Efficient Computation of Dendritic Microstructures Using Adaptive Mesh Refinement

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We study dendritic microstructure evolution using an adaptive grid, finite element method applied to a phase-field model. The computational complexity of our algorithm, per unit time, scales linearly with system size, allowing simulations on very large lattices. We present computations on a $2^{17} \times 2^{17}$ lattice, but note that this is not an upper limit. Time-dependent calculations in two dimensions are in good agreement with the predictions of solvability theory for high undercoolings, but predict higher values of velocity than solvability theory at low undercooling, where transients dominate, in accord with a heuristic criterion which we derive.

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Dendrites are the primary component of solidification microstructures in metals. Their properties have been a topic of intense study in the past 10–15 years. Experiments by Glicksman and co-workers [1,2] on succinonitrile (SCN) and other transparent analogs of metals have provided tests of theories of dendritic growth, and have stimulated considerable theoretical progress [3–5]. The experiments have demonstrated clearly that naturally growing dendrites possess a unique steady state tip, characterized by its velocity, radius of curvature, and shape, which leads to a time-dependent sidebranched dendrite as it propagates.

Insight into the steady state dendrite problem was first obtained from local models [6–9] describing the evolution of the interface, and incorporating the features of the bulk phases into the governing equation of motion for the interface. These models showed that a nonzero dendrite velocity is obtained only if a source of anisotropy—for example, anisotropic interfacial energy—is present in the description of dendritic evolution. It was then shown that the spectrum of allowed steady state velocities is discrete, not continuous, and the role of anisotropy was understood theoretically, both in the local models and the full moving boundary problem [5,10,11]. Moreover, only the fastest of a spectrum of steady state velocities is stable, thus forming the operating state of the dendrite. It is widely believed that sidebranching is generated by thermal or other statistical fluctuations on a microscopic scale, which are amplified by advective diffusion. This body of theoretical work is generally known as solvability theory.

Brute force solution of the time-dependent Stefan problem requires front tracking and lattice deformation to contain the interface at predefined locations on the grid [12]. The phase-field model avoids this problem by introducing an auxiliary continuous order parameter $\phi(\mathbf{r})$ that couples to the evolution of the thermal field. The phase field interpolates between the solid and liquid phases, attaining two different constant values in either phase, with a rapid transition region in the vicinity of the solidification front. The level set of $\phi(\mathbf{r}) = 0$ is identified with the solidification front, and the dynamics of $\phi$ are designed to follow the evolving solidification front [13–19]. The phase-field parameters can be derived from parameters of the Stefan problem [13,20]; however, this mapping is not very sensitive to the precise form of the phase-field model [21].

While the phase-field model finesse the problem of front tracking, it is still prohibitively expensive for large systems, because the grid spacing must be small enough everywhere that the phase-field model converges to the sharp interface limit [13–20]. Karma and Rappel [20] showed rigorously that the phase-field model converges to the sharp interface limit when the interface width (and hence the grid spacing) is much smaller than the capillary length. This result is necessary for acceptance of the phase-field model, but is not sufficient for computational tractability in the experimentally relevant regime.

However, more recently, Karma and Rappel [20] presented a different asymptotic analysis in powers of the ratio of the interface width to the diffusion length. Their procedure allows the selection of parameters such that the phase-field model corresponds to the sharp interface limit when the interface width (and hence the grid spacing) is of the order of the capillary length—a much more tractable regime. Furthermore, their improved analysis allows the kinetic coefficient to be tuned to zero, which corresponds to the experimentally realized situation at low undercooling in succinonitrile [2]. Karma and Rappel’s numerical results are in excellent agreement with solvability theory at dimensionless undercoolings as low as 0.30, but fail to access the range of experimentally realizable undercoolings near 0.1. What is needed is an effective adaptive technique [23] which dynamically coarsens the grid spacing away from the front.

