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LETTER TO THE EDITOR

Precise determination of the critical threshold and exponents in a three-dimensional continuum percolation model

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Abstract. We present a large-scale computer simulation of the prototypical three-dimensional continuum percolation model consisting of a distribution of overlapping (spatially uncorrelated) spheres. By using simulations of up to 10^5 particles and studying the finite-size scaling of various effective percolation thresholds, we obtain a value of $p_c = 0.2895 \pm 0.0005$. This value is significantly smaller than the values obtained for simulations that have been carried out using smaller systems. Employing this value of p_c and systems of size $L = 160$ (relative to a sphere of unit radius), we also obtain estimates of the critical exponents ν, β, and γ for the continuum system and show that the values are different than those obtained using previous values of p_c.

1. Introduction

Continuum percolation studies have become increasingly common in the literature, as they contain many of the same interesting mathematical properties of lattice percolation and often are more realistic models of a variety of disordered materials [1–16]. Such materials include porous media, composite materials, and colloids. Accordingly, it is important to have a clear understanding of the behaviour of these systems, especially in the critical region near the percolation threshold.

A simple class of continuum percolation models can be defined by considering a system of d-dimensional hyperspheres of radius a. In the prototypical model of 'overlapping spheres' the hyperspheres are spatially uncorrelated. At low concentrations of the overlapping hyperspheres (which we will heretofore just refer to as 'spheres'), there is little overlap between the spheres, except for the occasional two- or three-particle cluster. A cluster is defined by particle overlap, so if two particle centres are within a distance $2a$ of each other, they belong to the same cluster. As the concentration of spheres increases, the spheres begin to form larger and larger connected clusters until at some critical concentration the largest cluster percolates in a manner completely analogous to lattice percolation. Continuum percolation has also been studied in cases in which the particles are spatially correlated, for example, hard-core [5, 7, 9] or attractive interactions [3, 10].

Percolation systems are generally characterized by a power-law divergence of one or more geometrical–statistical properties in the vicinity of the percolation threshold [17]. In general, most of the precisely known percolation thresholds and critical exponents are associated with lattice percolation due, in part, to the fact that it has been studied more

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extensively, and many of the quantities that characterize lattice percolation can be solved exactly. However, the lattice values are also much easier to simulate, due to the ordered nature of their underlying structures. From a computational point of view, it is much easier to associate the lattice site with entries in a matrix than to store the location of a list of particles with arbitrary coordinates. The problem of determining bonds and connectivity is also much easier to solve when dealing with a lattice system than a continuum system.

One important result which connects lattice and continuum percolation is that the geometrical–statistical critical exponents β, γ, and ν appear to be the same for the two systems due to universality [1, 2, 6]. This universality argument is the same one which dictates that the exponents on different lattices with the same dimensionality should be similar. Unfortunately, it is difficult to test whether or not the exponents for continuum and lattice percolation are the same with any high degree of precision due to the difficulty in determining the continuum exponents. The reason for this is that while lattice simulations have been performed on lattices with more than 10^8 sites, most continuum simulations have been concerned with systems of less than 10^5 particles, especially in three dimensions. The primary numerical evidence for universality comes from two-dimensional examples, and there is very little high-quality numerical data that would be needed to extract the exponents for the three-dimensional continuum system.

In order to better determine the values of critical exponents for the continuum system, one must first have a very precise value for the percolation threshold p_c in the system. This is due to the fact that the scaling laws that describe the behaviour of some quantity X are of the form

$$X \propto |p - p_c|^b \tag{1}$$

where b is the critical exponent. Having an incorrect value of p_c, especially in the case where b is negative, can often lead to a serious misinterpretation of the data and an error in the estimation of b. In many cases, one can also scale the data not by p but by the size of the system L. However, this too involves knowing a precise value for p_c.

In this letter, we propose to determine p_c for the three-dimensional continuum percolation system in a very precise and self-consistent way, and use this value to determine precise values for some of the critical exponents associated with the system.

