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1984 J. Phys. A: Math. Gen. 17 L129

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LETTER TO THE EDITOR

Monte Carlo study of invasion percolation clusters in two and three dimensions

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Received 15 November 1983

Abstract. We consider the process of growing invasion percolation clusters from a point into an infinite medium. Invasion percolation is a modified form of percolation in which cluster growth proceeds dynamically along a path of least resistance. The form considered here is the simplest one in which the cluster is permitted to grow into regions it has previously surrounded. It is shown that this process can yield extremely good Monte Carlo estimates of the percolation threshold p_c . For the square, triangular and match-square lattices we obtain p_c values of 0.5925 ± 0.0003 , 0.5000 ± 0.0003 and 0.4072 ± 0.0002 , and for the simple cubic lattice 0.31158 ± 0.00006 . The errors quoted are purely statistical, and represent one standard deviation. Two critical exponents are obtained which we suggest should be identified in terms of the fractal dimension D and gap exponent Δ of ordinary percolation. Based on these identifications we obtain values for $1/D$ and $1/\Delta$ of 0.527 ± 0.002 and 0.393 ± 0.004 in two dimensions and 0.402 ± 0.003 and 0.454 ± 0.005 in three dimensions. These results are consistent with known exact results and best series and Monte Carlo estimates, suggesting that the form of invasion percolation considered here is probably in the same universality class as ordinary percolation.

Invasion percolation is a dynamic growth process which was originally developed to describe the displacement of one fluid by another from a porous medium in the presence of capillary (surface tension) forces (Chandler *et al* 1982, Wilkinson and Willemsen 1983, Koplik *et al* 1983). In this model the displacing fluid advances in a sequence of discrete jumps whose locations are chosen by a criterion of least capillary resistance (or greatest capillary drive). In the fluid problem there is a trapping rule which prevents the displacing fluid from invading a region it has previously surrounded, this representing physically the incompressibility of the displaced phase.

Here we will consider a simpler form of invasion percolation in which the growing cluster is permitted to enter such trapped regions, as would be appropriate if the displaced fluid were compressible. The process of growing a cluster from a point into an infinite lattice is defined by the following rules.

(1) Consider an infinite lattice of sites and connecting bonds in which each site is assigned a random number r , drawn from a uniform distribution on the unit interval $0 \leq r < 1$.

(2) Choose a site (the 'origin') to be occupied as the seed of the cluster. At any stage, define the boundary to be those unoccupied sites which are nearest neighbours of sites in the cluster.

(3) At each time step increase the number of sites in the cluster by one, by occupying that boundary site which has the smallest random number.

Cluster growth according to rules (1)–(3) has recently been solved exactly for the case of a Cayley tree of arbitrary coordination number (Nickel and Wilkinson 1983).

The analogous algorithm for growing a single cluster in ordinary percolation at occupation probability p is to take rules 1 and 2 above but replace rule 3 by (Leath 1976a, b, Leath and Reich 1978, Alexandrowicz 1980)

(3') At each time step the current boundary sites are examined and those with random number $r < p$ are accepted into the cluster. The cluster terminates when no sites with random number $< p$ remain on the boundary.

As is well known there is a critical percolation probability p_c such that for $p < p_c$ the cluster always terminates, but for $p > p_c$ there is a finite probability that the cluster grows indefinitely. By contrast in invasion percolation there is no temperature-like variable analogous to the occupation probability, but rather the control parameter is the size n of the cluster. Thus in invasion percolation the cluster may be grown to any desired size.

The close connection between the two forms of percolation is demonstrated by the following fundamental property of invasion percolation. Let us define the 'acceptance profile' $a_n(r)$ such that $a_n(r) dr$ is the probability that the random number chosen at the n th step is in the interval $[r, r + dr]$. Then as $n \rightarrow \infty$ it is found that the profile approaches a step function of the form

$$a_\infty(r) = \begin{cases} p_c^{-1} & \text{if } r < p_c, \\ 0 & \text{if } r > p_c. \end{cases} \quad (1)$$

Although from the point of view of this paper this property is merely a conjecture strongly supported by Monte Carlo evidence, we have been informed by C Newman (private communication) that this is in fact a rigorous theorem.

