Monte Carlo experiments on percolation: the influence of boundary conditions

1985 J. Phys. A: Math. Gen. 18 L175

(http://iopscience.iop.org/0305-4470/18/3/014)

J. Phys. A: Math. Gen. 18 (1985) L175-L179. Printed in Great Britain

LETTER TO THE EDITOR

Monte Carlo experiments on percolation: The influence of boundary conditions

D C Rapaport

Department of Physics, Bar-Ilan University, Ramat-Gan, Israel

Received 24 October 1984

Abstract. The slow convergence of the cluster size distribution observed in recent Monte Carlo simulations of two-dimensional site percolation is shown to be due to the use of free boundary conditions. When periodic boundaries are employed the convergence is improved considerably to the extent that the integrated size distribution for large (typically 10^{10} site) lattices is essentially flat over a range of cluster sizes spanning three orders of magnitude. The existence of this plateau, originally predicted by scaling theory, leads to an improved estimate of the critical probability for the square lattice. The observed correction to scaling is not readily characterised by a single additive term, a fact which helps one to understand the wide range of published exponent estimates.

As part of the continuing effort to understand the problem of two-dimensional percolation at and near the critical probability, a series of Monte Carlo studies involving lattices of ever-increasing size have been carried out in recent years (e.g. Hoshen and Kopelman 1976, Hoshen *et al* 1979, Margolina *et al* 1984). However, despite the fact that the latest work involves extremely large lattices—the biggest containing over 10^{10} sites—the results for one of the key quantities, the cluster size distribution, remain subject to pronounced finite-size effects. The consequence of this lack of convergence is that the evidence on which percolation scaling theory is based (Stauffer 1979) remains somewhat less than convincing.

A common feature of these Monte Carlo calculations is that they employ free boundary conditions. The failure to use periodic boundaries distorts the distribution of cluster sizes in an uncontrolled manner by fragmenting clusters that touch the perimeter sites, with appropriate consequences for scaling analysis. When, as will become apparent below, the calculations are carried out subject to periodic boundary conditions, a much sharper picture of the scaling behaviour emerges. This is not unexpected since, in the periodic case, the size distribution for clusters not large enough to span the lattice is that of the infinite system, a result which does not hold if the clusters must be truncated at the free boundaries.

The technical aspects of simulating percolation by means of a Monte Carlo approach are comparatively well known and will only be briefly mentioned here. The so-called 'cluster multiple labelling' method (Hoshen and Kopelman 1976) is used, together with the modification that only a single row of lattice sites is represented in the computer at each step of the calculation (Margolina *et al* 1984). A novel feature of the present approach is that the lattice is not generated *in toto*, but constructed by combining separately generated slabs. Each slab is a square of $10^4 \times 10^4$ sites; by combining sets of slabs a series of lattices of various sizes can be constructed with either periodic or

0305-4470/85/030175+05$02.25

free boundary conditions. The information which must be retained for each slab, to facilitate later combination, is the size histogram for complete clusters that do not extend to the slab perimeter and a list of the (tentatively) incomplete clusters to which the occupied perimeter sites belong.

The lattices constructed cover a range of sizes, the biggest having edges of length $L = 1.6 \times 10^5$—a lattice of 2.56×10^{10} sites, the largest generated to date. A particular economy of the slab approach is that while constructing a lattice of edge length L the method also produces 4 lattices with edge $\frac{1}{2}L$, 16 with edge $\frac{1}{4}L$, and so on. The random number generator used to determine site occupancy is of the shift-register type (Kirkpatrick and Stoll 1981). Construction of a single slab requires approximately 5.5 minutes on an IBM 3081 computer; the time required for combining the slabs is negligible by comparison with the overall generation time. The problem of the limited (32 bit) integer word size of IBM computers raised by Margolina *et al* (1984) does not occur here; the reason for this is that cluster sizes within a single slab cannot exceed the maximum integer value, whereas the relatively short computations involved in slab combination employ double-precision floating-point (with a 56 bit mantissa) arithmetic.

The focus of the present letter is on the nature of the cluster size distribution at (or, strictly speaking, very close to) the critical concentration p_c of the square lattice. The current best Monte Carlo estimate for p_c on this lattice is 0.5927 ± 0.0003 (Hoshen *et al* 1978) based on a lattice with $L = 4000$. A similar value was obtained recently by Gebele (1984). The simulations described here support this value of p_c but with smaller uncertainty limits.