2. Definition of mathematical quantities

The correlation length exponent ν can be defined by the relation

$$\xi(p) \propto |p - p_c|^\nu \tag{2}$$

where $\xi(p)$ is a correlation length which describes the typical radii of clusters in the system for $p < p_c$. For $p > p_c$, $\xi(p)$ represents a length scale over which the macroscopic properties of the system are homogeneous. These definitions are primarily useful in understanding the physical significance of ν, but are really not suited to a precise numerical calculation of its value.

In practice, ν is more often calculated by considering the finite-size scaling of one or more of the properties of the system. In our case, this is best done by studying the value of the *effective* percolation threshold for a system of linear size L, $p_c^{\mathrm{eff}}(L)$. For the infinite system, p_c is defined as the smallest volume fraction of spheres for which an infinite cluster forms. For a finite system, however, we must use some other definition to calculate $p_c^{\mathrm{eff}}(L)$. One common way is to require a certain fraction (often 0.5) of realizations to *span* the system in one or more directions. In this context, a cluster that spans the system is

one which crosses the cluster completely from one side to an opposite side, without the imposition of periodic boundary conditions. Another way is to require a certain fraction to *wrap* from one side of a system to another. This is similar to spanning except that the cluster must not only span, but the spanning ends must overlap if periodic boundary conditions are imposed.

The precise value of $p_c^{\mathrm{eff}}(L)$ is usually calculated by plotting the spanning (or wrapping) probability as a function of p. The resulting curve has a sigmiodal shape and the point at which the spanning probability crosses 0.5 can be obtained by fitting a curve with a similar shape to the data, such as $\{1 + \mathrm{erf}[(p - p_c^{\mathrm{eff}}(L))/\Delta(L)]\}/2$ or $\{1+\tanh[(p-p_c^{\mathrm{eff}}(L))/\Delta(L)]\}/2$. Besides giving a very statistically accurate determination of $p_c^{\mathrm{eff}}(L)$ for a system of size L, one also obtains the width of the percolation transition $\Delta(L)$. This width scales as a function of system size L as

$$\Delta(L) \propto L^{1/\nu}. \tag{3}$$

This often yields a very accurate value for ν due to the statistical nature of the way that $\Delta(L)$ is calculated.

Once ν is estimated, one can now estimate p_c from the scaling relation

$$p_c^{\mathrm{eff}}(L) - p_c \propto L^{-1/\nu}. \tag{4}$$

Thus, if $p_c^{\mathrm{eff}}(L)$ is plotted against $L^{-1/\nu}$, the result should be a straight line that intercepts the y-axis at a value of p_c. This scaling is general enough that it should apply to any of the definitions for effective percolation in a finite system.

The exponent that is related to the probability of a sphere belonging to the largest cluster in the system is β. It is most commonly defined as

$$P(p, \infty) \propto |p - p_c|^{\beta} \tag{5}$$

where $P(p, \infty)$ is the probability that a randomly chosen site belongs to the infinite (in this case the largest) cluster in an infinitely large system. By applying finite-size scaling techniques to equation (5), one can show that

$$P(p_c, L) \propto L^{-\beta/\nu} \tag{6}$$

where ν is just the correlation length exponent defined above. Equation (6) generally allows for a more precise numerical estimate of β due to the fact that the expression is not quite as sensitive to the estimated value of p_c. From equation (6), it is easily shown that the fractal dimension D of the system at p_c is just given by

$$D = d - \beta/\nu. \tag{7}$$

Finally, we will look at the mean cluster size exponent γ, which is defined by the expression

$$S(p, \infty) \propto |p - p_c|^{-\gamma} \tag{8}$$

where $S(p, L)$ is the mean cluster size of a realization of size L at volume fraction p. The mean cluster size is defined by

$$S(p, L) = \frac{\sum_s s^2 n_s}{\sum_s n_s} \tag{9}$$

where n_s is the probability of a single particle belonging to a cluster of s particles and the sums are over all clusters for $p < p_c$ and exclude the largest, or 'infinite' cluster for $p > p_c$. In practice, one also applies finite-size scaling to equation (8) to obtain

$$S(p_c, L) \propto L^{\gamma/\nu}. \tag{10}$$

Like the case for β, it is generally easier to obtain a precise estimate of γ using equation (10) than equation (8).

