Precise determination of the critical percolation threshold for the three-dimensional ''Swiss cheese'' model using a growth algorithm

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Precise values for the critical threshold for the three-dimensional ''Swiss cheese'' continuum percolation model have been calculated using extensive Monte Carlo simulations. These simulations used a growth algorithm and memory blocking scheme similar to what we used previously in three-dimensional lattice percolation. The simulations yield a value for the critical number density $n_c = 0.652\,960 \pm 0.000\,005$, which confirms recent work but extends the precision by two significant figures. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1338506]

I. INTRODUCTION

Continuum percolation is an interesting model because it shares many of the mathematical properties with lattice percolation, yet is a more accurate model of many disordered materials (i.e., porous media, composite materials, polymers, and colloids). Different types of continuum percolation have been the topic of recent literature including the distribution of rods,[1–4] the distribution of squares,[5] and the distribution of disks or spheres.[6–23]

In this paper, we study the continuum model that consists of a system of spatially uncorrelated, equal-sized spheres, whose centers are distributed by a Poisson process within the three-dimensional $L \times L \times L$ system. If the spheres are thought to be removed from the system, it can be seen why this has been given the nickname, the ''Swiss cheese'' model.

The spheres form clusters when they contact, or overlap, neighboring spheres. These clusters then form the porous path or conducting trail through the system. The density of spheres which causes a cluster to span the system is of particular interest and is called the critical density. In the literature, there are three common ways of expressing the critical density: the volume fraction ϕ_c [sometimes referred to as the percolation threshold p_c (Ref. 21)], the reduced number density η_c [which has also been referred to as the percolation threshold p_c (Ref. 24)], and the number density n_c. These three quantities are related to one another in the following fashion (for two- and three-dimensional systems):

$$\begin{aligned} \phi_c &= 1 - e^{-\eta_c}, \\ \eta_c &= (\pi/4) n_c \quad [2\mathrm{D}], \\ \eta_c &= (\pi/6) n_c \quad [3\mathrm{D}], \\ n_c &= N(2R)^2/L^2 \quad [2\mathrm{D}], \\ n_c &= N(2R)^3/L^2 \quad [3\mathrm{D}], \end{aligned} \tag{1}$$

where R is the radius of the sphere and N is the number of spheres placed in the system. Some other definitions of the critical density have also been used.

For example, the following is a summary of some of the different ways the transition point has been reported in the literature for two-dimensional systems. The critical threshold has been reported as $\phi_c = 0.676 \pm 0.003$,[22] $\phi_c = 0.6764 \pm 0.0009$,[16] $\phi_c = 0.676 \pm 0.0005$,[23] $\phi_c = 0.6764 \pm 0.0010$ and $\eta_c = 1.1283 \pm 0.0011$,[19] and $\phi_c = 0.67637 \pm 0.00005$.[13] Asikainen and Ala-Nissila[15] reported the two-dimensional threshold as $\eta_c = 0.36 \pm 0.01$, where $\eta_c = NR^2/L^2$, which is different by a factor of π from the definition given above. Balberg[17] reported the threshold as the actual number of disks N with a certain radius R that are required in order to form a percolating cluster in a system with size $L \times L$. With a density of spheres $n = N/L^2$ set equal to 1, the minimum distance between the centers of these spheres $r_c = 2R = \sqrt{n_c}$ is yet another way of reporting the critical threshold; Nguyen and Canessa[18] found that $r_c = 1.991 \pm 0.001$. A very precise value of the threshold [$\phi_c = 0.676\,339 \pm 0.000\,006$ (Ref. 20)] was found using the gradient percolation method. This method, however, is not applicable to 3D percolation.[25] A summary of some other determinations of the 2D transition point is given in Quintanilla *et al.*[20]

For 3D, a summary of the previous values of the critical number density is given in Table I. In all cases except Saven *et al.*,[34] the value for the critical threshold was reported in another form, which we converted to the number density n_c. The earliest values of the critical thresholds[26–28] were reported as the concentration parameter t_c, which in three dimensions is related to the number density by $t_c = n_c/8$. Other authors[30,31] reported the critical threshold in terms of the mean number of points W_c in a sphere, which corresponds to $W_c = 4\pi n_c/3$. The critical threshold was reported in terms of the scaled density ρ_c by Haan and Zwanzig,[32] where in three dimensions $\rho_c = 4\eta_c$. The other values were reported as either the volume fraction ϕ_c (Refs. 16, 21, 29) or the reduced number density η_c.[24,33]

In the remainder of this paper, we present our growth algorithm for the 3D Swiss cheese model, and compare the value of the critical threshold that we found using our algorithm to the previous works.

