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LETTER TO THE EDITOR

Monte Carlo simulation of a kinetic Ising model for dendritic growth

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Abstract. We have developed a Monte Carlo method for the interfacial dynamics of a two-phase Ising-like system made unstable by a temperature gradient. Dendritic shapes form and rapidly reach an asymptotic regime in which their tip velocities are approximately constant with time. A power-spectrum analysis of interfacial fluctuations in the asymptotic regime is consistent with roughening.

Over the last few years there has been important progress in the study of pattern formation during crystal growth [1-8]. The most well known example is the growth of dendritic crystals, such as snowflakes. In this case, a single crystal in an undercooled melt grows by the diffusion of latent heat from the crystal to the melt into a complex dendritic structure. For a given undercooling, experiments show that the tips of the branches of the dendrite grow at a particular constant velocity v and a particular radius of curvature $1/R$, whereas simple theories find that only the product vR is selected. The challenge, then, has been to determine how a particular curvature and velocity are selected in the asymptotic steady-state regime [1, 2]. The problem has usually been formulated in terms of the diffusion equation for temperature in the supercooled melt with moving boundary conditions at the crystal-melt interface. It is then argued [1] that selection in dendritic growth is determined by 'microscopic solvability', where a small length scale causes a singular perturbation to the continuum equations. The physical idea is that the surface tension determines short wavelength fluctuations, and that these fluctuations determine the long wavelength properties of dendrites. The predictions of microscopic solvability are in reasonable agreement with experimental data [1, 3, 4], but it remains the subject of current investigations [5].

Because this is a moving boundary-value problem, analytic methods are difficult. Another approach is through numerical modelling. There, typically, one either solves the continuum equations on a discrete mesh or uses lattice-gas automata which model the continuum equations by means of a prescription for small length scales. While these methods have been useful, and have led to important insights, they have an inherent weakness, since microscopic solvability has established that the continuum equations are singular on small length scales. Thus, for example, unusual behaviour on small length scales in lattice-gas automata need not be physically meaningful. For this and other reasons, numerical studies are used most often only for two-dimensional investigations of steady-state behaviour, or involve approximating the full diffusion equation by the Laplace equation for the temperature field.

However, if behaviour is sensitive to fluctuations on small length scales, it is natural to develop a fully microscopic description. Thus, for the first time, we have introduced

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a Monte Carlo method to simulate the unstable dynamics of a simple microscopic Ising-like Hamiltonian. In this way, we need take no special care to ensure the moving boundary is behaving correctly. Furthermore, we can investigate the sensitivity of dendritic growth to behaviour on small length scales in a manner independent of the mathematical technique of microscopic solvability.

Our algorithm is an adaptation of the microcanonical Monte Carlo method of Creutz [9]. If differs from existing Monte Carlo-like methods for this problem [6-8] in that it introduces an effective way to control the temperature by including thermal fields in a natural way [10]; the calculation closest to ours was a study of coarsening by Guo and Jasnow [6]. By contrast, the usual Monte Carlo algorithm fixes the temperature by a prescribed interaction of the dynamical system with a heat bath, a useful approximation if the time scales over which thermal diffusion occurs are very fast. But, in crystal growth, where the dynamical processes are controlled by local variations in temperature, it is clearly inadequate.

We apply the algorithm to simulate the Mullins-Sekerka instability of crystal growth, and demonstrate that we quickly reach the asymptotic regime in which dendrites grow at constant velocities. We do *not* find that dendrites are sensitive to short-length-scale behaviour: they actually support large spontaneous roughening fluctuations on small length scales. This implies that the algorithm successfully simulates correct physics on all length scales.

The Hamiltonian is the two-dimensional ferromagnetic Ising model in a constant field, modified so that each spin-up term is $\mathscr{D}$-fold degenerate [10]:

$$\mathscr{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \delta \sum_i \sigma_i$$

where J is the interaction constant, δ is the field, the sums $\langle ij \rangle$ run over distinct nearest-neighbour pairs, and the spins take on a value of $\sigma_i = \pm 1$. With a degeneracy $\mathscr{D}$ for the $\sigma = +1$ states, it is then easy to show that there is a first-order phase transition at the temperature $T_m = 2\delta / \ln \mathscr{D}$ (so long as T_m is less than the critical temperature $T_c \simeq 2.269J$ of the underlying Ising model), and that the latent heat of the transition is approximately 2δ (so long as the equilibrium magnetisation at T_m is close to unity). With this Hamiltonian, $\sigma = +1$ corresponds to the 'liquid' phase, and $\sigma = -1$ to the 'solid'. Since $\mathscr{D}$ need not be an integer, an appropriate choice of δ and $\mathscr{D}$ allows us to minimise computational problems: we choose $\delta = J$ so that all energy changes can be measured in units of 2δ, and $\mathscr{D} = 3.01$ so that T_m is $0.8T_c$ and the dynamics are fast enough for acceptable run times. Note, in particular, that since we have a well defined microscopic Hamiltonian, quantities such as anisotropic surface tension enter in a natural way.

