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Phase field benchmark problems for dendritic growth and linear elasticity

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ABSTRACT

We present the second set of benchmark problems for phase field models that are being jointly developed by the Center for Hierarchical Materials Design (CHiMaD) and the National Institute of Standards and Technology (NIST) along with input from other members in the phase field community. As the integrated computational materials engineering (ICME) approach to materials design has gained traction, there is an increasing need for quantitative phase field results. New algorithms and numerical implementations increase computational capabilities, necessitating standard problems to evaluate their impact on simulated microstructure evolution as well as their computational performance. We propose one benchmark problem for solidification and dendritic growth in a single-component system, and one problem for linear elasticity via the shape evolution of an elastically constrained precipitate. We demonstrate the utility and sensitivity of the benchmark problems by comparing the results of (1) dendritic growth simulations performed with different time integrators and (2) elastically constrained precipitate simulations with different precipitate sizes, initial conditions, and elastic moduli. These numerical benchmark problems will provide a consistent basis for evaluating different algorithms, both existing and those to be developed in the future, for accuracy and computational efficiency when applied to simulate physics often incorporated in phase field models.

1. Introduction

Over the past decade, the concept of integrated computational materials engineering (ICME) has firmly taken root within the materials science and engineering community. In the ICME approach, a material is described and modeled at different fundamental length and time scales; information is linked across these scales to fully capture material behavior and to develop the processing-structure-properties relationships used by materials engineers [1]. The ICME approach may be applied to achieve different goals, such as the development of wholly new materials for specific applications or the tuning of an existing material's composition to meet multiple, unrelated (e.g., color and strength) design criteria. The ICME approach has engendered multiple successes thus far, including the development of new alloys for aerospace [2,3], automotive [4,5], and coinage [6] applications.

The phase field approach is one modeling technique that is commonly included in ICME frameworks. Phase field modeling is a continuum method that is applied to study phenomena occurring on diffusive length and time scales (nanometers to micrometers and microseconds or longer). In a phase field model, certain field variables are defined (e.g., solute concentration) that are continuous across the computational domain and that vary smoothly across phase interfaces. A free energy of the system is defined based on these field variables, and the evolution of the system is driven by a reduction of the free energy. Unlike mean-field models, which average out spatial variations in microstructure, phase field models resolve microstructure evolution in space, elucidating how variations within a microstructure form and interact. Historically, phase field models have tended to be more qualitative in nature, providing insights into potential microstructure evolution mechanisms. However, with the integration of realistic energetics (e.g., CALPHAD-based free energies [7]), phase field models are now being crafted to quantitatively describe real materials. They have been applied to study a range of phenomena, such as the "rhenium effect" in nickel-based superalloys [8] and the formation of gas bubble superlattices in uranium-molybdenum nuclear fuel [9]. For comprehensive descriptions and reviews of phase field modeling, see Refs. [10–17].

Error and uncertainty in models and simulation results are

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important considerations when applying the ICME approach to materials design [18]. Error, broadly speaking, is the deviation in modeled results from physical reality, while uncertainty is the likelihood of the model and implementation to reproduce the physical phenomenon in question with some variation in parameters. Some degree of error and uncertainty exist within any model results, and the linked nature of ICME frameworks means that error and uncertainty at one level may propagate through the results at different length and time scales. While error analyses for phase field models and algorithms are published on occasion (e.g., Refs. [19–21]), the proliferation of scientific publications can make it difficult for new modelers to fully familiarize themselves with existing analyses on the subject, which are often a part of a larger publication on a different topic. The development of new solver frameworks combined with the growing popularity of the phase field approach and a desire for "turnkey" simulation software means that a common basis is needed for performing error analyses and uncertainty quantification; new numerical methods must be evaluated for their accuracy with respect to phase field model physics.

To help address these issues, the Center for Hierarchical Materials Design (CHiMaD) and the National Institute of Standards and Technology (NIST) are developing a suite of numerical benchmark problems that will allow the uniform testing of phase field algorithms and implementations. We choose problem formulations and benchmark metrics that balance the need for nontrivial solutions with computational resource requirements and the investment of human effort, and we intend that these problems are used by the community to understand how numerical methods impact results by comparing different results (see Ref. [22] for a detailed discussion). Importantly, the benchmark problem effort includes significant community involvement regarding problem proposal, design and vetting. These numerical benchmark problems are a necessary precursor before validating a model to experimental results, as the correctness of the numerical method must be verified for validation studies to be useful. Each of these benchmark problems targets a specific aspect of physics commonly found in phase field models. In particular, we address models that include coupled physics, as these can pose significant numerical challenges. The first set of problems focus on the diffusion of solute and the growth of a second phase [22], while this set involves solidification and dendritic growth as well as linear elasticity. To support community involvement, we have developed a website (https://pages.nist.gov/pfhub/), which serves as a repository for the problem statements and the results from different numerical implementations.