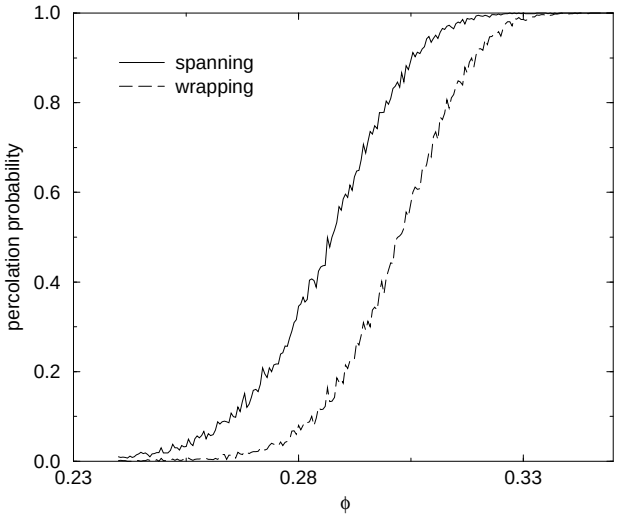

Figure 1. Percolation probabilities as a function of volume fraction ϕ for both the spanning (full curve) and wrapping (dashed curve) definitions of percolation for a system of size $L = 32$.

3. Computer simulation details

We have estimated p_c by taking systems of size L and generating a large number of configurations for various values of p. Next, the clusters were identified and then the fraction of configurations containing at least one cluster that both spanned and wrapped in at least one direction were tabulated for each value of p. This resulted in two different curves from which $p_c^{\mathrm{eff}}(L)$ and $\Delta(L)$ could be extracted. An example of such a set of curves for $L = 32$ is shown in figure 1. The realizations at each L were generated for a wide enough range of p to enclose both curves, in steps of $\Delta p = 5 \times 10^{-4}$. The number of realizations for each value of p varied from 1000 for $L = 32$ to 200 for $L = 160$. The values of $p_c^{\mathrm{eff}}(L)$ and $\Delta(L)$ were extracted by fitting each curve to the function $\{1 + \mathrm{erf}[(p - p_c^{\mathrm{eff}}(L))/\Delta(L)]\}/2$. We found that the curve more closely resembled that of the error function than the hyperbolic tangent, although fitting to the hyperbolic tangent form did not change the results significantly, especially in the case of $p_c^{\mathrm{eff}}(L)$.

Once an accurate estimate of p_c was established, $P(p_c, L)$ and $S(p_c, L)$ were then simulated for various values of L where $32 \leqslant L \leqslant 160$. These curves were then plotted on a log–log plot and the values for the exponents was extracted using the value of ν obtained from the width scaling of the curves.

4. Results

Figure 2 shows a log–log plot of $\Delta(L)$ against L for the transition widths associated with the different definitions of the effective percolation threshold. They are both basically parallel to each other, which is to be expected since they should both have the same slope. The slopes of both curves are 1.12 ± 0.01. This yields a values of $\nu = 0.89 \pm 0.01$, which is very much in line with previous estimates.

The plots of the $p_c^{\mathrm{eff}}(L)$ as a function of $L^{-1/\nu}$ are shown in figure 3. Most of the different effective percolation definitions show a smooth approach to the $L = \infty$ value of

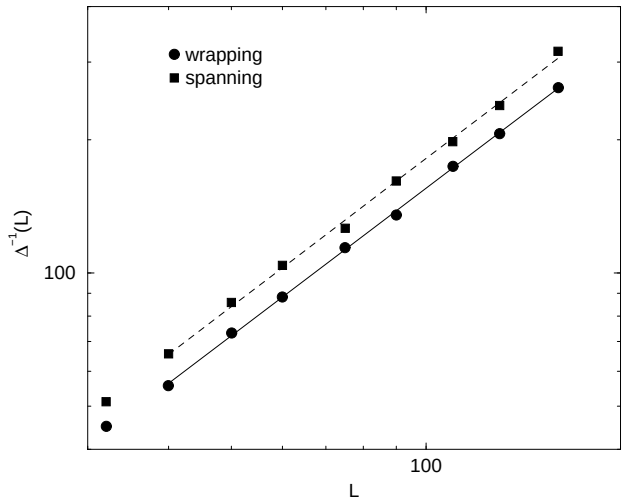

Figure 2. Inverse transition width $\Delta(L)$ plotted as a function of L for $32 \leqslant L \leqslant 160$. The straight lines are the best power-law fit for $L \geqslant 40$. Both lines have a slope of 1.12 ± 0.01, indicating a value of $\nu = 0.89 \pm 0.01$.