In this Letter we show how the phase-field model can be solved in a computationally efficient manner that opens a new large-scale simulational window on solidification
physics. Our method uses a finite element, adaptive-grid formulation, and exploits the fact that the phase and temperature fields vary significantly only near the interface. We illustrate how our method allows efficient simulation of phase-field models in very large systems, and verify the predictions of solvability theory at intermediate undercooling. We then present new results at low undercoolings that suggest that solvability theory may not give the correct tip speed in that regime.

We model solidification using the phase-field model used by Karma and Rappel [20]. We rescale temperature $T$ by $U = c_p(T - T_M)/L$, where $c_p$ is the specific heat at constant pressure, $L$ is the latent heat of fusion, and $T_M$ is the melting temperature. The order parameter is defined by $\phi$, with $\phi = 1$ in the solid and $\phi = -1$ in the liquid. The interface is defined by $\phi = 0$. We rescale time by $\tau_0$, a time characterizing atomic movement in the interface, and length by $W_0$, a length characterizing the liquid–solid interface. The model is given by

$$\frac{\partial U}{\partial t} = D \nabla^2 U + \frac{1}{2} \frac{\partial \phi}{\partial t},$$

$$A^2(n) \frac{\partial \phi}{\partial t} = \nabla \cdot [A^2(n) \nabla \phi] + [\phi - \lambda U(1 - \phi^2)](1 - \phi^2) + \frac{\partial}{\partial x} \left( |\nabla \phi|^2 A(n) \frac{\partial A(n)}{\partial \phi_x} \right) + \frac{\partial}{\partial y} \left( |\nabla \phi|^2 A(n) \frac{\partial A(n)}{\partial \phi_y} \right),$$

where $D = \alpha \tau_0/W_0^2$ and $\alpha$ is the thermal diffusivity, and where $\lambda$ controls the coupling of $U$ and $\phi$. Anisotropy has been introduced in Eqs. (1) by defining the width of the interface to be $W(n) = W_0A(n)$ and the characteristic time by $\tau(n) = \tau_0 A^2(n)$ [20], with $A(n) \in [0, 1]$, and $A(n) = (1 - 3\epsilon)(1 + \epsilon)$, where $\epsilon = \theta/(\theta + 1)$. The vector $\vec{n} = (\phi_x, \phi_y)/(|\phi_x|^2 + |\phi_y|^2)^{1/2}$ is the normal to the contours of $\phi$, and $\phi_x$ and $\phi_y$ represent partial derivatives with respect to $x$ and $y$. The constant $\epsilon$ parametrizes the deviation of $W(n)$ from $W_0$. We expect the results to be similar for other definitions of anisotropy [13].

We use the asymptotic relationships given in [20] to select the parameters in Eqs. (1) such that it operates in a regime similar for other definitions of anisotropy [13]. We use the grid formulation, and exploits the fact that the phase and temperature fields vary significantly only near the interface. We then present new results at low undercoolings that suggest that solvability theory may not give the correct tip speed in that regime.

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FIG. 1. A dendrite grown using the adaptive-grid method for $\Delta = 0.55$, $D = 2$, and $\epsilon = 0.05$. Clockwise, beginning at the upper right, the figure shows contours of the $U$ field, the contour $\phi = 0$, contours of the $\phi$ field, and the current mesh.

dendrite tip moves at a constant velocity $V_n$, then $R^a_{\text{tip}} = [R_0^a D V_n^2 \Delta x_m^2] L_B^2$, where $R_0^a$ is a constant that depends on the implementation. The CPU time $R^a_{\text{tip}}$ needed to compute the same case on a uniform grid scales as $R^a_{\text{tip}} = [R_0^a (V_n \Delta x_m^2)] L_B^3$. For large system sizes, $R^a_{\text{tip}} / R^a_{\text{sys}} \sim L_B$.

We tested the effective anisotropy of our dynamically adapting lattice in two ways. Following the method outlined by Karma [20], we find an equilibrium shape for the interface when the background field is adjusted dynamically so as to maintain the velocity of the interface at zero. The effective anisotropy is inferred by fitting an equation to the computed interface. We found $\epsilon_{\text{eff}}$ to be within 5% of the intended value for input $\epsilon = 0.02-0.04$.