We choose dendritic growth as a subject both because of the importance of the physical phenomenon in controlling materials properties [23] and because of the sensitivity of simulation results on phase field model formulations and implementations (see, for example, Refs. [19,24]). Historically, dendritic growth is one of the first applications of phase field modeling [25,26], and remains a significant area of research today. Sharp interface limit [26–30] and thin interface limit [19,31–33] analyses show that the diffuse-interface phase field formulation is asymptotically equivalent to the sharp-interface Stefan formulation. With the introduction of an "anti-trapping current" to correct for solute trapping due to the jump in chemical potential at the solid/liquid interface [33,34], quantitative phase field modeling of alloy solidification can be performed using unphysically large diffuse interface widths. Today, massive increases in computing power and the advent of scientific computing on graphical processing units (GPUs) enable large-scale, quantitative 3D phase field simulations (see, for example, Refs. [35,36] and reviews [37,38]).

Similar considerations drive our choice for the selection of linear elasticity as the subject of the second benchmark problem. Like dendrites, precipitates are a key microstructural feature impacting the strength of alloys [39], and they are often elastically stressed, which affects their shape and their microstructure evolution during service. Elasticity has long been incorporated into phase field models: indeed, Cahn's seminal paper on spinodal decomposition [40] incorporates elastic strains due to composition fluctuations. Eshelby presents an analytical solution for the elastic field of a single coherent, elastically stressed precipitate in an infinite matrix [41], but the generalized problem of multiple interacting precipitates in a matrix with arbitrary crystal structure, lattice parameter misfit and elastic stiffnesses can only be solved numerically. Sharp-interface approaches provide insight into equilibrium elastic shapes and coarsening under the influence of elastic stress [42–46], but these approaches have difficulty simulating precipitate splitting or merging. Early phase field formulations studying elastically stressed precipitates demonstrate the power of the method (e.g., Refs. [47–49]), and present-day studies have expanded to 3D simulations (e.g., Refs. [50–53]) and formulations that include plasticity (e.g., Refs. [54–56]).

In this work, we present the second set of community-driven benchmark problems developed by CHiMaD and NIST. One problem targets solidification by modeling dendritic growth for a single-component system, and the other targets linear elasticity by simulating the equilibrium shape of an elastically stressed precipitate. We discuss the importance of these problems for evaluating new numerical algorithms, a growing concern given the rise of generalized numerical solver frameworks that may include new algorithms that may not be suitable for phase field model physics. We demonstrate the utility of the dendritic growth problem by performing the same simulations with different time integration algorithms. In addition, we discuss how the problems may be modified to test small variations in model formulation or parameterization, and show how the shape of an elastically constrained precipitate is affected by these variations. Finally, we urge researchers to provide feedback on the existing benchmark problem set, contribute their results to the website, and make suggestions for modifications or future benchmark problem topics.

2. Benchmark problem formulations

The phase field approach is well suited for modeling multiphysics problems, that is, phenomena driven by more than one physical factor, e.g., diffusion in an electric potential field. In a phase field model, a microstructure is defined by one or more field variables, or "order parameters," which exist over the entire computational domain and which evolve in time. Multiphysics models may define additional field variables, such as temperature, that are needed to describe the system but not the microstructure itself. The total system free energy, $\mathscr{F}$, is a functional of different local free energy density contributions that depend on the field variables. These different free energy densities capture different energetic contributions to the system, such as bulk chemical energy, interfacial energy and elastic energy. The time evolution of the order parameters is governed by functional derivatives of the free energy as driving forces (Onsager non-equilibrium thermodynamics), though additional field variables may be driven by different dynamics (e.g., thermal diffusion). If the relaxation dynamics of one field variable is orders of magnitude faster than another, the model may be formulated using a quasi-static approximation, that is the time-independent solution for the rapidly-evolving variable is computed at each time step of the slower-changing variable's evolution.

The two benchmark problem formulations presented in Section 2 involve multiphysics coupling: the model for solidification and dendritic growth incorporates anisotropic interfacial energy and the release of latent heat, and the model for the elastically constrained precipitate adds the physics of linear elastic solid mechanics to the Cahn-Hilliard equation. We discuss each model formulation and parameterization, as well as our choices for computational domain sizes and initial and boundary conditions. Both models are restricted to two dimensions to capture essential physics and potential computational pitfalls without requiring the use of significant computational resources.