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LETTER TO THE EDITOR

The fractal dimension of percolation cluster hulls

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Abstract. Large simulations of 2D site percolation on a square lattice provide several estimates of the fractal dimension D_h of the 'hull' or outer boundary of percolation clusters close to criticality. Statistical estimates based on an ensemble of more than 10^6 clusters with varying sizes yield $D_h = 1.74 \pm 0.02$. Geometrical measurements of the hull two-point correlation for individual clusters with more than 10^5 sites give $D_h = 1.76 \pm 0.01$. The observed scaling behaviour is the same both slightly above and below p_c .

The recent interest in the geometrical aspects of phase transitions has been stimulated by the success of Mandelbrot's (1982) fractal geometry in both understanding and quantifying complicated shapes and providing a geometric basis for many physical relations. The idealised percolation problem, in which a random mixture of conducting (fraction p) and insulating (fraction $1-p$) material abruptly exhibits long-range conduction (connectivity) at a critical concentration $p = p_c$, has proven to be a fruitful analogue for many phase transition problems (see, for example, the excellent review by Stauffer 1979 or the articles in Deutscher *et al* 1983). In this case, the phase transition is obviously geometric and the connection between the 'universal' exponents and geometrical scaling quantities (typically, a fractal dimension) has been established (Mandelbrot 1982, Stauffer 1979 (and references therein), Voss *et al* 1982, 1983). The percolation problem is, moreover, ideally suited to large scale computer simulations. To date, many of the detailed studies of scaling behaviour (for example, Leath 1976, Leath and Reich 1978, Stanley 1977, Stauffer 1979) have come from such computer 'experiments'. This letter presents the results of new simulations designed to measure the fractal dimension of percolation cluster 'hulls' or outer perimeters in 2D.

Most of the fractal studies of percolation have concentrated on the fractal dimension D of the largest ('infinite') cluster at p_c (see, for example, Kapitulnik *et al* 1983 or Stauffer 1979). Both computer simulations and geometric measurements of actual metal film micrographs (Voss *et al* 1982, 1983, Kapitulnik and Deutscher 1983, Deutscher *et al* 1983) show that $D \approx 1.9$. This is in agreement with theoretical calculations that relate D to the universal exponents (Mandelbrot 1982, Stauffer 1979). In 2D, $D = 2 - \beta/\nu = \frac{1}{2}(2 + \gamma/\nu) = 2 - \frac{1}{2}\eta$. Other fractal dimensions are, however, important in the percolation problem and are expected to be of physical significance. Collectively, the boundary of all clusters is a space-filling fractal with $D_{\text{all}} = 2$ (Mandelbrot 1982, Voss *et al* 1982, 1983). This fractal dimension governs the perimeter against area scaling and, together with D of an individual cluster, determines the cluster size scaling exponent τ at p_c , $\tau = 1 + D_{\text{all}}/D$. The fractal dimension of the percolation

cluster 'backbone' or bi-connected component ($D_b \approx 1.7$) is also of physical interest (Kirkpatrick 1979).

Another apparently scaling quantity is the cluster external perimeter or 'hull' (a descriptive term first applied by Mandelbrot 1982). Early investigations suggest that the hull H varies with the cluster size s (area in 2D) as $H \propto s^{0.9}$ (Leath and Reich 1978). The physical significance of the hull may be related to that of a surface energy. Several different methods are used here with large 2D simulations to demonstrate the scaling behaviour of percolation cluster hulls and to estimate their fractal dimension, D_h .

The simulations approximated 2D site percolation using a 1024 by 1024 square lattice with periodic boundary conditions. For each sample a random number generator was used to independently occupy each site with probability p . A fast algorithm was used to find all connected clusters. Connectivity required occupation of at least one of the four neighbour sites (two horizontal and two vertical). Once determined, the cluster statistics were averaged over clusters having similar areas $s \pm \Delta s$ (number of sites). The quantities measured were $N(s)$, the number of clusters with s sites; $\lambda(s)$, the average size of an s -site cluster defined as $\lambda = (\Delta X \Delta Y)^{1/2}$; and $P(s)$ the average s -site cluster perimeter, where P = number of occupied sites neighbouring an unoccupied site.

Measurement of the cluster hulls required additional computation. In a similar fashion to the analysis of the occupied sites, the empty-site 'holes' were determined with connectivity based on eight neighbour sites (two horizontal, two vertical and four corners). The use of eight-neighbour connectivity for the empty sites preserves the occupied-empty symmetry about p_c . For $p < p_c$ there is long-range hole connectivity while for $p > p_c$ there is only long-range cluster connectivity. Each occupied-site cluster could then be associated with a number of neighbouring empty-site holes. The cluster hull or external perimeter is defined here as the number of occupied sites that neighbour the largest hole. For finite clusters the largest hole is the obvious cluster exterior. Above p_c (or for occasional large clusters below p_c that span the finite periodic sample) the hull is the boundary with the largest interior hole. It was, thus, possible to estimate $H(s)$, the average number of hull sites, and $A_{\text{tot}}(s)$, the total area (number of sites) enclosed by the hull, for an s -site cluster.

