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LETTER TO THE EDITOR

Percolation threshold of a random array of discs: a numerical simulation

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Abstract. We have evaluated numerically the percolation threshold of a 3D assembly of widthless monodisperse discs (radius R, number per unit volume N) in terms of the quasi-invariant NR^3. The value obtained is consistent with previous estimates. This model should apply to the permeability problem of fractured rocks.

Several attempts have been made to apply percolation theory to the hydrogeology of weakly fractured rocks, when the number of fractures is not large enough to create a well connected network inside the rock volume.

Computer simulations have been performed to relate the connectivity in random arrays of elements to fractured rock permeability, treating the fractures as random lines [1, 2] in two dimensions and as discs [1] or cracks [3] in three dimensions. Wilke *et al* [4], modelling fractures as widthless unit squares on a cubic lattice, verified that the problem corresponds to the same universality class as usual bond percolation and this general result obtained in other domains for that class of problem should apply to fractured rock hydrology.

Further attention was given to the determination of permeability thresholds. These are of practical importance as a basis for probabilistic analysis in problems dealing with waste storage in fractured rocks [5]. More generally, the homogenisation techniques fail to describe the transport properties in the neighbourhood of the permeability threshold.

A model of random widthless discs was discussed by Charlaix and co-workers [6, 7] and it was shown that the percolation threshold can be given by a critical value $(NR^3)_c$ of the dimensionless number NR^3, N being the number of discs of radius R by unit volume. A numerical value of $(NR^3)_c$ was estimated from the properties of the 'quasi-invariants' of percolation as the critical coordination or critical excluded volume (to be defined later).

After describing the recent developments on the existence and numerical values of quasi-invariants, we present a Monte Carlo simulation of a random system of widthless discs; the percolation threshold is determined using a finite-size scaling technique.

The near invariance at percolation threshold p_c of critical quantities such as the critical coordination for bond percolation ($zp_{cb} = 2$ (2D), 1.5 (3D)) or the critical volume fraction for site percolation ($\Phi = fp_{cs} = 0.44$ (2D), 0.15 (3D)) was first established [8] on regular lattices with nearest-neighbour interactions. (Here z is the coordination of the lattice and f is the packing fraction of spheres in contact.) The critical volume fraction was also shown to be a good invariant parameter to characterise the percolation threshold of random mixtures of hard core objects [9].

For percolation of overlapping objects in a continuous medium, Pike and Seager [8] introduced the mean number of intersections, B, as a generalisation to continuous media of the effective coordination zp_b of a bond problem (zp_b is also the mean number of active bonds per site). However the numerical value of B_c is not the same as the previous one: $B_c = 2.7$ for spheres (3D) and 4.5 for discs (2D). Further studies on regular lattices but with longer range interactions (i.e. larger z) showed increased numerical values of zp_{cb} in bond percolation [7], but always below 2.7 (3D) and 4.5 (2D). Ottavi [10] showed that a bond percolation problem can be mapped onto a site percolation on a 'covering lattice', the coordinations being related by $z_b = 2z_s - 2$. Similarly, continuous percolation of overlapping objects is a site percolation problem on an infinite coordination network. Ottavi proposed a new criterion for both site and bond percolation on lattices:

$$p_{c(s,b)}(z_{s,b}+3) = 4.5 \qquad (2D)$$

$$p_{c(s,b)}(z_{s,b}+1) = 2.7 \qquad (3D)$$

$$z_s = 1 + z_b/2$$

which accounts for the values of zp_c found in high coordination networks and continuous sphere (discs) percolation. A similar criterion was independently proposed by Roberts [11].

Balberg *et al* (see [12]) used the mean excluded volume $\langle V_{ex}\rangle$ (or area $\langle A_{ex}\rangle$) as an invariant parameter for the percolation of overlapping objects. These quantities are identical to B but are expressed in terms of geometrical parameters. For objects of simple shape, they showed that the excluded volume can account for anisotropic percolation once its critical value is known for the isotropic system. However, this latter is shape dependent and is maximum for isotropic objects: discs in 2D, spheres in 3D. Using objects of variable shape, Balberg [13, 14] found a general percolation threshold criterion for a continuous isotropic system of convex overlapping objects:

$$\begin{aligned} &3.2 < (\langle A_{ex}\rangle)_c < 4.5 \qquad (2D)\\ &0.7 < (\langle V_{ex}\rangle)_c < 2.8 \qquad (3D). \end{aligned} \tag{1}$$

Our simulation is performed on a VAX 750 computer and uses finite-size scaling techniques on cubic samples of size L (4–16); the parameter of percolation is the number of discs N per unit volume.

