterned after figures 22 and 23 in [lang92b].

As λ is increased from its minimal to maximal values (see figure 12.16), a path is effectively traced in the rule space that progresses from fixed point behavior to simple periodicity to evolutions with longer and longer periods with increasing transients, passes through an intermediate transition region at a critical value $\lambda = \lambda_c$, crosses over into a chaotic regime of steadily diminishing complexity until, eventually, the behavior is again completely predictable at the maximal value of λ and complexity falls back to zero. The transition region is a complex subspace. Some parts of this region act as simple boundaries between periodic and chaotic rules, such that all paths passing through such boundaries yield abrupt first-order

transition-like changes in statistical measures of the dynamics. These parts have essentially zero measure and hence harbor no rules within them. Other parts of the transition region have a finite measure and paths passing through them give rise to smooth second-order transition like changes in statistical measures.

Langton found that the most complex rules, those capable of supporting universal computation, appear to all be located within the second-order transition region, citing as evidence the fact that (1) all rules within this region possess Wolfram class c4-like characteristics (long transients, propagating soliton-like structures, large correlation lengths, etc.); (2) because of the arbitrarily long transients of rules within the transition region, it may be effectively undecidable – read: *Turing undecidable*, as in Turing’s Halting Theorem – whether their behavior will eventually settle down to one with fixed period or chaos; (3) the site-correlations induced by rules within the transition region are of precisely the right strength necessary to support computation.[†]

Langton’s ([lang90], [lang91], [lang92b]) tentative answer to the question with which we opened this section is therefore: “We expect that information processing can emerge spontaneously and come to dominate the dynamics of a physical system in the vicinity of a critical phase transition.”[‡] Langton speculates that the dynamics of phase transitions is fundamentally equivalent to the dynamics of information processing. Despite our CA universe being a decidedly artificial material substrate (a crude example of Toffoli’s “programmable matter” [toff91]) and not *real* matter, it cannot simply be a coincidence, so Langton argues, that the behavior of both systems is characterized by two universality classes (solid and fluid) separated by a phase transition.[§] “Thus, we are safe in assuming that these fundamental classes of dynamical behavior do not adhere in material *per se*, but rather in the way in which the material is organized.” [lang92] Since, as the λ -parameterization suggests, the dynamics of systems near the transition region support an embedded computation, there is also a third category of behavior; one that effectively avoids going into either the solid or fluid phase by maintaining itself within the transition on an indefinitely long transient.

If a fundamental equivalence between the dynamics of phase transitions and information processing along the lines suggested by Langton really exists, it would also lend support to the Church-Turing hypothesis [lang92]:

“The fact that physical systems having to “decide” between two qualitatively different

[†]If correlations between separated sites are too small, sites evolve essentially independently of one another and little or no transmission of information can take place. On the other hand, if the correlations are too strong, distant sites may cooperate so strongly so as to effectively mimic each others behavior and thus again preclude effective computation. It is only within the transition region that information can propagate freely over long distances without appreciable decay.

[‡]For a recent critical re-examination of this view see [mitch93b].

[§]As it is possible to continuously transform liquids into gases and vice versa without passing through a phase transition, Langton lumps liquid and gas phases into the more general *fluid* phase.

physical states can take arbitrarily long to make the “decision” – the phenomenon of critical slowing down – suggests that physical systems in general are bound by the same *in principle* limitations as computing devices. In fact, it is perhaps misleading to claim that the phenomenology of phase transitions explains the phenomenology of computation when, in fact, one could equally well claim that the phenomenology of computation explains the phenomenology of phase transitions... we could equally well say that the phenomenon of critical slowing down is simply a manifestation of the halting problem.”

12.8.4 *A Simple Coincidence or is Something Really Interesting Going on Here?*

The physicist Eugene P. Wigner once wrote [wigner60] a provocative short essay entitled, “The Unreasonable Effectiveness of Mathematics in the Natural Sciences.” In it, he argues that the real reason why mathematics appears to be so effective remains a mystery, concluding his essay with these words:

“The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve. We should be grateful for it and hope that it will remain valid in future research and that it will extend, for better or for worse, to our pleasure even though perhaps also to our bafflement, to wide branches of learning.”

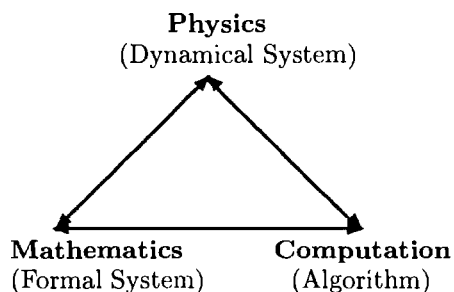


Fig. 12.17 Physics–Mathematics–Computation; *Equivalent Formalisms?*

The more one thinks about Wigner’s problem, the greater one’s suspicion that somewhere, not too far off, must lurk some form of the *Anthropic Principle*: the idea that the reason the universe appears to us the way it does, with all its myriad complexities and finely-tuned physical constants, is because it is the *only* such universe that could have spawned the sentient beings capable of gazing inquiringly at it. “Our existence imposes a stringent condition effect upon the type of universe we could ever expect to observe and document. Many observations of the natural world, although remarkable *a priori*, can be seen in this light as inevitable consequences of our own existence.” [barr86][†]

[†]Barrow and Tipler’s treatise, *The Anthropic Cosmological Principle* [barr86], is in many ways a

Although there are more than a few alternative definitions of the anthropic principle – our own rendition above most closely resembles its so-called *weak form* – they are united by the fact that they are all conceptual relatives of the “incompleteness” or “undecidability” theorems of mathematics and computation. Just as Gödel’s theorem makes use of logical self-reference to prove the existence of unprovable truths within a mathematical system, and Turing’s theorem makes use of algorithmic self-reference to show that a computer cannot fully encompass, or understand, itself, the anthropic principle limits the perceived structure of the universe by the fact that the universe is effectively perceiving itself. Weakening our “weak” anthropic principle still further, we might also say that we can only look at the universe with the apparatus and a level of description or understanding that the universe itself has either supplied us with or has allowed us to develop. Paraphrasing the countless retorts by Mr. Spock to Kirk’s queries about some strange new phenomenon on the television series *Star Trek*: “Captain, our sensors are able to measure only what they were *designed to measure!*”

So what does all of this have to do with our current topic of discussion, computability and physics? Going back to Wigner’s problem of deciding why mathematics is so unreasonably effective in describing the natural world, one might argue that it is something of a misnomer to label this a “problem,” for it is in reality much closer to being a tautology. That is to say, mathematics is not so much *unreasonable* in its effectiveness, as it just happens to be the form of expression that our species is currently using to describe the natural world.

Taking as a given that we are clearly intelligent enough as a species to look out into the world and articulate a bit of the order and complexity we perceive in it *in some form* – a form that we call “mathematics” or “physics” – Wigner’s problem becomes essentially rhetorical: why does our mathematics appear to be so good as a particular means of articulation? In a deep sense, it is *neither* “good” nor “bad,” as it both defines the manner in which we currently compartmentalize and “understand” the universe and the tool that we use to “define” what we mean by “universe.” That it appears to be “unreasonably effective” in its ability to describe the world should therefore come as no great surprise, as it effectively *defines* what we mistake to be something that it just only *describes*. As hinted by our paraphrasing of Spock’s frequent retorts to Kirk above, the universe can only appear to us in a way that our intellectual and perceptual abilities are designed to interpret and understand it. Understood in this light, “unreasonable effectiveness” is nothing more than the tautological identification of mathematics as our particular means of understanding. Really, the more interesting question to ponder is the nature of the relationship between the larger global system – the universe – and the smaller subset, our minds – or individual consciousnesses – that are both an integral part of it and a mechanism by which the universe is able to gaze out onto itself.

In the context of the above preamble, consider the listing of the analogous elements in physics, computation theory and mathematics given in table 12.3.

All three systems are characterized chiefly by some sort of “processing” of ele-

brilliant, *tour-de-force* treatment of this subject. Highly recommended.

Physics	Computation	Mathematics
Space-Time	Computer Circuit	Formal System
Matter/Energy States	Information; Bit-Strings	Propositions; Strings
Initial Conditions	Program Input	Set of Axioms
Dynamical "Laws"	Algorithm	Rules of Inference
Dynamical Constraints	Admissible Syntax	Grammar
Dynamical Evolution	Computation	Derivation
Final State; Attractor ("Observables")	Program Output	Theorem
Measurability	Computability	Provability
<i>Deterministic Unpredictability;</i> <i>Quantum Incompleteness?</i>	<i>Halting Theorem</i>	<i>Godel's Theorem</i>

Table 12.3 A few suggestive corresponding elements in *Physics*, *Computation* and *Mathematics*.

mentary entities that reside in a processing "arena," starting from some initial set of those entities and proceeding in a consistent fashion towards a climax of sorts that is the outcome of the processing. Mathematics uses formal axiomatic systems as its arena of activity, computation relies on the general purpose computer to carry out the steps of some algorithm, and physics of course takes place in space-time. Where mathematical logic uses rules-of-inference to navigate in a consistent fashion from proposition to proposition, computers have their algorithms and physics its dynamical laws. A "logical derivation" is a "computation" is a "dynamical evolution." Provability and "truth" in mathematics is directly analogous to computability for computers and the measurability of the final-state outcome of a dynamical evolution in physics. It is interesting that, at the deepest level of all three systems, emerges an apparently fundamental limitation on what can be expressed in the given system. Mathematics has its Godel's Theorem, computation is limited by Turing's Halting Theorem, and physics...? While there has not yet been found a direct analogue in physics of Godel's or Turing's theorems, it is tempting to speculate that it is somehow latent in the fundamental unpredictability found in deterministic chaotic systems, or maybe in the inevitability of all supposedly "complete" physical theories like quantum mechanics being fundamentally incomplete?

What must not be overlooked is the fact that physics, computation and mathematics share at least two additional traits: (1) they are each separate products of a given species' (namely, our own) attempt to articulate its perceptions of the universe (and, as such, they possess a common *conceptual* origin); (2) Godelian-like incompleteness – at least in the case of computation and mathematical logic – originates in a system's inherent ability to *perceive itself* (in the form of a logical self-reference in the case of mathematics, and a computational self-reference in the case of computation; the jury is still out on self-reference in physics). The possibility that both of these traits are true implies one last, and as yet unanswerable, question: *Is Godelian incompleteness solely a reflection of our limited capacity, as parts of a whole, to understand the universe (albeit, in a way that is consistent*

with the laws governing the universe), or is it a deeper limitation governing the knowability of the universe that is imposed on the universe itself by the nature of its very existence? Even more succinctly: Does nature contain any fundamentally unprovable, noncomputable, “truths?”

12.9 Have We Gone Far Enough or is the World Crazier Still?

Fredkin’s universe is a universe in which there is only a finite amount of information and, for want of a better or more suggestive metaphor, is thought to evolve according to some underlying local CA rule. While the information content of the universe is assumed to be finite, it is also tacitly assumed that all of that information resides on an underlying lattice, whose own existence comes, so to speak, “free-of-charge.” This underlying lattice supplies an arena for an informational dynamics to take place in, but, except for its role as “dynamical mediator,” it itself remains effectively uninvolved in that dynamics. Clusters of information may form and dissipate and all sorts of interactions may take place within it, but the lattice remains separate and fixed.

An intriguing possibility thus presents itself. If some kind of a primordial information, and not higher-level “constructs” such as mass, energy, spin, and so forth, is indeed the real substance out of which all “stuff” is made – leaving aside for the moment, the question of *form* of that information – is it not natural to suppose that a discrete space-time structure, our heretofore pre-defined and static dynamical mediator, is itself built out of the same substance?; i.e. to suppose that space-time is not just a backdrop for information processing, there only to define what is local and what is not and where to and where from information is allowed to flow, but is itself a construct of primordial information? This supposition is not entirely without precedent.

12.9.1 A Discrete Form of Geometrodynamics?

“Space acts on matter, telling it how to move. In turn, matter reacts back on space, telling it how to curve.” So is the central lesson of Einstein’s *Geometrodynamics* as explained by Misner, Thorne and Wheeler in their classic text on Gravitation [misner73]. The idea that space or space-time are more than just passive backdrops “on top” of which the real dynamics takes place, can be traced at least as far back as 1870, when W.K. Clifford, speaking to the Cambridge Philosophical Society, offered these four views of his “Space Theory of Matter” [cliff79]:

- Small portions of space are in fact of a nature analogous to little hills on a surface which is on average flat; namely that the ordinary laws of geometry are not valid in them.
- This property of being curved or distorted is continually being passed on from one position of space to another after the manner of a wave.

- This variation of the curvature of space is what really happens in that phenomenon which we call the motion of matter, whether ponderable or ethereal.
- In the physical world nothing else takes place but this variation, subject (possibly) to the law of continuity.

Earlier we discussed Wheeler's conception of a *pregeometry*, or a set of basic elements out of which what we conventionally think of spacetime is built, but which are themselves devoid of a specific dimensionality (section 12.4.4). Wheeler was led to explore the possibility of a pregeometry because of the fundamental incompatibility between quantum uncertainty and the notion of a deterministic classical history of space evolving in time: "no prediction of spacetime, therefore no meaning for spacetime, is the verdict of the quantum principle..." [misner73]. While spacetime is a useful concept, it is really valid only as a classical approximation to whatever is the deeper, quantum, reality. Wheeler [wheel62] also proposed the idea that particles could be looked at as geometric disturbances of spacetime, called *geometrodynamic excitons*.

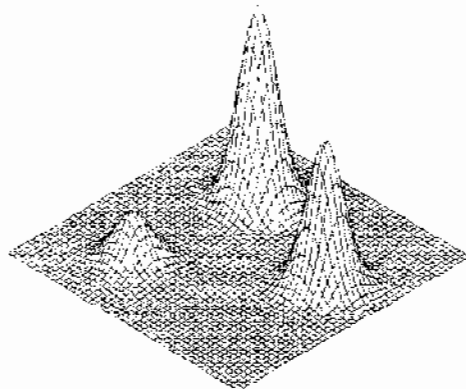


Fig. 12.18 Schematic representation of particles built up from a space-time lattice; i.e. *geometrodynamic solitons*.

Intentionally mistating Misner, *et.al.*'s quote with which we began this section, one is tempted to speculate, instead, that "*Neither matter nor space tells the other how to act, for both are nothing other than constructs of information.*" There is no such thing as spacetime, only information. Sometimes it acts like space, sometimes it acts like matter; and sometimes it simultaneously acts as both. In many ways, this would be an ideal marriage between the central lesson of gravity – namely, the proposition that spacetime is not just a static backdrop on top of which dynamics takes place but is an active coupled participant in that dynamics – and the notion that, underneath it all, fundamentally, all is information.

The idea that matter and spacetime might be built from the same "stuff" has been entertained, in a variety of guises, many times, beginning with Einstein himself. Einstein was unhappy with the models of particles that were prevalent in his

time – such as the Lorentz model of the electron – that contained singularities, and wondered if particles were really built out of the geometry of spacetime. Einstein fruitlessly searched for years for particle-like soliton solutions of the classical field equation; we now know, of course, of “no-go” theorems telling us that such solutions cannot exist. However, as Gibbons [gibbg84] points out in his short survey of recent progress in viewing geometry as particles and particles as geometry, all may not be lost. There are interesting “coincidences,” for example, between certain Klein-Kaluza theories and monopole models that suggest that, in some quantum mechanical sense, spacetime and the particles in it might be indistinguishable. Gibbons also speculates that the fact that a fluctuating quantum spacetime may be described effectively as a gas of colliding particles (albeit in three dimensions, in which it is known that spacetime locally has a trivially flat metric), is, at the very least, “very suggestive.” Might something more interesting happen, for example, in four or five dimensions where the field equations are less trivial?

12.9.2 *A Small Sampling of “Crazier Still...” Ideas*

A number of original speculations have been proposed in recent years in hopes of forging a deeper relationship among matter, dynamics and spacetime. Recall, for example, Zuse’s idea that an interdependence of mass, energy and curvature of space might be a consequence of a discrete spacetime lattice (see section 12.6.3). We give the reader a flavor of some these speculations with the following (far from complete) sampling.