Figure 1 shows a typical largest cluster (in grey) from one sample with $p = 0.592$ just below p_c . This cluster spans the sample in one direction. Occupied sites that belong to the hull are shown in black. Figure 1 shows that even for a very large cluster (more than 10^5 sites) many of the seemingly interior sites actually border the exterior through intricate fjords.

Figure 2 shows the variation of the number of sites in the hull with cluster size below ($p = 0.590$), above ($p = 0.595$) and close to p_c ($p = 0.593$). Each set of points represents an average over 20 to 50 1024 by 1024 samples. As discussed above, the hulls H of all clusters with size $s \pm \Delta s$ are averaged to give an estimate of $H(s)$. $\Delta s \propto s$ to give uniform spacing in log s . The full line shows a fit of the data to the form $H(s) \propto s^{0.89 \pm 0.02}$ in excellent agreement with the smaller simulations of Leath and Reich (1978). There is no significant difference in the results above, below or close to p_c .

The dependence shown in figure 2 is not, however, directly related to the fractal dimension D_h of the hulls. Figure 3 shows two alternative demonstrations of hull scaling behaviour that are directly related to D_h . One of the most common uses of the fractal dimension D has been to describe the variation of the amount or 'mass' M

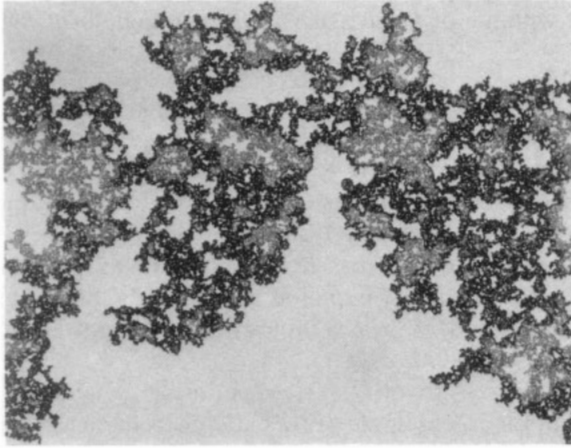


Figure 1. Largest cluster (grey) and its hull or external perimeter (black) for a typical 1024 by 1024 sample of 2D square lattice site percolation with $p = 0.592$ just below p_c .

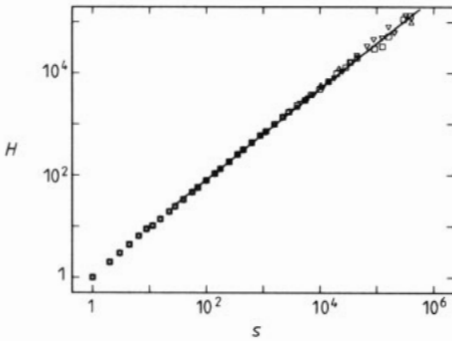


Figure 2. Hull against area scaling for the ensemble of all clusters from multiple 1024 by 1024 samples near p_c . The full line shows the least-squares fit to a power-law dependence ($H \propto s^{0.89 \pm 0.02}$). The values of p are: Δ , 0.595; \square , 0.593; ∇ , 0.590.

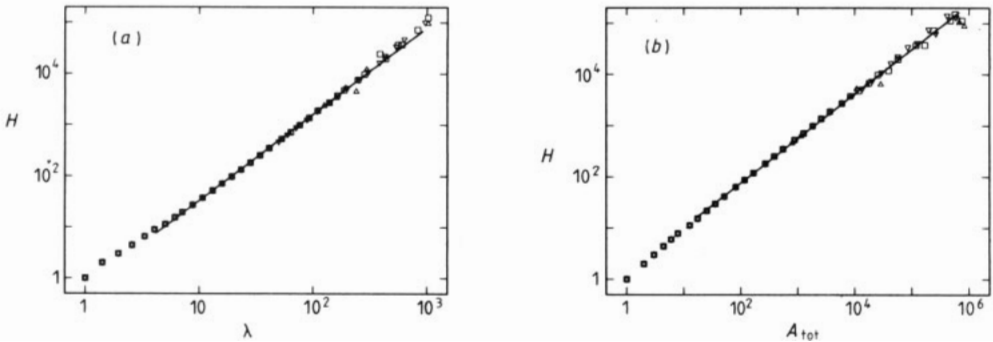


Figure 3. Ensemble estimates of the hull fractal dimension D_h from the same clusters as figure 2. Full lines show power-law fits. (a) Hull against characteristic cluster size $\lambda = (\Delta X \Delta Y)^{1/2}$ ($H \propto \lambda^{1.72 \pm 0.04}$). (b) Hull against enclosed area, A_{tot} ($H \propto A_{tot}^{0.870 \pm 0.015}$). The values of p are: Δ , 0.595; \square , 0.593; ∇ , 0.590.