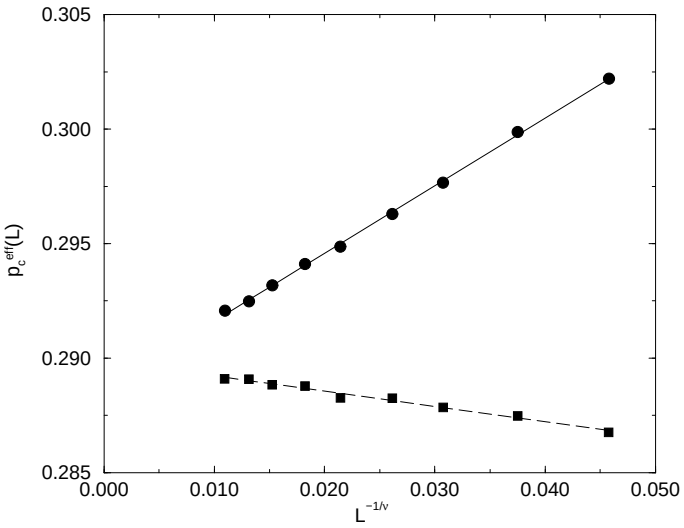

Figure 3. A plot of the different percolation probabilities as a function of $L^{-1/\nu}$, with accompanying linear fits to the data. Scaling laws predict that they should both intercept the y-axis at the percolation threshold for the infinite system.

$p_c(L)$ from above, indicating that the larger sizes allow for greater connectivity. However, the case in which spanning was required in at least one direction shows a somewhat different behaviour. In this case, the percolation threshold rose slightly as L increased. This behaviour is somewhat fortuitous as it allows the value of p_c to be more precisely determined since there exist curves which bound it from above and below. From a linear fit to the data in the figure, we estimate a value of 0.2895 ± 0.0005. The plots of the data are also shown extrapolated to $L^{-1/\nu} = 0$.

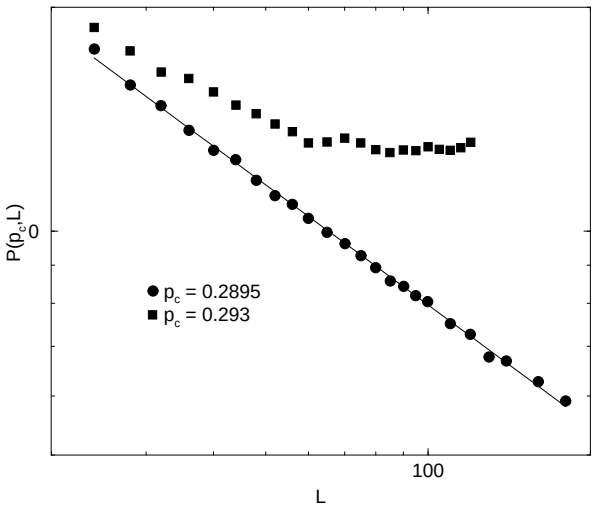

Figure 4. A plot of $P(p_c, L)$ for two different values of p_c. For $p_c = 0.293$, the figure diverges from a power-law behaviour as the length scale of the system becomes larger, indicating non-fractal behaviour. For our predicted value of $p_c = 0.2895$, the system shows a power-law behaviour for all L. The line indicates a power-law fit to the data for $L \geqslant 32$.