12.9.2.1 *DiMarzio*

DiMarzio ([dim77a], [dim77b]) derives an interesting set of equations for a fundamental “field” $\vec{\rho}$ using four assumptions: (1) there exists, in all of nature, velocity of only one magnitude (equal to the velocity of light, c); (2) relativistic covariance of the equations governing $\vec{\rho}$; (3) the principle of contiguous action (i.e. only “stuff” at the same spacetime point can interact); and (4) a (local) conservation principle on the total amount of $\vec{\rho}$ in the universe. With these four assumptions, DiMarzio derives an equation for $\vec{\rho}$, some of whose properties include (i) reducing to Maxwell’s equations when $\vec{\rho}$ is small, (ii) a natural quantization of the field into a set of discrete particle, (iii) a consistent relationship between the basic equation describing $\vec{\rho}$ and the laws of gravitation (in the second of his two papers DiMarzio suggests a tentative relationship between $\vec{\rho}$ and the spacetime metric). The view that emerges from DiMarzio’s analysis is that of fundamental particles as “extended” objects, and matter in general as a field that at each spacetime point travels in all directions with speed c . While there is no CA-like discretization in this theory, the idea that a consistent field-theoretic framework can be built upon otherwise very much CA-like basic principles (unit speed, locality, conservation – of information? – and so forth) is encouraging.

12.9.2.2 *Jourjine*

Jourjine [jour85] generalizes Euclidean lattice field theory on a d -dimensional lattice to a cell complex. He uses homology theory to replace points by cells of various dimensions and fields by functions on cells, the cochains, in hopes of developing a formalism that treats space-time as a dynamical variable and describes the change in the dimension of space-time as a phase transition (see figure 12.19).

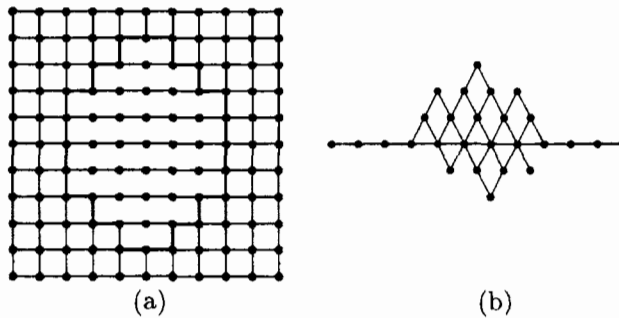


Fig. 12.19 Examples of dimensional phase transitions in Jourjine's model [jour85]: (a) one-dimensional phases inside of a two-dimensional phase, (b) a "bubble" of a two-dimensional phase inside of a one-dimensional phase.

12.9.2.3 *Kaplunovsky and Weinstein*

Kaplunovsky and Weinstein [kaplu85] develop a field-theoretic formalism that treats the topology and dimension of the spacetime continuum as dynamically generated variables. Dimensionality is introduced out of the characteristic behavior of the energy spectrum of a system of a large number of coupled oscillators.

12.9.2.4 *Chew and Stapp*

Chew and Stapp ([stapp71], [stapp72], [chew87a]) circumvent the ubiquitous transition between the classical and quantum worlds which becomes most apparent during an act of quantum "measurement" by trying to erect quantum theory exclusively on quantum principles, with all classical concepts, including the three-dimensional continuum, as derivative objects. They look for a discrete quantum mechanical precursor to spacetime geometry with the following set of features: (1) the theory is fundamentally quantum mechanical, and starts with a small set of quantum entities, devoid of spacetime properties, obeying a unitary law of evolution; (2) the coupling constants satisfy symmetry conditions allowing a graphical representation of evolution to be naturally embedded in a two-dimensional space (so that topological features analogous to those found in particle physics and string theory are embedded at a fundamental level); (3) spacetime is not just an arena for dynamics but emerges from the structural features of the conglomerate of quantum

entities (in the limit where the number of those entities becomes large). Postulating a Fock space built from the combinations of some finite set of unvalued labels $a, b, \dots$, the basic entities – or the “elementary events” – of Chew’s and Stapp’s theory are the vertices of what they call “causal graphs,” or ordered cubic graphs with consistently-oriented labeled arcs. What is exciting is that their approach has at its core the notion of self-organization, as fundamental particles are described essentially in terms of patterns and relationships that are not *a priori* embedded in space-time. Stapp, as quoted by Capra [capra88], reflects that he is “...looking for some guiding principle – maybe some kind of self-reference of the system, or some self-organization that gives the system a kind of autonomy in its environment.”

12.9.2.5 *Dadic and Pisk*

Dadic and Pisk [dadic79] introduce a self-generating discrete-space model that is based on the local quantum-mechanics of graphs. As in the Structurally Dynamic CA (SDCA) model discussed in section ?? (see below), Dadic and Pisk’s spatial structure is discrete but not static: it is fundamentally amorphous and changes dynamically in time. The metric is a familiar function from elementary graph theory: the distance between two points is set equal to the number of links on the shortest path between them, and is generalized to unlabeled graphs by referring to the topological description of the node positions rather than their arbitrary labels. Dadic and Pisk define a “quantum mechanical” graph dynamics using a symmetrized Fock space that is local in terms of this metric: (1) the interaction involves only those processes involving a minimal change to the distance structure, and (2) the interaction depends only on the local properties of the graph structure. An important consequence of their theory is that the dimension of a graph is a scale dependent quantity that is generated by the dynamics. One possibility is therefore to have a ground state of a system have (the phenomenologically observed) dimension $d = 3$ and define particles as spatially extended low-lying excited states generated by the same interaction as the ground state but differing from the ground state in local structural peculiarities. For example, a particle’s dimension might be different from that of the ground state. It is also interesting to speculate that in this picture of particles and ground-state-like structures spanned between them, observables such as distances, momentum, and so forth, are quasi-statistical constructs that can be defined only for many-particle states.

12.9.2.6 *Caianiello*

Caianiello ([caian83], [caian87b] and [caian88]) has been quietly developing a purely geometrical representation of quantum mechanics that is based on relative information measures (i.e. Kullback, or cross, entropy and the Fisher metric; see [brill56], [blahut87] and [guiasu77]) and in which “uncertainty” appears as “curvature” in a relativistic phase space. The Heisenberg uncertainty relations, for example, emerge naturally (or more precisely, formally), from the so-called Cramer-Rao information

theoretic inequalities.[†] While the theory is far from developed – Caianiello himself ambitiously conceives its application to quantum mechanics as merely being a special case of a “geometrization” of general systems theory – what is perhaps most significant about his theory is the philosophy it expounds, with not-too-distant echoes of Wheeler’s mantra, “no bit is a bit until it is a *measured* bit”: the notion that all parameters of any systemic model (including social, econometric, etc.) are fundamentally *model dependent* and have no “real” existence of their own; they exist only within the formal framework of the model. Classical notions such as “space”, in Caianiello’s view, are fundamentally model dependent and have no real existence or meaning before actually being “measured”; i.e. the act of measurement creates the thing it measures. Geometricized information theory is introduced to essentially provide a set of logical uncertainty conditions regulating the consistency of all measured quantities.

12.9.2.7 *Structurally Dynamic Cellular Automata (SDCA)*

The SDCA model ([ilach86], [ilach87] and [ilach88]), in which conventional CA dynamics is generalized to include dynamic changes to the underlying lattice structure, was motivated, in part, by a desire to find a formalism appropriate for describing a fundamental physics respecting two key assumptions: (1) information is finite, and (2) geometry and matter are dynamically coupled. The coupling between the lattice and local site-values treats geometry and value configurations on an approximately equal footing: the structure is altered locally as a function of individual site neighborhood value-states and geometries, while local site-connectivity supports the site-value evolution in exactly the same way as in conventional CA models defined on random lattices. The microphysical view of physics that emerges from this construction is one in which a fundamentally discrete pregeometry continually evolves in time as an amorphous structure but with a globally well-defined dimensionality. Particles are constructs of that amorphous structure and can be viewed as locally persistent substructures – i.e. geometrical or topological solitons – with dimensions that differ from the surrounding value (see figure 12.18).

While SDCA takes one step toward coupling “matter” (site variables σ) with “geometry” (link variables l_{ij}), the coupling is still incomplete, even in this toy model. What is missing is a mechanism for making both “matter” and “geometry” indistinguishable from the other; i.e. if both elements of reality stem from the same primordial source of information, they must each come into and out-of existence according to whatever is the underlying, primordial, dynamics. A generalized SDCA model must therefore add the following two provisions:

- Both matter-like (σ) and geometry-like (l_{ij}) information must be dynamical constructs of primordial “bits” of information; value and link dynamics must not just “mimic” one-another via a weak coupling, rather they must, in a sense, “tap from the same informational source” when it comes to their mutual creation and/or annihilation.

[†]See C.R.Rao, *Linear Statistical Inference and its Applications*, Wiley (1973).

- *the dynamics must be strictly reversible, so that the overall information content of the system is always conserved.*

The difference between SDCA and its generalized version may appear slight at first – after all, both σ and l_{ij} are already built of “bits” and putting a constraint on the rule set should be no big deal – but the difference in the way we interpret their respective behaviors is not. Unlike the basic SDCA model, in which bits of value and bits of geometry each change according to some arbitrary function of both, there is in the generalized SDCA model something akin to an uncertainty-relationship-like connection between value-bits and geometry-bits: lattice size and/or complexity can increase or decrease at the expense of local site-value information; and, likewise, site-value information can increase or decrease at the expense of lattice size and/or complexity. Put another way, a fixed finite amount of information continually flows in and out of both value-like and geometry-like channels. The two extremes of this dynamics occur either when there is only a pure value-like “ball” of static information, with no remaining geometry upon which to flow and interact, or when all of the primordial information has been converted into pure geometry, and only a static lattice remains, unchanging, with no remaining value-like information to flow and interact upon it. The stuff of physics is what lies sandwiched between these two extremes.

12.10 Final Musings & Speculations

“The division of the perceived universe into parts and wholes is convenient and may be necessary, but no necessity determines how it shall be done.” – Gregory Bateson[†]

In chapter one, we answered the basic question – *Why Study CA?*[‡] – by offering four motivations, ordered roughly according to their theoretical significance; namely, the use of CA...(1) as powerful computational engines, (2) as discrete dynamical system simulators, and (3) as conceptual vehicles for studying general pattern formation and complexity, and (4) as fundamental models of nature. We have seen many examples of each of these motivations throughout the book, and have focused on the fourth – and arguably the deepest – motivation in this concluding chapter, where we have examined some serious attempts to develop a discrete CA-like physics. In this final section, we take a bold step beyond even this highly speculative proposition to muse about a possible new CA-inspired physics. We ask, *“If nature, at its core, is truly a CA, what would a physics that describes such a reality look like?”*

In order to address this intriguing question, we must first of all be clear about what we mean by “physics.” According to the CD-ROM edition of the *American Heritage Dictionary*,[§] physics is the “science of matter and energy and of interactions

[†]Gregory Bateson, *Mind and Nature: A Necessary Unity*, Bantam Books (1979), chapter 2.

[‡]See section 1.2.2.

[§]*The American Heritage Dictionary*, Fourth Edition, CD-ROM, Houghton Mifflin Company, 2000.

between the two.” While this definition adequately describes what (conventional) physics studies, it says nothing about its epistemology. To facilitate the ensuing discussion, we thus refine this definition to one where “physics” is understood to be a description of natural phenomena that consists of the following two ingredients: (1) partitioning the world, in a self-consistent manner, into a set of objects and a set of relationships among those objects, and (2) using (or developing) a specialized language with which such partitions and relationships can be described. We contend that the physics that we learn about in textbooks today is but one (albeit rich) example, predicated on experimentation and mathematics, of a much broader set of alternative physics. It is this broader set of physics – and therefore a broader set of associated partitions and languages – about which we will muse in this closing section.

Old versus New

Figure 12.20 illustrates what (we will argue below) is the fundamental difference between conventional physics (shown on the left) and the conceptual cornerstone of a generalized new physics built upon the precepts of CA and the dynamics of complex adaptive systems (illustrated at right).

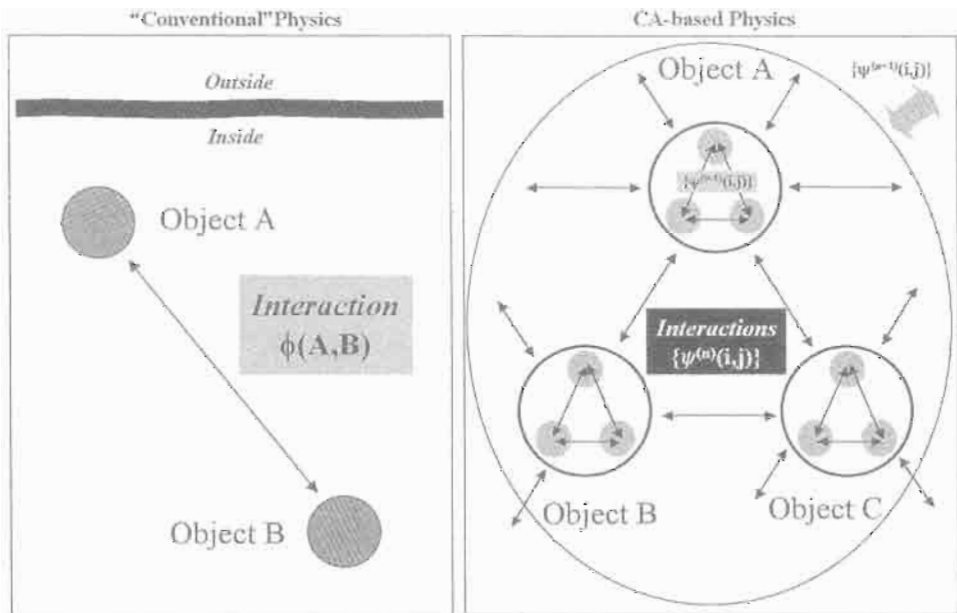


Fig. 12.20 Schematic distinction between conventional “physics” and a proposed generalized new CA-based physics; see text.

While the figure obviously grossly oversimplifies how we understand nature, it highlights the salient points we are trying to make in this section:

(1) Conventional physics tends to understand phenomena by first stripping away layers of complexity by isolating the “inside” of a system from an “outside.” It

then focuses its attention on sets of pairwise interactions $\phi(A, B)$ between separate objects, A and B . Physics, understandably, tries to simplify systems in this way in order to focus on relevant features of a problem and/or to render the problem mathematically tractable; on the other hand, we must appreciate that physics *does not* do so because of any particularly deep philosophical insight into how nature works.

(2) The real universe makes no absolute distinctions between objects and their environment, and must always deal – simultaneously – with a myriad of intertwined, multilayered webs of many-object interactions.

(3) Objects, however they are defined, possess both an *internal structure*, consisting of low-level interactions among lower-level constituents, and *external interactions* within a context provided for by higher-level constructs. For example, think of biological cells, that simultaneously harbor an enormously complicated inner world (that consists of enzymes, lipids, DNA, ...) and are vital components of a very complicated outer world; or human beings, whose viability as conscious organisms depends profoundly on the stability of a complicated inner world of highly interconnected cells, and whose mutual interaction, on a higher level, creates whole cultures.[†]

The dynamics of complex adaptive systems, in general, and of CA in particular, suggest that (i) most interesting phenomena arise precisely because of an irreducible, coupling between object and environment (so that any distinction between inside and outside is artificial and not representative of how real systems are fundamentally structured [atman93]), and (ii) “objects” are really semantic constructs that are functions of the local context within which their existence, or nonexistence, is assigned meaning, rather than independently – and objectively – existing entities within a system. We will elaborate on what we mean by both of these statements below.

Given that, historically, new developments in mathematics and physics have always been closely aligned, we can anticipate a strong need to develop a (possibly radically) new mathematics in order to effectively deal with these issues.

A Glimpse of Emerging Hierarchies

Let us focus our attention, for a moment, on “gliders” and other patterns, that frequently arise in Conway’s *Life* universe (see section 3.4.4). Such structures represent notional informational constructs that are meaningful *only on some “level” that lies above the individual ON/OFF bit-level on which the dynamical rules are defined*. Certainly, the emergence of such higher-level constructs cannot be inferred directly from the microscopic rules. Indeed, one can argue that part of the reason why such structures are interesting is that, *as a class*, they appear to interact among themselves according to an entirely different set of higher-level interaction rules.