According to the scaling hypothesis (Stauffer 1979) the cluster size distribution can be represented as

$$n_s(p) = s^{-\tau} f_0(z), \qquad z = (p_c - p)s^{\sigma} \tag{1}$$

where $n_s(p)$ is the mean number of clusters per site of size s and p is the site occupation probability. The accepted values for the two exponents appearing in (1) follow immediately from the conjectured thermal and magnetic Potts model exponents (den Nijs 1979, Pearson 1980) and are $\sigma = \frac{36}{91}$, $\tau = \frac{187}{91}$. Deviations from the scaling form (1) at small values of s are accommodated by an additive correction term (Hoshen *et al* 1979), namely

$$n_s(p) = s^{-\tau}(f_0(z) + s^{-\Omega} f_1(z)). \tag{2}$$

The measured cluster distributions are analysed by the approach adopted in earlier work (Hoshen *et al* 1979, Margolina *et al* 1984): the distribution is expressed as a histogram in which the kth bin contains the number of clusters in the range $2^{k-1} \leq s < 2^k$ ($k \geq 1$), and the quantities N_s based on partial sums of the bin contents

$$N_s = s^{\tau - 1} \sum_{s' \geq s} n_{s'} \qquad (s = 2^k) \tag{3}$$

are plotted against the geometric means of the bin limits $s = [2^{k-1}(2^k - 1)]^{1/2}$. If scaling is correct then the integration of (2) corresponding to the partial sum (3) at p_c ($z = 0$) yields

$$N_s = \frac{q_0}{1 - \tau} - \frac{q_1}{\Omega + \tau - 1} s^{-\Omega} \tag{4}$$

where $q_i = f_i(0)$; the implication of (4) is that N_s should tend to independence of s for s sufficiently large.

The measured s-dependence of N_s at p_c for both free and periodic boundary conditions is shown in figures 1 and 2. The results are based on a single lattice realisation for $L = 1.6 \times 10^5$, four lattices with $L = 8 \times 10^4$, etc. Figure 1 is typical of previously published results, especially those of Margolina *et al* (1984) for the triangular lattice; it shows that notwithstanding the extreme lattice sizes there is a lack of convergence for clusters containing more than about 1000 sites (i.e. $\log_2 s > 10$) and, furthermore, there is only the slightest hint of the s-independent plateau predicted by scaling theory, even for the largest of the lattices.

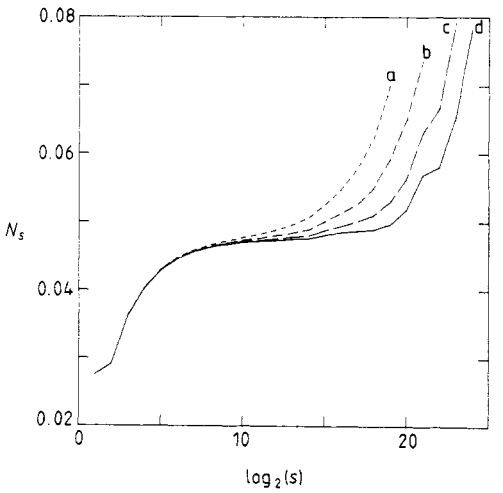

Figure 1. Dependence of the partial sums N_s on cluster size s for a series of square lattices (edge length L: a, 20 000; b, 40 000; c, 80 000; d, 160 000, subject to free boundary conditions ($p = 0.5927$).

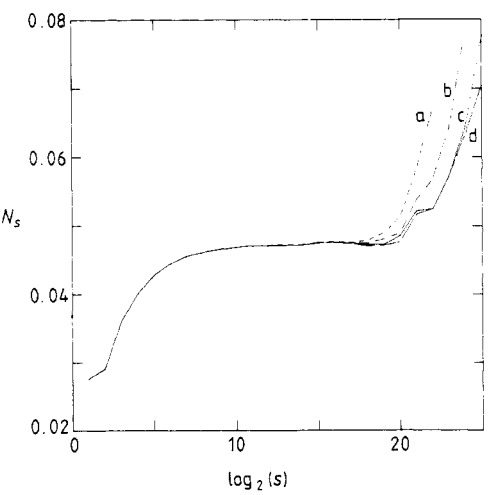

Figure 2. Dependence of N_s on s—as in figure 1—but for periodic boundaries.