Because our adaptation of the Creutz algorithm [10] places the Ising system in contact with a system of 'demons', with one demon per lattice site each carrying energy, the dynamics corresponds to model C in critical dynamics, although here we are considering a first-order transition. The two boundary temperatures are set at T_m and $0.2T_m$ respectively, so that the geometry is of a solid at its melting temperature in contact with a supercooled liquid. In addition, to increase the diffusion length and reduce the run time, each spin accesses the demon on its own site and those of its nearest neighbours. We consider lattices of size of 1024×128, large enough that finite size effects are unimportant for the structures we observe, and employ 100 independent runs of duration 10^4 Monte Carlo steps (MCS) per spin. Runs were begun with a flat interface parallel to the boundaries, with 10% of the rows set solid. The initial demon

energy distributions were chosen to be consistent with uniform temperatures of T_m and $0.2T_m$ in the solid and liquid, respectively.

Typical results for the development of the interface with time are shown in figure 1. It is clear that even at very early times ($t \sim 10^3$ MCS) the interface shows precursors of the dendritic structures which form more fully at a later stage. In particular, the characteristic spacing between dendrites, approximately 70, is already evident at early times (lengths are in units of lattice spacings). We also note that there is relatively little sidebranching. The most interesting feature of these results, the large fluctuations, will be discussed later. First, however, we establish that we are in the asymptotic regime by computing the velocity of the dendrites, comparing our results with simple theories, and looking for scaling. In particular, figure 2 demonstrates that, after an initial period of rapid growth, the length of the interface s increases at a constant rate. We have also computed the tip velocity of typical dendrites, and found $v \sim 6 \times 10^{-3}$ per MCS, which is consistent with this rate.

It is useful to compare our data with the predictions of simple theory for the late-stage regime [2]. Agreement is good. To see this, we estimate† the capillary length

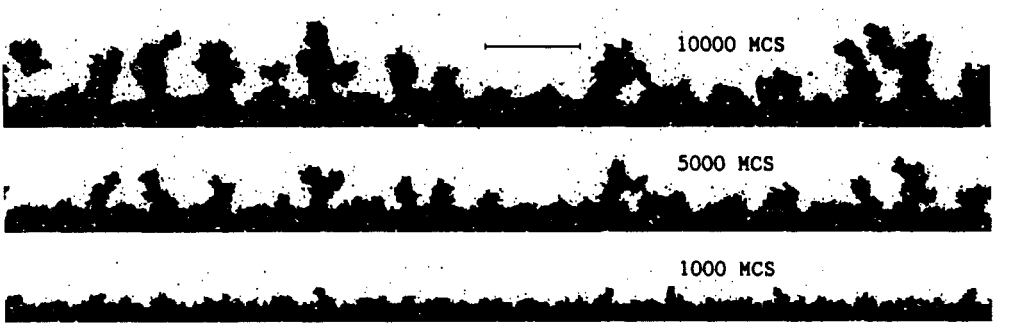

Figure 1. Evolution of typical interface. Horizontal bar shows 100 lattice spacings.

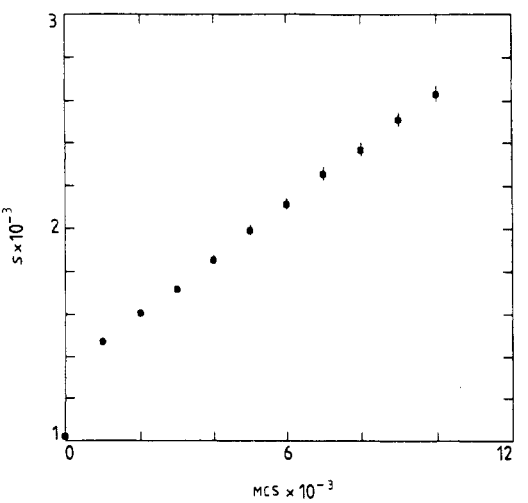

Figure 2. Interface length s against time. Note the data point at MCS = 0.