The fundamental result (1) indicates that the invasion percolation algorithm can be used to obtain a Monte Carlo estimate of p_c . In computer simulations it is more convenient to employ a cumulative acceptance profile $b_n(r)$ defined by

$$b_n(r) = \frac{\langle \text{no of random numbers in } [r, r + dr] \text{ accepted into cluster} \rangle_n}{\langle \text{no of random numbers in } [r, r + dr] \text{ considered} \rangle_n}, \quad (2)$$

where $\langle \rangle_n$ denotes an ensemble average over clusters of size n . In terms of $a_n(r)$ we have

$$b_n(r) = (n + \langle n_b \rangle_n - 1)^{-1} \sum_{m=1}^n a_m(r), \quad (3)$$

where $\langle n_b \rangle_n$ is the expected number of sites on the boundary immediately before the n th site is chosen. It is clear from its definition that $b_n(r)$ is normalised such that $b_n(0)$ is unity. Thus as $n \rightarrow \infty$, $b_n(r)$ has the asymptotic behaviour

$$b_\infty(r) = \begin{cases} 1 & \text{if } r < p_c, \\ 0 & \text{if } r > p_c. \end{cases} \quad (4)$$

In order to use (4) to estimate p_c it is necessary to make some assumption about the way the limiting form (4) is approached as $n \rightarrow \infty$. Following Wilkinson and Willemsen we define $B_1(n)$ and $B_2(n)$ by

$$B_1(n) = \int_0^{p_c} [1 - b_n(r)] dr, \quad B_2(n) = \int_{p_c}^1 b_n(r) dr, \quad (5a, b)$$

which represent the deviation of $b_n(r)$ from the step function (4). We assume that as $n \rightarrow \infty$ these have the power law behaviour

$$B_1(n) \sim b_1 n^{-1/\Delta}, \quad B_2(n) \sim b_2 n^{-1/\Delta}, \quad (6a, b)$$

with a common exponent Δ . This is consistent with the exact results on the Cayley tree, for which Δ is found to be 2. Our conjecture, supported by the Monte Carlo results of this paper, is that in general Δ should be identified with the gap exponent $\beta + \gamma$ of ordinary percolation. Our precise algorithm for determining p_c and Δ is to compute, for a set of r -values close to the percolation threshold p_c , the quantity

$$B_n(r) = \int_0^r b_n(r') dr', \quad (7)$$

which is just $(n + \langle n_b \rangle_n - 1)^{-1}$ times the expected number of chosen random numbers in the interval $0 \leq r' < r$. For a given guess for p_c the quantity $B_n(p_c)$ is found by interpolation and the corresponding $B_1(n)$ and $B_2(n)$ computed from

$$B_1(n) = p_c - B_n(p_c), \quad B_2(n) = p - B_n(p_c), \quad (8a, b)$$

where p is given by

$$p = B_n(1) = n / (n + \langle n_b \rangle_n - 1). \quad (9)$$

The value of p_c is then adjusted until a least squares fit of $\ln B_1(n)$ and $\ln B_2(n)$ against $\ln n$ yields a common slope $-1/\Delta$.

In addition to the exponent Δ we may also obtain a fractal dimension associated with the geometrical shape of the cluster. Let us define the root mean square cluster radius as

$$R(n) = \left(\left\langle \sum_{m=1}^n R_m^2 \right\rangle_n \right)^{1/2}, \quad (10)$$

where R_m is the Euclidean distance of the m th chosen site from the origin, and the average is taken over all clusters of size n . Then we expect that for large n

$$R(n) \sim n^{1/D}, \quad (11)$$

where D is the fractal dimension of the cluster. This is consistent with the results on the Cayley tree, for which D is found to be 4. Our conjecture, again supported by the Monte Carlo results of this paper, is that D is the same as the fractal dimension in ordinary percolation.

We now present Monte Carlo results for cluster growth in 2D and 3D according to the invasion percolation rules (1)–(3) given above. In 2D we have studied the square (SQ), triangular (TR) and match-square (MS) lattices with coordination numbers 4, 6 and 8 respectively, and in 3D the simple cubic (SC) lattice with coordination number 6. The match-square lattice is obtained by including all the diagonals on the square lattice; it is the so-called matching lattice to the square lattice and has the property (Sykes and Essam 1963, 1964)