These results should be contrasted with figure 2 from which a very different picture emerges. The use of periodic boundaries produces a broad, relatively smooth plateau spanning almost three orders of magnitude in cluster size (a result contrary to the expectations of Margolina *et al* 1984); the finite size effects are only noticeable for very large (typically $s > 2^{18}$) clusters. The fact that the plateau is obtained for the conjectured exact value of τ provides additional support for its correctness.

The numbers of small clusters appearing in the Monte Carlo generated lattices (with periodic boundaries) can be compared with the exact values (Sykes and Glen 1976). If the measured fraction of occupied sites (= 0.592 702) is taken as the effective value of p for comparison purposes, the number of isolated sites differs from the exact value by only 0.005%, and the number of 2 and 3 site clusters by 0.008%. The difference between cluster numbers arising from the choice of boundary conditions affects even the smallest clusters—there is a 0.004% increase in isolated sites if free boundaries are used, and a 0.008% increase in 2 and 3 site clusters. The effect of the boundaries on large clusters is apparent from figures 1 and 2. The large-s deviation from the plateau reflects the dearth of sufficient big ($>2^{19}$) clusters in a lattice which, though extremely large, is still of limited extent.

An analysis similar to that leading to figure 2 can be used to improve the precision of the square lattice p_c estimate. Figure 3 shows the partial sums N_s both at p_c and at two nearby values $p_c \pm \Delta p$, where $\Delta p/p_c \approx 2 \times 10^{-4}$, for a lattice with $L = 8 \times 10^4$. The observed transition of N_s from a monotonically increasing function of s to one with a maximum reflects the merging of numerous large but finite clusters into a single 'infinite' cluster that occurs at p_c. The broad plateau is present only at the intermediate value of p; thus if the scaling hypothesis is correct and τ is as conjectured, figure 3 suggests the estimate

$$p_c = 0.5927 \pm 0.0001.$$

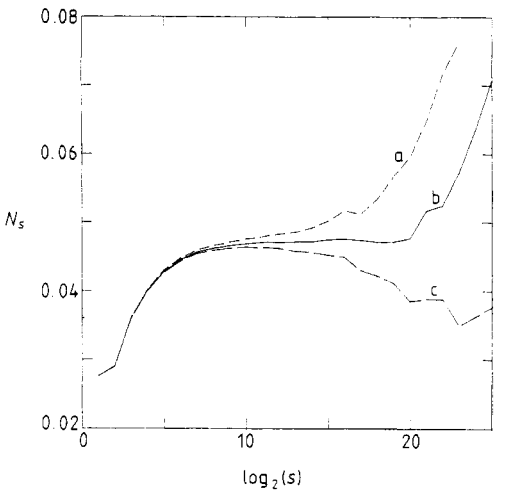

Figure 3. The s-dependence of the partial sums in the neighbourhood of p_c ($= 0.5927$) for $L = 80\,000$ and periodic boundaries. The plateau only appears at p_c. a, $p = 0.5926$; b, $p = 0.5927$; c, $p = 0.5928$.

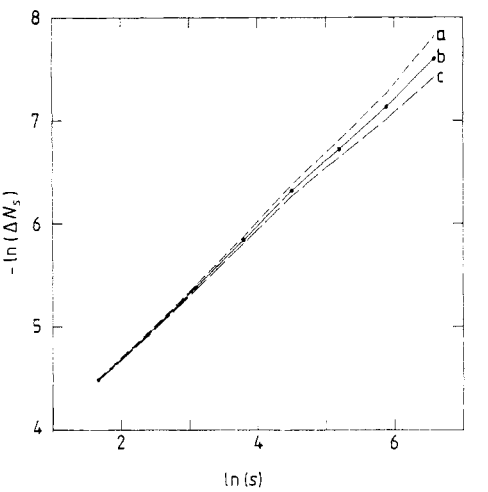

Figure 4. Log–log plot of the small-s deviations (ΔN_s) from the plateau for three possible plateau values $N^{(0)}$ (a, 0.0473; b, 0.0474; c, 0.0475).

The sensitivity to p apparent in figure 3 indicates that a further reduction in the error limits, with a possible minor adjustment to the value itself, would result from additional simulations close to the present value of p_c.

