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1983 J. Phys. A: Math. Gen. 16 L611

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LETTER TO THE EDITOR

The moles' labyrinth: a growth model

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Received 25 July 1983

Abstract. We present a simple model for the simultaneous growth of many clusters. A phenomenological theory and simulations in two and three dimensions for this model are presented which describe the critical point where, for the first time, an infinitely large cluster is formed by the coalescence of individual clusters. This critical point is not in the universality class of standard percolation.

Geometrical growth models are of practical importance in many areas but only recently has one begun to study them in the context of critical phenomena (Stanley *et al* 1983). For the growth of a single cluster several models that show the generic problems of the time dependence have been studied (Amit *et al* 1983, Witten and Sander 1982, 1983, Savada *et al* 1982, Chandler *et al* 1982). For these models the critical phenomenon occurs in the limit of infinite time and is described by the fractal dimension of the cluster. The other case of practical interest is the simultaneous growth of many clusters (polymerisation, coagulation, antigen-antibody reaction etc). In this case the critical point is the time t_c at which for the first time an infinitely large cluster is formed. The former belief that this critical point is always of percolation type has been ruled out by two different types of studies (Herrmann *et al* 1982, 1983, Ziff *et al* 1982a, b). But unfortunately the models studied there and subsequently investigated similar models for additive polymerisation (Bansil *et al* 1983, Rushton *et al* 1983, Pandey *et al* 1983)—although they have explained many experimental details—are not very helpful for an understanding of the growth as a critical phenomenon because they are too complicated. So we present in this letter a simple model which already contains typical features encountered in previously studied growth models of many clusters.

In a D -dimensional lattice of size L^D we choose (regularly or at random) $C_1 L^D$ sites from each of which we start a random walk. The paths formed by the walks will be considered (figure 1) and the question is asked when the system formed by the paths percolates, i.e. when there is a cluster of paths formed which spans over the whole lattice. The case $L \rightarrow \infty$ and $C_1 \ll 1$ is of particular interest.

This model can be interpreted in two dimensions as a description of the labyrinth formed by moles. One places moles with an (average) distance of $1/\sqrt{C_1}$ in the earth at a given depth. Simultaneously they then dig runs in a random way and without changing the depth. The moles have a vital interest in the critical time t_c at which for the first time their runs have intersected each other enough so that there exists one network of paths through which they could escape as far as they want. (At t_c , of course, not yet all the moles will have direct connection to this network).

Keeping the language of moles on the lattice we define one growth step of the labyrinth as follows: choose a mole randomly; choose one direction randomly and

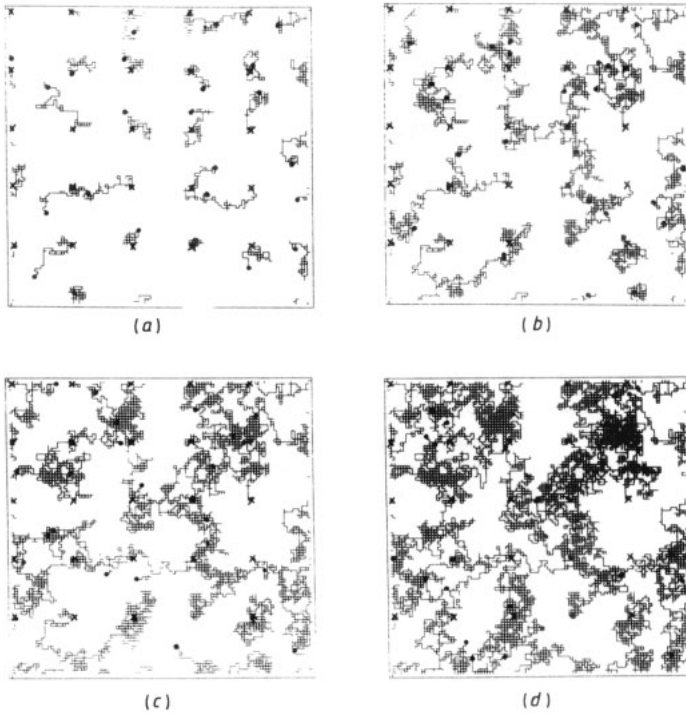


Figure 1. Different stages of the growth of a labyrinth on a 100×100 lattice with periodic boundary conditions. The moles are marked by a full circle. The initial positions of the moles (crosses) are regularly distributed with a concentration $C_1 = 0.0025$. (a), $t = 100$, $m = 0.121$, $P_\infty = 0.073$; (b), $t = 280$, $m = 0.273$, $P_\infty = 0.246$; (c), $t = 440 \approx t_c$, $m = 0.380$, $P_\infty = 0.880$; (d), $t = 720$, $m = 0.526$, $P_\infty = 1.0$.

