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First and second order numerical methods based on a new convex splitting for phase-field crystal equation

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ABSTRACT

The phase-field crystal equation derived from the Swift–Hohenberg energy functional is a sixth order nonlinear equation. We propose numerical methods based on a new convex splitting for the phase-field crystal equation. The first order convex splitting method based on the proposed splitting is unconditionally gradient stable, which means that the discrete energy is non-increasing for any time step. The second order scheme is unconditionally weakly energy stable, which means that the discrete energy is bounded by its initial value for any time step. We prove mass conservation, unique solvability, energy stability, and the order of truncation error for the proposed methods. Numerical experiments are presented to show the accuracy and stability of the proposed splitting methods compared to the existing other splitting methods. Numerical tests indicate that the proposed convex splitting is a good choice for numerical methods of the phase-field crystal equation.

1. Introduction

Phase-field models have emerged as a powerful approach for modeling and predicting mesoscale morphological and microstructural evolution in materials. Many of such models try to minimize an energy functional $\mathcal{E}(\phi)$ associated with a phase field function $\phi(\mathbf{x}, t)$. In general, the phase field equation is modeled by gradient flows for $\mathcal{E}(\phi)$,

$$\frac{\partial \phi}{\partial t} = -\text{grad}\, \mathcal{E}(\phi), \tag{1}$$

where the symbol "grad" denotes the gradient in the sense of the Gâteaux derivative. For example, the Allen–Cahn and Cahn–Hilliard equations are gradient flows of the Ginzburg–Landau free energy [1,2]. It is worth to note that the energy functional $\mathcal{E}(\phi)$ is non-increasing in time since (1) is of gradient type.

The main difficulty developing a numerical method for phase field equations is a severe stability restriction on the time step due to nonlinear terms and high order differential ones. There have been many numerical attempts to overcome the stability restriction. The convex splitting (CS) methods have been revitalized by the work of Eyre [3], which are originally attributed to Elliott and Stuart [4]. Recently, many researchers [5–11] have developed noteworthy schemes by using CS idea where an energy functional $\mathcal{E}(\phi)$ is split into two convex functionals (so called contractive and expansive parts),

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$\mathcal{E}(\phi) = \mathcal{E}^c(\phi) - \mathcal{E}^e(\phi)$. The energy of the first order numerical solution by a convex splitting method monotonically decreases when $\mathcal{E}^c(\phi)$ is numerically treated implicitly and $\mathcal{E}^e(\phi)$ explicitly, i.e.,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = -\text{grad}\, \mathcal{E}^c(\phi^{n+1}) + \text{grad}\, \mathcal{E}^e(\phi^n). \tag{2}$$

The convex splitting methods allusively indicate that we might have many kinds of energy splittings.

The phase-field crystal (PFC) model, which is the main subject of this paper, has been suggested to study the microstructural evolution of two-phase systems on atomic length and diffusive time scales. Elder et al. [12,13] introduce the PFC model to minimize the Swift–Hohenberg free energy functional [14],

$$\mathcal{E}(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 + \frac{1}{2}\phi \left(-\epsilon + (1+\Delta)^2 \right) \phi \right) d\mathbf{x}, \tag{3}$$

where ϕ is the density field and ϵ is a positive bifurcation constant with physical significance. Here, Δ is the Laplacian operator and $(1+\Delta)^2 = 1 + 2\Delta + \Delta^2$. For the interested readers, we refer to [14] for a detailed physical meaning of the functional. In particular, $(1+\Delta)^2$ of free energy is from fitting to an experimental structure factor [13]. The PFC equation arising from $\mathcal{E}(\phi)$ under the constraint of mass conservation can be written as follows:

$$\frac{\partial \phi}{\partial t} = \Delta \mu = \Delta \left(\phi^3 - \epsilon\phi + (1+\Delta)^2 \phi \right), \tag{4}$$

where μ is the chemical potential defined as $\mu = \frac{\delta \mathcal{E}}{\delta \phi}$ and $\frac{\delta}{\delta \phi}$ denotes the variational derivative with respect to ϕ. Since it is originally modeled to produce the periodic states [12], we assume that the density field ϕ is periodic on Ω.

Some researchers try to use a convex splitting method based on the following form of the Swift–Hohenberg energy functional,

$$\mathcal{E}(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 - |\nabla \phi|^2 + \frac{1}{2}(\Delta \phi)^2 \right) d\mathbf{x} \tag{5}$$

which is identical to (3) and can be easily split into two convex functionals,

$$\mathcal{E}^c_{DF}(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 + \frac{1}{2}(\Delta \phi)^2 \right) d\mathbf{x}, \quad \mathcal{E}^e_{DF}(\phi) = \int_\Omega |\nabla \phi|^2 d\mathbf{x}, \tag{6}$$

with $\epsilon \leq 1$. Here, the diffusion (DF) term is used for the expansive part. Wise et al. [5] propose a first order and unconditionally gradient stable scheme based on the convex splitting (6),

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Delta \mu^{n+1}, \tag{7}$$

$$\mu^{n+1} = \left(\phi^{n+1} \right)^3 + (1-\epsilon)\phi^{n+1} + \Delta^2 \phi^{n+1} + 2\Delta \phi^n, \tag{8}$$

which we are going to refer to as $\text{CS}_{DF}(1)$. Hu et al. [6] propose a second order convex splitting method, which is weakly energy stable. The second order method can be written as

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \Delta \mu^{n+\frac{1}{2}}, \tag{9}$$

$$\mu^{n+\frac{1}{2}} = \Lambda \left(\phi^{n+1} \right) + \frac{1-\epsilon}{2} \left(\phi^{n+1} + \phi^n \right) + \frac{1}{2}\Delta^2 \left(\phi^{n+1} + \phi^n \right) + \Delta \left(3\phi^n - \phi^{n-1} \right), \tag{10}$$

where $\Lambda\left(\phi^{n+1}\right) = \frac{1}{4}\left(\phi^{n+1} + \phi^n\right)\left(\left(\phi^{n+1}\right)^2 + \left(\phi^n\right)^2\right)$ and $\phi^{-1} = \phi^0$, which we are going to refer to as $\text{CS}_{DF}(2)$. We can give an account for this method as a multi-step implicit–explicit method [15]. The implicit part is designed with a secant-type difference method like as in [16] and explicit part is from a second order Adams–Bashford method. The secant-type difference is second order accurate and plays an important role for the proof of the energy stability.

In order to solve the PFC equation accurately and efficiently, we propose new numerical methods based on the following convex splitting

$$\mathcal{E}^c_{BF}(\phi) = \int_\Omega \left(\Psi_c(\phi) + \frac{1}{2}\phi \left(1+\Delta\right)^2 \phi \right) d\mathbf{x}, \quad \mathcal{E}^e_{BF}(\phi) = \int_\Omega \Psi_e(\phi) d\mathbf{x}, \tag{11}$$

where $\Psi_c(\phi) = \frac{1}{4}\phi^4$ and $\Psi_e(\phi) = \frac{\epsilon}{2}\phi^2$. Note that (11) has a different form to (6) but it is closely related to the original form (3). Here, the bifurcation (BF) term is used for the expansive part. We can easily show that (11) is a convex splitting and the detailed proof is presented in Appendix A.