Several other recent estimates of p_c are available with which the above result can be compared. Series analysis leads to the values 0.593 ± 0.002 (Sykes *et al* 1976) and, more recently, 0.5923 ± 0.0007 (Djordjevic *et al* 1982). Different kinds of spatial renormalisation techniques yield 0.5927 ± 0.0002 (Derrida and de Seze 1982) and 0.5931 ± 0.0006 (Reynolds *et al* 1980).

The correction-to-scaling exponent Ω defined in (2) provides a measure of the small-s deviation of N_s from the plateau. If the plateau value is denoted by $N^{(0)}$ and the deviation by ΔN_s, where

$$N^{(0)} = q_0/(1-\tau), \qquad \Delta N_s = N^{(0)} - N_s,$$

then (4) is equivalent to

$$\ln(\Delta N_s) = \text{constant} - \Omega \ln s. \tag{5}$$

If (5) holds, then Ω is the gradient of the log–log plot of ΔN_s against s. The deviations are plotted in figure 4; due to the slight uncertainty in the precise value of

$N^{(0)}$, plots for three closely spaced vaues are shown. The best choice of $N^{(0)}$ is the one for which the plot is closest to linear, namely $N^{(0)} = 0.0474$; as $N^{(0)}$ moves away from this value the curvature (which may be positive or negative) of the plots gradually increases. The actual range of s covered is 2^3 to 2^{10} and the results are independent of lattice size; at larger s the ΔN_s become dominated by statistical fluctuations in the cluster data. It is clearly impossible to arrive at a particularly precise estimate of Ω from the graph; a visual fit to the points for $N^{(0)} = 0.0474$ yields $\Omega = 0.64$, although individual near-linear segments correspond to Ω between 0.58 and 0.66—it is far from obvious that a linear fit is justified.

Other estimates of the exponent Ω exist that are obtained from Monte Carlo, series and renormalisation group calculations, but there is little overall agreement between the values which are spread over the range 0.46 to 0.75. The recent Monte Carlo study on the triangular lattice (Margolina *et al* 1984) concluded that $\Omega = 0.6 \pm 0.08$ on the basis of a series of linear fits; however, it is only when one examines a plot of the actual data (as in figure 4) that the reason for the low quality of the fit becomes apparent.

The relative merits of the different values for the exponent Ω have been discussed at some length by Adler *et al* (1983) and Margolina *et al* (1984), and the proposal made that the correction to scaling actually consists of two or more terms with similar exponents. While the presence of competing confluent singularities would certainly be a sufficient reason for the discrepancies between the various results, it also implies that accurate numerical analysis is very difficult, if not impossible, on the basis of data currently available. The inability to arrive at a reasonably confident estimate of the correction exponent, depite the very large lattice sizes used in the present work, is further evidence that a single additive term does not adequately describe the corrections to scaling.

References

Adler J, Moshe M and Privman V 1983 in *Percolation Structures and Processes* ed G Deutcher, R Zallen and J Adler (Bristol: Adam Hilger) p 397
den Nijs M P M 1979 *J Phys A: Math. Gen.* **12** 1857
Derrida B and de Seze L 1982 *J. Physique* **43** 475
Djordjevic Z V, Stanley H E and Margolina A 1982 *J. Phys. A: Math. Gen.* **15** L405
Gebele T 1984 *J. Phys. A: Math Gen.* **17** L51
Hoshen J and Kopelman R 1976 *Phys. Rev.* B **14** 3438
Hoshen J, Kopelman R and Monberg E M 1978 *J. Stat. Phys.* **19** 219
Hoshen J, Stauffer D, Bishop G H, Harrison R J and Quinn G D 1979 *J. Phys. A: Math. Gen.* **12** 1285
Kirkpatrick S and Stoll E P 1981 *J. Comp. Phys.* **40** 517
Margolina A, Nakanishi H, Stauffer D and Stanley H E 1984 *J. Phys. A: Math. Gen.* **17** 1683
Pearson R B 1980 *Phys. Rev.* B **22** 2579
Reynolds P J, Stanley H E and Klein W 1980 *Phys. Rev.* B **21** 1223
Stauffer D 1979 *Phys. Rep.* **54** 1
Sykes M F, Gaunt D S and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 97
Sykes M F and Glen M 1976 *J. Phys. A: Math. Gen.* **9** 87