

# Monte-Carlo renormalisation group for continuum percolation with excluded-volume interactions

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**Abstract.** The critical properties of a continuum percolation system with excluded-volume interactions are studied by Monte-Carlo position-space renormalisation group methods. The model system considered is comprised of oriented squares of unit side with concentric square hard-core regions of side  $L_{hc}$ . These elements are randomly distributed in a square planar region at a concentration  $x$ . For eight values of  $L_{hc}$ , the percolation threshold  $x^*$  is estimated. Additionally, for two of these eight values, the connectedness-length exponent  $\nu$  is computed. A monotonic dependence of  $x^*$  upon  $L_{hc}$  is observed and our estimates are close to those of the lattice and freely overlapping continuum percolation problems. However, the accuracy of these estimates is not sufficiently precise to determine whether there is universality of continuum systems with respect to the size of the hard cores.

## 1. Introduction

Freely overlapping (or ordinary) continuum percolation has been found to have the same critical properties as lattice percolation, dispelling possible concerns that these two problems might be in different universality classes (Haan and Zwanzig 1977, Vicsek and Kertész 1981, Gawlinski and Stanley 1981). A natural question arises as to what effects, if any, excluded-volume interactions may have on the critical properties of a continuum percolation system. In addition to this theoretical motivation, the study of such a model may also be of relevance for describing phenomena in nature that have both topological disorder and excluded-volume interactions. Two examples of such phenomena are conductivity in metal-insulator mixtures (Deutscher *et al* 1978) and gelation (Skal and Shklovskii 1974, de Gennes 1979). In this paper, we investigate the critical properties of a simple two-dimensional continuum percolation system with excluded-volume interactions and compare our results with those of the lattice and ordinary continuum problems.

In the ordinary continuum percolation process, completely interpenetrable geometric elements (e.g. discs, squares, spheres, etc) are distributed randomly in space at a given concentration,  $x$ , and a bond is said to exist between two such elements if they overlap. At a critical concentration,  $x^*$ , the onset of an infinite connected network of bonds occurs and the system displays a percolation threshold.

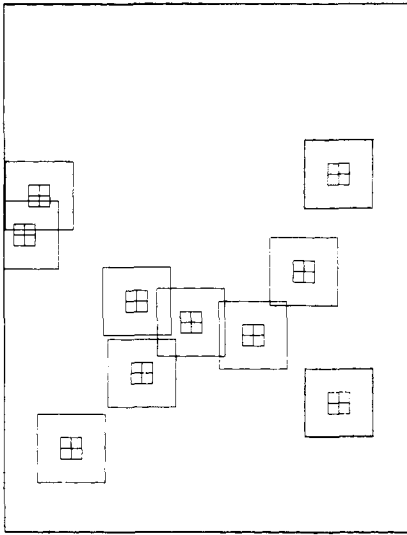
To incorporate excluded-volume interactions, we define each element to contain a concentric hard core that cannot be penetrated by that of any other element. With

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this additional constraint, the elements may resemble more closely the fundamental constituents (e.g. monomers, impurities, etc) of the particular system that we may be interested in representing.

The model system we choose to study is comprised of oriented squares each with unit side, that is, squares whose centres are positioned randomly in a plane, but whose sides are constrained to remain parallel. Within each square, another concentric and aligned square with side  $L_{hc} < 1$  is introduced to define the region of excluded volume. A square, rather than a disc or some other shape, was chosen for consistency in defining the renormalisation group transformation (see below) and for more economical usage of available computer resources. By definition, the hard-core regions exclude only other hard cores but do admit the 'soft' external region of other squares (figure 1). It is convenient to introduce a hard-core area fraction (hereafter called the 'core fraction'),  $\psi = L_{hc}^2$ , and our basic goal is to study the effects of varying this parameter on various quantities which typify critical behaviour, such as  $x^*$  and the connectedness-length exponent,  $\nu$ .

The technique we use for determination of  $x^*$  and  $\nu$  is the Monte-Carlo position-space renormalisation group (MCPSRG) (Reynolds *et al* 1978, 1980; for a recent review see Stanley *et al* 1982). In the following section, we give a brief review of this technique and a description of how it was applied to the problem at hand.



