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Surface effects in invasion percolation

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Boundary effects for invasion percolation are introduced and discussed here. The presence of boundaries determines a set of critical exponents characteristic of the boundary. In this paper we present numerical simulations showing a remarkably different fractal dimension for the region of the percolating cluster near the boundary. In fact, near the surface we find a value of $D^{sur} = 1.67 \pm 0.03$, with respect to the bulk value of $D^{bul} = 1.87 \pm 0.01$. Furthermore, we are able to present a theoretical computation of the fractal dimension near the boundary in fairly good agreement with numerical data. [S1063-651X(97)51108-1]

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A large effort has recently been dedicated to the study of invasion percolation (IP) [1,2], since this simple cellular model takes into account many characteristics of the capillary displacement of a fluid in porous medium [3]. Notwithstanding the extreme simplicity of the model, standard IP is able to explain many properties occurring in real situations; nevertheless we think that the simple ingredient of the presence of a surface (boundary) in the system could make the model properties even closer to the experimental results. The study of the more realistic case of systems in which boundaries are explicitly considered then becomes of great importance not only from a theoretical point of view, but also from a technological one.

In the standard theory of critical phenomena, the role of boundaries has been intensively analyzed [4], and for many physical situations ranging from Ising models to the more

recent class of self-organized models [5,6] their presence can be accounted for by the introduction of a different set of critical indices. The main reason for the behavior consists of the lack of the neighbor microscopical layer for the system. This changes dramatically the microscopic interactions of the surface region of the system, eventually yielding a macroscopically observable peculiar behavior.

In this work we present some numerical and theoretical evidence that the above situation applies also to IP. From an intuitive point of view this can be easily understood by considering that boundary sites have fewer neighbors and hence fewer chances to invade a new region than bulk ones. From a quantitative point of view, this is shown by considering an intersection of the percolation cluster with straight lines parallel to the external boundary. This subset of the percolating cluster has a fractal dimension (hence, a set of critical indi-

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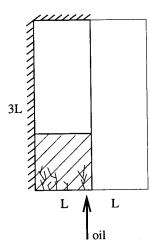


FIG. 1. Setup of numerical simulations. An invading, not yet percolating, cluster is shown. Only the bottom left part of the cluster will be considered, after it will have percolated the entire system.

ces) that varies with the distance from the boundary. Using some theoretical tools that were introduced for the study of fractal growth processes, the run time statistics (RTS) [7] and the fixed scale transformation (FST) [8], we are able to compute analytically the peculiar behavior, with a result that is in fairly good agreement with the numerical one.

Our results are shown in the following order. First, we present the definition of the model and the set up of our computer simulations, followed by a review of the numerical data. Second, we briefly describe the concepts underlying RTS and FST, and we present the result of analytical computations. A detailed description will be published elsewhere [9]. In the last part we give a summary of the main topics.

IP models the medium as a network of bonds. In this system there is an interface between two different fluids (e.g., oil and water), i.e., some bond belongs to the oil cluster and the others belong to water. Let us assume, now, that the oil cluster begins to invade the water one. Under the condition of a low and constant flow rate the interface will move one step at time. One mimics this behavior by assigning a random number x_i (here we take a uniform distribution in [0,1]) to each bond i of the medium. The invading cluster evolves by occupying the bond with the smallest x_i on its perimeter.

Usually, in any numerical simulations the boundaries of the system are present. We want to point out that at these



FIG. 2. This pictures corresponds to the entire cluster. The region of interest in which statistics is token is the lower one.

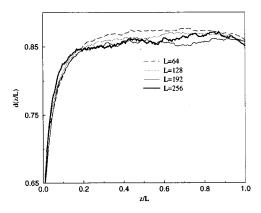


FIG. 3. Behavior of the fractal dimension of the intersection set versus the normalized distance z/L from the boundary. z and L are lattice distances, henceforth the normalized distance is dimensionless

boundaries a new behavior takes place. To study this new behavior we realised some numerical simulation in the system shown in Fig. 1. To ensure isolation from the right boundary (which has the same effect on the fractal properties as the left one) the whole system was size $3L\times 2L$, and the initial oil cluster is composed of the first L bonds of the bottom line. The simulation is stopped as soon as the cluster has percolated the system, i.e., reached the upper line. One typical realization of the process is shown in Fig. 2. The region of interest is the bottom-left one in Fig. 1, where we can assume that the region is "frozen" with respect to the invasion process, i.e., the asymptotic fractal properties of the percolating cluster are well defined. In the region in which we collect statistics, we study the fractal dimension of the sets of points obtained intersecting the spanning cluster with a line parallel to the boundary. In this way, we are able to follow the crossover of the fractal dimension of the cluster from the boundary to the bulk. The behavior of the fractal dimension d of the intersection as a function of the normalized distance z/L from the left boundary is presented in Fig. 3.