The percolation of a sample is decided by the following procedure: the number of discs centred in each given unit cube is chosen at random according to a Poisson law; the discs have the same unit diameter and are centred and oriented randomly. Intersections are searched in the present and neighbouring unit cubes. Periodic conditions are assigned on the six faces and percolation is looked for only between two given opposite faces (i.e. in a fixed direction). With this method the total number of discs in the sample is not constant but the standard deviation is not larger than 2%. This technique is similar both to the usual simulations on lattices where each bond or site is decided separately, and to the possible simulations of rock sites where the total number of fractures may not be known but a fracture density may be estimated from geostatistical analysis [6].

For each size L, about 2000 realisations have been performed. The finite-size percolation threshold $N_c(L)$ (defined as giving a $\frac{1}{2}$ probability of percolation) and the standard root mean square deviation $\Delta N(L)$ are given in table 1.

Table 1. The percolation threshold $N_c(L)$ for a cube of size L and its root mean square deviation $\Delta N(L)$.

L	$N_c(L)$	$\Delta N(L)$
4	1.7292 ± 0.0113	0.3627
6	1.6074 ± 0.0085	0.2412
8	1.5554 ± 0.0074	0.1743
10	1.5450 ± 0.0066	0.1383
12	1.5364 ± 0.0059	0.1193
16	1.5187 ± 0.0051	0.0785

One observes that $N_c(L)$ decreases as the size of the sample increases. Thus for a given density N, the larger the sample is, the higher are the chances of finding a continuous path. This can be of interest in the statistical analysis of sites with fracture densities below the percolation threshold.

At large L values, $N_c(L)$ converges towards the infinite percolation threshold N_c with a first-order term in $L^{-1/\nu}$, ν being the universal exponent of percolation for the correlation length which also describes the scaling of the standard deviation: $\Delta N(L) = wL^{-1/\nu}$. A log-log plot of $\Delta N(L)$ against L gives $\nu = 0.907 \pm 0.05$, in good agreement with the result obtained by Wilke *et al* [4]. However, the accuracy of the present work is not sufficient to study, as has been done in [4], the regular drift of the finite-size exponent $\nu((L_1 + L_2)/2)$ obtained from two successive values $\Delta N(L_1)$ and $\Delta N(L_2)$.

The main purpose of this letter is the determination of the percolation threshold N_c. It is usually determined by extrapolating towards $L = \infty$ the variation of $N_c(L)$ with $L^{-1/\nu}$. However, in our range of sizes ν has not yet reached its asymptotic value. Instead we consider the variation of $N_c(L)$ with $\Delta N(L)$. Since $\Delta N(L)$ and $N_c(L) - N_c$ both vary as $L^{-1/\nu}$ at large L, we take N_c equal to the limit of $N_c(L)$ as $\Delta N(L)$ goes to zero. A parabolic fit of the data (figure 1) gives the value $N_c = 1.48 \pm 0.02$.

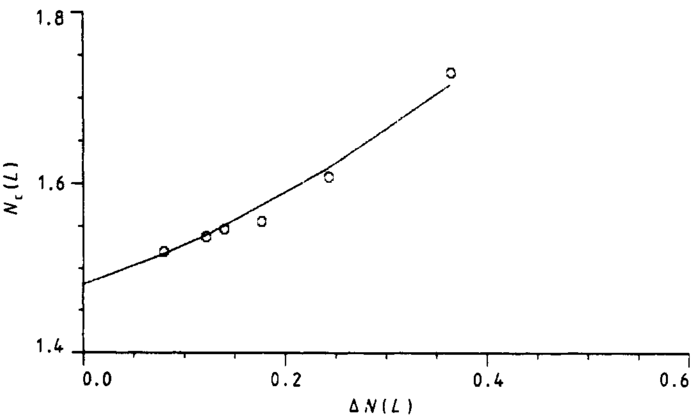

Figure 1. Variation of the finite percolation threshold $N_c(L)$ against standard deviation $\Delta N(L)$ for $L = 4, 6, 8, 10, 12, 16$. A quadratic fit (full curve) gives the infinite percolation threshold N_c.

The discs' radii being $\frac{1}{2}$, this value corresponds to a critical mean excluded volume (or mean number of intersections per disc):

$$(N\langle V_{ex}\rangle)_c = \pi^2 N_c R^3 = 1.80.$$

This value agrees with the Balberg criterion (1) and is not very far from that found by Robinson [2] for the percolation of randomly centred unit squares oriented along three orthogonal directions ($\langle V_{ex}\rangle_c = 2.09$).

Thus the excluded volume theory gives reliable numerical predictions for the permeability threshold of random monodisperse cracks, taking into account the size dependence. Further developments will deal with anisotropic systems (in which the excluded volume criterion is expected to apply) and with the important problem of multiple size fractures.

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