**Figure 1.** A 'snapshot' of a  $5 \times 5$  system of oriented squares with the concentric hard cores shown shaded. Squares may overlap, and this overlapping defines the criterion for bonding. However, the hard cores may not intersect each other.  $\psi = 0.10$ ,  $x = 0.40$ , 20 shuffles.

## 2. MCPSRG method

We begin by considering a  $b \times b$  planar region within which  $N$  oriented squares of unit edge length and core fraction  $\psi$  are randomly distributed according to a procedure to be discussed below. A rescaling is performed in which a  $b \times b$  cell is mapped into a  $1 \times 1$  square with the same core fraction  $\psi$ . Thus we consider a one-parameter group

with  $\psi$  held fixed. One can easily envisage a two-parameter transformation in which the core fraction itself is renormalised. We have not yet explored in detail the possibility of treating  $\psi$  as a relevant variable. However, in § 5, we discuss what we anticipate to be the outcome of such a calculation.

The most natural 'rule' for the one-parameter transformation is to occupy the renormalised square with probability equal to the overall area fraction  $s$  (not to be confused with the core fraction) covered by the squares in the initial  $b \times b$  cell (Vicsek and Kertész 1981). Specifically

$$s' = R(s; b) \tag{1}$$

where  $s'$  is identified as the probability of a randomly chosen  $b \times b$  area being occupied by a square of side  $b$  and core fraction  $\psi$ , and  $R(s; b)$  is the probability of spanning a  $b \times b$  cell with squares of unit side covering an area  $sb^2$ . From the fixed point  $s^*$  of equation (1), the eigenvalue  $\lambda_b^{(s)}$  is defined by

$$\lambda_b^{(s)} = \left. \frac{\partial R(s; b)}{\partial s} \right|_{s=s^*} \tag{2}$$

from which we determine the exponent  $\nu$  through

$$\ln \lambda_b^{(s)} = (1/\nu^{(\lambda)}) \ln b + \text{constant.} \tag{3}$$

For our purpose, this formulation has a drawback in that  $s$  is not an easily controllable parameter; the independent variable for this problem is the concentration  $x = N/b^2$ . The exact dependence of  $s$  upon  $x$  is known only in the limit of  $\psi = 0$ , where the spatial distribution is governed by Poisson statistics and the two variables are related by  $s = 1 - e^{-x}$ . One can, in principle, compute the dependence of the area fraction on the concentration for  $\psi \neq 0$  from the pair-correlation function  $g(r)$ . This function has been studied in great detail for the hard-sphere system (see, e.g., Barker and Henderson 1971 and references therein), but much less is known about the hard-square system, especially in the fluid phase.

Thus we must resort to formulating the PSRG in terms of  $x$ . To accomplish this, we first define  $R(x; b)$  to be the spanning probability. We then determine the underlying distribution  $L(x; b)$  from (Levinshtein *et al* 1975, Reynolds *et al* 1980)

$$R(x; b) = \int_0^x L(x'; b) dx'. \tag{4}$$

It is easily seen that  $L(x; b) dx$  is the probability of *first* spanning a  $b \times b$  cell when squares are being added to the cell continuously to bring the concentration to a value between  $x$  and  $x + dx$ . Provided that the cell is reasonably large, we can approximate the fixed point for the concentration by the maximum of  $L(x; b)$ , i.e. the most probable concentration at which spanning first occurs. Therefore we approximate the fixed point by  $x^* = x_{\max}$ , the concentration at which the derivative of  $L(x; b)$  with respect to  $x$  vanishes, and the eigenvalue by

$$\lambda_b^{(x)} = \left. \frac{\partial R(x; b)}{\partial x} \right|_{x=x^*} \tag{5}$$

This alternative definition of the eigenvalue in terms of  $x$  does not affect the determination of the connectedness-length exponent  $\nu$ . We can see this most easily by returning to the standard formulation in terms of  $s$ . The area fraction,  $s(x)$ , is an

analytic function of concentration near  $x^*$ . Thus from equations (2) and (5), the eigenvalues in the two formulations are proportional. Therefore, from the logarithm of  $\lambda_b^{(x)}$ , we determine  $\nu$  through equation (3) with only a shift in the additive constant.