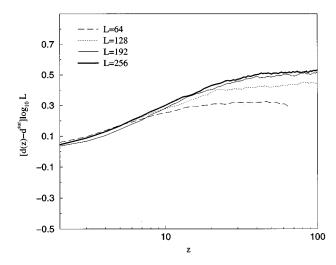


FIG. 4. Collapse plot of $[d(z)-d^{sur}]\log_{10}(L)$ for the different sizes, in \log_{10} linear scale. L and z are in lattice units.

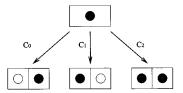


FIG. 5. Fine graining transformation for occupied cells.

The main result is that the fractal dimension of this subset of the cluster passes from $d^{sur} = D^{sur} - 1 = 0.67 \pm 0.03$ on the boundary to $d^{bul} = D^{bul} - 1 = 0.87 \pm 0.01$ in the bulk (at a distance $z/L \sim 0.4$ from the boundary).

The slow crossover behavior from d^{sur} to d^{bulk} could be explained by hypothesizing the following finite-size scaling form for the number of occupied boxes N(z,L):

$$N(z,L) = L^{d^{bul}} f(z/L), \qquad (1)$$

where one has $f(z/L) \sim (z/L)^{(d^{bul} - d^{sur})}$ for $z \ll L$ and $f(z/L) = \text{const for } z \gg L$. Then in the first region we should have

$$d(z) \simeq d^{sur} + (d^{bul} - d^{sur})\log_{10}(z)/\log_{10}(L)$$
. (2)

To test this scaling hypothesis we collapsed the curves relative to different L by plotting $[d(z)-d^{sur}]\log_{10}(L)$ as a function of z. The result depicted in Fig. 4 shows a fairly good collapse in the small z region.

We have also checked the asymptotic behavior of the distribution of the random numbers x_i associated to the perimeter bonds on the border of the system. It is known that for the bulk IP, this histogram distribution self-organizes into a θ function with a discontinuity at a critical value x_c^{bulk} which depends on the details of the model and on the embedding dimension [1]. For the 2D bond IP model one has $x_c^{bulk} = \frac{1}{2}$. Our simulations show that the border distribution of the x_i self-organizes into a theta function, too, and the critical threshold is again x_c^{bulk} [9]. This is not surprising, being the value of the border critical threshold dependent on the dynamical evolution of the whole percolating cluster.

Now, we turn to our analytical calculation of the boundary fractal dimension d^{sur} of the infinite IP cluster. Our strategy combines fixed scale transformation (FST) [8] and run time statistics (RTS) [7,2].

FST is a lattice path integral scheme allowing one to evaluate the spatial correlation properties of the intersection between the infinite cluster and a straight line through the statistical weights of growth path in a growth column. In particular, it allows one to calculate the fine graining probabilities C_0 , C_1 , and C_2 for the basic configurations shown in Fig. 5. Obviously, the normalization condition holds,

$$C_0 + C_1 + C_2 = 1. (3)$$

This approach is based on the statistical invariance of the correlation properties for vertical translations in the growth column. For this reason we have to take the column parallel to the boundary. Knowing the correlation probabilities in Eq. (3) of the intersection between a straight line and the cluster we can compute [8] the fractal dimension of this intersection set through the equation

$$d = \frac{\log(C_0 + C_1 + 2C_2)}{\log 2} = \frac{\log(1 + C_2)}{\log 2}.$$
 (4)

One has to note, however, that C_2 in Eq. (4) represents the correlation between two consecutive sites on a line perpendicular to the boundary. However, this value can be considered equal to the correlation between sites on the intersection parallel to the boundary, because, as can be seen from the numerical results, the fractal dimension of these intersections vary very slowly with the distance from the boundary.

Since the probabilities C_0 , C_1 , and C_2 are computed from growth paths, the use of FST is straightforward whenever a simple calculation of the statistical weights of time ordered paths of growth on the lattice is possible.

However, for IP (as for any other quenched-extremal dynamics) this calculation is extremely difficult, because the weight of a path cannot be written as the product of the probabilities of the single steps composing the path. This problem can be overcome by introducing the RTS transformation. The latter transformation maps a quenched-extremal process into a stochastic representation. Here we perform the RTS transformation following the approach in [2], by using the same conditional probability theorems.

