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LETTER TO THE EDITOR

Monte Carlo approach to dendritic growth

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Abstract. The connection between diffusion-limited aggregation and the equations of dendritic growth is critically examined. A different type of Monte Carlo simulation is proposed and used to construct two-dimensional dendrite-like patterns. The wavelength occurring for short times is in good agreement with the linear stability analysis. The time dependence of the characteristic wavelengths is also determined.

Many nonlinear processes leading to pattern formation can be described by linear equations of diffusion, where the nonlinearity is due to the moving boundaries determined by the pattern itself. Such phenomena include dendritic growth from supercooled molten or oversaturated solutions (Langer 1980), two-fluid displacement in porous media (Paterson 1984), aggregation clusters (Witten and Sander 1981) or electrical breakdown (Sawada *et al* 1982). The common reason for inhomogeneous solutions is the instability to fluctuations.

Since the introduction of the diffusion-limited aggregation (DLA) model (Witten and Sander 1981) the Monte Carlo (MC) approach to these problems has attracted great interest (Witten and Sander 1981, 1983, Sawada *et al* 1982, Rikvold 1982, Meakin 1983, 1984, Rácz and Vicsek 1983, Paterson 1984, Vicsek 1984). In the DLA model, particles diffuse from infinity and the stick on the boundary thereby changing its shape. In this letter we want to examine the DLA-based approach to dendritic growth and propose a different MC method.

Let us now recall the equations of dendritic growth using the approximation that the temperature is constant in the solid phase (Langer 1980):

$$\partial_t u - d \Delta u = 0 \quad (1a)$$

$$u(\mathbf{r}_\xi) = -d_0 k(\mathbf{r}_\xi) \quad (1b)$$

$$v_n(\mathbf{r}_\xi) = -d(\nabla u) \cdot \mathbf{n}(\mathbf{r}_\xi) \quad (1c)$$

$$\text{boundary condition at infinity} \quad (1d)$$

where u is the dimensionless temperature in the liquid, d is the diffusion constant and d_0 is the capillary length. The vector \mathbf{r}_ξ represents a point of the solidification front parameterised by ξ (we restrict ourselves to two-dimensional problems), k is the curvature at such a point, \mathbf{n} is the normal and v_n is the normal velocity of the interface. In order to get instabilities, perturbations to (1) should be supposed, but here we do not have to consider them explicitly, since we shall deal with MC simulations, where fluctuations are in any case present.

In the case when diffusive relaxation is much faster than the growth of the crystal, the time derivative in (1a) can be neglected (Witten and Sander 1981). Thus we consider the following set of equations:

$$\Delta u = 0 \quad (2a)$$

$$u(\mathbf{r}_\xi) = -d_0 k(\mathbf{r}_\xi) \quad (2b)$$

$$v_n(\mathbf{r}_\xi) = -d(\nabla u) \mathbf{n}(\mathbf{r}_\xi) \quad (2c)$$

$$u(y_0) = g y_0 \quad (2d)$$

where y_0 is some large distance to be specified later. We take the coordinate system fixed to the laboratory frame. In the stationary case a planar interface along the x direction will move with constant velocity in the y direction and the stationary solution will be $u(x, y; t) = -(y - vt)g$. The boundary condition (2d) is chosen accordingly; using (2c), $v = dg$ is obtained. Langer (1980) reviewed stationary solutions on the basis of (1) where the temperature field is exponentially varying along y . Near to the interface, i.e. from the point of view of the pattern, our solutions can be fitted to those of Langer by fitting the parameter g .

Let us take first in (2b) $d_0 = 0$ corresponding to the limit of zero surface tension. u in (2) can be identified with the probability of finding a randomly walking particle at site \mathbf{r} at time t if the particles have a source at y_0 and the interface \mathbf{r}_ξ is a sink.

In this representation DLA can be considered as a MC realisation of (2). However, there are the following problems with this approach.

(1) In a MC determination of the probability u one should take an average over many runs. But in DLA every single run is taken as an independent contribution to the change of the surface without averaging. Since the problem is sensitive to any kind of perturbation, many microfluctuations, which would be averaged out, influence the shape of the pattern, resulting in a very ramified cluster (Witten and Sander 1981, 1983, Meaking 1983, 1984, Rácz and Vicsek 1984).

