

Continuum percolation threshold for interpenetrating squares and cubes

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Monte Carlo simulations are performed to determine the critical percolation threshold for interpenetrating square objects in two dimensions and cubic objects in three dimensions. Simulations are performed for two cases: (i) objects whose edges are aligned parallel to one another and (ii) randomly oriented objects. For squares whose edges are aligned, the critical area fraction at the percolation threshold $\phi_c = 0.6666 \pm 0.0004$, while for randomly oriented squares $\phi_c = 0.6254 \pm 0.0002$, 6% smaller. For cubes whose edges are aligned, the critical volume fraction at the percolation threshold $\phi_c = 0.2773 \pm 0.0002$, while for randomly oriented cubes $\phi_c = 0.2168 \pm 0.0002$, 22% smaller.

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I. INTRODUCTION

Lattice percolation is often used for the statistical modeling of transport in porous media [1–4]. The requirement that sites, and the bonds between them, be constrained to a fixed lattice may not, however, be an appropriate model for natural porous media [1–4]. The characteristics of site and bond percolation potentially limit their applicability to modeling of natural phenomena such as oil and groundwater flow and extraction of melt from super-solidus regions deep inside a planetary body.

Continuum percolation offers two advantages for describing porous media.

(i) The objects that form clusters are not restricted to points on a fixed lattice; they can be placed anywhere within the volume studied and either be barred from interpenetration or allowed to interpenetrate, i.e., they can have either “hard” or “soft” cores [4]. Because of the freedom of placement inside the system, the connections between soft core objects can range from very small to very large, depending upon the extent of interpenetration.

(ii) The objects can be of any shape. In two dimensions the continuum percolation of discs is often investigated [2,4]. In most studies of continuum percolation in three dimensions, spheres are used as the objects, leading to the “Swiss cheese” nomenclature for continuum percolation [2,4]. Other frequently used shapes are rods and ellipsoids of revolution [5]. In a few cases, the continuum percolation of cubes has been considered [6].

Here we determine the threshold for continuum percolation of soft core squares in two dimensions (2D) and cubes in three dimensions (3D) whose edges are aligned parallel to, or oriented at random angles to, the axes of the system. Continuum percolation is believed to belong to the same universality class as site and bond percolation [7,8]; once we have determined the continuum threshold for an object of a specific shape, we can apply many of the characteristics of site and bond percolation, e.g., critical exponents, to describe the continuum percolation cluster.

II. METHODS

We construct 2D and 3D Monte Carlo simulations for the determination of the percolation threshold based upon the

Leath method [9] and the methods Lorenz and Ziff [10] used in their study of the continuum percolation of spheres.

We perform 2D simulations with squares whose edges are of unit length. In 3D we perform simulations with cubes of three different edge lengths: $1/\sqrt{3}$, 0.75, and 1.0; the length L of each axis of the simulation box in the 2D simulations is 301, and in 3D is 101 in simulations using cubes with edge lengths of $1/\sqrt{3}$ and 0.75, and is 161 in simulations with the unit cube [11]. We subdivide the system into either a 2D or 3D grid of unit area squares or unit volume cubes; an illustrative 12×12 2D version of our system is shown in Fig. 1.

The cluster begins in the center grid volume and objects are added to it based upon a Poisson distribution centered about the average number of objects per unit area or volume, N/L^d , chosen for the simulation of dimension d [10]. The product of this value and the individual object’s area or volume, v , is the reduced number density

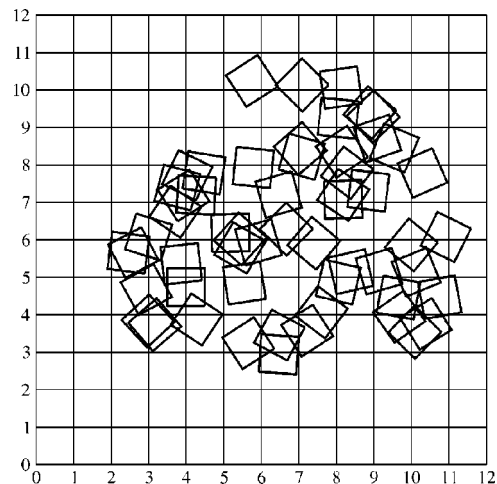


FIG. 1. Two-dimensional, 12×12 example of a percolation cluster of unit-length square objects (thick lines) for the case of randomly oriented squares. The system is divided by a series of grid lines (thin lines) that create unit areas in this 2D system. Note that the upper two objects of the cluster in the center of the system intersect each other even though their centers are placed in next-nearest-neighbor areas of the grid. The real 2D and 3D systems of our study are much larger than this system.

