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Massively Parallel Methods for Simulating the Phase-Field Model

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Massively Parallel Methods for Simulating the Phase-Field Model

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ABSTRACT

Prediction of the evolution of microstructures in weapons systems is critical to meeting the objectives of stockpile stewardship in accordance with the Nuclear Weapons Test Ban Treaty. For example, accurate simulation of microstructural evolution in solder joints, cermets, PZT power generators, etc. is necessary for predicting the performance, aging, and reliability both of individual components and of entire weapons systems. A recently developed but promising approach called the "Phase-Field Model" (PFM) has the potential of allowing the accurate quantitative prediction of microstructural evolution, with all the spatial and thermodynamic complexity of a real microstructure. Simulating with the PFM requires solving a set of coupled nonlinear differential equations, one for each material variable (e.g., grain orientation, phase, composition, stresses, anisotropy, etc.). While the PFM is versatile and is able to incorporate the necessary complexity for modeling real material systems, it is very computationally intensive, and it has been a difficult and major challenge to formulate an efficient algorithmic implementation of the approach.

We found that second order in space algorithm is more stable and leads to more accurate results. However, the computational requirements still remain high, so we have developed a single field algorithm to reduce the computations by 2 orders of magnitude. We have created a 3-D parallel version of the basic phase-field (PF model) and benchmarked it performance. Preliminary results indicate that we will be able to run very large problems effectively with the new parallel code. Microstructural evolution in a diffusion couple was simulated using PFM to simultaneously simulate grain growth, diffusion and phase transformation. Solute drag in a variable composition material, a process no other model can simulate, was successfully simulated using the phase-field model. The phase field model was used to study the evolution of fractal high curvature

structures to show that these structures have very different morphological and kinetic behaviors than those of equi-axed structures.

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Contents

Introduction 7
Model description 7
Objective 10
Numerical algorithms 10
Parallelization and extension to 3-D 11
Complex microstructural evolution simulations 11
Conclusions 14
References 15
Distribution 16

Introduction

Microstructural features control the properties and performance of engineering components to a large extent. Thus, it is vital that engineers tailor the microstructures of the components they fabricate to the components' applications. However, controlling microstructural evolution during processing is a challenging problem because of the large number of variables that must be understood and controlled. Therefore, predictive modeling techniques are necessary for tailoring microstructures to their applications.

Coarsening models are the most numerous and most mature of the microstructural evolution models. Many investigators have used a number of different numerical techniques to simulate coarsening by processes such as grain growth and Ostwald ripening. Among the numerical models used are the Potts model[1,2], the phase-field model[3,4,5], front tracking model[6,7,8], Voronoi tessellation[9], and vertex model[10]. While each of these models is vastly different in how it incorporates the physics of coarsening, they all give similar results. Among these models, the Potts and phase-field[11,12] are arguably the most robust and versatile and certainly the most highly developed and widely applied.

In this study, we focus on the phase-field model as incorporation of additional microstructural complexity beyond coarsening is straightforward in this model. The phase-field model[13] is based on the early field theory models[14] that in turn are based on the Cahn-Hilliard equation for a diffuse interface[15]. The phase-field model employs parameters called order parameters to represent microstructure. These field variables are continuum functions of spatial coordinates **r** and time **t** and are used to characterize a heterogeneous state consisting of phases with different composition and/or structure. Continuous fields of composition and long-range order parameters that characterize structural heterogeneities of a system are typical examples of such field variables. The evolution of these field variables in space with time gives detailed information about metastable and unstable microstructural states that occur during microstructural evolution. The combination of developments in the numerical techniques and computation power has allowed many investigators to develop the phase-field model to study a wide variety of microstructural evolution processes and progressively more complex problems. Some of these applications have been normal grain growth[3,4], Ostwald ripening[16], combined grain growth and Ostwald ripening[17], microstructural evolution with coherent strain[18,19,20], twin formations[21,22] and ferroelectric domain switching[23].