As the cell size becomes infinite,  $R(x; b)$  and  $L(x; b)$  approach a step function and a delta function respectively. If  $\sigma$  is the width of  $L(x; b)$ , we expect from finite-size scaling arguments (Levinshtein *et al* 1975) that

$$\sigma \sim b^{-1/\nu(\sigma)}. \quad (6)$$

The slope of  $\lg \sigma$  against  $\lg b$  then gives another independent estimate of  $\nu$ .

### 3. Monte-Carlo method and determination of $R(x; b)$

For a particular concentration  $x$  and core fraction  $\psi$ , we employ a Monte-Carlo simulation based on an importance-sampling procedure (see, e.g., Wood 1975, Levesque *et al* 1979 and references therein). We begin by generating an initial state in which squares are positioned on the sites of a regular square lattice.

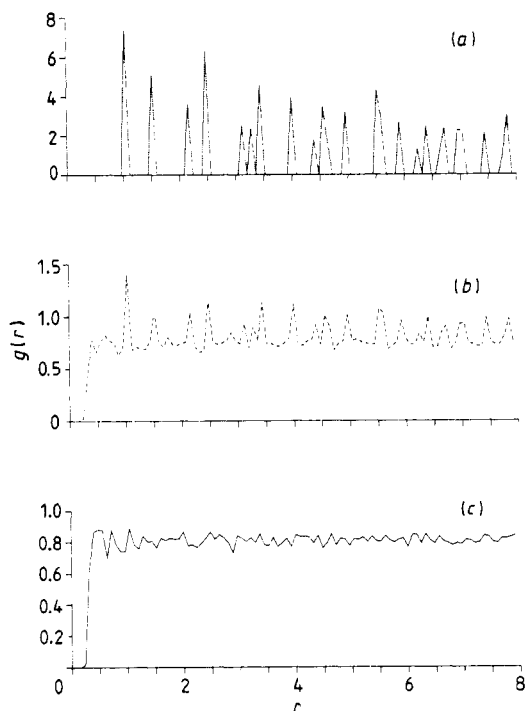
In order to generate the desired hard-square fluid from the initial hard-square 'crystal', one possibility is to attempt to move each square into a new position anywhere in the system with a probability equal to the Boltzmann factor for the particle at this new position. For the hard-core potential this sampling technique is trivial: all points in the system with both  $x$  and  $y$  coordinates within  $L_{hc}$  of the centre of any other square are occupied with zero probability, while all other points are occupied with unit probability. Except at low concentrations, it is extremely inefficient to attempt to move particles entirely at random. It is more useful to move particles only a small distance of the order of the mean free path  $r_0$ . This is quite similar to the methods employed for simulating spin systems with continuous degrees of freedom where a spin flip is defined to be only a small angular deviation from an initial state (see, e.g., Binder and Stauffer 1979).

In the course of moving particles from one position to another, it is possible that two cores may pass through each other. The occurrence of this event is of no concern as we are only interested in attaining the proper *static* distribution.

To equilibrate in the fluid phase, we scan sequentially through the lattice and attempt to move particles one at a time. A trial move is made for each square by first moving it in a randomly chosen direction and by a distance chosen from a uniform distribution which is bounded from above by  $r_0$ . This particular upper limit is chosen to increase the likelihood of a successful move. If the final position for a particular square is such that its hard core does not penetrate that of any other square, the move is accepted, otherwise the particle remains in its initial position. For the duration of this simulation process, periodic boundary conditions are in effect.

We have varied  $r_0$  so that the success rate for moving ranges typically from 10 to 60% depending on the concentration and core fraction. One scan through the entire lattice, attempting to move each square, will hereafter be referred to as one 'shuffle'.

