Parallel Implementation of Phase Field Modeling for Solidification

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Background

Solidification continues to be of great importance in materials science and materials processing. Engineering alloys cast from the melt undergo extreme microstructural changes during the solidification process, and the resulting morphological and topological characteristics direct subsequent work on the material, which ultimately determines its properties. Small variations in composition and cooling rates can have profound effects on the resulting solidified microstructure, for example, the grain size distribution, the appearance of columnar grains, or the growth of dendrites. The ability to efficiently and accurately predict solidification microstructures helps engineers increase the rate of development of new materials and materials processing techniques.

The phase field method has been successfully applied in studying various types of microstructure evolution, including solidification, solid-state phase transformations, grain growth, and dislocation dynamics [1]. The method describes a microstructure via a set of "order parameters" $\phi_i(\boldsymbol{x}, t)$, which must sum to 1, and together represent the "phase state" at time t at location $\boldsymbol{x}$ in the microstructure [2]. For example, if there are three phases in the microstructure, and at location $\boldsymbol{x}$, $\phi_1 = \phi_2 = 0$ and $\phi_3 = 1$, then the microstructure at $\boldsymbol{x}$ is completely phase three. If, at another location $\boldsymbol{x}'$, $\phi_1 = 0$, $\phi_2 = 0.25$, and $\phi_3 = 0.75$, then $\boldsymbol{x}'$ would be located at an interface between phases two and three. Sharp interphase boundaries are avoided by letting the ϕ_i functions vary continuously, and interface movement can be modeled without tracking interfaces explicitly—interface velocity simply arises due to the $\phi_i(\boldsymbol{x})$ parameters changing through time.

For basic solidification problems, there are only two phases present: solid and liquid. Since in this case $\phi_1 = 1 - \phi_2$ always, the equations are usually written in terms of a single order parameter ϕ, representing the solid phase.

The time change of ϕ is modeled as proportional to the variation in a free energy functional,

$$\frac{\partial \phi(\boldsymbol{x}, t)}{\partial t} = M \frac{\delta F}{\delta \phi(\boldsymbol{x}, t)}, \tag{1}$$

where M is related to the mobility of the phase, and F is an appropriately chosen free energy; for solidification the Helmholtz free energy is often used. The variation of F provides the driving force for the interface movement. Increasingly complex expressions for F can capture bulk free energy, interfacial free energy, and free energy contributions from longer range interactions, such as elastic (mechanical) and electrostatic interactions between phases [1]. Diffusion equations and the effects of temperature gradients can be solved simultaneously with Eqn. (1). Given initial and boundary conditions, Eqn. (1) can be solved for all $\boldsymbol{x}$ at each timestep to track the growth and shape of the solidifying precipitates.

Project Description

The goal of this project is to implement a parallelized version of the phase field model. Since the bulk of the effort will be focused on building the infrastructure, the problem space will be limited to a basic solidification problem in, e.g., a Cu-Al system. Since the project will focus on such a well-studied system, there should be sufficient microstructural data and materials parameters available in the literature. However, the code should be sufficiently modular so that it can be later extended; for example, more advanced treatments of the free energy functional could be plugged in, or more phases could be added.

Traditionally, Eqn. (1) has been solved using finite difference methods, though other methods are possible, e.g., Fourier transform methods [1]. For this project, I intend to use the finite difference method. Since Eqn. (1) is over a spatial domain, it should parallelize quite naturally over a computer cluster, where each node communicates at its boundary. One advanced technique that I would like to pursue, if time permits, is an adaptive mesh over the spatial domain. Since the most interesting parts of the simulation are the interphase regions; that is, where ϕ transitions from 0 to 1, it would be ideal if $\boldsymbol{x}$ was discretized such that it had the finest mesh size in those locations. These areas of finer mesh would travel with the interfaces.

Final deliverables include the parallelized phase field method code, any post-processing or visualization code, and the final report.

References

[1] L. Q. Chen, Phase-Field Models for Microstructure Evolution, Annual Review of Materials Research 32 (1) (2002) 113–140.

[2] M. Ode, S. G. Kim, T. Suzuki, Recent Advances in the Phase-field Model for Solidification, Iron and Steel Inst. of Japan, International 41 (10) (2001) 1076–1082.