$$\eta \equiv \frac{vN}{L^d}. \quad (1)$$

If the number of objects n generated from the Poisson distribution is nonzero, then these n objects are placed at random locations inside the grid volume. To fix the orientation of each individual object, random numbers are generated to determine the one angle of rotation in the 2D simulations and the three Euler angles of rotation in the 3D simulations. The one angle in 2D and two of the angles in 3D vary from 0 to 2π and are drawn from a uniform distribution. The third angle in 3D varies between 0 and π and is drawn from a cosine distribution in order to yield an isotropic distribution of orientations. The locations of the 4 (2D) or 8 (3D) corners and the center of each object are stored in a data structure, along with a flag indicating that the grid area (2D) or volume (3D) was visited and populated during the realization. The nearest neighbors and next-nearest neighbors of this grid area or volume are then populated in a similar manner and the intersection between squares or cubes is tested.

To determine whether or not two squares intersect, we choose one square in the cluster as the reference square and another square in the simulation as the test square. We use an algorithm for the intersection of two lines [12] to test if any of the four edges of the reference square intersect the four edges of the test square. To determine if two cubes intersect, we choose one cube in the cluster as the reference cube and another in the simulation as the test cube. We use an algorithm for the intersection of a line and a facet [13] to test if any of the edges of the reference cube intersect the faces of the test cube. In this algorithm, the location of each of the 12 edges of the reference cube are compared to the location of the 12 triangular facets that describe the locations of all faces on the test cube using the corners and diagonal of each face. If the test object intersects the reference object, it is added to the growing cluster. This process is repeated for each new square or cube added to the system until the cluster can no longer grow. Intersections between squares or cubes in grid areas or volumes up to two units away can occur for edge lengths 0.75 and 1, as exemplified in 2D for squares of unit edge (Fig. 1), but cubes of edge $1/\sqrt{3}$ can only intersect if they are in the same or neighboring volumes of the grid, which reduces the number of grid volumes that must be checked for cube overlap in simulations with cubes of this smallest size.

The cumulative distribution of cluster sizes is calculated from the cluster size of each realization, s , by binning the cluster sizes such that all bins in the range of 2^0 to $2^{s+1} - 1$ are incremented by 1. In order to estimate finite-size effects of the simulation, objects in each cluster are tested to determine whether they touch the edge of the simulation. If so, the cluster size is compared to the smallest cluster size in previous realizations that touch the edge and the smaller value is stored. Bins of sizes greater than the smallest cluster that touched the edge of the system are not used in the determination of the percolation threshold.

At the end of the simulation, the value of each bin is divided by the number of realizations, from 10 000 to 50 000,

to yield the probability of achieving a cluster of size s , $P(s|\eta)$, for a given value of η . Power law behavior of the probability as a function of the bin size is interpreted to indicate the critical percolation threshold $\eta = \eta_c$ [2,4]. To accurately determine the threshold, we follow the techniques of Ref. [10]. The probability of generating a cluster size greater than s at a specified η is [2,4]

$$P(s|\eta) \sim A s^{2-\tau} f[(\eta - \eta_c) s^\sigma], \quad (2)$$

where both τ and σ are universal exponents and A is a non-universal constant. In 2D the values of these exponents are 187/91 and 36/91 [4], respectively. In 3D the values of τ and σ are $2.189\,06 \pm 0.000\,06$ and 0.4522 ± 0.0008 , respectively [14]. Near the percolation threshold the scaling function $f(x)$ can be expanded in a Taylor series:

$$f(x) = 1 + Bx + \mathcal{O}(x^2). \quad (3)$$

Combining Eqs. (2) and (3),

$$P(s|\eta) s^{\tau-2} \sim A + AB(\eta - \eta_c) s^\sigma + \dots, \quad (4)$$

which demonstrates that $P(s|\eta) s^{\tau-2}$ becomes constant at the percolation threshold as s becomes asymptotically large.