$$p_c(\text{SQ}) + p_c(\text{MS}) = 1. \quad (12)$$

The triangular lattice is self-matching in this sense and so

$$p_c(\text{TR}) = \frac{1}{2}. \quad (13)$$

Since the algorithm for invasion percolation involves searching for the smallest random number of the current boundary sites, the computer time required to grow a cluster of n sites grows at least as fast as $n \ln n$, since the number of boundary sites is of order n . We actually use a simpler search technique which causes the computing time to grow as $n^{3/2}$; this method appears competitive with a logarithmic search for the cluster sizes considered here. Our Monte Carlo algorithm is implemented on a CDC Cyber 750 computer and represents the coordinates of a lattice point in a single 60-bit word. The actual locations of the current occupied and boundary sites are stored using a hashing technique (see e.g. Knuth 1973). The total number of occupied and boundary sites $n + n_b$ is currently limited to around 100 000. Since $n \rightarrow \infty$ we have

$$n/(n + \langle n_b \rangle_n) \sim p_c, \quad (14)$$

the maximum cluster size attainable depends on the percolation threshold for the lattice in question. The maximum cluster size used for each of the four lattices is listed in the column n_{\max} of table 1.

Table 1. Results of Monte Carlo simulations of invasion percolation for four different lattices. For each lattice is shown the range of cluster sizes n used to fit the data, the number of realisations used, and the obtained percolation threshold p_c and exponents $1/\Delta$ and $1/D$.

Lattice	n_{\min}	n_{\max}	Number grown	p_c	$1/\Delta$	$1/D$
SQ	1000	60 000	1800	0.5925 ± 0.0003	0.395 ± 0.007	0.529 ± 0.003
TR	1000	50 000	1800	1.5000 ± 0.0003	0.390 ± 0.007	0.531 ± 0.004
MS	1000	40 000	1800	0.4072 ± 0.0002	0.395 ± 0.005	0.521 ± 0.003
SC	1000	30 000	2500	$0.311\ 58 \pm 0.000\ 06$	0.454 ± 0.004	0.402 ± 0.003

When obtaining exponents from Monte Carlo data, it is necessary to decide the range of values of the independent variable, here n , to use. Naturally it makes sense to use the maximum cluster size n_{\max} as the upper end of the range, but the lower end n_{\min} is not so easy to decide. For fixed n_{\max} , as n_{\min} increases the statistical errors increase, but the systematic errors due to the use of finite n -values presumably decrease. Here we have made the choice $n_{\min} = 1000$ for each of the four lattices; this choice is clearly arbitrary, but has the property that it limits the statistical errors in the exponents to around 0.005.

In table 1 we present our results for the percolation threshold p_c and exponents $1/\Delta$ and $1/D$. The errors quoted are one standard deviation statistical errors estimated by dividing the data for each lattice into ten groups and observing the standard deviation between the ten sets of results. No attempt has been made to estimate the systematic errors, and so the errors quoted may be over-optimistic. Nevertheless the results in 2D are quite encouraging. The value $p_c = \frac{1}{2}$ for the TR lattice is obtained exactly, while for the SQ and MS lattices we obtain

$$p_c(\text{SQ}) + p_c(\text{MS}) = 0.9997 \pm 0.0005, \quad (15)$$

clearly consistent with (12), and suggesting that the p_c values obtained for these lattices are correct within the quoted errors. Assuming (12) we may combine the results for

the two lattices to obtain the improved estimate

$$p_c(\text{SQ}) = 0.5927 \pm 0.0002, \quad p_c(\text{MS}) = 0.4073 \pm 0.0002, \quad (16)$$

which is consistent with previous results for the SQ lattice of $p_c = 0.5923 \pm 0.0007$ (Djordjevic *et al* 1982) and $p_c = 0.5927 \pm 0.0002$ (Derrida and de Seze 1982).

To within two standard deviations, the critical exponents obtained for the three 2D lattices are consistent with each other (universality), and yield the combined results

$$1/\Delta = 0.393 \pm 0.004, \quad 1/D = 0.527 \pm 0.002. \quad (17)$$

These results are also consistent with the hypothesis that these exponents should be identified with the corresponding ones in ordinary percolation. The den Nijs values (den Nijs 1979, Nienhuis *et al* 1980, Pearson 1980), which are thought to be exact, are

$$1/\Delta = \frac{36}{91} = 0.3956, \quad 1/D = \frac{48}{91} = 0.5275. \quad (18)$$