The first 20 shuffles at each concentration are used to allow for the decay of any transient behaviour. To test whether an equilibrium fluid state is reached within this time, the pair-correlation function was measured over a range of concentrations and core fractions. It was observed that after only a few shuffles, all memory of the initial crystalline structure was apparently eliminated (see figure 2). At this point, the system is tested for spanning. We continue to shuffle the particles and test for spanning in



**Figure 2.** The two-particle correlation function  $g(r)$  for a  $50 \times 50$  system at various stages in the shuffling procedure. (a) The correlation function of the initial crystalline state, (b) after one shuffle and (c) after 20 shuffles. The initial crystallinity appears to be entirely eliminated after 20 shuffles. Note the different vertical scales for the initial correlation function and those after shuffling has taken place.  $\psi = 0.10$ ,  $x = 0.8$ .

sequential order for a large, predetermined number of times. The fraction of spanning realisations is then recorded for input to the PSRG calculation.

As a check that the shuffling procedure generates realisations which are statistically independent, we tested for possible correlations in the spanning states of different realisations (either yes or no). We observed that the movement of only a small fraction of the squares in a single shuffle was necessary to change the geometrical structure of the system significantly. Thus one shuffle, or at most two shuffles in the most extreme situations, is adequate to ensure statistical independence between realisations.

Once a realisation has been generated, we ascertain whether a spanning cluster exists by employing a cluster multi-labelling scheme (Hoshen and Kopelman 1976) that can determine whether a connected path spans the system. Unfortunately, because of the necessity of storing the coordinates of all the squares for the purpose of shuffling, we are not able to exploit the full power of the Hoshen–Kopelman algorithm—that being the storage and manipulation of only a small fraction of the system at any given time. This limits us to a study of system sizes that are considerably smaller than those examined in previous work on lattice percolation and ordinary continuum percolation. However, by choosing a square as the percolating element, rather than a disc as has been done generally for continuum percolation, we were able to decrease both data storage space and computer execution time. This permitted the study of larger systems with more realisations than would have been possible with a system comprised of discs.

#### 4. Calculations and results

We examined eight core fractions between  $\psi = 10^{-4}$  and  $\psi = 0.6$  (higher core fractions lead to some interesting problems which will be discussed below). The run at  $\psi = 10^{-4}$  was made to check whether the results of ordinary continuum percolation would be reproduced. Limitations in computer resources confined us to a detailed study of only two of these core fractions,  $\psi = 0.1$  and  $\psi = 0.5$ . For these two, we took data at eleven concentrations, each for six different cell sizes ranging from  $b = 6$  to  $b = 85$ . At  $b = 6$ , 45 000 realisations were generated for each concentration, decreasing to 1500 realisations for  $b = 85$ . In addition, for one cell size,  $b = 20$ , 1000 realisations were run at each of eleven concentrations for the six remaining core fractions in order to estimate  $x^*$ . Implicit in these estimates is the fact that, for  $b \geq 10$ ,  $x^*$  differs by less than 1% from its limit as  $b \rightarrow \infty$ .

For the purpose of determining exponents, we assume that  $L(x; b)$  can be described accurately by a beta distribution. This is a two-parameter canonical form for normalised distributions defined on the unit interval—precisely the situation we encounter if we measure the concentration relative to the close-packing concentration. The beta, rather than the Gaussian, distribution was chosen because the former has been shown to be more representative of  $L(x; b)$  for small  $b$  where the distribution can be skewed (Reynolds *et al* 1980). Raw data for  $R(x; b)$  against  $x$  for  $\psi = 0.1$  and  $\psi = 0.5$  have been fitted to the integral of the beta distribution as shown in figure 3. Expressions for  $x^*$ ,  $\lambda$  and  $\sigma$  are easily found in terms of the fitting parameters, and the numbers reported here are calculated accordingly (see figure 4). Uncertainties in the fitting parameters are computed from the standard deviation taken over all realisations and these uncertainties are propagated down to the relevant quantities according to standard procedures.