II. METHOD

We utilized a Monte Carlo simulation which is similar to the one that we had used in studies of three-dimensional

TABLE I. Values of n_c for the three-dimensional ''Swiss cheese'' model.

Author(s)	Year	n_c	Error
Roberts and Storey[a]	1968	0.711	0.019
Domb[b]	1972	0.65	0.05[h]
Holcomb *et al.*[c]	1972	0.56	
Pike and Seager[d]	1974	0.64	0.02[b]
Goyda and Ottavi[e]	1974	0.62	0.02
Kurkijärvi[c]	1974	0.66	0.02
Fremlin[g]	1976	0.64	0.02
Haan and Zwanzig[h]	1977	0.67	0.05
Chiew and Stell[i]	1989	0.644	
Saven *et al.*[j]	1991	0.646	0.007
B. Lorenz *et al.*[k]	1993	0.673	0.016
Rintoul and Torquato[l]	1997	0.6528	0.0011
Present work	2000	0.652 960	0.000 005

[a]Reference 26.
[b]Reference 27.
[c]Reference 28.
[d]Reference 29.
[e]Reference 30.
[f]Reference 24.
[g]Reference 31.
[h]Reference 32.
[i]Reference 33.
[j]Reference 34.
[k]Reference 16.
[l]Reference 21.

lattice percolation.[35–37] The simulation employed a growth algorithm to generate clusters of the spheres, whose radius R is equal to 0.5. The system, which was of size $1024\times1024\times1024$, was divided into cubes of unit volume. A Poisson function was used to determine how many sphere centers were in each of the cubes, where the probability P_n that there are n particles in a given volume V is given by

$$P_n=\frac{1}{n!}(\rho V)^n e^{-\rho V}. \tag{2}$$

Here ρ is the density of sphere centers in the cube and $V=1$ for the unit cubes in our system. The algorithms in Ref. 38 were used to generate numbers with this distribution.

We started our growth algorithm in the center unit cube of our system. In order to determine the number of spheres inside of this cube, a random number n was generated according to Eq. (2). If $n>0$, then n spheres were randomly placed within the cube. We stored the x-, y-, and z-coordinates of each sphere into three one-dimensional coordinate arrays, which were indexed by the order that the spheres were distributed (i.e., the first sphere placed is numbered 0, the second is numbered 1,...). We also stored the index of the first and last sphere distributed in the cube in two one-dimensional pointer arrays. Then each of the neighboring 26 cubes were checked for spheres. Whenever a previously unvisited cube was accessed, a new random number n was generated by Eq. (2) and the n spheres were randomly placed within the cube. We used the index of the first and last spheres placed in the cube to find from the coordinate list the spatial coordinates of the spheres whose centers are inside the current cube. Then, we calculated the distance between the first sphere placed in the cube and each of the spheres in its cube and also each sphere in the neighboring 26 cubes. We performed the same distance calculations for the 2nd, 3rd,... sphere placed in a cube, until we reached the last sphere in the cube. If the distance between any two spheres was less than or equal to $2R$, then the two were considered to be in the same cluster. The coordinates of each sphere in the cluster were stored in three one-dimensional list arrays, which were indexed by the order that the spheres were determined to be part of the cluster. After each of the spheres in the center cube were checked for overlapping neighbors, then spheres on the list arrays were checked, in the order that they were placed on the list, for overlapping neighbors. This process was continued until a cluster stopped growing, or reached the upper cutoff size (defined as the number of overlapping spheres) of 2^{15} (32 768), at which point the growth was stopped. The coordinate arrays were thus of length 32 768.

If we made complete arrays for the two pointers in a 1024^3 system, we would have needed many gigabytes of memory. Therefore, for these arrays, we used a data-blocking scheme[39] to grow such large clusters in our system. In our simulation, this scheme was used to divide the large system ($1024\times1024\times1024$) into 2^{21} (2 097 152) smaller blocks whose dimensions were $8\times8\times8$. Memory was not assigned to a specific block of pointers until the cluster grew into it. We also used bit mapping to reduce the memory load required for the large lattices. The upper seven bits of each coordinate were used to determine where in the memory each block was mapped. The lower three bits of each coordinate told us the word, or ''address'' in the block, which maps to that location. We then used this ''address'' as an index for the pointer arrays where the index of the first and last sphere in each cube was stored. By using a large system and the previously stated cutoff, the cluster never saw the system boundary, so there were no boundary effects in our results.