Our results for the SC lattice are also in good agreement with best known values in ordinary percolation. Our value $p_c = 0.31158 \pm 0.00006$ is certainly consistent with the value

$$p_c = 0.3117 \pm 0.0003 \quad (19)$$

obtained by Monte Carlo methods (Heermann and Stauffer 1981), though we believe that in this case our error estimate is certainly too optimistic (see below). The exponents for the SC lattice in table 1 are also consistent with the most recent series estimates (Gaunt and Sykes 1983)

$$1/\Delta = 0.459 \pm 0.009, \quad 1/D = 0.403 \pm 0.002, \quad (20)$$

and with the values given by Heermann and Stauffer

$$1/\Delta = 0.457, \quad 1/D = 0.402. \quad (21)$$

As emphasised above, the percolation threshold and exponent estimates made in this paper have been obtained by straightforward fitting of the data; no attempt has been made to estimate or correct for the systematic errors which are always present when one tries to fit asymptotic laws with data which are obtained over a finite range of parameters. However, it is possible to modify the predictions somewhat by making more subjective judgements. For example, the method of determining p_c by finding a common exponent in (6a) and (6b) is equivalent to finding that value for which the ratio B_2/B_1 is 'most constant' over the chosen range of n -values. In figure 1 we plot this ratio for the SC lattice for $1000 \leq n \leq 30\,000$ for various values of p_c . While our value $p_c = 0.31158$ clearly gives a reasonably constant ratio B_2/B_1 over the whole range, a human eye, seeing the trend in the data, would probably pick $p_c = 0.3118$ as the best value. Clearly our purely statistical error of 0.00006 is too optimistic in this case.

We have demonstrated that invasion percolation can provide an excellent algorithm for determining the percolation threshold p_c . While our actual method makes use of the unproved assumption of a common exponent in (6a) and (6b), the close agreement with accepted percolation thresholds for the lattices considered clearly indicates that this assumption is correct. Although the algorithm for invasion percolation requires computer time of order at least $n \ln n$ as opposed to the order n time for ordinary percolation, it seems likely that invasion percolation is a better p_c algorithm because (a) the critical point is found automatically without the need for trials at different

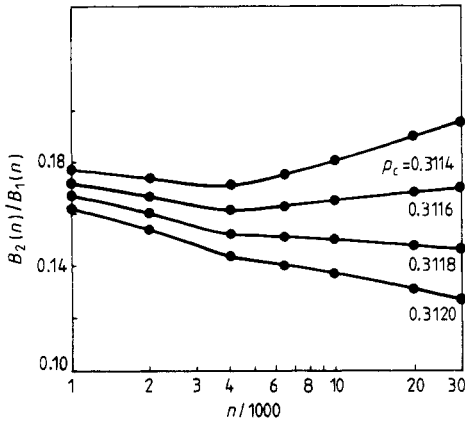


Figure 1. Plot of the ratio $B_2(n)/B_1(n)$ (see (5)) for $1000 \leq n \leq 30\,000$ for the SC lattice for various choices of p_c . The correct p_c is that for which the ratio is 'most constant'.

values of the occupation probability p , and (b) every cluster can be grown to a chosen size without risk that some clusters will grow too large to handle, as happens in ordinary percolation as p approaches p_c .

The good agreement between our critical exponents and those of ordinary percolation both in 2D and 3D strongly suggests that we have made the correct identifications and that the form of invasion percolation considered here is in the same universality class as ordinary percolation. As observed above, these hypotheses are also consistent with the exact results on the Cayley tree, for which $\Delta = 2$ and $D = 4$. Given these identifications, the exponent values obtained here appear competitive with best previous Monte Carlo and series work in ordinary percolation.

The results described here apply only to the simplified form of invasion percolation in which the cluster is allowed to grow into regions it has surrounded. The version in which this is not permitted is much more complicated to simulate because of the necessity of checking after each step whether a trap has taken place. Although the Monte Carlo work for this version is not therefore of the same quality as that presented here, there is considerable evidence that, at least in 2D, invasion percolation with trapping is in a different universality class from ordinary percolation (Chandler *et al* 1982, Wilkinson and Willemsen 1983). The underlying reason for this is not understood, and poses an interesting theoretical problem. Indeed a field theoretic formulation of even the simple form of invasion percolation considered here, analogous to the mapping of ordinary percolation onto the Potts model, is completely lacking at present.

It is a pleasure to thank J Willemsen and B Nickel for useful discussions.

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