(2) When trying to handle the case of non-vanishing surface tension ($d_0 \neq 0$) on the DLA framework one usually operates with the sticking probability s . Witten and Sander (1983) argued, that with $s < 1$ one simulates the surface tension. However, it seems to us that this is rather a rough way of the above mentioned averaging. The generated clusters remain fractals (scale invariant objects, Mandelbrot 1982) on a scale, above a length determined by s (Witten and Sander 1983). Vicsek (1984) introduced, in addition to the curvature-dependent sticking probabilities of the particles, a relaxation of their position corresponding to surface diffusion. In this way he succeeded in generalising DLA, in that he obtained dendrite-like patterns; in fact Vicsek's algorithm somehow takes both averaging and stabilising effects into account. However, the connection with physical parameters is not clear and in any method in which the sticking probability determines u at the boundary, $u(\mathbf{r}_\xi) \propto g$ – a result not compatible with (2b).

As a different simulation approach from DLA, we propose a MC model in which the above mentioned problems can be handled. In the standard MC method (Shreider 1963), solving the Laplace equation $\Delta u = 0$ on a region ρ with the boundary condition $u(\mathbf{r}_\xi)$, randomly walking particles start at $\mathbf{r} \in \rho$ and the average is calculated over the values $u(\mathbf{r}_\xi^i)$, \mathbf{r}_ξ^i being the point where the i th particle hits the boundary.

On this basis we construct the following simulation. We start from a straight solidification front of length L on the square lattice at $Y = 0$. (The lattice constant is

taken as unit length.) Let us call the points belonging to the solidification front boundary points (B) and the points of the liquid having neighbours on B perimeter points (P). (Henceforth the quantities in the model calculations are denoted by capital letters.)

First let us show how to determine the value of U on the perimeter. N particles are started at every $W_i \in P$ and

$$U(W_i) = \frac{1}{N} \sum_j U(Z_{ij}) \quad (3)$$

is taken, where $Z_{ij} \in B$ is the terminating point of the walk started at W_i and $U(Z_{ij})$ is determined by the discrete version of the RHS of (2b). The curvature is calculated by a method similar to that of Vicsek (1984), from the occupation of a 7×7 square around Z_{ij} .

When changing the solidification front a point of P becomes one of B and new perimeter sites are created at the same time. This means that to every perimeter site W_i a boundary site Z_i can be assigned, namely that which has borne it, $Z_i(W_i)$. Like in the mother-child relationship this assignment does not work in the opposite direction. Having determined $U(W_i)$, the discrete version of $\nabla U = U(W_i) - U(Z_i)$ can be taken and the solidification front can be moved according to (2c). Denoting the velocity of the solidification front at W_i by $V(W_i)$,

$$V(W_i) = (1 \text{ lattice unit})/(\Delta T)$$

where ΔT is the time which has elapsed since the lattice site at $Z_i(W_i)$ was occupied. The time is measured in MC step/site, i.e. going once along the perimeter P takes one time unit.

At this point a technical remark is necessary. If the maximal extent of the developed pattern in the Y direction is denoted by Y_m , it has no sense to follow the walking particles for $Y > Y_m$. If it just leaves the domain of interest $Y = Y_m + 1$, it has two possibilities: either it reaches Y_0 —then the sum on the RHS of (3) would have a contribution $U_0 = GY_0$ —or it turns back to $Y = Y_m$. Since the probability that the walking particle reaches Y_0 is approximately $(1/Y_0)$ ($Y_0 \gg Y_m$ is assumed), we give the weight $(1/Y_0)$ to this event and the weight $(Y_0 - 1)/Y_0 \sim 1$ to the event where it comes back to a point with $Y = Y_m$. Therefore, if the Y coordinate of the particle exceeds Y_m , the sum in (3) is enhanced by G and the particle is put back to $Y = Y_m$ with an X coordinate chosen from a proper distribution. It is clear from this consideration that the value of Y_0 is irrelevant if $Y_0 \gg Y_m$ is fulfilled during the whole process.