III. RESULTS

The percolation threshold can be expressed as either the critical reduced number density, η_c , or the critical area (or volume) fraction, ϕ_c , which are related to each other by [15]

$$\phi_c = 1 - e^{-\eta_c}. \quad (5)$$

A. Two dimensions

For square objects aligned parallel to each other in the 2D system we find

$$\eta_c = 1.098 \pm 0.001 \quad (6a)$$

or, from (5),

$$\phi_c = 0.6666 \pm 0.0004 \quad (6b)$$

[see Fig. 2(a)]. Our value of ϕ_c is within the error bars of two previous determinations by Monte Carlo techniques, where $\phi_c = 0.668 \pm 0.003$ [16] and $\phi_c = 0.65 \pm 0.02$ [17]. However, our determination of ϕ_c is slightly lower than that calculated in [6], whose Monte Carlo simulations produced $\phi_c = 0.6753 \pm 0.0008$, and whose application of the direct-connectedness expansion method yielded $\phi_c = 0.6912$. In contrast, our value of ϕ_c is significantly higher than the experimental one of [18] whose average for nine trials is $\phi_c = 0.613 \pm 0.013$.

We find that for randomly oriented square objects in 2D,

$$\eta_c = 0.9819 \pm 0.0006 \quad (7a)$$

or

$$\phi_c = 0.6254 \pm 0.0002 \quad (7b)$$

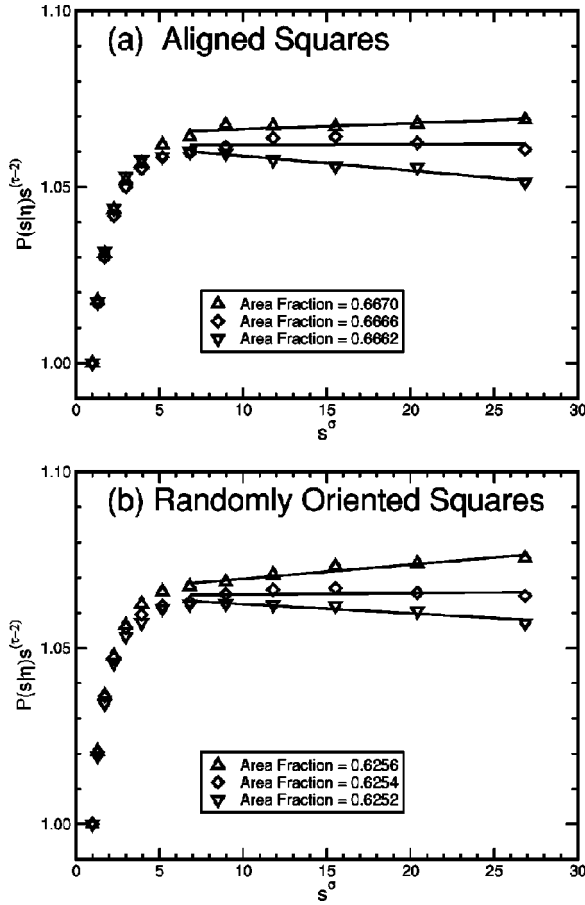


FIG. 2. Power-law scaled plots for determination of percolation threshold for squares of unit size in a 301×301 system based upon 50 000 realizations at each area fraction. At the threshold $\eta = \eta_c$, $P(s|\eta)s^{\tau-2}$ is independent of s^σ , which allows for accurate determination of η_c , which is related to ϕ_c by Eq. (5). (a) Squares whose edges are aligned parallel to each other, for which case we estimate $\eta_c = 1.098 \pm 0.001$, so $\phi_c = 0.6666 \pm 0.0004$ by Eq. (5). (b) Squares that are randomly oriented as shown in Fig. 1, for which we estimate $\eta_c = 0.9819 \pm 0.0006$, so $\phi_c = 0.6254 \pm 0.0002$.

[see Fig. 2(b)].

