Editor's Choice

Benchmark problems for numerical implementations of phase field models

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ABSTRACT

We present the first set of benchmark problems for phase field models that are being developed by the Center for Hierarchical Materials Design (CHiMaD) and the National Institute of Standards and Technology (NIST). While many scientific research areas use a limited set of well-established software, the growing phase field community continues to develop a wide variety of codes and lacks benchmark problems to consistently evaluate the numerical performance of new implementations. Phase field modeling has become significantly more popular as computational power has increased and is now becoming mainstream, driving the need for benchmark problems to validate and verify new implementations. We follow the example set by the micromagnetics community to develop an evolving set of benchmark problems that test the usability, computational resources, numerical capabilities and physical scope of phase field simulation codes. In this paper, we propose two benchmark problems that cover the physics of solute diffusion and growth and coarsening of a second phase via a simple spinodal decomposition model and a more complex Ostwald ripening model. We demonstrate the utility of benchmark problems by comparing the results of simulations performed with two different adaptive time stepping techniques, and we discuss the needs of future benchmark problems. The development of benchmark problems will enable the results of quantitative phase field models to be confidently incorporated into integrated computational materials science and engineering (ICME), an important goal of the Materials Genome Initiative.

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1. Introduction

Many important processes in materials microstructural evolution, such as coarsening, solidification, polycrystalline grain evolution, and magnetic and ferroelectric domain formation and motion, occur on mesoscopic length and time scales. The "mesoscale" is the scale "in between;" in this case, in between atomistic scales of the order of sub-nanometers and femto- to picoseconds, and macroscopic scales of the order of micrometers and microseconds and larger. Mesoscale processes can strongly impact materials properties and performance in engineering applications, providing strong motivation to develop accurate mesoscale microstructure evolution models.

Two general mesoscale modeling approaches exist, with the primary difference being how interfaces are handled [1–3]. Sharp-interface approaches, which treat interfaces as mathematically sharp, can be very efficient numerically when simulating the evolution of simple microstructural geometries. However, interface tracking with complex geometries (e.g., during dendritic growth) and topology changes, such as particles merging or splitting, pose significant numerical challenges [3]. Diffuse-interface approaches, in which the interface has a finite width, avoid these issues [1–3]. However, they generally require more computational resources because the diffuse interface, which often has a width of a few nanometers, must be resolved even as other structural features may have length scales in the hundreds of nanometers or larger.

One popular diffuse-interface technique is the phase field approach, which has been used to study dendritic growth, spinodal decomposition, grain growth, ferroelectric domain formation, and

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other phenomena [1,2,4–9]. In a phase field model, a microstructure is described by one or more continuous fields, $\varphi(\mathbf{r}, t)$. The fields change smoothly over the computational domain and across interfaces. The field variables may be either a physical quantity, such as composition or density, or a phenomenological descriptor [1]. Originally [10,11], the fields were used to denote a local phase (hence the name *phase field*), with the value of φ at position $\mathbf{r}$ and time t indicating the phase. For example, a two-phase system can be described by a field φ that takes the values φ_α and φ_β in the bulk α and β phases, respectively, while at the α/β interface, the value of φ changes smoothly over a finite width. The use of phase field methods is now more diverse, with the phase field variable often representing other quantities or properties, such as concentration or density. The evolution of existing phases within the system is driven by the reduction of the free energy, which is described as a functional of the field variables. Depending on the physics being modeled, the field variables may be conserved or non-conserved. Finally, "sharp-interface limit" or "thin-interface limit" analyses have shown that phase field models are equivalent to their analogous sharp-interface models when the interface width is significantly smaller than the size of other characteristic length scales (reviewed in Refs. [1,2]). For comprehensive descriptions and reviews of phase field modeling, see Refs. [1,2,4–9].

Quantitative phase field models have been developed to study technologically important phenomena in real materials systems as part of integrated computational materials engineering (ICME) [12–14]. In ICME, models at different length scales are linked together to design materials for technological applications. A few selected references of recent quantitative phase field studies include solidification in Al alloys [15–17], precipitation in Ni-based superalloys [18–20], recrystallization in Ti [21] and Mg [22] alloys, quantum dot formation in InAs/GaAs [23], and semiconducting core-shell nanoparticles [24]. The phase field approach continues to be applied to novel materials systems and phenomena, and a growing number of scientists are adopting the technique.