For example, think of the complicated 13-glider collision producing a glider gun shown in figure 3.79. One might also ask whether it is more (or less) appropriate

[†]See H. Bloom, *The Lucifer Principle*, The Atlantic Monthly Press (1995).

to think of a *glider-gun* (which is a considerably more complicated structure than a simple glider, requiring many more individual “bits” to define), as an individual object, rather than a composite of simpler parts, that, when acting in concert – as separate objects – spew out gliders in regular fashion. In any case, whether the construct is a glider or glider-gun, or some other still more complicated object, the construct at time t is different, on the bit-level, from the pattern that existed at $t - 1$; it is also likely to be different from the patterns that will appear at times $t + 1$, $t + 2$ and so on. Thus, we ask, *Where is the object?* and *What is real?*

The short answer is that the ON/OFF bits are “real” on the microscopic level and the objects are “real” on a higher, emergent level. A glider is a specific pattern of lower-level bits that, unless it comes into “contact” with other patterns, is faithfully reproduced in a diagonally displaced position every four iterations. The deeper answer is that both questions are ill-posed because neither “object” nor “real” can be objectively defined. Both terms can be understood only when interpreted *modulo* a specific dynamical level.

To illustrate this, consider a complicated circuit consisting of combinations of NOT, AND and OR gates, such as the one shown in figure 3.84. We call this a “circuit” because – within the implicit context – we know it performs a certain “function” on higher-level bits of information (i.e. gliders). Recall that Conway’s *Life* rule is universal; that is, it has the same computational power as any general purpose computer.[†] The specific set of operations that are executed, and thus the specific function that is computed, is a function of the initial, bit-level, information. Now, there is nothing preventing us from initializing the system in such a way that *Life* effectively computes a sequence of say *3D Life* states for some special initial state. For example, we may choose to use the (two-dimensional) *Life*’s universal computing ability to update sites for the *3D Life* rule.[‡] The interesting question now is, *Which gliders are real?* The 2D gliders that are primitive parts of the 2D “computer” or the 3D gliders that exist on a considerably higher, virtual, level within the emergent informational constructs that define the virtual *3D Life* universe? Of course, we are free to use *Life* to reproduce the behavior of any other rules that harbor other kinds of higher-level emergent behaviors as well.

By insisting on isolating systems from an “outside,” and by treating fundamental processes as though they are merely linearly additive strings of simple two-point interactions, conventional physics thus strips away much of the universe’s nonlinear richness. Certainly, such a program fails to capture subtle nuances of behavior, that can be revealed only when the full integrity of system complexity – with all of its interconnected hierarchy of interactions – is retained and respected.

The main philosophical lesson that one ought to walk away with from a study of CA and complexity is this: just as what we label as being a “glider” in Conway’s *Life* depends on us recognizing the fact that its underlying bit pattern repeats in a

[†]The proof of *Life*’s universality is outlined in section 3.4.5. The proof proceeds by observing that each of the primitive elements of computation – i.e., the *storage*, *transmission*, and *processing* of information – can be implemented by evolving an appropriate set of *Life* patterns.

[‡]Several possible forms for *3D Life* are discussed in section 3.4.6.

regular fashion every four steps, an "object," in a more general sense, is said to exist only if we can identify some regularity within its local context. An object's existence thus depends on the physicist's innate pattern recognition skills at establishing an objective, self-consistent, local context. As contexts change, and as the levels on which their characteristics take on meaning change, any given object can take on varying characteristics and identities.

Two New Axioms

How is physics, as it is currently practiced, deficient in its description of nature? Certainly, as popularizations of physics frequently remind us, theories such as *Quantum Electrodynamics* are "successful" to a remarkable degree in predicting the results of experiments. However, any reasonable measure of success requires that we add the caveat, "...in the domain (or domains) for which the theory was developed." For example, classical Newtonian physics is perfectly "correct" in its description of slow-moving, macroscopic objects, but is fundamentally incorrect in its description of quantum and/or relativistic systems.

As the foregoing discussion suggests, our contention is not that today's science or physics is wrong *per se*; rather, that the domain of phenomena to which physics has been traditionally applied has been unnecessarily restricted. Physics is deficient not in its explanatory and predictive powers within the domains for which it has been developed, but in its presumptive disregard of an additional set of deeper axioms that would otherwise lead to a comprehensive description of a much broader class of phenomena.

Inspired by characteristic features of the emergent behavior in complex systems and CA that we have examined in this book, we therefore suggest the following two axioms to augment those already subsumed in conventional physics:

1. *Information is primitive.* Information is a fundamental characteristic of physical systems, on an equal footing with matter and energy. To which we add the fundamental postulates that the total information content of the universe is finite and strictly conserved.
2. *The distinction between "objects" is fundamentally subjective.* Objects have no meaning (or reality) in isolation. The identity and characteristics of an object are functions of the total web of inter-relationships that object has with all other objects, on all (emergent) levels of a system. Objects may take on different identities and characteristics that depend on their local context.

Primitive Information

What is information? It is the incorporeal abstraction of how corporeal substance is organized. What "energy" is to matter, "information" is to how matter is organized. It follows that there is not only a hierarchy of matter-forms and interactions (i.e. thought of as conduits of energy), but a hierarchy of information as well. As *matter* is to *substance*; *energy* is to *process*; and *information* is to *pattern*. A

simple example is a network system whose (1) matter consists of its physical sites (“information receptacles”) – parameterized by quantity N and site-vector $\vec{\sigma}_i$; (2) energy consists of the dynamics between sites; and (3) information consists of the network’s topology, as expressed, say, by its adjacency matrix.

We have already seen hints of the kinds of theories that are possible using the first axiom; see Kantor’s *Information Mechanics* (section 12.4.5), Stonier’s *Information Physics* (section 12.4.6) and Frieden’s *Extreme Physics Information Principle* (section 12.4.7). Minsky, Zuse and Fredkin, among many others, have speculated on a CA-like dynamics of primitive information (see section 12.6).

Physical matter is conventionally thought of as both consisting of, and being a “conduit” for, energy. Sometimes it simply transfers energy (as when a body of water acts as a medium for propagating waves), sometimes it acts as a medium that dissipates, transforms, and/or reacts with incoming energy (such as when a tomato is squashed against a wall).

Symbolically – letting $\mathcal{O}$ represent matter (or an “object”), $\mathcal{E}$ represent energy and $\mathcal{T}$ a “transformation” – we can write $\mathcal{E} \rightarrow \mathcal{O} \xrightarrow{\mathcal{T}} \mathcal{E}'$, where time implicitly flows from left to right. Also implicit is the fact that the transformation $\mathcal{T}$ acts *only* on the incoming external energy $\mathcal{E}$ and does not involve any internal energy of $\mathcal{O}$. Now suppose that – fundamentally – matter is not merely a conduit for energy (with which it may or may not interact), but acts, in general, as an *information processing agent* that uses its own store of energy to encode an outgoing “message” in response to incoming messages encoded and/or transmitted via the incoming energy. Letting $\mathcal{I}[\mathcal{E}_{\text{ext}}]$ represent information $\mathcal{I}$ encoded using external energy $\mathcal{E}_{\text{ext}}$, $\mathcal{E}_{\text{int}}$ represent an internal energy and $\mathcal{C}$ an encoding of information, we now have the more general expression: $\mathcal{I}[\mathcal{E}_{\text{ext}}] \rightarrow \mathcal{O} \xrightarrow{\mathcal{C}} \mathcal{I}[\mathcal{E}_{\text{int}}]$.

Primitive Objects

The second axiom, which is reminiscent of *Mach’s principle*,[†] also contains the seeds of Leibniz’s *Monads* [resch91]. “All is process. That is to say, there is ‘no thing’ in the universe. Things, objects, entities, are abstractions of what is relatively constant from a process of movement and transformation. They are like the shapes that children like to see in the clouds.”[‡] The Einstein-Podolsky-Rosen correlations (see section 12.7.1) remind us that what we empirically accept as fundamental particles – electrons, atoms, molecules, etc. – actually never exist in total isolation. Moreover, recalling von Neumann’s uniqueness theorem for canonical commutation relations (which asserts that for locally compact phase spaces all Hilbert-space representations of the canonical commutation relations are physically equivalent), we note that for systems with non-locally-compact phase spaces, the uniqueness theorem fails, and therefore *there must be infinitely many physically inequivalent and*

[†]Mach’s principle, as formulated by Wheeler [wheel64a], states that the inertial properties of an object are determined by the energy-momentum distribution throughout all of space.

[‡]David Bohm, “Further remarks on order,” in *Towards a Theoretical Biology*, edited by C.H. Waddington, Aldine Publishing (1970).

physically relevant representations.[†]

While we do not have the space in the remaining pages of this book to describe the full epistemological ramifications of adding these two axioms to conventional physics, we will briefly map out a possible strategy for developing a generalized new physics that is based on them. We begin by again asking the basic question, *What is real?*

12.10.1 What is Real?

Western science has traditionally emphasized reductionism as the road to understanding. Reductionism, of course, is a process that involves the systematic labeling, categorizing and compartmentalizing of objects. Unfortunately, the western world has also somewhere along the line lost sight of the fact that the universe is *one*, *essentially unfragmented, whole*.

As Watanabe's *Ugly Duckling Theorem*[‡] reminds us, there can never be a rigorously objective way to ascribe a measure of similarity (or dissimilarity) between any two randomly chosen subsets of a given set. An asymmetry can be induced only via some external aesthetic measure. The absolute validity of any partitioning of the world into a specific set of *objects* and *relations* – which, as we have argued, constitutes the very essence of physics – is therefore, fundamentally, arbitrary.[§]

As far as an external aesthetic is concerned, we do have two important clues to help guide us: (1) *chaos theory*, from which we learn that natural processes that appear complicated can often be well understood using relatively simple rules, and (2) *complex systems theory*, from which we learn that interesting phenomena often emerge on higher levels from parts that are mutually interacting on the lower levels of a hierarchy.

Of course, physics has long used the idea of arbitrary labeling to its advantage in solving problems. Consider, for example, the following system of equations: $dx_i/dt = \sum_{j=1}^n \alpha_{ij}x_j$, $i = 1, \dots, n$. This system may describe the reaction of n chemicals with x_i representing concentrations of the reactants and α_{ij} representing the various rate constants.[¶] Depending on the rate-constant matrix α_{ij} , the solution to this set of coupled equations can be quite complicated. Suppose there exists an invertible matrix T_{ij} such that (1) $\eta_i = \sum_{j=1}^n T_{ij}x_j$ and (2) the rate constants α'_{ij} for the system defined by the “effective” concentrations η_i is *diagonal* (i.e. $\alpha'_{ij} = a_{ij}\delta_{ij}$),

[†]See Hans Primas, “Endo- and Exo-Theories of Matter,” *Inside versus Outside*, H. Atmanspacher and G.J.Dalenoot, editors, Springer-verlag (1994).

[‡]See section 12.3.3.

[§]Recall also the sentiments of Ludwig Wittgenstein, taken from his *Tractatus Logico-Philosophicus*: “All propositions are of equal value.” (Proposition #6.4) and “The sense of the world must lie outside the world. In the world everything is as it is, and everything happens as it does happen: in it no value exists – and if it did exist, it would have no value.” (Proposition #6.41).

[¶]This example is taken from R. Rosen, “Complexity as a system property,” *Int. Jour. Gen. Sys*, **3** (1977) 227-232.

so that $d\eta_i/dt = \alpha_{ii}\eta_i$, $i = 1, \dots, n$. In contrast to the “real” physical system, the effective system is uncoupled and therefore trivial to solve.

The question of interest in our current context is “Which system is more fundamental?” That is, which variables – x_i or η_i – are real? Or, which system more naturally describes the real physics? In either case, as is also true for any of an infinite number of other possible effective concentration variables y_i that we could have chosen, the physical system remains the same, of course. The labels, or variables, with which we choose to describe that system are not fundamental. One is tempted to ask whether substantially greater depths of truth can be mined by considering the set of all possible transformations T_{ij} (from one consistent set of variables to another) rather than the set of all possible variables (as is typically done)?

An even deeper dilemma confronts an honest physicist when trying to understand what “really” happens during a quantum measurement. Despite using (macroscopically) intuitive descriptions of the quantum-entangled “objects,” what really happens remains a deep mystery.[†] Or, consider the following simple thought experiment using CA.

A Thought Experiment

Consider a two-dimensional CA system with the usual Euclidean lattice and some simple set of nearest-neighbor rules. Suppose that, for some set of initial states, the system appears random, with no discernible patterns or correlations. Now start playing with the ordering of the individual sites of the lattice: $(x, y) = (13, 40)$ becomes $(x', y') = (27, 50)$, the site $(22, 115)$ becomes $(0, 0)$, and so on. Maybe you tinker with your definitions of the local state variables, so that $\sigma \in \{0, 1, \dots, k\}$ becomes $\sigma' \in \{0, 1, \dots, k'\}$. Maybe you partition the lattice using some peculiar tiling; maybe you use a Penrose tiling, whatever that would be like. The point is, you take your original system, and redefine it *without adding or subtracting any information and by maintaining the overall integrity of the entire system*. You are allowed only to use whatever latent information already exists within the system to reorganize its parts internally. Now examine the behavior of your reorganized system, using your new labels, site variables, rules, and/or whatever else you have altered the prescription for.

Presto! Conway-like gliders are everywhere! In particular, gliders are streaming across your “effective” (i.e. internally relabeled/redefined virtual) computer screen – which may consist of “pixels” that are grossly nonlocally connected relative to their original coordinates of the “real” screen – *where none had been seen in the “real” (i.e. original) system*. *Are the gliders real?* What about locality? Is it perhaps an ill-formed concept, taking on meaning only with respect to a particular physics and not to the fundamental reality the physics supposedly describes? Suppose the gliders are real. What is the real dynamics underlying their existence? Is the dynamics itself a mere artifact of the physics used to describe the underlying reality,

[†]See *Interpreting Bodies: Classical and Quantum Objects in Modern Physics*, edited by Elana Castellani, Princeton University Press, 1998.

being devoid of any real fundamental meaning?

Suppose further that there is another partitioning of the same lattice that gives rise to an entirely different set of Conway-Life-like gliders, obeying a different set of higher-level rules. Now what is really going on? Which set of gliders are the ones that “really” exist in this system, the first set or the second? *Or has reality itself become a vague concept?*

As you pay homage to the diversity of behavior that emerges across the spectrum of all possible representations of all possible systems, you inevitably conclude that (1) there can be no objectively privileged system for which the emergent structures are “real,” and such that all other structures, for all other derived systems, are less real, and (2) *reality*, or the emergence and identity of particular sets of objects and their interactions, is wholly dependent on the arbitrary dynamical labels that prescribe a particular system. In short, reality loses its objectivity, and takes on a more tentative, ineffably relative facade. You begin to wonder if the best that you can do to get a hold on “objective reality” is to look for whatever remains fixed - i.e. what is *universal* - within the space of *all possible representations, all possible rules, and all possible emergent structures*.

Ω -Wholeness

Bohm [bohm80], Capra [capra88], Jantsch [jant80], Koestler [koest78], Wilber [wil95] and others have argued that reality is fundamentally whole and unfragmented. An object has no real meaning except when interpreted within the context of *all other objects in the universe*. We suggest a generalization to this idea – an Ω -wholeness: an object has no real meaning except when interpreted not just in terms of all other objects, but in terms of *all possible patterns of organization among all other objects*.

Stated another way, (i) what an entity is can only be defined relative to all other entities that are (in a static, bean-counting, manner); (ii) what an entity does can only be defined relative to what all other entities do (which depends on how they are all “interconnected”); (iii) what fundamental role an entity plays in the “world” can only be defined relative to the roles that all other entities play in the world (which depends on the role all entities play on each level of the hierarchy).

Whatever understanding of $\mathcal{O}$ can come about by confining $\mathcal{O}$ (and $\mathcal{O}$ ’s role in the “world”) to a single level – even while formally acknowledging the existence of other levels – is necessarily incomplete. In order to fully understand an observer $\mathcal{O}$, one must (1) understand $\mathcal{O}$ ’s context within the level on which the agent that is trying to understand $\mathcal{O}$ himself lives (i.e. relative to all other observers/agents with whom $\mathcal{O}$ communicates), and (2) $\mathcal{O}$ ’s role within – and relative to – the entire hierarchy of levels, *above and below* the level on which the agent has (arbitrarily?) identified one element of his partition of $\Omega^{(n)}$ as $\mathcal{O}$. This view is clearly consistent with Koestler’s cosmogony, which uses *holons* as primitive ingredients of a nested hierarchy [koest78].