† We estimate the diffusion length from observation of the temperature fields. To estimate the dimensionless undercooling, we require a value of the specific heat, which is approximately 1.2.

$d_0 \sim 1$, the diffusion length $l \sim 100$, and the undercooling $\Delta \sim 0.8$. The velocity v_0 of the interface itself is $v_0 \sim 6 \times 10^{-4}$ per MCS, and the tip radius $R \sim 6$. Thus, if we calculate the characteristic wavelength using

$$\lambda = 2\pi\sqrt{ld_0}$$

we obtain $\lambda \sim 60$, compared with 70 for the simulation. If we calculate the tip velocity using the simple expression

$$v = \frac{D}{R}\left(\Delta - \frac{2d_0}{R}\right)$$

taking the diffusion constant $D = v_0 l/2$, we obtain $v/v_0 \sim 4$, compared with the value of 10 we observe. These values for λ and v also confirm that we have reached the asymptotic regime.

Further insight comes from the power spectrum $P(q)$ of fluctuations of the interface, shown in figure 3 as a function of wavenumber q. For this analysis, overhangs of the interface were eliminated by projecting them onto the horizontal plane parallel to the original interface†. In figure 3(a) we show that the $q \to 0$ part of this spectrum scales with the growing length s of the interface, as one would expect, in the late stages of growth. All these results imply that the Monte Carlo algorithm is successfully simulating the growth of dendrites from the initial instability to the late-time asymptotic regime.

The most striking feature of our results is that the dendrites support short-wavelength fluctuations which can be interpreted as roughening: notice the large fluctuations in figure 1, and $P(q)$ in figure 3(b). In the latter figure, we see that the interface fluctuations

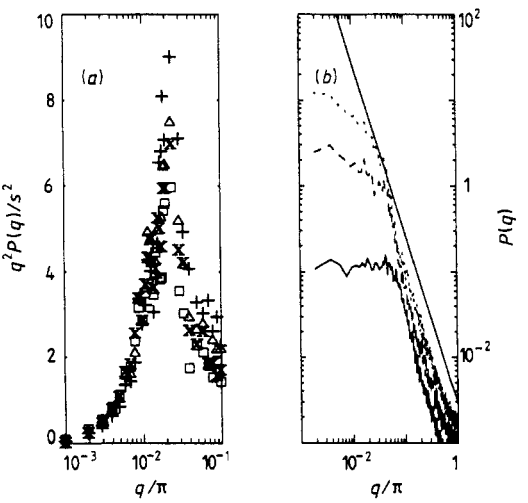

Figure 3. Power spectra $P(q)$ against wavenumber q for selected times: (a) low q, late-time data, scaled with $(q/s)^2$, □ 10 000 MCS, × 8000 MCS, △ 7000 MCS, + 5000 MCS; (b) high q data, line of slope −2 added to guide the eye, dotted curve 10 000 MCS, broken curve 5000 MCS, full curve 1000 MCS.

† To check that this did not bias our results, we have also parametrised the interfaces in terms of arc length and local orientation coordinates, and carried out a power spectrum analysis with respect to a wavevector conjugate to the arc length. These spectra are similar to those from the projection ansatz, and we will present them in a future paper.

on the dendrite have the $1/q^2$ spectrum of equilibrium capillary-wave roughening†. As far as we can tell, they play no direct role in controlling the instability.

In conclusion, we have simulated a microscopic model of dendritic growth with a Monte Carlo algorithm. After a short transient growth following the initial instability, the dendrites grow at constant velocity. The relationship between tip velocity and tip radius is found to be in accord with simple arguments, and the late stages can be characterised by scaling behaviour. Our most interesting result is that the growing dendrites support large roughening fluctuations, which appear to be in local thermodynamic equilibrium. We are currently extending the algorithm to study pattern formation during both directional solidification and three-dimensional dendritic growth, and are investigating the detailed predictions of microscopic solvability.

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† At low q, there are deviations from the $1/q^2$ behaviour showing enhanced spectral weight. These enhancements occur with maximum weight in the vicinity of $2\pi/70$, which is the wavenumber characteristic of the visible pattern. The data is consistent with our analysis of interface roughening in equilibrium [11].