While the phase-field model is highly versatile, it is computationally very intensive and becomes increasingly so as additional physics is introduced. The goal of this investigation was to develop numerically efficient algorithms while preserving the versatility of the phase-field model.

Model description

The phase-field model is a thermodynamic model, which uses a field representation for microstructure. As an example, consider a 2D grain structure and phase-field description of a polycrystal. The continuum grain and grain boundary structure is mapped onto a discrete square lattice using a set of order parameters, $\{\eta_i(r)\}$ where $i = \{1, 2, \ldots Q\}$, which may be conceptualized as membership of site r in Q different grains. This set of order parameters is allowed to evolve with time at each

lattice point *r* to simulate microstructural evolution. Figure 1 is a schematic diagram showing how the order parameters vary continuously from one grain to its neighbor to form diffuse grain boundaries. For the grain interior site, all order parameters have values of 0.0 except one; it has a value of 1.0. This may be interpreted as that site having exclusive and full membership in the grain represented by that particular order parameter and in no other grains. A site at an interface between two grains has partial membership in the two grains on both sides of it and no membership in any other grains. The order parameters are nonconserved parameters, thus they need not sum to any particular value locally at any given site or globally at all sites. This type of representation leads to diffuse interfaces as described by Cahn and Hilliard[15].

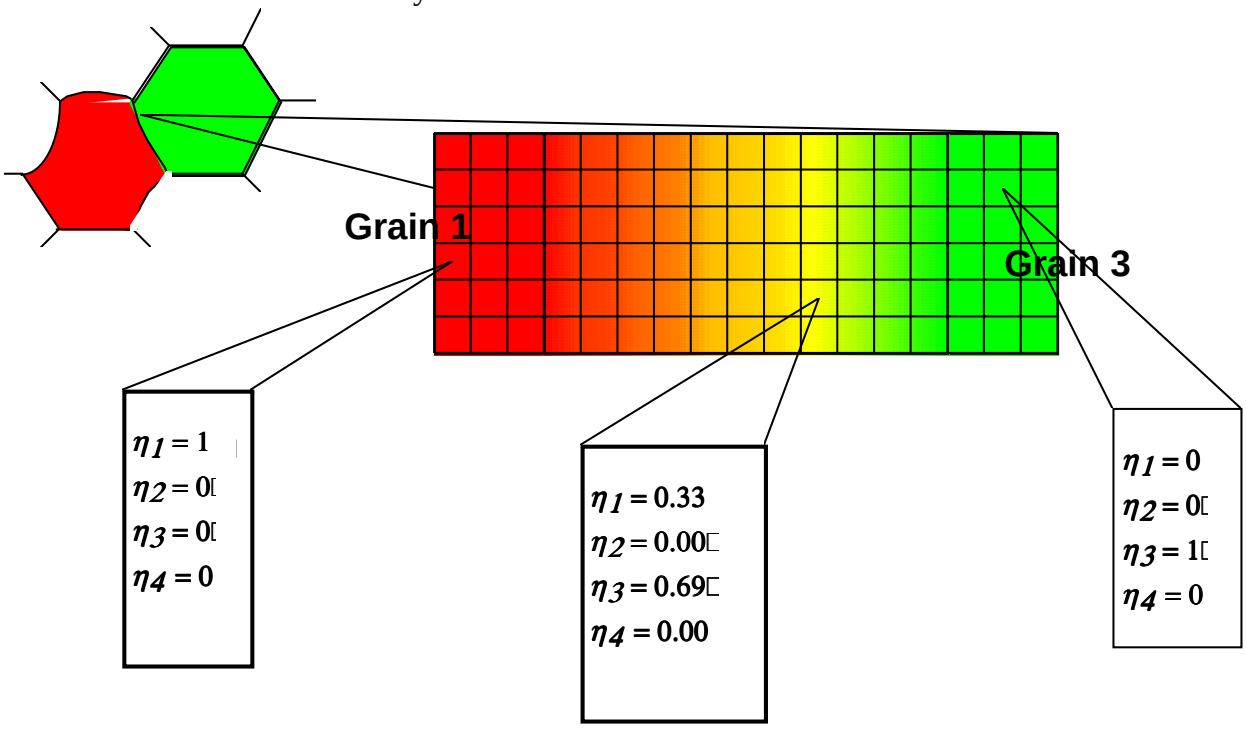

Figure 1. Microstructural representation of the phase-field model.