We implemented the following algorithm. During the simulation the starting straight line develops into a pattern. Helical boundary conditions are taken in the X direction. For every point $W_i \in P$ a function $F(W_i)$ is defined, which has the value zero at the beginning. A $W_i \in P$ is taken as a starting point of a random walk. If the walker leaves the domain of interest ($Y \leq Y_m$) the value DG is added to $F(W_i)$ and the particle is put back to a point as described above. If the walk terminates at Z_{ij} , the value of $F(W_i)$ is enhanced by $D(U(Z_i) - U(Z_{ij}))$. Then a new walker starts at W_i and the procedure is repeated until all points of P are taken. Going N times along the perimeter, F will contain an approximate value of $ND\nabla U$. If F becomes unity at a point W_i this point is converted to an element of the solidification front B and at the same time it bears new perimeter sites. Identifying N by ΔT when $F = 1$, (2c) is fulfilled. After moving the interface, the value of F at the new perimeter sites is set to be zero.

In the computer simulation of this model we investigated how the instabilities occur and develop to dendrites when started from a planar interface and keeping the parameters D , D_0 and G constant. This phenomenon has been investigated both theoretically and experimentally by several authors (see, for example, Langer 1980, Trivedi and Somboonsuk 1984), but we are not aware of quantitative results concerning the time dependence of the characteristic lengths.

In figure 1 $D = 0.12$, $D_0 = 0.12$ and $G = 0.03$ were taken in order to have a relatively large averaging and to get a nice pattern within reasonable computing time. The width of the sample is $L = 256$ lattice units. The exact solution in the absence of noise would be the stationary motion of a planar interface. However, this motion is unstable against fluctuations always present in a MC simulation. Due to this noise instabilities occur at the initial stage of the growth (figures 1(a) and 1(b)). After some time a characteristic length becomes observable (figures 1(c) and 1(d)), reminiscent of the cellular structure. The amplitude differences become gradually stronger (figures 1(d) and 1(e)). The larger forms screen the smaller ones in a 'struggle for life' which leads to an appearance of longer characteristic wavelengths (figures 1(d), 1(e) and 1(g)). Later side branches develop showing the onset of the dendritic structure (figure 1(g)). The short wavelength roughness is caused by the MC noise. In figure 2 the characteristic wavelengths as a function of time are displayed determined from the maximal Fourier amplitudes of two set of figures like figure 1. We consider these as preliminary results and we intend to decrease the errors by statistics.

The linear stability analysis (Langer 1980) of this model shows that the amplification rate—the sign of which determines the stability—vanishes at a wavenumber

$$Q_s = (G/D_0)^{1/2}. \quad (4)$$

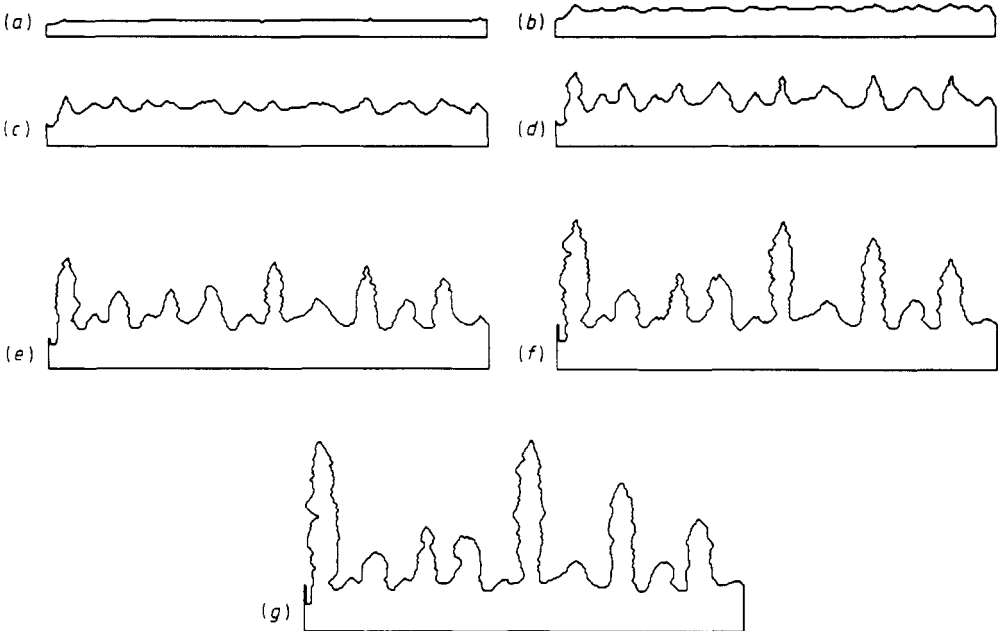


Figure 1. Pattern formation in our MC model. The parameters are given in the text. the time elapsed between the shown snapshots is 2000 MC step/site. The form in (g) contains 10 612 occupied sites.