These values for the continuum percolation threshold for aligned and randomly oriented squares are lower than for discs, $\phi_c = 0.676339 \pm 0.000004$ [19], by a maximum of $\approx 1\%$ for aligned squares and $\approx 7\%$ for randomly oriented squares. We attribute the significant difference in ϕ_c between discs and randomly oriented squares to the possibility of randomly oriented squares intersecting other squares whose centers are located at distances up to the diagonal length of the square (see Fig. 1), whereas two discs can only intersect if their centers are no further than one diameter away from each other. The similarity of ϕ_c for aligned squares and discs may occur because both objects only have the potential to intersect other objects whose centers are separated by at most either the edge length of the square or the diameter of the disc.

B. Three dimensions

For cubic objects aligned parallel to each other in the 3D system,

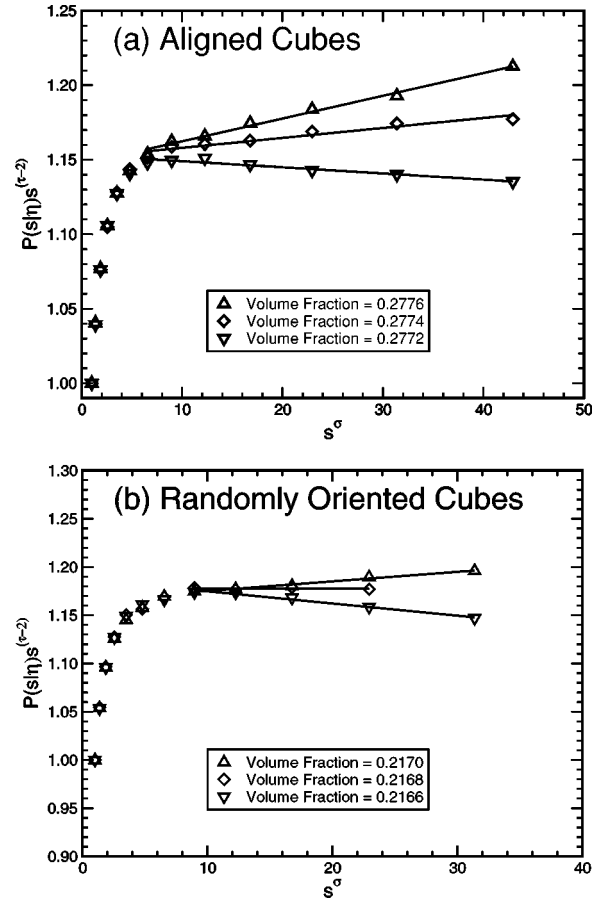


FIG. 3. Power-law scaled plots for determination of percolation threshold for cubes of unit size in a $161 \times 161 \times 161$ 3D system based upon 50 000 realizations for each volume fraction. At the threshold $\eta = \eta_c$, $P(s|\eta)s^{\tau-2}$ is independent of s^σ , which allows for accurate determination of η_c , which is related to ϕ_c by Eq. (5). (a) Cubes whose faces are aligned parallel to each other, for which case we estimate $\eta_c = 0.3248 \pm 0.0003$, so by (5) $\phi_c = 0.2773 \pm 0.0002$. (b) Cubes that are randomly oriented, for which we estimate $\eta_c = 0.2444 \pm 0.0003$, so $\phi_c = 0.2168 \pm 0.0002$.

$$\eta_c = 0.3248 \pm 0.0003 \quad (8a)$$

or

$$\phi_c = 0.2773 \pm 0.0002 \quad (8b)$$

[see Fig. 3(a)]. The precision of this result is greater than the most precise previous determination $\phi_c = 0.280 \pm 0.005$ [6]. The critical volume fraction is significantly less when cubic objects are allowed to have random orientations,

$$\eta_c = 0.2444 \pm 0.0003 \quad (9a)$$

or

$$\phi_c = 0.2168 \pm 0.0002 \quad (9b)$$

[see Fig. 3(b)]. The result for randomly oriented cubes is the same for cubes of edge lengths $1/\sqrt{3}$, 0.75, and 1. Thus, as expected, the percolation threshold is independent of the cube and system size used. Our value of ϕ_c for the con-

TABLE I. Percolation threshold, excluded areas and volumes, and average bond numbers.