The equation of state for the simulation is a free energy function, *F*, which is a function of the order parameters. It defines the energy of the system given any combination of order parameters η_i's. The order parameters, η_i's, are locally and globally non-conserved parameters. Since the free energy is defined for all possible combination of η_i's, the combination of these parameters which gives the lowest *F* is the equilibrium state of the system.

The free energy for normal grain growth is

$$F = \int \left[f_o\left(\eta_1(r),\ldots,\eta_p(r)\right) + \sum_{i=1}^{p} \frac{\kappa_i}{2} \left(\nabla \eta_i(r)\right)^2 \right] d^3r \qquad \textit{eq. 1}$$

where f_o is the bulk chemical free energy,

$$f_o = -\frac{\alpha}{2}\sum_{i=1}^{p}\eta_i^2 + \frac{\beta}{4}\left|\sum_{i=1}^{p}\eta_i^2\right|^2 + \left(\gamma - \frac{\beta}{2}\right)\sum_{i=1}^{p}\sum_{j\neq i}^{p}\eta_i^2\eta_j^2 \qquad \textit{eq. 2}$$

with $\alpha=1$, $\beta=1$ and $\gamma=1$

In this model the interfacial energy consists of the excess free energy in the interface and the terms quadratic in the gradients of the order parameters, $2\kappa_i(\nabla\eta_i)^2$, where κ_i are the gradient coefficients of the order parameters. Thus, at grain boundaries and triple junctions, where order parameters change spatially, the free energy of the system is increased.

The driving force for microstructural evolution is the reduction of total free energy of a system. In this case, the total interfacial energy is decreased as the microstructure evolves. Kinetics for microstructural evolution is introduced by the time-dependent Ginzburg-Landau equations.

$$\frac{d\eta_i(r,t)}{dt} = -L_i\frac{\delta F(r,t)}{\delta\eta_i} = -L_i\frac{\partial f_o(r,t)}{\partial\eta_i} + L_i\kappa_i\nabla^2\eta_i(r,t) \qquad \textit{eq. 3}$$

where L_i is the kinetic rate coefficient related to interface mobility and diffusivity. Equation 3 determines the evolution of the order parameters and, hence, the grain structure.

The starting microstructures for this study were initialized by assigning small random numbers between *-0.001* and *0.001* for each order parameter at each site at time $t = 0.0$. This microstructure is analogous to a supercooled liquid. Once the microstructure is initialized, grain growth is simulated by repetitive calculation of order parameters at each site for the next time increment $t = t+\Delta t$ or $\eta_i(r,t+\Delta t)$ which is calculated using the forward Euler technique,

$$\eta_i(r,t+\Delta t) = \eta_i(r,t) + \frac{\partial\eta_i(r,t)}{\partial t}\Delta t \qquad \textit{eq. 4}$$

where the quantity $\frac{\partial\eta_i}{\partial t}$ is determined using *eq. 3*. The Laplacians used in *eq. 3* were calculated for a discretized system as

$$\nabla^2\eta = \frac{1}{(\Delta x)^2}\left|\frac{1}{2}\sum_{i}\left(\eta_i - \eta_r\right) + \frac{1}{4}\sum_{j}\left(\eta_j - \eta_r\right)\right| \qquad \textit{eq. 5}$$

where Δx is the grid size, i is the set of first nearest neighbors of site r, and j is the set of second nearest neighbors of site r.