We propose that the basic principle underlying the dynamics on all possible levels of the universal hierarchy $\Omega = \Omega^{(1)} \subseteq \Omega^{(2)} \subseteq \dots \subseteq \Omega^{(N)}$ that we call “the universe” is *information (or language) processing*. That is to say, on each level

of the hierarchy, arbitrarily partitioned observers interact with the remainder of the universe (i.e. all other observers) according to their respective “languages,” or internally consistent, filtered, representations of what they perceive (interpret) as being the external “reality.” The real reality is fundamentally whole, undifferentiated, and structureless but attains an apparently consistent form and structure when filtered through a given language *qua* observer.

A strong caveat to all of this, of course, is that the notion of *partition* itself depends on an arbitrary set of symbols and images that represent the de-facto “natural” partitioning of Ω . More concrete notions such as *language, meaning, context, information, energy, matter, pattern, process, reality* – and the notion that these notions are all legitimate, well-defined, meaningful notions! – all depend on the natural partitioning of Ω that Ω has “forced” upon us through millions of years of co-adaptive evolution.

We suggest that just as a human child learns to exist within, interact with, and adapt to a constantly changing environment, so every possible “observer” of the world – as defined by every possible partition of the world (i.e. in a maximally relativistic observer-independent partitioning of Ω) – do the same, on all appropriate levels of the hierarchy. Every galactic cluster, every galaxy, every planetary ecosystem, every cultural “superorganism,” every biological entity, every molecule, every atom, every particle, every node of the space-time foam,...is in its own way performing exactly the same core set of information processing functions: *making distinctions, observing, filtering, processing/ assimilating, communicating*.

Where Western science has heretofore been predicated on (1) static partitions of Ω (modulo our co-evolved senses and language), and (2) simple, linear chains of *cause* $\leftrightarrow$ *effect*, the generalized CA-based physics represents a paradigm shift to (1) *causal webs*, and (2) *fully coevolving object* $\leftrightarrow$ *interaction hierarchies and dynamic partitions*.

What kind of new physics must be developed in order to understand Ω -wholeness? Whatever form it ultimately takes, we suggest that this new physics must be fundamentally built upon hierarchical relationships and be maximally relativistic.

Hierarchical Physics

Each entity on a given level of a hierarchy is simultaneously subject to N separate forces acting on each of the levels of the hierarchy. As is true of Koestler’s *holons* [koest78], each object has both a *self-assertive* tendency to affirm, and preserve, its individuality as a semi-autonomous whole, and an *integrative* tendency to function as a coordinated part of an existing (or evolving) larger whole. It is this polarity between the self-assertive and integrative tendencies that defines the hierarchy, and is arguably a fundamental characteristic of life. It is tempting to speculate that quantum indeterminacy may be nothing more than a consequence of effectively ignoring *all but one level* of interactions in the space of all possible interactions on all possible levels.

Consider the n^{th} level, $\Omega^{(n)} \subset \Omega$, of a hierarchy Ω . Suppose $\Omega^{(n)}$ consists of N_n “observers” (or entities) $\Omega^{(n)} = \{\mathcal{O}_1^{(n)}, \mathcal{O}_2^{(n)}, \dots, \mathcal{O}_{N_n}^{(n)}\}$. Each observer, $\mathcal{O}_i^{(n)} \subset \Omega^{(n)}$,

evolves in what he perceives as an n^{th} level time $t^{(n)}$ according to a dynamics, $\mathcal{D}^{(n)} = \mathcal{D}^{(n)}(\Omega^{(n)} - \mathcal{O}_i^{(n)})$, that is (in the Libnizian/Machian view) a function of all other level- n observers: $\mathcal{O}_i^{(n)}(t^{(n)}) \xrightarrow{\mathcal{D}^{(n)}} \mathcal{O}_i^{(n)}(t^{(n)} + \delta^{(n)}t)$. But the total dynamics of each observer $\Omega^{(n)}$ must be determined by considering the dynamics on *all possible* levels of Ω . That is to say, $\Omega^{(n)}$ is simultaneously subject to the n^{th} level dynamics $\mathcal{D}^{(n)}$, the $(n-1)^{\text{st}}$ dynamics $\mathcal{D}^{(n-1)}$, the $(n+1)^{\text{st}}$ dynamics $\mathcal{D}^{(n+1)}$, *and all other levels*. Each level of dynamics must, of course, be properly interpreted in a manner consistent with the level of “observers” to which it is applied. For example, if $\mathcal{O}^{(n)} \subset \mathcal{O}^{(n+1)} \subset \Omega^{(n+1)}$, what $\mathcal{O}^{(n)}$ “does” (i.e. what its next “state” will be as a part of the total dynamics $\Omega \rightarrow \Omega'$) will depend, in part, on what the observer $\mathcal{O}^{(n+1)}$ that contains $\mathcal{O}^{(n)}$ does according to the dynamics $\mathcal{D}^{(n+1)}$ it is following on level $(n+1)$.

Maximally Relativistic Physics

There is no unique articulable law or set of laws that any observer contained in the universe Ω can construct – even in principle – that describes Ω exactly. It therefore behooves us to develop a primal physics P that is *maximally relativistic*; not in a generically Einsteinian sense, but in an informational sense. That is, to develop a physics in which the meaning of any object or process exists only relative to something (ideally, everything) else.

P should also minimize distinctions between conventionally distinct but “atomic” primitives (such as space, mass, time, etc.). The vision is to take one more step along the metaphoric road *remove man from the center of the universe* $\rightarrow$ *remove all privileged frames of reference* $\rightarrow$ *remove all absolutes* $\rightarrow$ *remove all distinction between space and matter* $\rightarrow$ *remove all distinction (?)* Start by eliminating the tacit assumption that whatever physics is self-organizing itself out of the “soup” of the current crop of physicists is the physics of this universe; in short, go from a solipsistic physics to a fundamentally relativistic physics, wherein even “physics” itself becomes a set (an infinite hierarchical set?) of self-consistent world-views rather than a prescribed set of exactly/uniquely prescribed “laws” operating independently of all observers.

The apparent merging of heretofore disjoint – or only partially overlapping – disciplines (physics, chemistry, biology, ecology, psychology, etc.) is consistent with the ideas that (1) they are all somehow analogous to one another, despite the fact that the objects of their discourse and methodologies may appear very different, and (2) as the fuzzy boundaries of their respective domains continue expanding, the growing overlaps increasingly point to a heretofore hidden skeletal substructure that unifies those domains. The science that is struggling to emerge will almost certainly require an entirely new methodology; a methodology that builds fundamentally upon information theory, hierarchy and maximal relativity.

12.10.2 A Glimpse of a New Physics?

Consider a simple formalization of a conventional dynamical system. Define (1) a dynamical arena – i.e. the space-time background on “top” of which everything occurs – $\mathcal{A}$; (2) a set of dynamical variables $\vec{V} = \{\sigma_1, \dots, \sigma_N\}$ describing the “objects” undergoing a dynamical change; $\vec{V}$ lives in the phase-space Γ ; (3) a dynamics $\mathcal{D} : \Gamma \rightarrow \Gamma$, where (either implicitly or explicitly) $\mathcal{D} = \mathcal{D}(t)$ and t is a “time” parameter; and (4) a set of “appropriate” filter(s), $\vec{\mathcal{F}} = \{\mathcal{F}_1, \dots, \mathcal{F}_N\}$, to “interpret” the orbits $\mathcal{O}_{\mathcal{D}}$ of $\mathcal{D}$.

Note that there is a potentially problematic self-referencing involved here: each of the four elements making up (an observer’s description) of the system $S - \mathcal{A}, \vec{V}, \mathcal{D}$, and $\vec{\mathcal{F}}$ – can only be conceived and articulated *modulo* the observer’s language $\mathcal{L}_{\mathcal{O}}$. But the observer’s language must of necessity itself be born of the prior manner in which $\mathcal{O}$ categorizes (i.e. partitions) Ω . That is, $\mathcal{O}$ ’s language is what it is because $\mathcal{O}$ partitions his view of the world according to what that language is then used to articulate $\mathcal{A}, \vec{V}, \mathcal{D}$, and $\vec{\mathcal{F}} \rightleftharpoons \mathcal{L}_{\mathcal{O}}$.

Conventionally, $\mathcal{A}$ supplies a static arena on top of which sit objects $\sigma \in \vec{V}$ whose internal state and/or external position in $\mathcal{A}$ change according to $\mathcal{D}$. Assuming that there is anything nontrivial worth describing at all, conventional physics arbitrarily chooses – ala Watanabe’s ugly-duckling theorem, albeit tailored by our evolved, and therefore, nonarbitrary perceptual/cognitive apparatus – a set of distinctions such that $\mathcal{D}$ displays particularly appealing properties (locality, unitarity, gauge-invariance, etc.). In principle, *the entire alphabet according to which $\mathcal{A}, \vec{V}$, and $\mathcal{D}$ are defined can be altered*, so long as whatever it is that the set $\{\mathcal{A}, \vec{V}, \mathcal{D}\}$ defines as existing (and/or “going on”) is itself left unaltered. That is, in principle, physics is a grand transformation theory; where “transformation” is understood to refer to all possible ways of defining all possible descriptions of what exists. One could say that conventional physics is an internal language describing a perceived external reality predicated on the desire to compress and simplify the appearance of the dynamics $\mathcal{D}$ as much as possible. The question is, *Is this the only compression scheme and simplification possible and/or is it the best?*

Consider $\Omega \Leftrightarrow \mathcal{I}(\Omega) \Leftrightarrow \{\mathcal{A}, \vec{V}, \mathcal{D}, \vec{\mathcal{F}}, \mathcal{L}_{\mathcal{O}}\}$, where $\mathcal{I}(\Omega)$ represents some irreducible “information” of the set Ω . Examine everything that must be specified in order to define a “system” – both explicit (like the system’s parts and their interactions) and implicit (like the existence of a space-time in which to embed it) – interpret it as being articulated modulo a particular language and accessibility to a given set of observations about the world, and then ask: *to what extent is what I have thus defined independent of all of the assumptions I have made (or have been constrained to make) to do so?* Just as conventional, relativistic physics teaches us that the real physics is what is independent of a particular inertial reference frame, so too our maximally relativistic physics teaches us that *the real physics is what is independent of a particular self-consistent way (i.e. language) of describing it*. The catch is that one is forced to use an arbitrary language $\mathcal{L}$ to articulate what is presumably independent of all languages.

The generalized new physics that we are using our two fundamental axioms to

help point the way towards, can perhaps be found by looking at... (1) all possible states of a system; (2) all possible partitions of each state; (3) all possible descriptions of dynamics for a given partition (template of templates); (4) all possible ways in which each element of a given partition can “represent” the information content of the remaining part of U so as to draw consistent inferences about U’s evolution (as seen from the element’s point of view) – i.e. *all possible consistent semantics based on all possible syntax*.

Four Basic Principles of a Generalized New Physics

We propose four basic principles of a generalized new physics that builds upon the two fundamental axioms listed earlier, as well as the notions of hierarchy and maximal relativity:

1st principle. *All useful information is fundamentally relative.* An individual entity E cannot be defined in any meaningful way without reference to at least one other entity E’ – $\mathcal{I}(\sigma_j \text{ relative to } \sigma_i)$ makes sense, $\mathcal{I}(\sigma_j)$ does not; $\mathcal{I}(\sigma_j \text{ relative to } \sigma_i) \neq$ (in general) $\mathcal{I}(\sigma_j \text{ relative to } \sigma_i \& \sigma_k)$. Strong Machian version: The information content of each system S in U must be defined in terms of all other systems S’ in U.

2nd principle. *Primitive bounded rationality: all usable information – and all information processing resources – are finite.* No part of a complex can “know” the remainder of the complex arbitrarily well.

3rd principle. *The sole function of every system S is to maximize its distinction from the remainder of its perceived universe (U - S), thereby increasing its own approximate knowledge of U.*

4th principle. *Systems evolve according to the principle of “maximum freedom” (or “minimal constraints”).* Each component of a system seeks to maximize its available degrees-of-freedom. As each system co-evolves with its environment, it tries to position itself (along its dynamic trajectory) so that its trajectory always points in the direction of the phase-space that yields it the greatest freedom to “explore.”

The third and fourth principles are patterned after Julian Barbour’s principle of *extremal variety* (see [barb82], [barb89] and [barb94]). Extremal variety, which Barbour uses as a foundation for a new cosmological quantum theory, refers to an extremization of a non-local and non-additive quantity – called variety – of a system. In Barbour’s view, all dynamical quantities are fundamentally relational, and the properties of individual objects (or *monads*) are meaningful only in the context of the set of these relational quantities. “Variety” measures how strongly each element of a system can be distinguished from other elements in terms of the relational variables. A system with extremal variety is one in which its parts are related to the whole in as distinct a way as possible. We might say that the CA/complexity-

like tension between order and chaos translates into the principle: each *Leibnizian monad seeks to simultaneously maximize self-knowledge (that is, knowledge of the remainder of Ω and therefore itself by distinction) and maximize diversity.*

Construction of a Toy Universe

Consider a “toy universe”, Ω . As described above, it is an a-priori formless, undifferentiated space that can be arbitrarily partitioned into 2^n atomic predicates. Suppose that Ω contains ‘m’ “observers” O_i , $i = 1, 2, \dots, m$, where the rank $R(O_i) = R_i$ is the number of atomic predicates defining O_i . Each observer “sees” an effective universe Ω_i , consisting of all possible predicates of all possible ranks but excluding the set of atomic predicates that defines itself. A particular realization (or categorization) of Ω_i by O_i is a partition of Ω_i into u disjoint subsets $S_{i1}, S_{i2}, \dots, S_{iu}$, where $u = u(i)$; Ω_i and Ω_j , where $i \neq j$, need not equal one another (i.e. world views of particular observers are in general different).

Each observer O_i (1) “knows” that ‘m-1’ other observers exist, but does not know anything about their internal construction (or “predicate skeletons”); (2) must balance two complementary “desires” – (i) the desire to create as unambiguous a language as possible to communicate as easily as possible with all other observers (which requires his world-view to be as *similar* to the world-views of other observers as possible); (ii) the desire to be as distinct – and therefore, as locally well-defined – as possible, relative to all other observers (which requires each observer to evolve as *different* a world-view from the world-views of his neighbors as possible). The “natural metric” of Ω , on any given level, measures the similarity (or difference) between the views that any two observers on that level have of the “rest-of” Ω . Two observers that have partitioned and connected Ω_i in almost exactly the same way are “objectively” closer (via the natural metric) than are some other two observers who have partitioned and connected Ω_i in very different (perhaps entirely distinct) ways.

Assume, as above, that the universe consists of a hierarchy of levels, $\Omega \equiv \Omega^{(1)} \subset \Omega^{(2)} \subset \dots \subset \Omega^{(N)}$, such that each element is simultaneously subject to N different levels of “forces” compelling it to act on N different levels (“elements” and “forces” must, of course, be interpreted in an appropriate context within the level on which they are each defined). An understanding of such a structure can come about in one of two ways: (1) by imposing an *external* order (such as by, say, defining a CA rule that implicitly yields an emergent N -level hierarchy), or (2) assuming that you – the observer – are already occupying some level (say level- n) of the hierarchy, and then inducing the overall structure from your *internal* observations of the n^{th} level. In this case – which is yet another example of Godelian self-reference – you must somehow step outside your level- n arena of existence (and vantage point) and induce the structure of the whole hierarchy – and – do so *while still under the simultaneous influence of N separate “forces”* (acting on the N different levels and on entities that both contain and are increasingly smaller parts of the observer).