displace the mole in this direction by one lattice spacing. After $C_1 L^D$ such growth steps on average every mole has moved once. So we define the 'time' by

$$t = N / C_1 L^D \quad (1)$$

where N is the total number of growth steps. The t defined in equation (1) is also the mean length of a path. In figure 1 we show a labyrinth grown from an initial regular distribution of moles at different times. One cluster is given by all lattice sites that are connected. Note that in figure 1, sites on opposite boundaries can be connected because we use periodic boundary conditions in the simulation. We denote by m the fraction of all the sites of the lattice that are touched by a path at a given time. The fraction of sites touched by a path that belongs to the largest cluster divided by m is P_∞ . In the thermodynamic limit ($L \rightarrow \infty$) $\langle P_\infty \rangle$ plays the role of the order parameter of the transition where $\langle \rangle$ denotes the average over all different possible growths. If the initial distribution is random one has to average in addition over all possible initial configurations. A quality which is suited for the study of the critical behaviour is the mean squared cluster size χ

$$\chi = \left\langle \sum_{cl} S^2 - S_\infty^2 \right\rangle / L^D \quad (2)$$

where the sum goes over all clusters and $S(S_\infty)$ is the number of sites in the (largest)

cluster. χ diverges at t_c like

$$\chi = C_{\pm}|t - t_c|^{-\gamma} \tag{3}$$

where C_+ is the value for $t > t_c$ and C_- the value for $t < t_c$. The exponent γ and the ratio

$$R = C_-/C_+ \tag{4}$$

are universal quantities for standard percolation in the renormalisation group sense (Stauffer 1979, Aharony 1980).

Before analysing χ in more detail we will study the location of the critical time t_c in dependence of the concentration C_1 for the case of a regular initial distribution of moles. Each path is an object of a mean square radius of $l \propto \sqrt{t}$. For $D \leq 4$ the critical time may be characterised by the time when these objects touch each other, i.e. when $l^D \propto 1/C_1$. Thus we have

$$t_c \propto C_1^{-2/D}. \tag{5}$$

Simulations made in $2D$ and $3D$ for values of C_1 over several orders of magnitude support equation (5) as shown in figure 2. Let us now determine t_c by a mean-field argument of the Flory-Stockmayer-type (Flory 1953). The critical time t_c is reached when the mean number X of times that one path crosses other paths is exactly one.

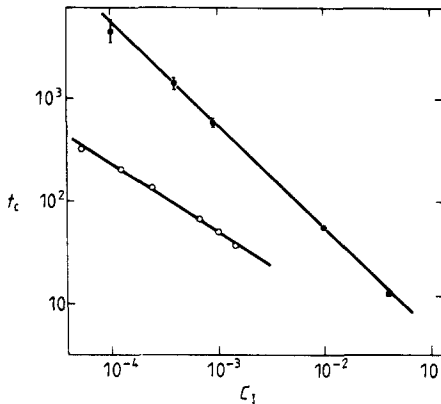


Figure 2. Log-log plot of the critical time t_c against concentration C_1 for the case of regular initiation. For two dimensions (full circles) the slope is -1 , for three dimensions (open circles) the slope is $-\frac{2}{3}$.