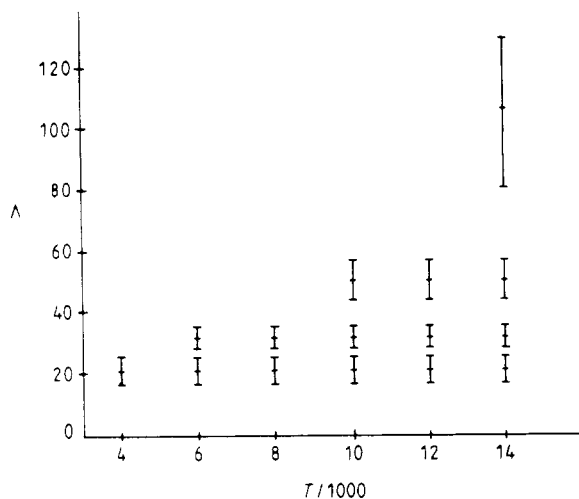


Figure 2. Characteristic wavelengths Λ as a function of time T . Λ is measured in lattice units, T in MC step/site. The parameters are the same as in figure 1.

Using the Fourier analysis of the initially developed solidification front the wavelength Λ^* belonging to the maximal amplitude can be determined. Physically $\Lambda^* = 2\pi/(Q_s/2)$ is expected: changing the D_0/G ratio by a factor of 4, Λ^* should be doubled. In runs with different growth rates (governed by G) we obtained the predicted Λ^* within 20%, in good agreement with (4).

Figure 3 shows a nice dendrite-like pattern in the limit, where the stabilising effect of the surface tension is negligible (small D_0 limit). We emphasise the difference of this figure compared to deposition patterns obtained by DLA (Meaking 1983, Rácz and Vicsek 1984): in our case the averaging due to D is still present.

The simulation was carried out on a microcomputer based on a Z-80 microprocessor. Coding in assembler speeded up the program so much that only a factor of 10 remained compared with a FORTRAN program on an IBM 370/3031. We used about hundred computing hours for this work.

In conclusion we investigated the MC simulation approach to the problem of pattern formation described by the diffusion equation and moving boundary conditions—essentially the problem of dendritic growth. One possible way is the generalisation of the DLA to include averaging and surface tension. Although we emphasise that DLA is interesting in its own right too, we believe we have defined a model where these effects can be more naturally introduced. The model is based on a well known MC



Figure 3. Dendrite like pattern. $D = 4 \times 10^{-1}$, $D_0 = 10^{-6}$, $G = 10^{-2}$, $t = 5 \times 10^3$, $L = 256$.

method of solving the Laplace equation (Shreider 1963). The averaging procedure—controlled by D if D_0 and G are fixed—is an inherent part of this method. The stabilising effect of the surface tension is taken into account via a direct discretisation of (2b) instead of operating with sticking probabilities. The motion of the interface satisfies (2c).

Due to the immediate connection of our method with equations (2)—which is underlined by using the corresponding capital letters for the model—the results can be related to other theoretical approaches or even to experiments. Here we have put emphasis on the time evaluation of the pattern—an aspect which has not yet been studied by MC simulations. We presented the time dependence of the characteristic wavelengths based on computer realisations of our model. The wavelength first appearing is in good agreement with the linear stability analysis.

Our model is suitable to incorporate further important physical effects like diffusion in the solid or on the surface. We intend to continue the investigation of this model from different aspects of pattern formation.

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Note added in proof. After completion of this work we learned about a preprint by L P Kadanoff (1985) which contains ideas somewhat similar to ours applied to a hydrodynamic instability.

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