The results of the normal grain growth simulation are given in figure 2 showing the microstructure at increasing times during grain growth. This simulation has all the necessary materials physics to simulate grain growth correctly. Grain boundaries moved

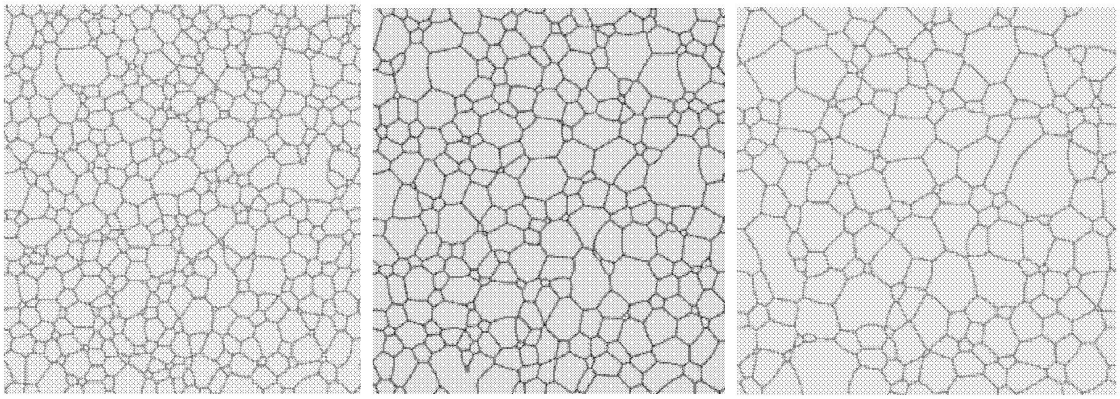

Figure 2. The microstructural evolution resulting from grain growth simulations

to their centers of curvature, the grain growth exponent, n, in the grain growth equation $R^n - R^n_o = kt$ was found to be $n = 2$ in agreement with grain growth theory and the grain size distributions at different times were self-similar.

Objectives

The grain growth example shown above can be used to demonstrate the huge computational demand of the phase-field model. The differential eq. 4 was solved at each lattice point (total simulation space was 1024 x 1024 sites) for 36 order parameters η_i at each time step (total simulation time was 100,000 time step). This is a huge number of calculations for a relatively simple coarsening simulations. The drawbacks of PFM simulations are that they (1) are very computationally intensive and become increasingly so with more complex materials behaviors and (2) require the difficult task of formulating of a set of differential equations that describe the materials phenomena and are numerically stable and efficient. The purpose of this investigation was (1) to develop numerically efficient algorithms to simulate microstructural evolution and to evaluate their numerical stability to address materials problems, (2) to extend the phase-field model to a massively parallel code to allow solving large 3D microstructures and, finally, (3) to demonstrate the versatility of the phase-field model by incorporating additional materials physics.

Numerical algorithms

In grain growth simulation shown above the number of order parameters (representing the number of different grain orientations) is Q = 36. One wishes the number Q of possible grain orientations to be as large as possible, since Q is actually physically infinite. However, initial implementations of the phase field grain growth algorithm scaled at least linearly with Q, presenting a bottleneck. Furthermore, the algorithm also became increasingly unstable with larger Q.

We developed an algorithmic approach that replaces the multiple phase fields by a single field, allowing the grain growth phase field method to scale independently of Q and hence removing the previous bottleneck. The new method also allows a different grain orientation to be initially associated with each discretized spatial point, giving the practical equivalent of the desired "infinite" number of grain orientations. This new approach was rigorously mapped to earlier ones. It reduces the number of differential

equations to be solved from Q to 2 at each lattice site and at each time step. In addition, we derived an accurate analytic estimate for the grain boundary width, allowing an *a priori* selection of the spatial discretization.

A variety of implementation issues were investigated. A speed-up technique that selectively ignores the less active grain interiors was developed by identifying regions where the gradients of the order parameters in the simulation space are high. We determined that a continuous single well was adequate for the grain growth functional, which may allow a reduction in operations count from the previous quartic functional. We next investigated discretization (or related alternative) approaches. One of the most efficient, the alternating direction implicit (ADI) version of the Crank-Nicholson method, routinely used for finite difference, is second order in both space and time discretization and is unconditionally stable for the related heat equation by the (standard) von Neumann criterion. However, it involves tridiagonal solves across the entire length of the simulated region. We have found a completely local and hence more efficient alternative to ADI which nonetheless retains ADI accuracy. This alternative is a second order in space algorithm that is more stable and leads to more accurate results. While simulation results obtained from second order in space discretization algorithms are highly accurate, the computational demand still remains very high because the time step for each microstructural evolution calculation is small.