It is this *inside versus outside* (see figure 12.20) tension that is at the core of all “observers” trying to fathom the meaning of their own existence. It is important

to appreciate the fact that while you are in the process of inducing your place in Ω , so too are each of the cells of your body and molecules that they are each composed of, as is the superorganism of which you are a part and the galaxy or cluster of which *Gaia* is herself immersed in. *Each "entity" seeks to find its place and meaning within different but complementary contexts, but does so consistently with the overall structure and self-meaning of Ω .*

Artificial Life $\longleftrightarrow$ Artificial Physics

We conclude by bridging the gulf between the highly speculative propositions outlined above, and the insights into the origins of complex behavior in nature that we have gleaned by exploring the dynamics of CA. CA provide a powerful starting point because they embody so well the quintessential lesson of complexity: start with simple parts, and simple rules that govern how those parts interact, and – if you stand back far enough away so that distinctions between the primitive parts begin to blur – you will likely witness interesting behavior emerge, *on a higher level*; behavior that you could not have anticipated by knowing just the parts and rules you started with.

In CA, the parts and rules are typically very simple. We keep them simple in order to help make our study of their behavior easier. In reality, of course, as we have seen repeatedly throughout this book, even the simplest CA systems can display remarkably complex behavior. To make matters even more complicated, the real world is messier still; it has many more parts than we can manage and obeys rules that we are still struggling to fully understand. So what are we to do? Artificial life research, that we touched on briefly in chapter 11, arguably comes to the forefront as a useful generalization of CA studies. In artificial life, individual cells (i.e. the "parts") are effectively endowed with an inner structure and dynamics, and the domain of the simple cell-cell interaction rules (as used by CA) is extended to include both the inner world of individual cells and an outer space of cell communities. Moreover, in artificial life, communication between cells can be mediated not only via simple CA-like information channels that depend on fixed lattice topology, but according to arbitrary semantic links between entire cell assemblages as well.

Proponents of the strong form of artificial life emphasize that artificial life is fundamentally about the exploration of "life as it could be," as compared to life as we know it [lang89]. It is an attempt to enlarge our currently meager set of examples of life in the set of all possible life – more precisely, our meager *one data point* of life as it has evolved on this planet (see figure 12.21) – in hopes abstracting the set of basic principles that are universal to all life forms.

Insofar as artificial life depends, in part, on the synthesis of self-contained worlds that obey a consistent physics, it is not a great leap to suggest that artificial life is a harbinger of a new kind of generative, *artificial physics*. In such a case, a strong form equivalent of the importance of CA is that it furnishes us with a way to explore

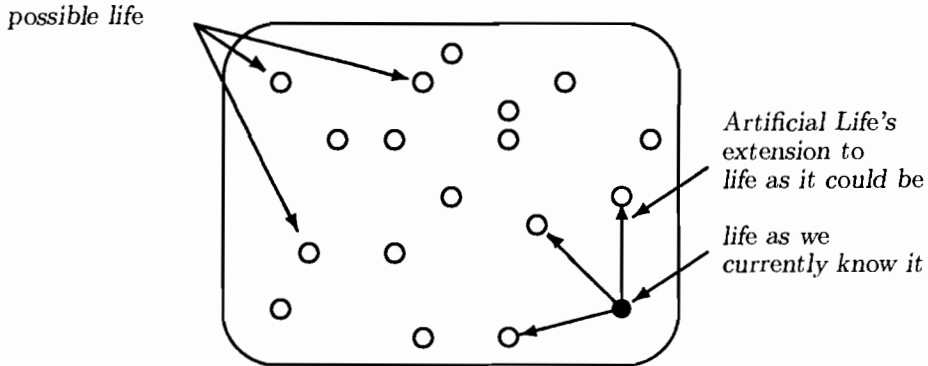


Fig. 12.21 Schematic representation of the set of all possible life and artificial life's (AL's) attempt to extend *life as we know it* to *life as it could be*. Might an analogous schematic be drawn for an artificial physics extending *physics as we know it* to *physics as it could be*? After Langton's opening plenary talk at the *Artificial Life IV* Conference [brooks94].

"*physics as it could be*" as compared to physics as we know it. It is an attempt to enlarge our currently meager set of examples of physics in the set of all possible physics – more precisely, our meager *one data point* of physics as it has evolved in this universe – in hopes of being able to abstract the set of basic principles universal to the evolution of all consistent self regulated co-evolving universes. Toffoli's and Margolus's work with "programmable matter," for example, suggests one promising avenue to take in this direction [toff91].

"Perhaps the world was actually different from the one I had begun to perceive. Every man who had ever lived became a contributor to the evolution of the earth, since his observations were a part of its growth. The world was thus a place entirely constructed from thought, ever changing, constantly renewing itself through the process of mankind's pondering its reality for themselves." – James Cowan, *A Mapmaker's Dream*

A Glimpse of a New Cosmogony?

Most importantly, artificial physics provides a practical means by which to explore the theoretical frontier of the CA/complexity-inspired science we have outlined above. It is only by systematically probing the boundaries of what we "know" to be real, what we "know" to be *foreground* and *background*, what we "know" to be *object* and *interaction*, that we will come to appreciate the fundamental ambiguity of conventional categories and attain a glimpse of a greater context in which everything can be seen as a subjective mirror of everything else.

Predicated on the dynamics of CA, the case studies of artificial life (and, in the coming years, the many provocative examples that are sure to come from artificial

physics), we propose a new cosmogony; a cosmogony in which our universe is viewed not as one “master arena” in which objectively real objects interact and events occur, but as a vast, amorphous, ineffable firmament where reality assumes an objective meaning only locally, and the nature of which varies according to local context. In this new cosmogony, the collective “we” – space-time, strings, quarks, atoms, cells, consciousness, planetary systems, galaxies, and all – are not so much a product of the universe, as active, autopoietically sustaining parts of the universe’s ongoing, open-ended, evolution. [†]

[†]For a richly textured discussion of similar ideas along these lines, see Lee Smolin’s provocative book [smolin97] (see also [smolin92]). It is intriguing that this cosmogony, born of the sciences of complexity and artificial life, should also be so similar in form to one of the most far-reaching, and controversial, interpretations of quantum mechanics: the *many-worlds interpretation* (or *relative-state formulation*) due to Everett [ever57]. (Detailed discussions of the *many-worlds interpretation* may be found in the collection of papers (including Everett’s original paper) edited by Dewitt and Graham [dewitt73] and Jammer’s [jam74] classic monograph on the interpretation of quantum mechanics.) Recall (see section 12.4.2) that the so-called “quantum measurement problem” is to reconcile the deterministic evolution of a system’s state vector with the apparently random projection of that state vector into a measured eigenvalue. Everett’s point-of-departure for this problem was to imagine that if one could write down a “wavefunction for the universe,” there would literally be no “outside observers” capable of reducing the wavefunction. He concluded that wavefunctions do not collapse, ever. This implies that each of the N possible outcomes of any measurement process, anywhere and everywhere in the universe, is realized for that process. That is to say, since no one outcome can be preferred over any other, and there is effectively no “observer” to collapse the wavefunction, each possible outcome of a measurement is in fact realized. Everett accounted for the fact that no one has ever witnessed an actual splitting of any measuring device into multiple copies of itself – each copy registering a different outcome – by boldly asserting that each of the N measurement-outcome possibilities induces the universe to *split into N parallel universes*. Since there are uncountably many “acts of measurement” taking place within each instant of time, this in turn implies that the universe is continually splitting into uncountably many parallel universes. While the inescapable fact that humans perceive only a single universe is left unaccounted for in Everett’s theory, this seemingly fantastic theory is favored by many physicists over the more conventional Copenhagen interpretation precisely because of its ability to solve the measurement problem without resorting to ad-hoc “privileged observers.”

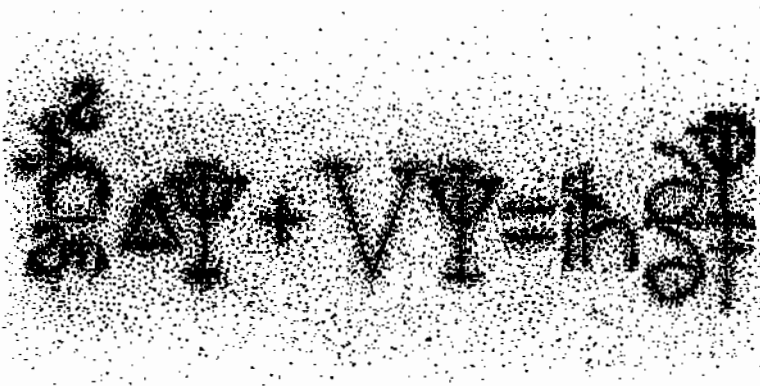
Postscript

Two last questions to ponder...

“If patterns of ones and zeroes were ‘like’ patterns of human lives and deaths, if everything about an individual could be represented in a computer record by a long string of ones and zeroes, then what kind of creature could be represented by a long string of lives and deaths?”

– Thomas Pynchon, *Vineland*

What CA rule leads to the emergence of the Schrödinger equation?



Appendix A

CA Research Tools

A.1 Hardware

In chapter 9 we argued that the use of dedicated lattice gas (LG) hardware represents one of the most promising *practical applications* of CA modeling. With the help of such hardware, many heretofore intractable but technologically important hydrodynamical problems such as fluid flow near and around airplane wings, are becoming computationally accessible for the first time. Weisbuch has aptly compared such dedicated CA processors to being the numerical equivalents of wind tunnels [weis91]. More ambitiously, Toffoli and Margolus foresee hardware implementations of CA systems as embodying the concept of *programmable matter* [toff91]; that is to say, a computationally amorphous “machine” that can be “programed” to act as a numerical wind tunnel one moment, or a sea of fermions the next. Their CAM-8 machine, a powerful new descendent of their earlier CAM-5 and CAM-6 CA simulators (see below), comes close to realizing this exciting possibility.

A.1.1 CAM-6

One the first special-purpose computers that was designed specifically to study CA systems and was also one of the first commercially available cellular automata machines (CAMs) was the CAM-6. It was designed and built by Toffoli and Margolus at the MIT Laboratory for Computer Science in the early 1980s [calif87]. A description of CAM-6 as well as an in-depth discussion of the kinds of physical modeling that is possible with it appear in Toffoli’s and Margolus’ excellent book *Cellular Automata Modeling: A New Environment for Modeling* [toff87]. A discussion of an earlier prototype (CAM-5) is described in [toff84b].

While CAM-6 is somewhat limited in its ability to perform large-scale simulations of physical systems (it is a much less capable system than its follow-on, the CAM-8, for example; see discussion below), its fundamental historical importance cannot be overstated. CAM-6 allowed researchers to directly experience, for the first time and in *real time*, the evolution of CA systems theretofore understood only as purely conceptual models. Margolus and Toffoli recall that when Pomeau, one of

the originators of the HPP lattice-gas model (see section 9.2.2), had seen his model running on their CAM-6, the experience had “made him realize that what had been conceived primarily as a *conceptual* model could indeed be turned, by using suitable hardware, into a *computationally accessible* model, and stimulated his interest in finding CA rules which would provide better models of fluids.” [marg90a]

A CAM-6 compatible plug-in board for IBM-PC compatible computers, the CAM-PC, is currently being distributed by *Automatrix, Inc.* of Rexford, NY. Its cost is approximately \$1900. The CAM-6 itself resides as a permanent exhibit at the Boston Computer Museum. A CAM-6 compatible software emulator called CAM-PC has also been developed by members of the *GENOME Project* at Eotvos University in Hungary (see discussion below). A collection of experiments that can be run using the CAM-PC can be downloaded from <http://delta.cs.cinvestav.mx/~mcintosh/oldweb/camex/camex.html>.

Physically, CAM-6 consists of a single plug-in module that fits into an IBM-PC compatible’s 8-bit slot. The control software is written in *Forth* and comes with the hardware. It was designed using a raster display architecture and with an eye towards facilitating the modeling of two-dimensional systems on a square lattice using the (first and second neighbor) *von Neumann* neighborhood. It allows for a 256×256 site “universe” with 4-bits per site[†] and updates the display 60 times per second. For the kinds of experiments that are possible with a CAM-6, its performance is roughly equivalent to that of a CRAY-1 [toff87].

To be a bit more specific about CAM-6’s design, each of its 65536 sites are mapped to individual pixels on a standard RGB monitor, with all 4 bits per site being retrieved in parallel. The array itself is scanned *sequentially* left-to-right and top-to-bottom. While such memory-mapped displays are fairly common, what CAM-6 brings that is new and CA-specific is a *pipeline buffer* that stores the data in a 3×3 site window. This makes all of the necessary neighborhood site values available *simultaneously* to the look-up table processors into which the buffer feeds the information. The output of the table is then written back into memory. Figure A.1 shows a schematic of the basic CAM-6 design.

Notice that CAM-6 is not a fully parallel device, since each site does not have an independent access to the look-up table processor. While the site updating is sequential, however, it is still a very fast time-sharing sequential system. At 60 updates a second, the time-window allotted for the processing of each site is only about 160 ns. It is possible to add external processors such as stand-alone random number generators or larger look-up tables and for linking several CAM-6 modules together,[‡] with the only constraint being that any external signals appropriate for individual sites must arrive within the allotted 160 ns wide “time-window.”

A public domain CAM-6 simulator is available via ftp from <ftp://ftp.lifesci.ucla.edu/pub/alife/public/cam.zip>.

[†]Up to 10 bits per site can be obtained by exploiting the *Margolous neighborhood* (see section 6.4.3).

[‡]By carefully stacking several individual CAM-6 modules, all ostensibly being two-dimensional simulators, a *three-dimensional* system can be modeled.

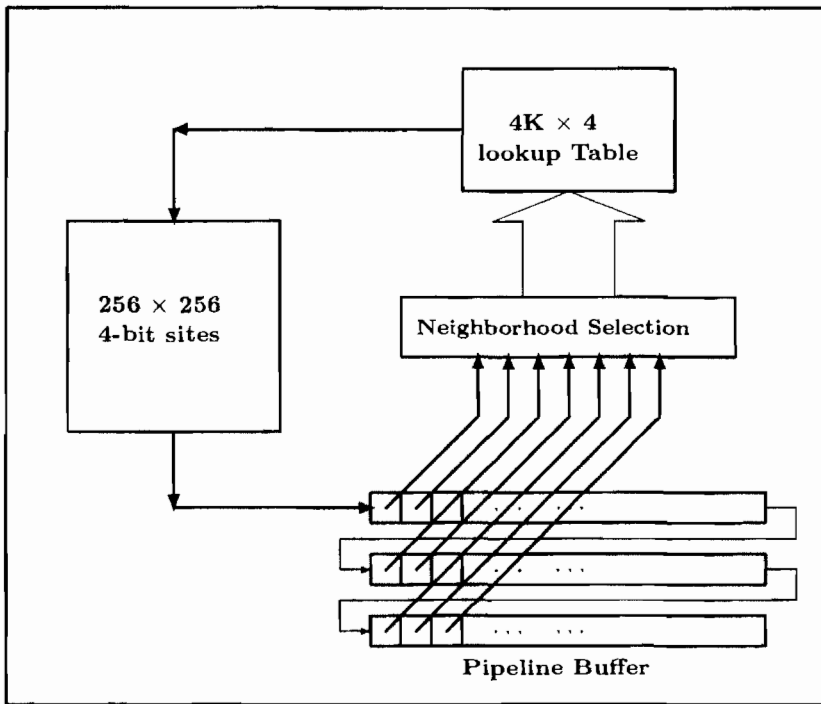


Fig. A.1 Schematic of the CAM-6 design (after figure 1 of [marg90a]).

A.1.2 CAM-8

The most recent incarnation of Toffoli's and Margolous' series of CAMs is the CAM-8, a considerably more powerful and versatile version of the CAM-6 discussed above. Where the CAM-6 is rather limited in its choice of local neighborhoods (it was designed primarily for modeling CA using conventional Moore and von Neumann neighborhoods), the number of bits available for its local state space (four) and the number of dimensions it can simulate, CAM-8 extends the size and speed of CAM-6's calculations by several orders of magnitude and effectively generalizes the notion of a local "neighborhood" to mean any neighborhood consisting of 16 bits selected from any of a few *million* nearest sites. In fact, the CAM-8 can be used to simulate a fully parallel synchronous updating of a system with *billions* of 16-bit sites. The trick is to use many (i.e. thousands) look-up table processors, each of which is shared among a millions sites. The actual computation speed depends on how many sites each processor services. Thus, while the nominal speed is about 25 updates/sec, the update speed can be effectively increased to about 25,000 times/sec by making each processor service only a thousand sites vice a million.