Object	V_{ex} for unit object	ϕ_c	N_c	B_c (calculated)	B_c (literature)
Discs	4	0.676 339 [19]	1.128059	4.51	4.5±0.1 [24] 4.7 [6]
Aligned squares	4	0.6666±0.0004	1.098±0.001	4.39±0.01	4.5±0.1 [24] 4.7 [6]
Random squares	4.547	0.6254±0.0002	0.9819±0.0006	4.46±0.01	
Spheres	8	0.289 573 [10]	0.341889	2.74	2.79 [6]
Aligned cubes	8	0.2773±0.0002	0.3248±0.0003	2.59±0.01	2.60 [6]
Random cubes	11	0.2168±0.0002	0.2444±0.0003	2.69±0.01	

tinuum percolation of randomly oriented cubes is significantly more precise than the previous one of 0.22 ± 0.01 [20].

Comparison of the critical volume at the percolation threshold for aligned cubes with that determined for spheres, $\phi_c = 0.289\,573 \pm 0.000\,002$ [10], demonstrates that the difference in shape between spheres and cubes affects ϕ_c by $\approx 4\%$ [6]. Allowing cubes to randomly orient lowers ϕ_c $\approx 22\%$. The difference between the randomly oriented cubes and spheres is due to the same process as discussed above for discs and squares, but in this case it is the greater length of the body diagonals of cubes compared to the diameter of spheres or the edge length of aligned cubes that enhances the probability of connectedness for randomly oriented cubes at any given volume fraction.

IV. DISCUSSION

The continuum percolation threshold can be approximated with excluded volume theory [6,21,22]:

$$N_c V_{\text{ex}} = B_c, \quad (10)$$

where N_c is the critical density of objects [23], V_{ex} is their excluded area or volume, and B_c is the average number of bonds per object [24]. Originally, B_c was thought to be one constant for all parallel (i.e., not randomly oriented) convex objects in 2D and another constant in 3D [24], but later B_c was determined to be different for spheres and for cubes in 3D [6]. The excluded area for discs and aligned squares of unit area is 4 and for randomly oriented unit squares 4.547 [21]. For both spheres and aligned cubes V_{ex} is equal to 8 times their volume in 3D. For randomly oriented cubes V_{ex} is 11 times their volume [25]. Calculated values of B_c in 2D and 3D are presented in Table I.

In 2D we determine that $B_c = 4.39 \pm 0.01$ for aligned squares and $B_c = 4.46 \pm 0.01$ for randomly oriented squares. The value for aligned squares is similar to that originally proposed by Balberg for discs and squares, $B_c = 4.5 \pm 0.1$

[24], and to the values for discs and squares calculated from Monte Carlo simulations: $B_c = 4.51$ [19] and $B_c = 4.5 \pm 0.1$ [6], respectively. On the other hand, our value for B_c is somewhat lower than that calculated by a series expansion technique, $B_c = 4.7$ [6]. Thus we confirm that B_c has the same value, within error, for discs and for aligned and randomly oriented squares in 2D.

Our Monte Carlo simulations yield $B_c = 2.59 \pm 0.01$ for aligned cubes, as is expected because of the agreement between our estimate of the percolation threshold and previous estimates. For randomly oriented cubes $B_c = 2.69 \pm 0.01$ is closer to the value of B_c for the continuum percolation of spheres (Ref. [6]) than is the value of B_c for aligned cubes. However, the B_c value for randomly oriented cubes does not exceed the limiting value predicted by the excluded volume theory of the continuum percolation threshold Ref. [21]. The increases in B_c and decreases in ϕ_c observed for both squares and cubes when they are randomly oriented compared to when they are aligned is consistent with the idea that increasing connectivity results in decreasing percolation thresholds for these objects.

Our results confirm previous research demonstrating the effect of object shape on the threshold for continuum percolation. We find, furthermore, that the incorporation of random orientations of objects in continuum percolation simulations significantly affects the percolation threshold. Most of these effects are predicted by the application of excluded volume theory to the calculation of the percolation threshold. Randomly oriented squares and cubes have B_c values similar to those determined by other researchers for discs and spheres, respectively.

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