Parallelization and extension to 3-D

Thus far during FY99, we have created a 3-D parallel version of the basic phase-field model. Computationally, the PF equations require local stencil operations on a regular 3-D grid to update the field variables in a coupled fashion for a single time step. Using a spatial-decomposition of the grid across processors, only sub-domain boundary information need be communicated between processors for each field variable. Although the computation per grid point per field variable is relatively modest in the basic phase-field model, we found this strategy to scale reasonably well to large numbers of processors.

To wit, we have performed the following benchmark calculations with the new parallel phase-field code on the Intel Paragon. For a small problem (50x50x50 grid with 10 order parameters) the code runs in 2.96 secs (per time step) on 1 processor, 0.07 secs on 64 procs, and 0.024 secs on 256 procs. This is fixed-size parallel efficiency of roughly 65% and 50% on 64 and 256 processors. A more typical production-scale problem (100x100x100 grid with 36 order parameters) runs in 1.45 secs (per time step) on 64 procs and 0.44 secs on 256 procs. This is a fixed-size parallel efficiency of 92% and 75% on 64 and 256 procs. Scaled-size speed-ups would undoubtedly be even better. These preliminary numbers indicate that we will be able to run very large problems effectively with the new parallel code.

Complex microstructural evolution simulations

Microstructural evolution in a diffusion couple

Several microstructural evolution problems of higher complexity than simple coarsening in a single phase material were investigated. The first was of simulating microstructural evolution in a diffusion couple, such as that found during joining processes. In this case, two materials are placed next to each other under high

temperature so that they join to form a single part. The system simulated was characterized by a two-component (A and B), two-phase (α and β) system with mutual solubility and diffusion of the two components in both phases. The active processes in such a system are diffusion, coarsening, and phase transformation, all occurring simultaneously. The phase field model used two sets of order parameters, one for each phase. Each set of order parameters had a free energy functional associated with it. The simulation of simultaneous coarsening, diffusion, and phase transformation gave qualitatively accurate results, with the proper materials physics. The resulting microstructures and composition profiles varied with the starting conditions of the simulation as one would expect and were consistent with diffusion theory. The example shown in figure 3 is simulation of grain growth and diffusion in a two-component, two-phase system with an initial composition in the α-phase region. On the left side of the simulation space, the α-phase nucleates homogeneously and grows. On the right side, the β-phase nucleates heterogeneously and grows in as columnar grains before other β-grains can nucleate. However, the simulations showed two unexpected results: 1. The coarsening rate was a function of composition, and 2. solute segregation was observed at grain boundaries. These two results are undesired artifacts of the free energy functional. This example highlights the need to carefully design the free energy functional to incorporate the thermodynamic and kinetic properties of a particular system without introducing any artifacts.