CAM-8 also eliminates CAM-6's need for pipeline buffering (see above) by using *partitioning cellular automata* (see section 8.1.3) as its basic neighborhood structure. Space is effectively subdivided into disjoint subsets of sites and each site is

updated independently of all other sites. In this way, sites can be updated in any desirable order and old values can be immediately replaced with their successors; there is no longer a need to temporally retain site values in a pipeline buffer. Details of the CAM-8 design can be found in [inarg90a] and [toff91].

CAM-8 comes very close to what Toffoli and Margolus call *programmable matter* [toff91]. They define programmable matter as a “three-dimensional, uniformly textured, fine-grained computing ‘medium’ having the following properties:

- It can be assembled into lumps of arbitrary size.
- It can be dynamically driven, in the sense that its dynamical evolution can be started, interrupted, and resumed at any moment in response to the occurrence of specified internal or external events.
- It is totally accessible to real-time observation, analysis and modification.”

More information can be found at MIT’s CAM-8 site: <http://www.im.lcs.mit.edu/cam8/>.

A.1.3 RAP1

The basic architecture of the RAP1 machine, designed by Clouquer and d’Humieres at the Ecole Normale Supérieure in the middle 1980s [clouq87], is very similar to the architecture of the CAM-6. The difference is that while the CAM-6 was designed primarily for simulating CA systems using two-dimensional Moore and von-Neumann neighborhoods, the RAP1 was optimized from the outset for studying lattice-gases.

For example, RAP1 replaces CAM-6’s neighborhood structures with *plane replacements*. Since it is no longer necessary to worry about generic two-dimensional CA neighborhood structures and updates, RAP1 dynamical updates are simplified by having to compute the successor state of a site using only the information at that given site on the previous time step. RAP1’s performance is comparable to that of CRAY-1 (it can process several million sites per second), and it provides a direct visualization of about 50 update steps per second [clouq87].

The actual computation is broken down into two steps: (1) A *Collision Step*, during which the value of a site is sent to a computation look-up table, with its input written to the display screen memory as in CAM-6. RAP1’s screen memory consists of $16\,256 \times 512$ planes. (2) A *Propagation Step*, during which the system is decomposed into a set of one-bit two-dimensional planes (one plane for each bit of each site), and the bits of each site are displaced to one of the site’s neighbors by a translation of the entire plane.

As with CAM-6, there is a provision for effectively enlarging the “size” of the lattice-gas universe by glueing together several RAP1 modules.

A.1.4 Connection Machine

One of the earliest hexagonal lattice-gas simulations of fluid flow [saletn86] was carried out on the Connection Machine (CM), designed by Hillis ([hill82], [hill84], [hill85] and [hill87]; see also [wayn88]).

The CM is a massively parallel-processing computer that consists of anywhere from $2^{12} = 4096$ to $2^{16} = 65536$ processors, each of which has 8192 bytes of memory and is linked with 12 neighbors. In the second generation version (CM-2), each processor can have from $2^{16} = 65536$ to $2^{18} = 262144$ bits of local memory and has its own floating-point chip to execute fast numerics. A conventional front-end computer (a Sun or VAX workstation, for example) is used to precompile a desired program and load the compiled code into the parallel processors. Each time step on a CM consists of a *communications* step between neighboring processors and a *computation* step. Details of its design are given by Hillis [hill85] and Boghosian [bog90b].

For LG simulations, the CM can be configured as a two-dimensional Euclidean plane with links between each processor and its four neighbors. However, the communications step must be specially rigged to simulate a hexagonal grid. Computation speed is on the order of 10^9 sites per second. The 16384-processor version of the latest generation CM, the CM-5, has a main memory of 512 GB and can achieve 2048 GFLOP/sec [hill93] (for comparison, 1 GFLOP/sec is roughly the peak rate attainable of a single processor on a CRAY Y-MP super computer). Interesting discussions of the kinds of computational physics problems that can be solved on the CM appear in [bog90c] and [sim92].

A.2 Software

While serious research of the behavior of CA systems demands the use of dedicated hardware, the often high cost of such hardware sometimes prevents its acquisition, particularly by young researchers and graduate students just entering this field of study. It is therefore important to realize that there are many excellent software-only solutions that can often be used very effectively for research. While the list provided below is by no means exhaustive, it gives some idea of the kind of packages that are currently available either commercially or via anonymous `ftp` over the Internet.

A.2.1 CA Lab

An inexpensive but powerful software package for IBM-PC compatible computers is *CA Lab* by Autodesk, Inc. [ruck89a]. Designed to be used in either text-mode (at 80×25 or 80×100 sites) or graphics-mode (at 320×200 sites and 8-bit color states), *CA Lab* updates the screen at a rate of about 1 screen per second on an AT-class computer and is fully programmable in BASIC, Pascal, C and assembly language. The program comes with a large sampling of predefined rule tables.

CA Lab is now in the public domain (and called *Cellab*) and can be downloaded from a number of sites, such as <http://www.geocities.com/CapeCanaveral/Launchpad/2833/software/cellab.zip> and from <http://www.mathcs.sjsu.edu/faculty/rucker/cellab.htm>.

A.2.2 CAM-PC

CAM-PC is a general purpose CA software simulation environment based on CAM-6. Designed by members of the *GENOME Project* at Eotvos University in Hungary, the first version of CAM-PC extends the possibilities of CAM-6 but is not yet fully compatible with it. The primary addition is support for 8 bit planes, increasing the size of CAM-6's cell-state alphabet to 256. The laudable purpose behind the project is to provide inexpensive but otherwise fully functional simulation tools for amateur researchers unable to afford faster dedicated hardware.

Like CAM-6's underlying control software, CAM-PC is programmed using an interactive FORTH interpreter. Its hardware requirements are modest: an IBM-PC compatible computer, MCGA or VGA display, about 188 KB of free memory to run and about 100 KB of storage space on the hard drive. Future releases will provide for full CAM-6 compatibility and will include a version of the program for Sun workstations. CAM-PC is available by anonymous ftp on the internet: <ftp://ftp.lifesci.ucla.edu/pub/alife/public/cam.zip>.

A.2.3 CAPOW

CAPOW (Cellular Automata & Electric Power) began as a research project headed by Rudy Rucker at San Jose State University. CAPOW runs under windows 95/98/NT and contains a powerful set of visualization tools for studying many different kinds of continuous-valued cellular automata. While designed initially for simulating the flow of electricity in a powergrid, it can be used to simulate a very large set of one-dimensional and two-dimensional cellular automata.

Among its many useful features is the ability to simulate both discrete and continuous CA, run in autorandomize and screensaver modes, display 1D CAs as color spacetime diagrams or as changing graphs, display 2D CAs either as flat color displays or as 3D surfaces in a virtual reality interface, file I/O, interactive seeding, a graph-view mode in which the user can select a sample point in a 1-D CA and track the point as a time-series, and automated *evolution* of CA behaviors.

Details about this powerful program, as well as free run-time versions, can be obtained from the CAPOW web site: <http://www.mathcs.sjsu.edu/capow/index.html>.

A.2.4 CellMaster

CellMaster, by Sinter Software, is an excellent menu-driven CA program for IBM compatibles [cellm90]. It provides for up to a 320×240 cellular space, comes with a large number of predefined rules and sets of initial patterns, and is programmable.

A.2.5 *Cellsim*

Cellsim is a public-domain simulator that runs on both Sun workstations and the CM2 Connection Machine. It is designed to allow the interactive specification, editing, running, and analysis of 1- and 2-D CA's. With the most recent version (2.5), *Cellsim* is now becoming a tool flexible enough to use for the exploration of lattice-based systems in general. Aside from providing simulation of conventional CAs, *Cellsim* allows one to run computed functions of up to 256 states per cell, use floating-point values, or run large ensembles of 1-D systems.

Cellsim's universe consists of a 512×512 array. The program itself is completely menu-driven and includes these features: (1) 256-state "computed-function" rules, in addition to lookup-tables, on both the Sun and CM; (2) creation of look-up tables using Langton's *lambda* parameter (see section 3.2); (3) the ability to save images in Sun raster format; and (4) the ability to generate lookup tables with standalone C code. *Cellsim* can be obtained via anonymous ftp on the Internet to think.com.

A.2.6 *Discrete Dynamics Lab*

A very powerful based CA simulation tool, many years in development, is Andy Wuensch's *Discrete Dynamics Lab* (DDLab). Versions for UNIX/XWindows/Sun, Linux/PC and DOS/PC can be downloaded from <http://www.ddlab.com/>.

DDLab is an interactive graphics program for studying many different kinds of discrete dynamical systems. Arbitrary architectures can be defined, ranging from 1d, 2d or 3d CA to random Boolean networks.

A particular strength of the program is that it can not only generate the usual space-time patterns, but can also run systems *backwards* to produce a predecessor states and thereby reconstruct the branching sub-trees of all ancestor patterns. DDLab also includes extensive provision for making quick on-the-fly changes, as well as collecting and displaying various statistical parameters.

A.2.7 *Fractint*

The IBM compatible public-domain program *Fractint*, created by The Waite Group [weg93], is arguably one of the most powerful fractal-generating programs available. While *Fractint* was designed primarily as a fractal-generating program – it contains built-in code for well over a hundred different types of fractals – its latest version (v20) contains code for generating evolutions of both L-systems[†] and one dimensional CA systems.

Various versions of *Fractint* (DOS, windows, Unix, Linux) can be downloaded from the URL address <http://spanky.triumf.ca/www/FRACTINT/fractint.html>.

[†]L-systems are discussed in chapter 11.

A.2.8 LCAU

LCAU is a set of DOS programs designed to allow the user to explore linear CA. It is accompanied with extensive help (in the form of text files). With LCAU, you can analyze (1) general rules (not just totalistic rules); (2) cell densities and block probabilities are calculated according to mean field theory and local structure theory; and (3) de Bruijn diagrams can be automatically generated. It can be downloaded from <http://delta.cs.cinvestav.mx/~mcintosh/oldweb/software.html> (a NeXTStep version is also available at this site).

A.2.9 Life32

Johan Bontes' Life32 is arguably the best software implementation of Conway's *Life* rule currently available. Its many features include (1) 1 million x 1 million universe; (2) user-definable speed; (3) supports all popular Life file formats: Life 1.05/1.06, RLE, Xlife 2.0, dbLife, ProLife; (4) uses Microsoft DirectX to accelerate drawing; (5) user-definable rules; (6) advanced editing features (cut and paste, drag and drop, etc.); (7) zoom from 10 pixels per cell down to 1/32 sub-pixel. It also includes extensive on-line help. Life32 can be downloaded from <http://psoup.math.wisc.edu/Life32.html>.

There are extensive collections of pre-defined starting patterns that can be used with Life32. Some of the better ones include: (1) Alan Hensel's collection (at <http://www.mindspring.com/~Ealanh/lifep.zip>); (2) David Bell's huge collection of patterns for various evolution rules (<ftp://sunsite.unc.edu/pub/Linux/games/amusements/life/dblifelib-2.tgz>); and (3) Dieter Leithner's collection of the smallest glider guns with period > 1000 (<http://www.mindspring.com/~Ealanh/guns.zip>).

A.2.10 Lifemn

A $k = 2$ two dimensional configurable neighborhood, mouse driven, CA rule explorer program for Windows 95/98 has recently been introduced into the public domain by Ben Schaeffer. It can be downloaded from: <http://www.effectnet.com/bens/lifemn.htm>

A.2.11 MCell

Mirek's Celebration (MCell) is one of the most powerful and complete 32-bit Windows CA programs currently available. With it, the user can explore existing rules (and create new rules) and patterns of 1-D and 2-D Cellular Automata. MCell supports eleven different CA rules: *Life*, *Generations*, *Weighted Life*, *Vote for Life*, *Rules tables*, *Cyclic CA*, *1-D totalistic CA*, *Neumann binary*, *Larger than Life*, *User DLLs*, and *Special rules*. MCell also supports various neighborhoods, including Moore 8 and 9, von Neumann 4 and 5, and allows you to define other neighbourhood ranges and properties. MCell includes many built-in rules, including Conway's

Life, HighLife, Day & Night, Long life, Diamoeba, Fredkin, Vote 4/5, Brian's Brain, Star Wars, RainZha, Swirl, HGlass, Midges, Sticks, Career, Venus, and many more. All rules come with a sampling of predefined initial patterns. MCell, written by Mirek Wojtowicz, can be downloaded from: <http://psoup.math.wisc.edu/mcell/download.html>.

A.2.12 *StarLogo*

StarLogo is a programming environment for exploring the dynamics of decentralized systems. StarLogo can model many real-life phenomena, including bird flocks, traffic jams, ant colonies, and market economies. StarLogo is a specialized version of the Logo programming language. With traditional versions of Logo, one can create drawings and animations by issuing commands to graphic "turtles" on the computer screen. In StarLogo, one can control *thousands* of graphic turtles in parallel. Moreover, StarLogo makes the turtles' world computationally active: *i.e.* one can write programs for thousands of "patches" that make up the turtles' environment. Turtles and patches can then interact with one another. For example, one can program the turtles to "sniff" around the world, and change their behaviors based on what they sense in the patches below. StarLogo is particularly well-suited for artificial-life and cellular-automata projects.

A Mac version of StarLogo (as well as a platform-independent StarLogo written in Java) can be downloaded from <http://starlogo.www.media.mit.edu/people/starlogo/>.

A.2.13 *WinCA*

WinCA is a CA modeling environment for windows developed by Robert Fisch and David Griffieath. Although the program is no longer in development, it is nonetheless quite powerful and is still available for public download from <http://math.wisc.edu/~griffieath/kitchen.html>. It comes with many predefined 2D CA rules and initial patterns. WinCA also allows you to define your own rules, neighborhoods and palettes (supporting 16 and 32 bit color).

A.2.14 *Symbolic Math Packages*

There is an entirely different class of programs from the ones discussed above that are also extremely useful for studying CA systems: namely, symbolic math packages like Wolfram Research, Inc.'s *Mathematica* [wolf91] and Waterloo Maple Software's *Maple V* [char92]. While such programs do not generally provide "fast" simulation environments (remember that these are interpreted-language systems and are by no means optimized for graphics simulation), their symbolic computation capability

provides a powerful tool for studying CA behavior *analytically*.[†] Their integrated graphics/ programming/ symbolic environments actually come close to providing an ideal research environment (particularly if combined with dedicated hardware simulators like the CAM-6).

Both *Mathematica* and *Maple V* run on virtually every available operating system/CPU platform (IBM-PC/DOS, VAX/VMS, Unix, CRAY, etc.). *Mathematica*'s online source of public-domain programs, *Mathsource*, contains a number of useful algorithms dealing with automata, and is readily accessible via ftp and http over the Internet. For example, look at the listings in the *Complexity* section at [http://www.mathsource.com/ Content/ Applications/ Complexity](http://www.mathsource.com/Content/Applications/Complexity). *Mathematica* itself comes bundled with several routines for generating and manipulating both 1D and 2D CA. Gaylord, *et al.* ([gay95] and [gay96]) have extensive collections of *Mathematica* CA source code accompanying their explanatory text.

[†]Anyone who has ever tried to factor a large polynomial over some finite field by hand (such as might be required by problems involving linear rules; see section 5.4), will attest to the welcome power of symbolic math packages.

Appendix B

Complex Systems Theory Resources

Appendix B provides a brief listing of information sources currently available on the World Wide Web (WWW), subject-sorted into a total of 91 WWW Universal Resource Locator (URL) links in 16 categories. Other links and information may be obtained from CA-related newsgroups such as `comp.theory.cell-auto`, `comp.ai`, `comp.ai.alife` and `comp.ai.genetic`. Additional resources may be found at the author's website at the Center for Naval Analyses: <http://www.cna.org/isaac>.