At time t a chain crosses in the mean $(C_1 L^D - 1)t/L^D$ other paths. So up to a time τ one path has crossed

$$X = (C_1 - 1/L^D) \sum_{t=1}^{\tau} t \tag{6}$$

other paths and thus t_c is given by

$$t_c \propto C_1^{-1/2} \tag{7}$$

in the limit $L \rightarrow \infty, C_1 \ll 1$. This is the same result as obtained for additive polymerisation with Flory-Stockmayer theory (Bansil *et al* 1983). Comparing equations (5) and (7) shows that the mean-field theory becomes correct for $D = 4$ thus implying that the

upper critical dimension for this problem is 4 and not 6 as for standard percolation. So already from this argument we see that our growth model is not in the same universality class as standard percolation thus supporting the picture obtained from other growth models (Herrmann 1982, Ziff *et al* 1982a, b, Rushton *et al* 1983). Let us point out here that also for self-avoiding walks the upper critical dimension is found to decrease (from 4 to 2) when, instead of giving all configurations the same weight, the walks are grown in a straightforward way (Amit *et al* 1983).

We will now present the results of a Monte Carlo simulation of our growth model to obtain the γ and R defined in equations (3) and (4) in a similar way to Herrmann *et al* (1982, 1983). First we will discuss the three-dimensional case. In figure 3(a) we plot double logarithmically χ against $|t-t_c|/t_c$ for $C_1=0.001$. The critical time t_c is obtained by the requirement that the slopes of the curves (i.e. γ) should be equal above and below t_c . We obtain $t_c=50\pm 1$. Every point in the curve is an average over 20 to 200 samples. Below t_c finite size effects become visible as a systematic deviation between the points of the 80^3 and the 60^3 lattice. Above t_c the asymptotic scaling region is smaller than below t_c and strong corrections to scaling are present. By plotting $\chi(100-t)$ against $(t-t_c)/t_c$ in figure 3(b) we expect to find the same slope γ as before but the deviations far from t_c are less strong and we can see a straight line over a wider range of values. The result of our analysis is $\gamma=2.4\pm 0.4$ and $R=7\pm 2$. Compared with the values $\gamma=1.8$ and $R\approx 10$ from standard percolation, γ is higher and R lower in our model but apparently only by an insignificant amount. However, making the same analysis for smaller C_1 ($C_1=0.000125$), as shown in figure 4(a), yields $\gamma=3.4\pm 0.6$ and $R=6\pm 3$. The deviation from the standard percolation values is in the same sense as for $C_1=0.001$ and the value for γ is significantly higher than the γ of standard percolation. If instead of a regular initial distribution of moles one takes a random initial distribution one obtains for $C_1=0.001$, figure 4(b) and the values $\gamma=2.6\pm 0.5$ and $R=2\pm 2$. Here R is noticeably smaller than the value for standard percolation. Summarising, we found a very similar picture to that found in the gelation model in $D=3$ (Herrmann *et al* 1982, 1983): compared with standard percolation there is a smaller R and larger γ and the effects depends on C_1 in the

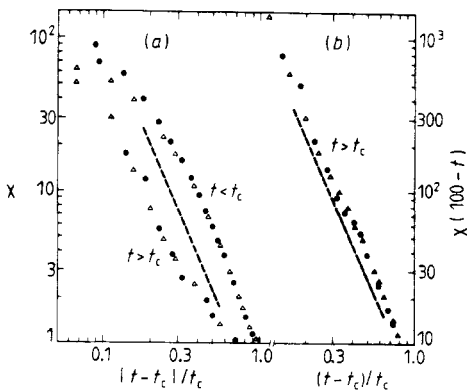


Figure 3. Log-log plot of: (a), χ and (b), $\chi(100-t)$ against $|t-t_c|/t_c$ for lattices of size 80^3 (●) and 60^3 (△). The broken lines are guides to the eye of slope 2.4. The critical time used is $t_c=50$.

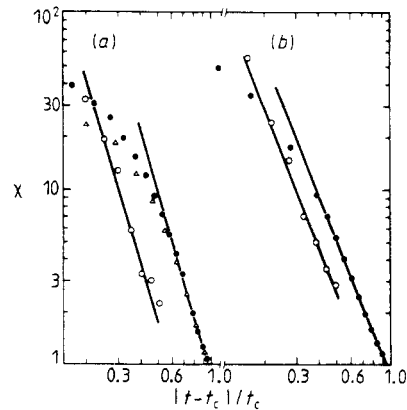


Figure 4. Log-log plot of χ against $|t-t_c|/t_c$ for lattices of size 80^3 (● for $t < t_c$ and ○ for $t > t_c$) and 60^3 (△). (a), Regular initial distribution, $C_1=0.000125$, $t_c=200$; (b), random initial distribution, $C_1=0.001$, $t_c=42.3$.

sense that it becomes stronger if C_1 is decreased. Apparently the case of random initial distribution comes closer to the gelation model.