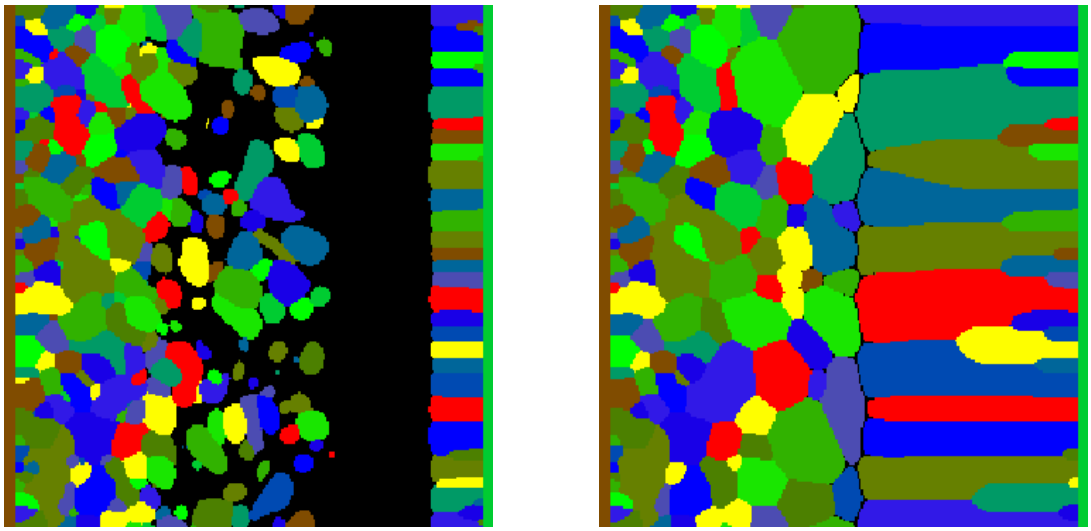

Figure 3. Microstructural evolution in a diffusion couple with simultaneous diffusion and coarsening.

Simulation of solute drag

The second materials problem studied was solute drag. Several important components that Sandia manufactures and maintains such as the PZT voltage bars, solder joints and cermet source feed throughs have compositional gradients at the grain boundaries. The grain boundary regions are regions of high entropy and can dissolve more impurities than grain interiors in many systems. The grain boundary compositional changes can influence the microstructural evolution of the components both during processing and during service by a process commonly know as solute drag[24,25]. The

understanding and prediction of solute drag is important for the design of many engineering components.

Solute drag was simulated by the phase-field model by designing a free energy functional for a two-component (A and B), single phase (α-phase) system with solute enrichment in the grain boundary region. Simultaneous coarsening and diffusion was simulated by coupling the free energy and solving the kinetic equations for grain growth and diffusion alternately. Figure 4a shows a circular grain in a homogeneous matrix shrinking uniformly while maintaining circular symmetry. However solute drag at the grain boundary caused the composition at the grain boundary to change as shown in figure 4b. Furthermore, the grain growth rate decreased with increasing solute enrichment at the grain boundary.

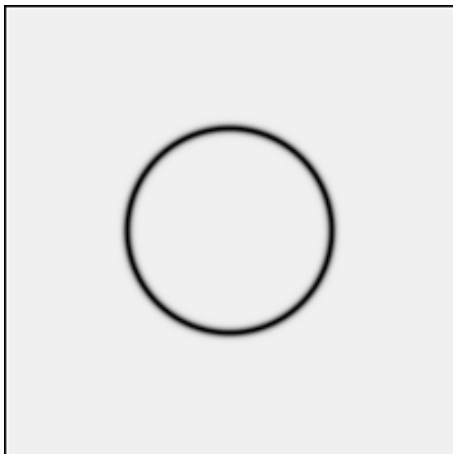

Figure 4a. Density of solute phase

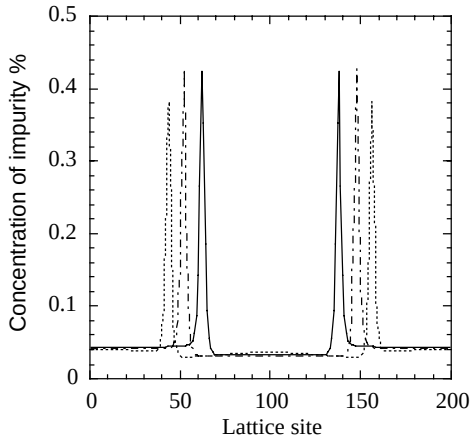

Figure 4b. Solute phase concentration across the center line in Figure 4a.

The ability to track solute enrichment at the grain boundaries as the microstructure evolves will be very useful for a number of Sandia projects. Furthermore, no other mesoscale microstructural model has the ability to treat solute drag at the grain boundaries.