B.1 General Sources

Santa Fe Institute:

<http://www.santafe.edu/>

Complex Systems Research at the Beckman Institute:

<http://www.ccsr.uiuc.edu/>

Complex Systems at Australia National University:

http://life.anu.edu.au:80/complex_systems/complex.html

The Chaos Network, applications of chaos theory to the social sciences:

<http://www-cse.ucsd.edu:80/users/rik/>

Complex Systems Bibliographies:

<ftp://ftp.cs.umanitoba.ca/pub/bibliographies/index.html>

Bibliography of Measures of Complexity:

<http://www.fmb.mmu.ac.uk/bruce/combib>

Complex Adaptive Systems Information:

<http://www.seas.upenn.edu/ale/cplxsys.html>

Principia Cybernetica:

<http://pespmc1.vub.ac.be/>

Complex Systems Information Network:

<http://www.csu.edu.au/complex/compsys.html>

Virtual Library on Complex Systems:

http://life.csu.edu.au/vl_complex/library1.html

B.2 Artificial Intelligence

Artificial Intelligence (Berkley):

<http://www.cs.berkeley.edu/~russell/ai.html>

Artificial Intelligence (Stanford):

<http://www-cs.stanford.edu/profile/ai.html>

Artificial Intelligence (University of Washington):

<http://www.cs.washington.edu/research/projects/ai/www/ai.html>

International's Artificial Intelligence Center:

<http://www.ai.sri.com:80/aic/>

Journal of Artificial Intelligence Research:

<http://www.cs.washington.edu/research/jair/home.html>

Artificial Intelligence (Georgia Institute of Technology):

<http://www.cc.gatech.edu/cogsci/ai.html>

Distributed Artificial Intelligence Laboratory (UMass):

<http://dis.cs.umass.edu/>

B.3 Artificial Life

Adaptive Systems and Artificial Life:

<http://doradus.einet.net/galaxy/Engineering-and-Technology.html>

Philosophy of Artificial Life Bibliography:

http://mugwump.ucsd.edu/bkeele/work-stuff/Alife_Bib.html

Artificial Life Bibliography:

<ftp://cognet.ucla.edu/pub/alife/papers/alife.bib.gz>

A Semi-annotated Artificial Life Bibliography:

<http://www.cogs.susx.ac.uk/users/ezequiel/alife-page/alife.html>

Artificial Life Digest:

<http://www.cogs.susx.ac.uk/users/ezequiel/alife-page/complexity.html>

Fundamental Algorithms of Artificial Life:

<http://alife.santafe.edu/alife/topics/simulators/dret/dret.html>

B.4 Artificial Life Simulation and Research Groups

Links to various Artificial Life Groups:

<http://www.krl.caltech.edu/brown/AL-groups.html>

Autonomous Agents/Alife Group at MIT:

<http://agents.www.media.mit.edu/groups/agents/>

Latent Energy Environments Project:

<http://www-cse.ucsd.edu:80/users/fil/>

The Avida Artificial Life group:

<http://www.krl.caltech.edu/avida/Avida.html>

Distributed Intelligent Agents Group:

<http://ai.eecs.umich.edu/diag/homepage.html>
Autonomous Agents Research Group:
<http://alpha.ces.cwru.edu/pub/agents/home/html>

B.5 Autonomous Agents

Autonomous Agents Group at MIT:
<http://agents.www.media.mit.edu/groups/agents/>
Autonomous Agents Group at Case Western Reserve University:
<http://yuggoth.ces.cwru.edu/>
Research on Autonomous Agents at Stanford:
<http://csli-www.stanford.edu/csli/9394reps/agents9394-nilsson.html>
Software Agents Mailing List:
<http://www.smlt.com/research/tcl/lists/AGENTS/index.html#163>
Autonomous Agents Research at Buffalo:
<http://www.cs.buffalo.edu/~jweber/autoagent.html>
Distributed Intelligent Agents Group at the University of Michigan:
<http://ai.eecs.umich.edu/diag/homepage.html>

B.6 Cellular Automata

Cellular Automata Frequently Asked Questions (FAQ):
<http://alife.santafe.edu/alife/topics/cas/ca-faq/ca-faq.html>
The Cellular Automata Simulation System:
<http://www.cs.runet.edu/~dana/ca/cellular.html>
Cellular Automata Web:
<http://alife.santafe.edu/alife/topics/ca/caweb>
Cellular Automata Bibliography Database:
<http://www.ima.umn.edu/bibtex/ca.bib>
Usenet Cellular Automata Newsgroup:
news:comp.theory.cell-automata
Evolving Cellular Automata:
<http://www.santafe.edu/projects/evca/>
CA Links:
http://psoup.math.wisc.edu/mcell/ca_links.html
CA JAVA applets:
<http://cgi.student.nada.kth.se/cgi-bin/d95-aeh/get/lifeeng>

B.7 Chaos

Applied Chaos Laboratory at Georgia Tech:
<http://acl1.physics.gatech.edu/aclhome.html>
Chaos Bibliography:

<http://www.uni-mainz.de/FB/Physik/Chaos/services.html>
Chaos e-Print Archive at Los Alamos:
<http://xxx.lanl.gov/archive/chao-dyn/>
Chaos Group at the University of Maryland at College Park:
<http://www-chaos.umd.edu/>
The Chaosgruppe (Munich):
http://www.nonlin.tu-muenchen.de/chaos/chaos_e.html

B.8 Fractals

Exploring Chaos and Fractals (MIT):
<http://www.lib.rmit.edu.au/fractals/exploring.html>
Fractals FAQ:
<http://www.cis.ohio-state.edu/hypertext/faq/usenet/fractal-faq/faq.html>
Fractal Images:
<http://www.acm.uiuc.edu:80/rml/Gifs/Fractal/>
Fractal Pictures and Animations:
<http://www.cnam.fr/fractals.html>
Fractal Explorer:
<http://www.vis.colostate.edu/user1209/fractals/index.html>
Fractal Database:
<http://spanky.triumf.ca/>

B.9 Fuzzy Logic

Fuzzy Logic Archive:
<http://www.quadralay.com/www/Fuzzy/Fuzzy.html>
Fuzzy Logic FAQ:
<http://www.cis.ohio-state.edu/hypertext/faq/usenet/fuzzy-logic/part1/faq.html>
Fuzzy Logic Repository:
<ftp://ntia.its.blrdoc.gov/pub/fuzzy>

B.10 Genetic Algorithms

Illinois Genetic Algorithm Repository:
<http://gal4.ge.uiuc.edu/>
Genetic Algorithms FAQ:
<http://www.cs.cmu.edu:8001/afs/cs.cmu.edu/project/ai-repository/ai/html/faqs/genetic/top.html>
Interactive Genetic Art:
<http://robocop.modmath.cs.cmu.edu:8001/htbin/mjwgenformI>
Genetic Music:
<http://nmt.edu/jefu/notes/notes.html>

Genetic Algorithm Digest Archives:

<ftp://ftp.aic.nrl.navy.mil/pub/galist>

Genetic Algorithms Tutorial:

<ftp://129.82.102.183/pub/TechReports/1993/tr-103.ps.Z>

B.11 Genetic Programming

Genetic Programming FAQ:

<http://wwwhost.cc.utexas.edu/cc/staff/mccoy/gp/FAQ-toc.html>

Genetic Programming Tutorial:

http://dcpu1.cs.york.ac.uk:6666/mark/top_ga.html

Genetic Programming in C++ FAQ:

<http://www.salford.ac.uk/docs/depts/eee/gpfaq.html>

Genetic Programming Source at UCL:

http://www.cs.ucl.ac.uk/intelligent_systems/genetic_programming.html

Genetic Programming Bibliography:

<ftp://cs.ucl.ac.uk/genetic/biblio/>

Genetic Programming FTP site:

<ftp://ftp.io.com/pub/genetic-programming>

B.12 Intelligent Software Agents

Software Agents:

<http://hitchhiker.space.lockheed.com/pub/AGENTS/htdocs/agent-home.html>

Intelligent Software Agents Resources:

<http://retriever.cs.umbc.edu:80/agents/>

Intelligent Agents Mailing List (by thread):

<http://www.smlt.com/research/tcl/lists/AGENTS/index.html#163>

MIT Media Lab:

<http://www.media.mit.edu/>

Intelligent Software Agents (University of Maryland Baltimore County) :

<http://www.cs.umbc.edu/agents/>

B.13 Neural Nets

A Basic Introduction To Neural Networks:

<http://ice.gis.uiuc.edu/Neural/neural.html>

An Introduction to Neural Nets:

<http://www.mindspring.com/~zsol/nnintro.html>

Neural Networks FAQ:

http://www.eeb.ele.tue.nl/neural/neural_FAQ.html

Collection of Neural Net Bibliographies:

<http://glimpse.cs.arizona.edu:1994/bib/Neural/>

IEEE Neural Networks Council:

<http://www.ieee.org:80/nnc/index.html>

International Neural Network Society:

<http://sharp.bu.edu/inns/>

B.14 Nonlinear Dynamics

Nonlinear Dynamics Archive:

<ftp://lyapunov.ucsd.edu/pub>

Nonlinear Dynamics e-print Archive at Los Alamos:

<http://xyz.lanl.gov/>

Nonlinear Dynamics and Topological Time Series:

<http://t13.lanl.gov/nxt/intro.html>

Institute of Nonlinear Science at UC San Diego:

<http://inls.ucsd.edu/>

Nonlinear Dynamics at UC Santa Cruz:

<http://noether.ucsc.edu/groups/nonlinear/research.html>

Nonlinear Dynamics Sites:

<http://www.ucl.ac.uk/ucesjph/resources/uk.html>

B.15 Software

Artificial Life Software at Santa Fe Institute:

<http://alife.santafe.edu/alife/software/>

Artificial Life Software Repository:

<http://www.cs.cmu.edu/afs/cs/project/ai-repository/ai/areas/alife/systems/0.html>

Cellular Automata Simulator for PC Windows:

<ftp://ftp.Germany.EU.net/pub/research/softcomp/Alife/rudy-rucker/>

Complex Systems Software Repository at Australian National University:

ftp://life.anu.edu.au/pub/complex_systems

WinLife (a PC Windows implementation John Conway's Life rule):

<ftp://ftp.Germany.EU.net/pub/research/softcomp/Alife/packages/winlife>

WinCA (a fast PC Windows simulator):

<ftp://ftp.Germany.EU.net/pub/research/softcomp/Alife/packages/winca>

PC Windows implementation of Craig Reynolds "Boids":

<ftp://ftp.Germany.EU.net/pub/research/softcomp/Alife/packages/boids/>

B.16 Time Series Analysis

Nonlinear Dynamics and Topological Time Series Analysis Archive:

<http://t13.lanl.gov/nxt/intro.html>

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Index

- 1/f noise, 437, 441
- n -dimensional discrete maps, 203
- “bucket of dust”, 639
- “it from bit”, 640
- Perceptrons* (book), 509
- 3D *Life* rule, 151
 - analogs of 2D *Life* patterns, 154
- abstract automata, 38
 - alphabet, 38
 - formal languages, 38
 - example, 39
 - strings, 38
- ADALINE, 514
- additive invariants, 378
- adjacency matrix, 33
- agent-based models, 564
 - versus traditional AI, 566
- algorithmic complexity, 624
- algorithmic randomness, 624
- algorithmically incompressible, 625
- AND logic gate, 313
- anthropic principle, 685
- area-preserving map, 193
- artificial life, 604, 708
 - combat models, 592
 - Lindenmeyer systems, 576
 - overview, 557
 - SWARM, 568
- associative memory, 518
- autonomous agent, 565
- autoplectic systems, 86
- backpropagation, 540
 - pseudo-code, 544
- Bak, Per, 437
- Baker-Campbell-Hausdorff series, 653
- basin complexity, 272
- BBMCA rule, 321
- Bell’s theorem, 677
- Belousov-Zhabotinski Reaction, 15, 419, 612, 630
- Bernoulli shift map, 172
- Billiard-Ball model (BBM), 317, 673, 681
- black holes, 636
- block blentropy, 216
- block probability, 217, 249, 720
- blocking transformation, 66, 70
- boids, 561
- Boltzman distribution, 326
- Boltzman’s equation, 459, 475, 494
- Boltzman’s H-theorem, 459, 479
- Boolean function, 312, 429, 430, 516
- Boolean logic gate, 318
- Boolean satisfiability, 624
- bottom-up, 558
- boundary conditions, 41
- box-counting algorithm, 213
- Brillouin, Louis, 310
- busy beaver function, 681
- CA and formal languages, 298
- CA lab, 717
- CA models of combat, 457
- CA Over $\mathcal{F}_p$ (p Prime), 245
- CA phase space, 46, 215
- CA simulations of spin models, 358
- CA-based cosmogony?, 694
- CA-like representation of real-valued maps, 198

- CAM-6, 128, 510, 713
- CAM-8, 714
- CAM-PC, 718
- canonical distribution, 385
- Cantor set, 26, 47
- Cantor's diagonal argument, 24
- CAPOW, 718
- Capra, Fritjof, 608
- cardinality, 23
- Cartesian product, 23
- CellMaster, 718
- Cellsim, 718
- cellular automata, 4
 - collective behaviors, 16
 - computation, 6
 - Conway's *Life* example (short), 13
 - embodiments of paradigm shift, 608
 - finite lattice dynamics, 47, 75
 - formal language theory, 298
 - fundamental physics, 9
 - lattice-gas example, 15
 - one-dimensional examples, 9
 - pattern formation, 8
 - powerful computational engines, 7
 - simulation tools, 8
 - topological characterization, 46
 - why study CA?, 7
 - Wolfram's behavioral classification, 98
- chaos, 167, 172, 177, 182, 192, 204, 390
- chaotic attractors, 175
- Chapman-Enskog expansion, 497
- Chomsky language hierarchy, 294
- Church's theorem, 679
- Church-Turing thesis, 682
- circle map, 387, 397
- circulant matrix, 237
- collective sorting, 561
- collectivism, 609
- color plates, 156
- combat models, 592
- combinatorial hierarchy, 641
- complex systems, 2, 611
 - chronology, 3
 - on-line resources, 722
- complexity, 611
 - algorithmic complexity, 624
 - as information, 615
 - computational complexity, 623
 - dynamic complexity, 614
 - graph complexity, 616
 - hierarchical systems, 620
 - logical depth, 626
 - simplicial complex, 619
 - static complexity, 614
 - thermodynamic depth, 627
 - topological complexity, 617
- complexity engineering, 248
- complexity science, 607, 611, 629
- computability, 176, 624
- computability and physics, 678
- computation and phase transitions, 682
- computational complexity, 623
- computational irreducibility, 680
- connected graph, 32
- connection machine, 716
- conservative logic circuits, 315
- context-free grammar, 296
- context-free languages, 296
- continuity equation, 465, 482, 496
- Conway's *Life* Rule, 3, 13, 129, 631, 720
 - proof of universality, 141
 - stochastic version, 363
 - three-dimensional version, 151
 - What's so Special About *Life*?, 131
 - zoology, 132
 - eaters, 136
 - flotillas, 136
 - garden-of-Eden configurations, 136
 - glider shuttle, 136
 - glider-glider collisions, 136
 - gliders, 135
 - puffer trains, guns and breeders, 138
 - R-pentomino, 135
 - simple seeds, 133
 - spaceships, 135
- Conway, John, 3, 6
- cooperative structures, 581
- correlation dimension, D_C , 211
- correlation function, 73, 334, 442
- coupled-map lattices, 51, 386
 - CA approximations, 401
 - first-order, 404
 - higher-order approximations, 405
- entropy, 395
- homogeneous solutions, 387
- inhomogeneous initial states, 388
- logistic equation, 443
- pattern distribution, 394
- quantitative measures, 393

- coupler link rules (for SDCA), 444
- Creutz's demons, 361
- critical behavior, 325, 344
- critical exponents, 329, 346
- cubic lattice, 151
- cycle length, 243
- cyclic CA, 158
- cyclic states, 280, 288
- cyclotomic polynomial, 243

