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First and second order operator splitting methods for the phase field crystal equation

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ABSTRACT

In this paper, we present operator splitting methods for solving the phase field crystal equation which is a model for the microstructural evolution of two-phase systems on atomic length and diffusive time scales. A core idea of the methods is to decompose the original equation into linear and nonlinear subequations, in which the linear subequation has a closed-form solution in the Fourier space. We apply a nonlinear Newton-type iterative method to solve the nonlinear subequation at the implicit time level and thus a considerably large time step can be used. By combining these subequations, we achieve the first- and second-order accuracy in time. We present numerical experiments to show the accuracy and efficiency of the proposed methods.

1. Introduction

Material properties at the meso- and macro-scales are to a large extent controlled by complex microstructures exhibiting topological defects, such as vacancies, grain boundaries, and dislocations. An understanding of formation and evolution of these defects is of great interest, and defects pose significant challenges to modeling and simulation because of the complexity they introduce. Recently, a new model called the phase field crystal (PFC) model for simulating defects has been proposed by Elder et al. [1,2]. This model describes the microstructure of two-phase systems on atomic length scales but on diffusive time scales, leading to significant computational savings compared to molecular dynamics simulations which are limited by atomic length scales and femtosecond time scales. In the PFC model, a phase-field formulation is introduced that accounts for the periodic structure of a crystal lattice through a free energy functional of Swift–Hohenberg type [3]

$$\mathcal{E}(\phi) := \int_{\Omega} \left(\frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}(\Delta\phi)^2 \right) d\mathbf{x}, \tag{1}$$

where $\phi : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ $(d = 1, 2, 3)$ is the density field, ϵ is a positive constant with physical significance, and ∇ and Δ are the gradient and Laplacian operators, respectively. The PFC equation is derived from the energy functional $\mathcal{E}(\phi)$ under the constraint of mass conservation:

$$\frac{\partial\phi}{\partial t} = \nabla \cdot (M(\phi)\nabla\mu), \tag{2}$$

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where $M(\phi) > 0$ is a mobility function and μ is the chemical potential defined as $\mu := \frac{\delta \mathcal{E}}{\delta \phi} = \phi^3 + (1-\epsilon)\phi + 2\Delta\phi + \Delta^2\phi$. $\frac{\delta \mathcal{E}}{\delta \phi}$ denotes the variational derivative of $\mathcal{E}$ with respect to ϕ. We assume that ϕ, $\Delta\phi$, and μ are periodic on Ω. Because (2) is of gradient type, it is easy to see that the energy functional $\mathcal{E}(\phi)$ is non-increasing in time. Taking $M(\phi) = 1$ for convenience, we obtain the PFC equation

$$\frac{\partial \phi}{\partial t} = \Delta(\phi^3 + (1-\epsilon)\phi + 2\Delta\phi + \Delta^2\phi). \tag{3}$$

The PFC equation is a sixth-order nonlinear partial differential equation. It is not easy to get an analytic solution in general, therefore, accurate and efficient numerical algorithms are essential in the computer simulations. Various computational algorithms [1,2,4–8] have been applied to solve the PFC equation numerically. In [1,2], Elder et al. use an explicit Euler method which is known to be unstable for time step Δt above a threshold proportional to $(\Delta x)^6$ where Δx is grid spacing. Thus, the explicit Euler method is computationally expensive to evolve large systems.

In [4], Cheng and Warren propose a method which improves the time step restriction considerably larger by splitting the linear terms into backward and forward pieces while treating the nonlinear term explicitly. In [5], Backofen et al. present a semi-implicit finite element method which is a backward Euler method, whereas the nonlinear term ϕ^3 in the chemical potential μ is linearized via $(\phi^{n+1})^3 \approx 3(\phi^n)^2\phi^{n+1} - 2(\phi^n)^3$. In [6], Hu et al. present first-order one-step and second-order two-step methods where a considerably large time step can be used by computing the nonlinear term at an implicit time level. However, an effective time step becomes smaller than the specified time step, as the authors observed for larger time steps.

We here present accurate and efficient operator splitting methods for solving the PFC equation that are first- and second-order time accurate. Operator splitting schemes have been and continue to be used for many types of evolution equations [9–12]. It is easy to construct a first-order solution $A(t^{n+1})$ of time evolution equation

$$\frac{\partial A}{\partial t} = f_1(A) + f_2(A)$$

by computing

$$A(t^n + \Delta t) \cong \left(\mathcal{S}_1^{\Delta t} \circ \mathcal{S}_2^{\Delta t}\right) A(t^n)$$

where $\mathcal{S}_1^{\Delta t}$ and $\mathcal{S}_2^{\Delta t}$ are the evolution operators for $\frac{\partial A}{\partial t} = f_1(A)$ and $\frac{\partial A}{\partial t} = f_2(A)$, respectively. Then a second-order scheme can be derived simply by symmetrizing the first-order scheme [10]:

$$A(t^n + \Delta t) \cong \left(\mathcal{S}_1^{\Delta t/2} \circ \mathcal{S}_2^{\Delta t} \circ \mathcal{S}_1^{\Delta t/2}\right) A(t^n).$$

A core idea of the proposed methods is to decompose the PFC equation into linear and nonlinear subequations, in which the linear subequation has a closed-form solution in the Fourier space. We apply a nonlinear Newton-type iterative method to solve the nonlinear subequation at the implicit time level and thus a considerably large time step can be used. In particular, we combine a half-time linear solver and a second-order nonlinear solver followed by a final half-time linear solver for a second-order method.

This paper is organized as follows. In Section 2, we propose new operator splitting methods for the PFC equation. Numerical experiments showing the accuracy and efficiency of the proposed methods are presented in Section 3. Finally, conclusions are drawn in Section 4.

2. Operator splitting methods for the phase field crystal equation

We consider the PFC equation (3) in two-dimensional space $\Omega = [0, L_1] \times [0, L_2]$. Let N_1 and N_2 be positive integers, $h_1 = L_1/N_1$ and $h_2 = L_2/N_2$ be uniform grid sizes, and Δt be the time step size. We denote $x_{l_1} = l_1 h_1$ and $y_{l_2} = l_2 h_2$ for $l_1 = 0, 1, \ldots, N_1 - 1$ and $l_2 = 0, 1, \ldots, N_2 - 1$. Let $\phi^n_{l_1 l_2}$ be the approximation of $\phi(x_{l_1}, y_{l_2}, t^n)$, where $t^n = n\Delta t$.

For simplicity of notation, we define the "*linear operator*" $\mathcal{L}^{\Delta t}$ as follows

$$\mathcal{L}^{\Delta t}(\phi(t^n)) := \phi(t^n + \Delta t), \tag{4}$$

where $\phi(t^n + \Delta t)$ is a solution of the linear differential equation

$$\frac{\partial \phi}{\partial t} = (1-\epsilon)\Delta\phi + 2\Delta^2\phi + \Delta^3\phi \tag{5}$$

with an initial condition $\phi(t^n)$. To solve the PFC equation with the periodic boundary condition, we employ the discrete Fourier transform $\widehat{\phi} = \mathcal{F}[\phi]$:

$$\widehat{\phi}_{k_1 k_2} = \sum_{l_1=0}^{N_1-1} \sum_{l_2=0}^{N_2-1} \phi_{l_1 l_2} e^{-i\left(x_{l_1}\xi_{k_1} + y_{l_2}\xi_{k_2}\right)}, \tag{6}$$