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Spectral implementation of an adaptive moving mesh method for phase-field equations

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Abstract

Phase-field simulations have been extensively applied to modeling microstructure evolution during various materials processes. However, large-scale simulations of three-dimensional (3D) microstructures are still computationally expensive. Among recent efforts to develop advanced numerical algorithms, the semi-implicit Fourier spectral method is found to be particularly efficient for systems involving long-range interactions as it is able to utilize the fast Fourier transforms (FFT) on uniform grids. In this paper, we report our recent progress in making grid points spatially adaptive in the physical domain via a moving mesh strategy, while maintaining a uniform grid in the computational domain for the spectral implementation. This approach not only provides more accurate treatment at the interfaces requiring higher resolution, but also retains the numerical efficiency of the semi-implicit Fourier spectral method. Numerical examples using the new adaptive moving mesh semi-implicit Fourier spectral method are presented for both two and three space dimensional microstructure simulations, and they are compared with those obtained by other methods. By maintaining a similar accuracy, the proposed method is shown to be far more efficient than the existing methods for microstructures with small ratios of interfacial widths to the domain size.
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1. Introduction

Phase-field method has been applied to modeling mesoscale morphological pattern formation and interface motion for many different materials processes [1]. It describes a microstructure using a set of spatially dependent field variables. The temporal evolution of the field variables is then governed by systems of time-dependent Ginzburg–Landau (TDGL) and Cahn–Hilliard (CH) equations. Numerical solutions to the phase-field

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equations yield the temporal and spatial evolution of the microstructures. However, most of the existing phase-field simulations employ the simple explicit Euler finite-difference scheme which has severe limitations on simulation time and system size. Consequently, a number of efforts have been made to develop and implement more advanced numerical algorithms for solving the phase-field equations. In general, existing algorithms are designed either to increase the numerical stability with respect to time or to achieve higher accuracy in spatial discretization. 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, 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 [2]. The spectral method and its semi-implicit implementation have proved particularly efficient for systems in which the morphologies and microstructures are dominated by long-range elastic interactions [3] while the adaptive mesh method is useful for microstructures with a very small interfacial width compared to the domain size. However, it is a technical challenge to efficiently combine the spectral method with an adaptive mesh. The main objective of this paper is to develop a FFT based spectral implementation of an adaptive mesh method for solving phase-field equations.

To achieve the adaptivity within the framework of Fourier-Spectral Semi-implicit methods, we employ the moving mesh approach while maintaining the same number of Fourier modes instead of using local refinement (either by adding extra grid points or enriching Fourier modes). The main idea of the moving mesh approach is to construct a time-dependent mapping $x(\xi,t)$ from the computational domain Ω_c (parameterized by ξ) to the physical domain Ω_p (parameterized by x), such that the representation $v(\xi,t)=u(x(\xi,t))$ of the physical solution $u(x(\xi,t))$ in the computational domain is "better behaved". The criteria for constructing the mapping are usually expressed as certain variational principles, whose solutions via gradient flow lead to the so-called moving mesh partial differential equations (MMPDEs) [4–9]. Similar domain or coordinate mapping ideas have been also used in [10,11] for the adaptive pseudo spectral approximation of reaction-diffusion and combustion problems. Other works on adaptive spectral methods can also be found in [12,13]. It turns out the semi-implicit Fourier spectral method can also be effectively used to solve the MMPDEs. Taking advantages of both the moving mesh method and the Fourier Spectral Semi-implicit scheme, larger time steps and larger system sizes can be used in phase-field simulations to gain computational efficiency without sacrificing the accuracy. In this paper, we demonstrate the performance of this new approach for the Phase-field equation in both two and three space dimensions for model problems. Similar improvement can also be expected for its application to the phase filed simulations of more realistic and complicated problems.

The rest of the paper is organized as follows: we first review the framework for the MMPDEs, and discuss its Fourier-Spectral implementation, in particular, for the Phase-field equation. We then present numerical simulation results and make comparisons with other existing methods. Some concluding remarks are given in the end.

2. Formulations of moving mesh PDEs and applications to Phase-field equations

We first present the variational formulations of the moving-mesh PDEs, then we discuss the applications to Phase-field equations and their spectral implementation.

2.1. The moving-mesh PDEs

Moving-mesh PDEs can be formulated either on a computational domain [14] or on a physical domain [15]. The former has the advantage of being simple and efficient, though bearing a lesser rigorous derivation. The latter is derived on a more rigorous basis, but the resulting MMPDE is slightly more complicated. More comparisons of the implementation based on the two different approaches are given in [16]. In this paper, we briefly discuss both approaches, although only the second approach, the physical domain variational formulation (PDVF), is implemented in the numerical simulations.

To explain the idea, we first describe the MMPDE in one dimension. Fig. 1 shows the discretization of a function in the physical domain and in the computational domain, respectively. One can achieve the high grid density in the high gradient region in the physical domain (Fig. 1, left) by smoothing the gradient in the computational domain (Fig. 1, right).

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