The number of phase field software implementations is proliferating with the growing application of phase field techniques, necessitating a means of benchmarking, validating, and verifying the numerical behavior of a diverse set of codes. Many research domains which apply computational modeling have converged around a small number of standard pieces of software and benchmarking sets (e.g., COMSOL [25] and ABAQUS [26] for engineering simulations, or VASP [27–30], Quantum ESPRESSO [31], and the G3/99 test set [32] for electronic structure calculations[1]), but this is not the case for the phase field community. A multitude of phase field software implementations exist, and numerical approaches abound. Phase field simulations have been performed using open-source codes such as MOOSE [33,34], FEniCS [35,36], OpenPhase [7], DUNE [37,38], FiPy [39,40], as well as with many proprietary codes, such as MICRESS [41,42], PACE 3D [43,44] and other in-house codes. Numerical implementations may employ finite difference, finite volume, finite element, or spectral methods to solve the evolution equations, direct or spectral methods for solid mechanics calculations, explicit or implicit time stepping, and adaptive or non-adaptive meshing. To confidently incorporate quantitative phase field results obtained from this wide variety of numerical methods into ICME, both physical models and numerical implementations must be validated and verified.

A set of standard benchmark problems allows the comparison of models, algorithms, and implementations, as well as the testing of solution accuracy, solver optimizations, and code modifications. While the phase field community ultimately needs validated experimental data sets to compare different models, we focus our effort here on first developing benchmark problems for numerical implementations, which is a necessary precursor for the comparison of model results; a model cannot be validated in a useful way until questions about the correctness of numerical implementations are resolved. The micromagnetics community created benchmark problems in the late 1990s to early 2000s to address a similar situation of multiple implementations and numerical methods [45], and these problems are still evolving today. Benchmark problems significantly aided the community in creating accurate micromagnetics codes [45], such as the Object Oriented MicroMagnetics Framework (OOMMF) [46], MuMax3 [47], and Magpar [48]. To aid in the development, validation, and verification of phase field modeling software, the Center for Hierarchical Design (CHiMaD) and the National Institute of Standards and Technology (NIST) are developing phase field benchmark problems. These problems are hosted on the NIST website [49] and are freely available. In addition, NIST will also host the solutions to the problems submitted by members of the phase field community so that the results from different implementations may be compared.

Phase field benchmark problems for numerical implementations should exhibit several key features, analogous to those in the micromagnetics benchmark problems. First, the problems should be nontrivial (i.e., not solvable without a computer) and should exhibit differing degrees of computational complexity, yet not require extensive computational resources. Second, simulation outputs must be defined in such a way that results are easily comparable. In addition to snapshots or videos of the evolution of the microstructure itself, the evolution of overall metrics such as the total energy of the system or the volume fraction of each phase should be quantified. Finally, the problems should test a simple, targeted aspect of either the numerical implementation or the physics. For example, simple physics could be used while complicated domain or boundary conditions are tested, or coupled physics could be tested on a simple domain. Numerical aspects that must be challenged include solver algorithms, mesh geometry, boundary conditions, and time integration. Benchmark problems could be especially useful when examining multiphysics coupling, including such behaviors as, e.g., diffusion, linear elasticity, fluid flow, anisotropic interfacial energy, and polarization.

In this paper, we present a first set of community-driven, benchmark problems for numerical implementations of phase field models and the efforts of NIST and CHiMaD to date. This first set of problems focuses on diffusion of a solute and phase separation; the second problem adds a coupled non-conserved order parameter. We discuss our choice of model formulations, parameterizations and initial conditions so that these considerations may be kept in mind while developing additional benchmark problems. Furthermore, we demonstrate the utility of benchmark problems by comparing simulation results obtained using two different time adaptivity algorithms. We also briefly review lessons learned from the first CHiMaD "Hackathon," an event in which different phase field codes within the community were challenged against model problems. Finally, we discuss the development of additional formulations for the future, and encourage community involvement in the entire process of problem design, development, and reporting of results.

2. Model formulations

In phase field models, field variables are evolved using dynamics derived from generalized forces. The field variable is often termed the "order parameter," and we adopt that terminology here.

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[1] Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.