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A Fourier Spectral Moving Mesh Method for the Cahn-Hilliard Equation with Elasticity

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Abstract. In recent years, Fourier spectral methods have emerged as competitive numerical methods for large-scale phase field simulations of microstructures in computational materials sciences. To further improve their effectiveness, we recently developed a new adaptive Fourier-spectral semi-implicit method (AFSIM) for solving the phase field equation by combining an adaptive moving mesh method and the semi-implicit Fourier spectral algorithm. In this paper, we present the application of AFSIM to the Cahn-Hilliard equation with inhomogeneous, anisotropic elasticity. Numerical implementations and test examples in both two and three dimensions are considered with a particular illustration using the well-studied example of mis-fitting particles in a solid as they approach to their equilibrium shapes. It is shown that significant savings in memory and computational time is achieved while accurate solutions are preserved.

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Key words: Phase field, diffuse interface, moving mesh, adaptive mesh, Fourier-spectral method, adaptive spectral method, Cahn-Hilliard equation, elasticity.

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1 Introduction

Phase field method has been extensively applied to modeling microstructure evolution for various materials processes including solidification, solid state phase transformations, grain or phase coarsening, etc. It is an attractive and popular approach since the evolution of different microstructural features can be predicted by means of a single set of equations, and there are no explicit boundary conditions defined at interfaces [2, 10].

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However, full three-dimensional computer simulations using the phase field method are still computationally challenging in both memory and computational time.

Much of the earlier phase field simulations employed numerical algorithms such as the explicit Euler finite difference method, which suffered severe limitations on the simulation time step and system size. More advanced numerical algorithms have been proposed recently. Generally, these algorithms are designed to increase the numerical stability and the accuracy. Implicit or semi-implicit methods are typically required to increase the time step and improve the stability [10, 14]. To achieve high accuracy in space, two types of approaches have been utilized. One is to employ a spectral representation of a continuous spatial profile of a field variable whenever applicable, e.g. using a Fourier series for a periodic system, and the other is the adaptive mesh approach in which dense grid points are used in the interfacial regions where the field variables have large gradients. The Fourier spectral method and its semi-implicit implementation have shown to be particularly efficient for systems in which the morphologies and microstructures are dominated by long-range elastic interactions [10, 11, 42].

Fourier-spectral methods are best defined for a fixed uniformly distributed spatial mesh. On the other hand, recent studies on adaptive meshing techniques have led to significant improvement of the computational efficiency of traditional fixed grid methods in many applications, including phase field modeling [6, 16, 26, 32, 39]. Particular examples of adaptivity include the mesh refinement and coarsening as well as mesh movement, and it is clear that adaptive mesh methods are useful for microstructures with a very small interfacial width compared to the domain size. An interesting question to be answered is how the efficiency of spectral methods can also be improved through adaptivity. Naturally, many approaches may be offered for different applications [3, 4, 18, 27, 28].

Recently, a new adaptive Fourier-spectral semi-implicit method (AFSIM) is developed which takes advantages of both the moving mesh method and the Fourier Spectral Semi-implicit scheme [17, 40]. With periodic boundary conditions, the key ingredients making the new adaptive method highly efficient and different from some traditional ones include the utilization of a varying physical domain cell for the Fourier spectral implementation and the coupling of iterative schemes with semi-implicit time discretization. A comparison of different ways to incorporate the moving mesh strategy was given in [40] along with some preliminary discussion on the application of AFSIM to various phase field models. Detailed implementation of AFSIM for the numerical solution of the Allen-Cahn equation has been presented in [17] which has demonstrated that it is possible to keep the high accuracy using AFSIM with larger time steps and fewer grid points than previous algorithms. Many solid state phase transformations and microstructure involve the solution of the Cahn-Hilliard diffusion equation and the elasticity equation. Furthermore, the elastic modulus is not only generally anisotropic, but also inhomogeneous, i.e. its magnitude and anisotropy depend on composition, and thus are spatially dependent. In these cases, the implementation of AFSIM is significantly more challenging.

The work here continues our earlier discussions and represents the first attempt, as