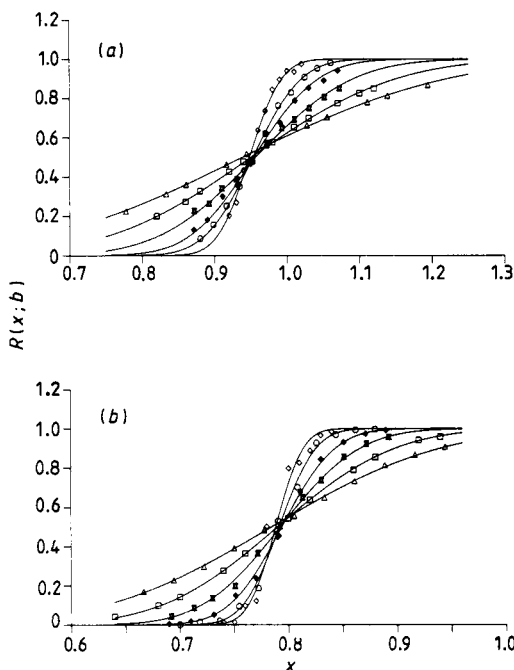
#### 5. Discussion and conclusion

In table 1, we list  $x^*$  and  $\nu$  for each core fraction investigated and compare these estimates, where possible, with previous results. The error bars on  $\nu$  indicate a slight discrepancy between systems with and without the hard-core interaction. However, our analysis does contain systematic errors which are hard to quantify, as well as the quoted statistical errors.

Due to the lack of any reasonable estimates for such systematic errors, we are unable to arrive at a definite conclusion concerning the possible universality or non-universality between continuum percolation with and without excluded-volume interactions. The answer to this question appears to require further study.

There are two interesting points that have not been fully addressed in this study. The first is that our investigations were limited to core fractions  $\psi \leq 0.6$ . For higher core fractions,  $x^*$  occurs above the concentration where the freezing transition for a gas of hard squares of side  $L_{hc}$  occurs; that is, at a concentration where percolation is expected to occur, there is little free volume available for particle movement. Consequently, the shuffling procedure becomes extremely inefficient in equilibrating the system. Starting with a crystalline initial state, it would take a prohibitive amount of time before a random distribution of particles was obtained.

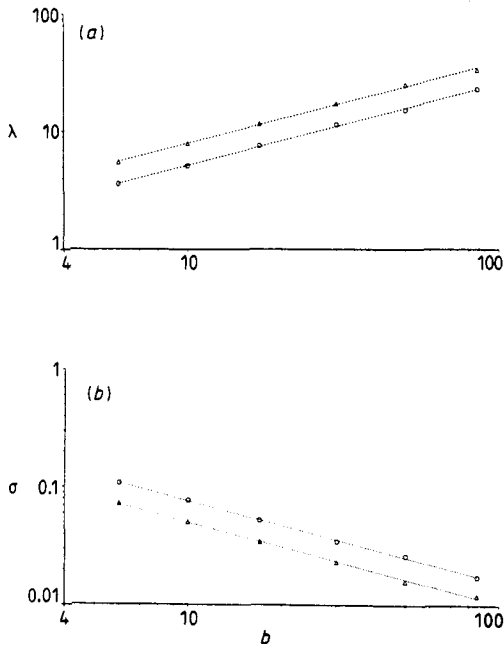
One possible solution is to start with an initial state which is in the fluid phase. To achieve this, one possibility is to start with the fluid phase at an intermediate



**Figure 3.** Raw data for the spanning probability  $R(x; b)$  for (a) core fraction  $\psi = 0.1$  and (b)  $\psi = 0.5$ . The data for  $b = 6-85$  are shown by the following symbols:  $b = 6$ ,  $\triangle$ ;  $b = 10$ ,  $\square$ ;  $b = 17$ ,  $\boxtimes$ ;  $b = 30$ ,  $\diamond$ ;  $b = 50$ ,  $\circ$ ;  $b = 85$ ,  $\diamond$ . The smooth curves through the data represent best fits to the integral of the normalised beta distribution. Notice that as the cell size increases,  $R(x; b)$  approaches a step function. Furthermore, for  $\psi = 0.5$ , the data appear to be considerably smoother than the data for  $\psi = 0.1$ . This appears to stem from the smaller available phase space at  $\psi = 0.5$  which can be sampled more thoroughly using fixed computer resources.

concentration. Thereby successively shuffling and compressing the system, it may be possible to arrive at the desired high concentration while still remaining in the fluid phase.