of an individual object within a distance λ as λ varies (Mandelbrot 1982). Thus,

$$M(\lambda) \propto \lambda^D. \quad (1)$$

This concept can be extended to an ensemble of scaling objects each of which is characterised by some largest length scale λ , provided all of the objects are examined with the same small scale resolution (in this case, the lattice size). Equation (1) then takes on a statistical meaning where $M(\lambda)$ becomes the average over all objects of similar characteristic size λ . Figure 3(a) shows a plot of average hull H against characteristic cluster size for the same samples as figure 2. The behaviour is obviously scaling and the fractal dimension D_h comes directly from the power-law fit shown as the full line. Here $D_h = 1.72 \pm 0.04$.

An alternative statistical measure of D_h is from perimeter, P against area, A scaling in the plane. Once again, for an ensemble of fractal objects of varying sizes examined with the same resolution (Mandelbrot 1982),

$$P \propto A^{D/2}, \quad (2)$$

where D is the fractal dimension of the perimeter. For common Euclidean shapes, such as a collection of various sized circles, the perimeters have $D = 1$ and equation (2) gives the familiar $P \propto A^{1/2}$. For the ensemble of all percolation clusters, $P \propto A$ leading to $D_{\text{all}} = 2$ (Voss *et al* 1982, 1983, Mandelbrot 1982) as discussed above. This relation has also been used to estimate the fractal dimension for 2D projections of cloud and rain areas (Lovejoy 1982). Figure 3(b) shows a plot of percolation cluster hull against total enclosed area A_{tot} for the same samples as figure 2. For a given cluster, A_{tot} is the sum of the occupied sites s , the interior holes, and all smaller clusters completely surrounded by the cluster in question. The scaling behaviour is again obvious and the fractal dimension D_h can be read directly from the power-law fit as $\frac{1}{2}D_h = 0.870 \pm 0.015$ in excellent agreement with figure 3(a).

Whereas figure 3 demonstrates the statistical determination of D_h from the ensemble of percolation clusters, D_h can also be estimated with equation (1) from the scaling properties of individual large clusters. A convenient method is based on the two-point correlation function $G(r)$. $G(r)$ is the probability that two points separated by a distance r are both in the same object (here, a given cluster's hull). For a fractal (Mandelbrot 1982), $M(r) \propto \int G(r) r \, dr$ and

$$G(r) \propto r^{2-D}. \quad (3)$$

A 2D fast Fourier transform (FFT) was used as a computationally efficient means of calculating $G(r)$ from an individual hull picture ($P(r) = 1$ if r is in the hull, 0 otherwise). The 2D inverse transform of the spectral density immediately yields $G(r)$ which was then averaged over all directions. Figure 4 shows the measured $G(r)$ averaged over the largest cluster hull in 20 samples slightly above and slightly below p_c . There is no appreciable difference in the scaling behaviour of $G(r)$ on either side of p_c and the measured $D_h = 2 - 0.234 \pm 0.003$ is in good agreement with that of the ensemble estimates of figure 3.

In summary, large simulations of 2D site percolation on a square lattice have been used to demonstrate the geometrical scaling behaviour of the hull or external perimeter of percolation clusters close to p_c . Different methods of estimating the hull fractal dimension D_h were presented. Ensemble estimates based on more than 10^6 clusters

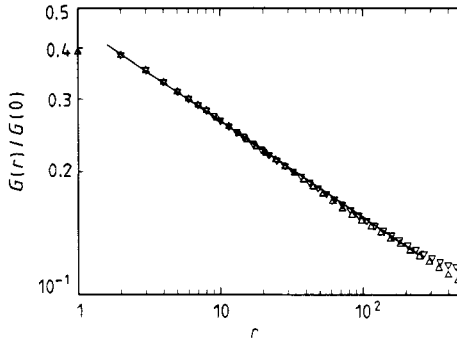


Figure 4. Estimate of the hull two-point correlation $G(r)$ against r for the largest cluster from each of 20 1024 by 1024 samples slightly above and below p_c . Full line shows power-law fit ($G(r) \propto r^{-0.234 \pm 0.003}$). The values of p are: \triangle , 0.594; ∇ , 0.592.

with varying sizes yield $D = 1.74 \pm 0.02$. Geometrical measurements of the hull two-point correlation $G(r)$ for large clusters with more than 10^5 sites give $D = 1.76 \pm 0.01$. No difference was observed in the scaling properties above and below p_c .

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