Using the value of p_c determined above, the finite-size scaling data for β is shown in figure 4. The log–log plot shows a smoothly decreasing behaviour with a slope corresponding to a value of $-\beta/\nu$ of -0.53 ± 0.01. Using the value of ν calculated above, this gives an estimate of $\beta = 0.472 \pm 0.015$. This value of β/ν is different than the estimate given by Grassberger [18] of 0.474 ± 0.006 for lattice systems. In order to carry out a more direct comparison of our results to similar lattice results, we performed nearly identical finite-size scaling simulations in which the probability of belonging to the largest cluster (using periodic boundary conditions) was plotted as a function of system size L for $8 \leqslant L \leqslant 384$. For this simulation, a value of $p_c = 0.311\,605 \pm 0.000\,010$ was used. This data gives a value of $\beta/\nu = 0.485 \pm 0.005$, more in line with the lattice value given in [18].

An estimate of γ for the continuum system can now also be determined by looking at a plot of the mean cluster size at concentration p_c as a function of L. Because the simulation is being done at p_c, the largest or 'infinite' cluster is excluded from the sum. The resulting plot is shown in figure 5. The slope of the power-law fit line is 1.94 ± 0.01 which gives a value of $\gamma = 1.725 \pm 0.015$. This is somewhat smaller than the best estimate for lattice percolation in three dimensions. However, this is to be expected given the value for β, and the fact that β, γ, and ν are related by the relation

$$d = 2\beta/\nu + \gamma/\nu. \tag{11}$$

It should be noted that the values calculated here for β/ν and γ/ν have been calculated independently of each other and satisfy equation (11) very well.

5. Discussion

The difference between the value of β/ν (and therefore the fractal dimension D) calculated in this continuum simulation and that calculated from lattice calculations differs by a small but significant amount. Because of the high precision of the estimate and the large scale of

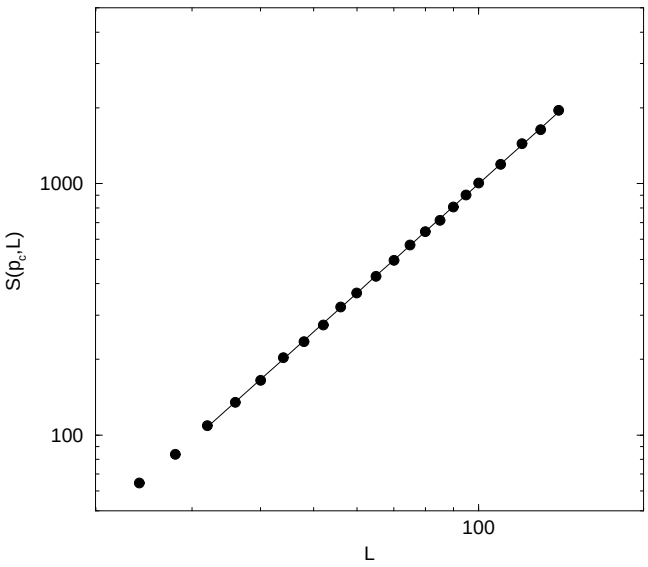

Figure 5. A plot of $S(p_c, L)$ for $p_c = 0.2895$. The line indicates a power-law fit to the data for $L \geqslant 32$. The slope of the line indicates a value of $\gamma = 1.725 \pm 0.015$.

the simulations in this work, the difference between the value obtained here and in previous works must be addressed. If we assume that universality arguments apply in this case, then there should be no difference between the true value of β/ν for the two different systems. If the difference is indeed a numerical one that is a result of the finite size of the simulation and the interpretation of the data, then this needs to be better understood.

However, given the data presented here, one can also speculate on whether universality holds in the three-dimensional case. It has already been shown numerically that universality does not apply to the case of the transport exponents in three dimensions [8]. This difference was seen because of the significant difference between the two exponents. Most of the previous numerical data which were used to establish universality of the geometrical–statistical exponents were of poor quality, and we would not have been able to see the small difference between the two values. It should also be noted that we have shown here that a small difference in the percolation threshold leads to a very different value of the exponents. We obtained results similar to earlier works when we used larger values of p_c.

6. Conclusions

We have presented here a new and more precise value of the percolation threshold for three-dimensional continuum percolation. By performing finite-size scaling calculations using this new value, we have obtained estimates of β and γ for three-dimensional continuum percolation. These values are different than previous lattice estimates, and we have demonstrated that this difference is due to the fact that previous estimates of p_c were too high. There is still a discrepancy between the value of β/ν measured here and the value estimated from lattice simulations that more extensive simulations must address.

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