A second point is that we have only considered a one-parameter renormalisation in which the core fraction remains constant. However, a two-parameter scheme in which both the concentration and the core fraction are renormalised could, in principle, be constructed easily. The inherent nature of the excluded-volume effect suggests the proper weight function for rescaling the core fraction. Since the hard cores do not overlap, the excluded-volume effect in any configuration should be additive. Thus, to find the rescaled core fraction, we should first add the areas of the cores for all particles in a configuration and divide by the rescaling factor. Since the ‘soft’ regions of the squares can overlap but the hard cores cannot, the above prescription suggests that the core fraction *increases* with renormalisation. Therefore, the critical point at  $\psi = 0$  should be unstable in the  $\psi$  direction with a critical line emanating from the  $\psi = 0$  fixed point and terminating at a stable fixed point located at  $\psi = 1$ . On these grounds, one should expect universality with respect to core fraction, with the critical behaviour controlled by a fixed point at  $\psi = 1$ . In the light of the difficulties encountered with the presence of the freezing transition, however, it is not clear how one might study the  $\psi = 1$  limit. Another difficulty with this limiting case is the extremely



**Figure 4.** Double logarithmic plots of  $\lambda$ , the eigenvalue of the renormalisation group transformation, and  $\sigma$ , the width of the underlying distribution, as functions of  $b$ . Data for two core fractions are shown:  $\psi = 0.1$  ( $\circ$ ) and  $\psi = 0.5$  ( $\triangle$ ). A linear least-squares fit is shown in (a) for  $\lambda$  and in (b) for  $\sigma$ . From the slopes of these lines we obtain the exponent estimates quoted in the text.

**Table 1.** Estimates of critical parameters for continuum percolation with hard-core interactions, and comparison with results from freely overlapping percolation. Superscripts ( $\lambda$ ) and ( $\sigma$ ) on the exponent  $\nu$  indicate that these values are determined from equations (3) and (6) respectively. For comparison, recent estimates of  $\nu$  for lattice percolation are  $\nu = 1.333 \pm 0.002$  (Blöte *et al* 1981),  $\nu = 1.342 \pm 0.004$  (Eschbach *et al* 1981) and  $\nu = 1.33 \pm 0.01$  (Stanley *et al* 1982).

$\psi$	$x^*$	$\nu^{(\lambda)}$	$\nu^{(\sigma)}$
0.0001	$1.11 \pm 0.04$	—	—
0.1	$0.96 \pm 0.01$	$1.44 \pm 0.09$	$1.47 \pm 0.08$
0.2	$0.87 \pm 0.04$	—	—
0.3	$0.81 \pm 0.03$	—	—
0.4	$0.80 \pm 0.03$	—	—
0.5	$0.79 \pm 0.01$	$1.39 \pm 0.07$	$1.41 \pm 0.05$
0.55	$0.78 \pm 0.02$	—	—
0.6	$0.79 \pm 0.02$	—	—
0.0 <sup>a</sup>	$0.74 \pm 0.01$	$1.35 \pm 0.07$	$1.33 \pm 0.05$
0.0 <sup>b</sup>	$0.718 \pm 0.003$	—	$1.343 \pm 0.019$
0.0 <sup>c</sup>	$1.1 \pm 0.1$	—	—

<sup>a</sup> Vicsek and Kertész (1981); MC PSRG calculation for overlapping discs.

<sup>b</sup> Gawlinski and Stanley (1981); Monte-Carlo simulation for overlapping discs. These authors determined only one estimate of  $\nu$ .

<sup>c</sup> Pike and Seager (1974) and H Nakanishi (private communication); Monte-Carlo simulation for overlapping squares.



stringent bonding criterion due to the vanishingly small 'soft' regions. We hope to consider these interesting questions in the near future and also to explore the possibility of extending our method to three dimensions, where good agreement between exponents for three-dimensional lattice percolation and percolation of bound water molecules interacting through an ST2 potential has been found by Geiger and Stanley (1982).

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