Applying these concepts we can introduce, at each time step t, an effective probability density $\rho_{i,t}(x)$ for the random number x_i associated to each bond i of the growing interface $\partial \mathcal{C}_t$. This density depends on the entire growth history of the dynamics. In fact, $\rho_{i,t}(x)dx$ gives the probability that the variable x_i for the bond i at time t is in the interval [x,x+dx], conditioned by the past growth dynamics of the cluster. When we know the densities $\rho_{i,t}(x)$ for each bond i on the interface, we can calculate the growth probability distribution $\{\mu_{i,t}\}$ (i.e., the probability of being the minimum on the interface) at that time step for each interface bond,

$$\mu_{i,t} = \int_0^1 dx \rho_{i,t}(x) \prod_{j \in \partial C_t - \{i\}} \left[\int_x^1 dy \rho_{j,t}(y) \right],$$
 (5)

where $\partial C_t - \{i\}$ represents the growth interface except for the bond i. The effective probability density of every surviving bond j at time t+1 on the interface must then be updated, conditional on the previous growth history at time t, i.e., the growth of the bond i. The corresponding equation is

$$\rho_{j,t+1}(x) = \frac{1}{\mu_{i,t}} \int_0^x dy \, \rho_{i,t}(y) \prod_{k \in \partial C_t - \{i,j\}} \left[\int_y^1 dz \, \rho_{k,t}(z) \right],$$
(6)

where $\partial C_t - \{i, j\}$ is the growth interface except for bonds i and j. New bonds added to the perimeter are assigned an effective probability density according to a uniform distribution in [0,1].

The above formalism allows us to write the statistical weight of a path as the product of the probabilities of the single steps. Following this RTS scheme one can perform the FST calculation of the asymptotic cluster fractal dimension (for technical details see [2]).

However, the application of the FST to our given problem involves some further peculiar difficulties. Because of the presence of a lateral surface, this model is intrinsically anisotropic, and consequently we have to introduce some modiR1294

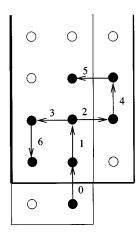


FIG. 6. This is a possible path of growth of the 6th order. The invasion follows the arrows, from one black point to another one. The number near arrows is the growth time.

fication to the usual way of performing the FST for the bulk IP. The anisotropy of the environment implies a breaking of symmetry in the FST basic configurations in Fig. 5: Due to the presence of the boundary, the probabilities C_0 and C_1 are not equal.

Consequently, the indices of the transfer matrix M_{ij} between these three configurations run from 0 to 2. The closure condition of this matrix can be written

$$\sum_{j=0}^{2} M_{ij} = 1 \quad \forall i. \tag{7}$$

Through the FST we calculate directly the matrix elements M_{ij} and from the relation

$$\begin{pmatrix} C_0 \\ C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} M_{00} & M_{10} & M_{20} \\ M_{01} & M_{11} & M_{21} \\ M_{02} & M_{12} & M_{22} \end{pmatrix} \begin{pmatrix} C_0 \\ C_1 \\ C_2 \end{pmatrix}$$
(8)

we can evaluate C_2 and, by using the Eq. (4), (D). In our case we have

TABLE I. Values of the boundary fractal dimension with respect to the order n of computation.

n	3	4	5	6	7	 ∞
$d^{sur}(n)$	0.576	0.632	0.657	0.671	0.679	 0.702

$$M_{01} = M_{10} = 0, (9)$$

so we obtain

$$C_2 = \frac{M_{12}M_{02}}{M_{12} + M_{21}(M_{02} - M_{12}) + M_{12}(M_{02} - M_{22})}.$$
 (10)

The anisotropy of the environment is also introduced in the lateral boundary condition of the growth column in which the FST calculation is performed. On the left-hand side of the column we impose the presence of a rigid wall and on the right-hand side the paths are allowed to go out and then to return inside, as can be seen in Fig. 6. In this way we have obtained the results shown in Table I, where the fractal dimension for increasing order n (the path length) of the FST computation is given. We used a power law fit to extrapolate $d^{sur}(n)$ to $n=\infty$ and obtained $d^{sur}_{FST} \approx 0.70$.

In summary, we have introduced, in analogy with usual critical phenomena, the study of boundary behavior in invasion percolation. Near a boundary one deals with a qualitatively different rate of occupation. This is reflected in a lower fractal dimension of this part of the cluster. Numerical simulations give a surface fractal dimension $d^{sur} = 0.67$. We are also able to present a theoretical tool to compute analytically this quantity; the result $d^{sur}_{FST} \approx 0.70$ is in fairly good agreement with the numerical data. Further developments of this work, which are currently in progress, will involve an analytical reproduction of the logarithmic crossover between surface and bulk fractal dimension through the RTS-FST approach and an analytical and numerical study of border avalanche dynamics.

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