- decoupler link rules (for SDCA), 444
- DeMorgan laws, 23
- descendent forcing structures, 433
- detailed balance, 328, 353–355
- deterministic finite automaton (DFA), 300
- deterministic randomness, 175
- difference patterns, 64
- difference space-time pattern
 - spreading rate, 100
- digital mechanics, 639, 666
- DIL systems, 579
- dimensional shadowing, 649
- dimer problem, 270
- discrete dynamics lab, 719
- discrete Green function, 64
- discrete physics, 610, 638
- discrete space-time, 653, 663, 688
- dissipative systems, 170
- DOL systems, 576
- Dresden, Max, xxiii, 460
- dynamical entropy, 396
- dynamical rules
 - additive rules, 45
 - aditive rules, 48
 - BBMCA rule, 321
 - billiard-ball rule, 320
 - brain CA, 162
 - CCA rule, 158
 - chaotic, 102
 - critical rules, 406
 - deduction of properties, 225
 - dependence on lattice topology, 107, 259
 - [3 : 3 : 3] profiles, 112, 114
 - general solution in $\mathcal{F}[q]$, 261
 - natural topology, 260
 - simplifications in $\mathcal{F}[2]$, 269
 - faders CA, 163
 - hodgepodge rule, 159
 - legal rules, 44
 - majority rules, 280
 - minimally diluted deterministic rules, 355
 - multithreshold rules, 284
 - notation, 40
 - nucleating rules, 125
 - outer-totalistic rules, 45
 - parity rule FA, 92
 - Park's glider-gun, 91
 - percolating rules, 125
 - reversible rules, 50
 - rule codes, 44
 - rule composition, 43
 - rule R110, 661
 - rule R150, 56
 - rule R178, 298
 - rule R18, 68, 236
 - rule R30, 84
 - rule R90, 55, 238
 - state transition graph, 298
 - stepping stone CA, 160
 - totalistic rules, 44
 - traffic CA, 157
 - voting rules, 124
- dynamical system theory, 167
 - Bernoulli shift map, 172
 - conservative systems, 171
 - integrability, 188
 - phase portraits, 190
 - standard map, 193
 - dissipative systems, 170
 - Hénon map, 184
 - Hamiltonian systems, 171
 - invariant measures, 207
 - logistic map, 177
 - Lyapunov exponents, 201
- edge-of-chaos, 106, 562, 683
- effective dimensionality, D_{effec} , 455
- effective-measure complexity, 219
- EINSTEIN combat model, 592
- Einstein, Podolsky and Rosen (EPR) paradox, 677
- elementary CA, 71
 - finite lattices, 75
 - global properties, 75
 - cyclic states, 76
 - entropy, 80
 - Garden-of-Eden states, 76
 - stability, 79

- statistical ensembles, 80
 - transient states, 76
- infinite lattices, 82
- local properties, 71
 - correlation function, 73
 - density, 71
 - mean-field approximation of
 - density, 73
- rule R110, 87, 661
- rule R150, 56
- rule R18, 68
- rule R22, 83
- rule R30, 84
- rule R90, 55
- elliptic points, 191
- emergence, 14, 400, 560, 606, 628, 631
- encryption, 95
- entropy, 100, 302, 637
 - dynamical entropy, 396
 - formal language theory, 302
 - pattern entropy, 395
- enumeration of limit cycles, 233
- Euler totient function, 243
- Euler's equation, 465, 482, 496
- extension field, 242
- feedback catastrophe, 359
- feedback shift register, 45, 236
- Feigenbaum constant, 182
- Feigenbaum, Mitchell, 177, 181
- field theory, 647
 - reformulated as a CA: I, 648
 - reformulated as a CA: II, 651
 - reformulated as a CA: III, 654
- fields, 36
- filter automata, 92
 - parity rule, 92
- finite automata, 38, 294
- finite lattice dynamics, 47, 75
- Fisher information, 646
- fitness landscape, 585
- flicker noise, 442
- fluid dynamics, 463
- forcing loops, 433
- forcing structures, 432
- formal language theory, 292
 - pumping lemma, 304
- fractal dimension, D_F , 26, 210
- fractals, 25
- Fredkin logic gate, 314, 673
- Fredkin reversibility, 94
- Fredkin's billiard-ball gas model, 317
- Fredkin, Ed, 94, 313, 665
- free energy, 327, 331, 336
- Frieden, Roy, 646
- Frobenius-Perron construction, 208
- frustration, 337, 431
- garbage bits, 315
- garden-of-Eden configurations, 48, 136
- generalized fractal dimensions, 212
- generalized threshold automata, 274
- genetic algorithms, 583
 - building-block hypothesis, 589
 - CA rule extraction, 591
 - example, 588
- genetic operators, 584
- geometrodynamics, 688
- Gödel's incompleteness theorem, 625, 632, 679
- graph theory, 30, 616
 - adjacency matrix, 33
 - automorphism, 617
 - complexity of a graph, 616
 - examples, 32
 - incidence matrix, 34
 - random graphs, 34
 - trees, 48
- Greenberg-Hastings model, 420
- groups, 35
- Hénon map, 184
- Halting theorem, 131
- halting theorem, 3, 679, 684
- Hamiltonian graph, 32
- Hamiltonian systems, 167, 171, 188
- Hamming distance, 79
- harmonic oscillator, 189
- heat-conduction equation, 485
- hexagonal lattice, 494
- hierarchical structures, 443, 620
- hodgepodge rule, 159, 422
- homoclinic points, 192
- homogeneous functions, 330
- homogeneous states, 231
- immunology, 425
- implicit deterministic structures, 228
- incidence matrix, 34
- infin, 645

- information capacity, 28
- information dimension, D_I , 210
- information mechanics, 643
- information physics, 634, 643
- information theory, 27, 603
 - Fisher information, 646
 - graph complexity, 616
 - mutual information, 104
 - Shannon information, 616
 - thermodynamics, 634
- input-free modular systems, 261
- intermittency, 397, 442, 475
- invariance matrix, 233
- invariant measures, 207
- invertibility versus time-reversal
 - invariance, 369
- irreversibility, 48, 60, 75, 82, 94, 170, 177, 188, 216, 311, 313, 372, 462, 634, 672
- irreversible rules, 48, 216
- ISAAC combat model, 592
- Ising model, 332, 358
 - mean-field approximation, 336
 - one-dimensional, 334
- isotropic growth, 161
- isotropic peripheral PCA, 354

- Kac-ring model, 458
 - origins of irreversibility, 462
- KAM theorem, 190
- KAM torus, 192
- Kauffman, Stuart, 3, 51, 429, 560, 563, 586
- kink diffusion, 391
- kink-annihilation, 68
- kink-antikink structures, 391
- Koch curve, 27
- Kolmogorov's theorem, 548
- Kolmogorov-Sinai entropy, 213
- Korteweg-de Vries equation, 92

- Landauer, Rolf, 311, 672
- Langton's λ Parameter, 98
- Langton's λ parameter, 683
- Langton's self-reproducing loop, 573
- Langton's self-reproducing loop, 164
- Langton's vants, 580
- Langton, Chris, 562, 683, 684
- lattice gas computers, 502
- lattice gas models
 - discrete systems, 486
 - equations for macroscopic behavior, 493
 - FHP model, 492
 - HPP model, 489, 714
 - short history, 488
- Laypunov functions, 275
- LCAU, 719
- Life32, 720
- limit cycles, 233
- Lindenmeyer systems, 576, 719
- linear PCA, 351
- linear peripheral CA, 351
- local conservation laws, 95, 383
- local structure theory (LST), 98, 247, 363
 - 0th-order LST, 253
 - 1st-order LST, 254
 - 2nd-order LST, 255
 - N^{th} -order LST, 256
 - Bayesian extension, 250
 - block probability functions, 249
 - CA action on probability measures, 249
 - local structure operator, 251
 - LST for d -dimensional lattices, $d > 1$, 258
- local versus global, 558
- localized demons, 361
- logic gates, 144, 311, 312
 - reversible, 313
- logical depth, 626
- logistic map, 177, 389
 - fixed-point solutions, 178
 - limit cycles, 180
 - universality, 181
- Louville's theorem, 476
- Lyapunov dimension, 213
- Lyapunov exponents, 201
 - CA analogs, 206
 - information-theoretic interpretation, 205
- Lyapunov functions, 521
 - threshold CA rules, 274

- majority rules, 280
- MapleV, 722
- marginal stability, 406
- Margolus, 129, 317, 375, 676, 713
- Margolus neighborhood, 320
- Mathematica, 722
- Maxwell's demon, 310, 635
- Maxwell-Boltzman distribution, 483
- McCulloch-Pitts artificial neuron, 510

- mean-field approximation, 101, 530
- mean-field theory, 338, 349, 358
- measure entropy, 215
- metastability, 528
- metric entropy, 213
- metric function, 24
- metrizability, 25
- Metropolis algorithm, 359
- microcanonical ensemble, 35, 359
- microscopic reversibility, 354
- minimal basis, 313
- minimal DFA, 300
- minimization algorithm, 300
- Minsky, Marvin, 509, 662
- Mobile CA, 457
- Moebius function, 243
- molecular chaos, 495
- momentum flux tensor, 466
- Monte Carlo dynamics, 328
- Moore neighborhood, 49
- multi-layered perceptrons, 536, 550
- multithreshold rules, 284
- Myhill-Nerode theorem, 300

- N-k landscapes, 430, 586
- NAND logic gate, 313
- natural topology, 107
- Navier-Stokes equations, 466, 483, 500
- NETtalk, 552
- neural networks
 - ADALINE, 514
 - adaptive resonance, 555
 - biological origins, 510
 - Boltzman machines, 531
 - learning rule, 534
 - connection with CA, 508
 - Hebbian learning rule, 512
 - Hopfield model, 518
 - capacity, 524
 - energy function, 520
 - learning rule, 522
 - pseudo-code, 527
 - spurious attractors, 524
 - McCulloch-Pitts model, 511
 - model development, 546
 - NETtalk, 552
 - overview, 507
 - stochastic models, 528
 - supervised learning, 555
- Noether's theorem, 378

- non-homogeneous CA, 51
- non-monotonic behavior, 598
- noncomputability, 681
- NP-complete problem, 532, 624

- one-dimensional CA, 41, 53
 - algebraic properties
 - cycle length distribution, 242
 - algebraic properties, 237
 - rule R90, 238
 - blocked space-time patterns, 70
 - blocking transformations, 66
 - critical-like behavior, 86
 - filter automata, 92
 - langton's λ parameter, 98
 - legal rules, 44
 - majority rules, 280
 - notation, 41
 - parity rule FA, 92
 - Park's glider-gun, 91
 - particle-like behavior, 87
 - reversible rules, 94
 - rule codes, 44
 - rule R110, 661
 - rule R150, 56
 - rule R18, 68
 - rule R90, 55
 - rule-space parameterization, 98
 - sandpile model, 438
 - solitons, 91
 - space-time patterns, 53
 - behavioral classes, 63
 - difference plots, 64
 - irregular growth, 59
 - random seeds, 59
 - simple seeds, 54
 - spatial and temporal measure
 - dimensions, 223
 - totalistic rule T20 ($r=2$), 89
 - totalistic rule T88 ($r=3$), 89
 - Wolfram's behavioral classification, 98
- one-dimensional random walk, 670
- order parameter, 339

- parable, 661
- parse trees, 297
- partition function, 326, 333, 530
- partitioning CA, 374, 715
- pattern entropy, 395
- perceptrons, 512

- learning rule, 514
- multi-layered, 536
- percolation, 332, 344, 355, 433
- period doubling, 184, 185, 357, 389
- periodicity of temporal sequences, 229
- peripheral PCA, 345
 - isotropic, 354
- peripheral probabilistic CA, 345
- phase space, 170, 211
- phase transition, 98, 325, 332, 346, 355, 357, 531, 691
- physical entropy, 626
- physics and information, 608, 632
- Poincaré Maps, 168
- Pomeau-Manneville intermittency, 397
- power spectra, 304, 394
 - Li's algorithm, 306
 - sandpile models, 441
- predictability, 175
- pregeometry, 639
- probabilistic CA, 50
- programmable matter, 713
- PSPACE-complete problem, 624
- pullback-technique, 203
- pumping lemma, 304
- push-down automata, 296
- quantum CA, 51, 406
 - QCA-I, 407
 - QCA-II, 411
- quantum measurement problem, 635
- quantum mechanical computers, 673
- Rényi entropy, 218
- Rényi information, 212
- random Boolean networks, 429
- random graphs, 34, 654
- random mappings, 435
- RAP1, 510, 716
- rational canonical form, 263
- reaction-diffusion systems, 419
- recursive growth models, 577
- reductionism, 608
- regular language complexity, 302
- regular languages, 293
- replica method, 338
- restricted totalistic rules, 446
- reversible CA, 94, 369, 606, 652
 - elementary reversible CA (ERCA), 376
 - historical overview, 371
 - synthesis techniques, 372
 - conserved landscape permutations, 374
 - Fredkin's construction, 374
 - partitioning, 375
- reversible computation, 50, 309, 315, 638
 - Feynman's challenge, 638
- reversible computers, 672
- reversible logic circuit, 316
- reversible logic gate, 313, 674
- reversible rules, 50, 94
- Reynold's number, 469
 - scaling, 505
- rings, 36
- roots of unity, 243
- sandpile CA model, 437
 - d-dimensional, 440
 - one-dimensional, 438
 - power-law scaling, 441
- Santa Fe Institute, 4, 607
- scalar fields, 657
- scale invariance, 55
- scaling behavior, 177
- scaling hypothesis, 330
- SDCA model, 444
- second law of thermodynamics, 559
- self organization, 8, 95, 559, 609, 692
- self organized criticality, 437, 441
- self similarity, 27
- self-reproducing automata, 570
- sequential updating, 285
- set theory, 21
- Shannon information, 29
- shift operator, 47
- shift transformations, 236
- simplicial complex, 619, 659
- simulated annealing, 532
- Smith canonical form, 263
- soliton collision theorem, 93
- solitons, 64, 91, 399
- Solomonov-Kolmogorov-Chaitin complexity, 624
- spatial block entropy, 83
- spatial domain structures, 390
- spatial set entropy, 215
- spatio-temporal intermittency, 397
- spatio-temporal measures for infinite lattices, 221
- spin glasses, 286, 337, 519

- equivalence with probabilistic CA, 341
- spinodal point, 128
- splitting field, 243
- standard map, 192
 - sample trajectories, 194
- state transition graph, 48, 81, 241, 295
- stochastic dynamics, 327
- stochastic neural nets, 531
- strange attractors, 171
 - 2D examples, 187
- structurally dynamic cellular automata (SDCA), 51, 443, 694
 - example, 447
 - neighborhood partitioning, 446
 - patterns, 451
- surface tension, 129
- SWARM system, 568
- symbolic dynamics, 195
- thermodynamic behavior, 385
- thermodynamic depth, 627
- threshold automata, 274
- time-reversal invariance, 94
- Toffoli, Tom, 4, 94, 129, 317, 610, 669, 713
- top-down, 558
- topological characterization of CA, 46
- topological dimension, 26
- topology (on a set), 24
- toss model, 363
- totalistic PCA, 348, 352
- totalistic peripheral CA, 348
- traffic CA, 157
- transfer matrix, 335
- TRANSIM, 566
- transitional lattice construction, 110
- turbulence, 399, 470
 - Feigenbaum route, 475
 - Landau-Hopf route, 472
 - Pomeau-Manneville route, 474
 - routes to turbulence, 472
 - Ruelle-Takens-Newhouse route, 473
- Turing machine, 149, 293, 679
- Turing's theorem, 3
- Turing's *Halting theorem*, 679
- turtle graphics, 579
- two-dimensional CA, 48, 116
 - combat models, 457
 - Conway's *Life* rule, 129
 - Greenberg-Hastings model, 420
 - hodgepodge rule, 422
 - infinite systems, 128
 - majority rules, 281
 - nucleating rules, 125
 - percolating rules, 125
 - random seeds, 123
 - simple seeds, 119
 - voting rules, 124
- ugly-duckling theorem, 629, 700
- ultrametric distribution, 339, 621
- undecidability, 684
- universal computation, 89, 141
- universal computer, 6, 293, 316, 624
- universal logic gates, 312
- universal reversible logic gate, 313
- universality, 50, 60, 69, 329
- universe as CA, 660
 - speculations I (Minsky), 662
 - speculations II (Zuse), 664
 - speculations III (Fredkin), 665
- virtual ants (vants), 580
- von Neumann, xxviii, 3, 4, 310, 570
- von Neumann neighborhood, 49
- voting rules, 128
- WinCA, 721
- Wolfram's behavioral classification, 63, 98, 683
 - local structure theory alternative, 247
 - refinement due to Culik and Dube, 64
- Wolfram, Stephen, xxvii, xxviii, 1, 3, 4, 47, 53, 91, 118, 161, 678, 680
- XOR function, 537
- XOR problem, 515, 548