We also tested for grid anisotropy by rotating the grid by 45°, which should represent the lowest accuracy for square elements. In this case, the steady state tip velocity was within 1% of its value in the original orientation.

We further verified our algorithm by comparing measured tip velocities and shapes for dendrites grown using the same undercoolings, parameter sets, and system sizes reported in [20]. We found very good agreement for $\Delta = 0.65$, 0.55, 0.45, and 0.30. We next investigated the effect of system size. Figure 3 shows the time evolution of tip velocity for several undercoolings and system dimensions. The two cases for $\Delta = 0.65$ are typical of results at intermediate $\Delta$, showing a relatively rapid leveling to an asymptotic speed within a few percent of that predicted by solvability theory.

At lower $\Delta$, however, we found that the tip velocity deviates from that predicted by solvability theory. Figure 3 also shows the evolution of the tip velocity for $\Delta = 0.25$ in two different sized boxes. Whereas the computed tip velocity falls a few percent below the solvability value in the $6400 \times 400$ box, it exceeds by 8% the solvability value in the $6400 \times 3200$ box. This effect is even larger at $\Delta = 0.1$, also shown in Fig. 3, where the tip speed is about 3 times larger than that predicted by solvability theory.

The explanation for this behavior is that, at low $\Delta$, the thermal fields of the two dendrite branches overlap, violating the assumptions of solvability theory, which model an isolated single dendrite. At large undercooling, each dendrite arm quickly outruns the other’s thermal boundary layer, and solvability theory should apply (see Fig. 1, $\Delta = 0.65$). The conditions of solvability theory can also be approximated at lower undercooling if simulations are performed in a domain which is small in one direction. For the simulation performed with $\Delta = 0.25$ in the small box ($6400 \times 400$), the branch in the $y$ direction is extinguished by its interaction with the wall, and agreement with solvability theory is obtained. However, when both

FIG. 2. CPU time vs the system size, illustrating the computing time for a dendrite to move through the system of linear dimension $L_B$ using our adaptive mesh method.

FIG. 3. The time evolution of the tip velocity for undercooling $\Delta = 0.65$, 0.25, and 0.10.
branches are present, as in the simulation with $\Delta = 0.25$ in the larger box ($6400 \times 3200$), their interaction leads to an increased tip velocity because the dendrites are embedded in a circular rather than parabolic diffusion field. This is seen clearly in Fig. 4, where the dendrite shape and its associated field are shown for $\Delta = 0.10$ ($D = 13$, $d_0 = 0.043$, $\epsilon = 0.05$, $\Delta x = 0.78$, $dt = 0.08$). The dendrite arms never became free of each other in this simulation, causing the observed deviation from solvability theory shown in Fig. 3. This latter simulation was performed in a $102400 \times 51200$ domain, chosen to contain about $10D/V_n$. We note that the ratio of the largest to smallest element size in this simulation is $2^{17}$. A fixed mesh having the same resolution would contain $9 \times 10^9$ grid points, clearly beyond current computing capability.

We can estimate the time $t^*$ when the growth of the dendrite tip crosses over from the transient regime where the branches interact to where they become independent by equating the length of the full diffusion field $3(Dt^*)^{1/2}$ to the length of a dendrite arm $V_n t^*$. This gives the crossover time as $t^* = 9D/V_n^2$. The values for $t^*$ corresponding to the cases $\Delta = 0.65$, $0.25$, and $0.10$ in Fig. 3 are $2.5 \times 10^3$, $1.6 \times 10^4$, and $5.9 \times 10^7$, respectively. Inspection of Fig. 3 confirms this scaling.

These results have important implications when comparing theory to experimental observations at low undercooling. We find that, in this regime, the appropriate theory to use is one which explicitly takes into account the long range effects of other branches [25]. In particular, the study of real dendrites with sidebranches, growing at low undercooling will require such treatment. An investigation of this effect, as well as results on directional solidification will appear in future publications.

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