The simulation accumulated the number of clusters that grew to a size within a range of $(2^n,2^{n+1}-1)$ for $n=0,1,...$ and recorded this number in the nth bin. If a cluster reached the upper cutoff, then it was counted in the last bin ($n=15$).

The random numbers used in these simulations were generated by the four-tap shift-register rule $x_n=x_{n-471}\oplus x_{n-1586}\oplus x_{n-6988}\oplus x_{n-9689}$, where $\oplus$ is the exclusive-or operation, which we have used in numerous previous studies.[35–37,40]

III. RESULTS

The probability $P(s,n)$ that a cluster will grow to a size greater than or equal to s at a certain number density $n\neq n_c$ is expected to behave as

$$P(s,n)\sim As^{2-\tau}f((n-n_c)s^{\sigma}) \tag{3}$$

in the scaling limit as $s\to\infty$ and $n\to n_c$ such that $(n-n_c)s^{\sigma}=$constant.[41] In Eq. (3), τ and σ are universal exponents which have the values 2.189 (Refs. 35,42,43) and 0.453 (Ref. 42) in 3D. The scaling function $f(x)$ in Eq. (3) can be expanded in a Taylor series when n is close to n_c,

$$f((n-n_c)s^{\sigma})\sim1+C(n-n_c)s^{\sigma}+\cdots. \tag{4}$$

Combining Eqs. (3) and (4), it follows that $s^{\tau-2}P(s,n)$ deviates from a constant for large s and n close to n_c. Figure 1 shows the plot of $s^{\tau-2}P(s,n)$ vs s^{σ} for the 3D Swiss cheese model. This plot shows a steep increase for small s, which is the finite-size effect, followed by a linear portion,

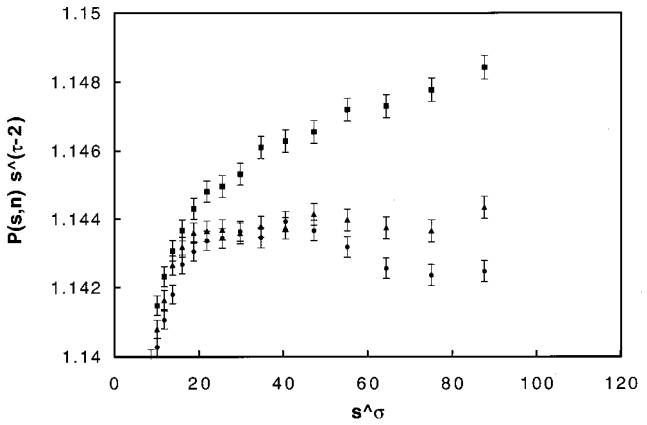

FIG. 1. Plot of $s^{\tau-2}P(s,n)$ vs s^{σ}. Each curve represents a different value of n: 0.652 970, 0.652 960, and 0.652 950 (from top to bottom). The value of n that yields the best horizontal fit is the critical threshold.

which as predicted by Eq. (4) becomes more horizontal as n gets closer to n_c. By interpolating from this plot, we determine the critical threshold to be

$$n_c = 0.652\,960 \pm 0.000\,005, \tag{5}$$

which corresponds to

$$\eta_c = 0.341\,889 \pm 0.000\,003,$$
$$\phi_c = 0.289\,573 \pm 0.000\,002. \tag{6}$$

Approximately 9×10^6 clusters were generated for each value of n in order to achieve the statistical error represented in Fig. 1. This required a total of a few months of workstation computer time.

IV. DISCUSSION OF RESULTS

Using a growth model to find the clusters in this 3D Swiss cheese model, we were able to find the critical threshold within an error of less than one part in 10^5, thus extending the known precision of this number by more than two significant figures. Our result confirms the recent value $\phi_c = 0.2895 \pm 0.0005$ found by Rintoul and Torquato,[11] and in fact shows that their central value is correct to less than 1 in the last digit, well within the error bars that they give. The high precision that we were able to obtain shows that the method used here, which is based upon the technique we had developed for lattice percolation, is also efficient for continuum percolation. The precise value of the critical threshold that we find will allow other problems on the 3D Swiss cheese model to be studied to equal precision.

One limitation of the growth method is finite-size effects, which must be overcome in order to accurately interpolate the value of the critical threshold. It was not clear in advance how the finite size effects for the continuum model would compare to those that we have seen for the lattice model. From Fig. 1, one can see that a cluster must be larger than about 10^3 spheres in size in order to overcome the finite size effects for the continuum model, which is about the same as for lattice models in 3D.[35–37] Consequently, we expect that the growth method should be applicable for other models of continuum percolation. Likewise, we expect it to be good for higher dimensions also.

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