Coarsening kinetics of dendritic structures

Many materials have high curvature, fractal structures such as dendrites in braze joints or eutectic colonies in solder joints. Microstructural evolution due to coarsening in these structures is very different from that in equi-axed structures. Not only is the morphology different, but the kinetics of coarsening are also very different. It is the kinetics that interests us more as it is not readily predictable and has implication for the engineering performance of these components as they age. The phase field model was used to study the evolution of high curvature structures such as the fractal structure similar to that of a dendrite (shown in figure 5a). The free energy functional used was the same as that for normal grain growth given by eq. 1. However, unlike normal grain growth only two order parameters are necessary, one for the matrix grain (blue region in figure 5a) and the other for the dendrite (the red feature in figure 5a). The results of this simulation are shown in figure 5. Figure 5b, a plot of dendrite interface length as a

function of time, shows that there are two distinct kinetic regions in such a system. At high curvature, the grain boundary length dependence on time is given by the power law with the exponent (1-Ds)/2 determined by on initial fractal dimension Ds of the grain boundaries. At low curvature the behavior approaches the normal grain growth behavior seen in the more equi-axed microstructures with a grain growth exponent n = 2. This behavior was compared to the results of a Potts model simulation and very good agreement was found between to the two systems.

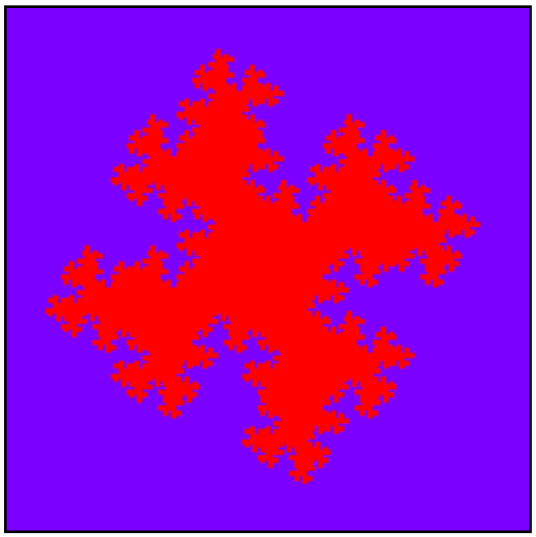

Figure 5a. Microstructural evolution of initial dendritic structure used to study coarsening.

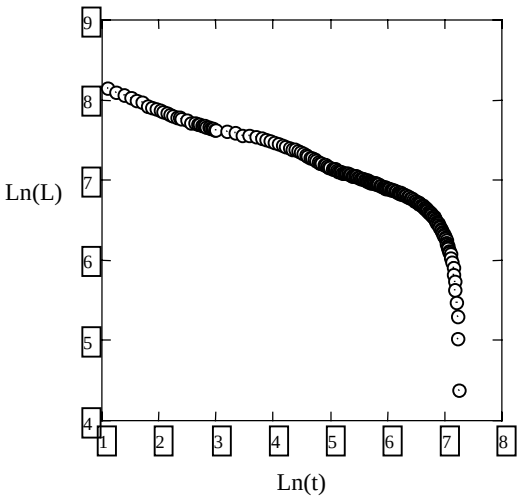

Figure 5b. Grain boundary length of dendrite as a function of time

Conclusions

The phase-field model is highly versatile and can simulate many problems of microstructural evolution rigorously. We determined a relatively simple implementation of the single-field algorithmic approach, which we expect to reduce computation by up to two orders of magnitude and to eliminate unphysical “coalescence” by using a single order parameter with infinite degenerate minima to represent different grain orientations. We explored a higher-order spatial finite-difference stencil, finding it more stable and accurate in some regimes. We created a 3-D parallel version of the basic phase-field model important for realistic simulations, and benchmarked its performance. Preliminary results indicate that we will be able to run very large problems efficiently with the parallel code. The phase-field model was used to simulate microstructural evolution in a diffusion couple with simultaneous diffusion, coarsening and phase transformation. The important problem of solute drag in variable composition materials was successfully simulated, a process no other model can simulate. The phase-field was used to study the evolution of fractal high-curvature structures, showing that these structures have very different morphological and kinetic behaviors than those of equi-axed structures.

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