The results of the two-dimensional simulation with a regular initial distribution are presented in figure 5. In figure 5(a) χ is double-logarithmically plotted against $|t - t_c|/t_c$ for $C_1 = 0.01$. The situation is similar to that in three dimensions with the difference that below t_c the limit of the asymptotic region cannot be estimated because the curvature produced by the correction terms is in the same sense as the finite-size effect. By plotting instead $\chi t C_1$ against $(t_c - t)/t$ below t_c and $\chi(2t_c - t)C_1$ against $(t - t_c)/(2t_c - t)$ above t_c in figure 5(b), the slope γ and ratio R should be preserved and the curve for $t < t_c$ is now slightly S-shaped, $t_c = 55 \pm 2$ yields parallel curves above and below t_c . From figure 5(b) we obtain $\gamma = 2.0 \pm 0.4$ and $R = 7 \pm 3$. The difference between the effective slope for $t < t_c$ in figure 5(a) and the γ obtained from figure 5(b) shows that in two dimensions much stronger corrections to scaling are present below t_c than in three dimensions. In figure 5(c) we make the same analysis as in figure 5(b) for $C_1 = 0.0004$ and obtain $t_c = 1375 \pm 50$, $\gamma = 2.3 \pm 0.4$ and $R = 18 \pm 10$. Compared to the values of standard percolation, $\gamma = 43/18$ and $R \approx 200$, only the ratios R of our model are distinguishably smaller. We note that in gelation models, different values of γ were also found (Rushton *et al* 1983).

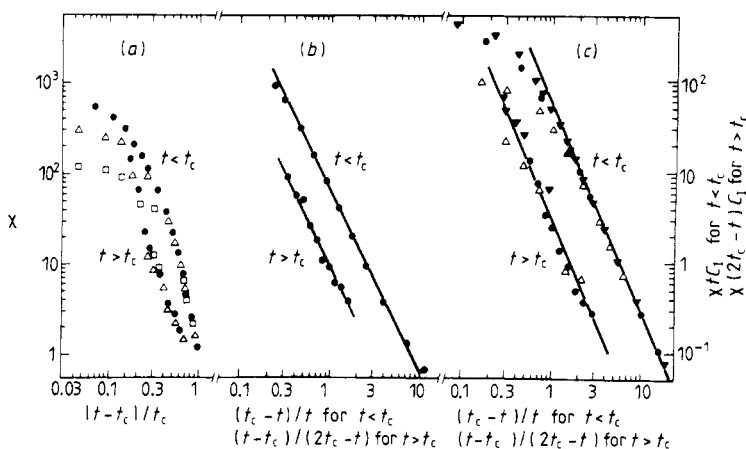


Figure 5. (a), Log-log plot of χ against $|t - t_c|/t_c$ (left axis); (b), and (c), for $t < t_c$: $\chi t C_1$ against $(t_c - t)/t$ and for $t > t_c$: $\chi(2t_c - t)C_1$ against $(t - t_c)/(2t_c - t)$ (right axis). Lattice sizes: 100^2 (\square), 200^2 (\triangle), 300^2 (\bullet) and 400^2 (\blacktriangledown), regular initial distribution. (a) and (b) are for $C_1 = 0.01$ and $t_c = 55$, (c) is for $C_1 = 0.004$ and $t_c = 1375$.

We have presented a simple growth model which, although it has a threshold in time where it percolates, does not belong to the universality class of standard percolation. It has upper critical dimension 4 and its critical exponent γ differs in 3D from the value of standard percolation. The ratio R of the critical amplitudes of the mean-square cluster size is smaller than the ratio of standard percolation in 2D and 3D. Under changes of the concentration C_1 the model has similar behaviour to 3D gelation models. Further studies on random initiation and repulsion are under way and will be presented elsewhere.

I thank J des Cloiseaux, J M Luck, J P Nadal and D Stauffer for interesting discussions.

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