NUMERICAL METHODS FOR PHASE-FIELD CRYSTAL EQUATION USING A NEW CONVEX SPLITTING

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ABSTRACT

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.

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 $E(\phi)$ associated with a phase field function $\phi(x, t)$. In general, the phase field equation is modeled by gradient flows for $E(\phi)$,

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

where the symbol “grad” denotes the gradient in the sense of the Gâteaux derivative. It is worth to note that $E(\phi)$ is non-increasing in time since (1) is of gradient type. The convex splitting (CS) methods have been revitalized by the work of Eyre [1], which are originally attributed to Elliott and Stuart [2]. The energy of numerical solution by the first order convex splitting method monotonically decreases when $E^c(\phi)$ is numerically treated implicitly and $E^e(\phi)$ explicitly, i.e.,

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

where $E(\phi)$ is split into two convex functionals, $E(\phi) = E^c(\phi) - E^e(\phi)$.

The phase-field crystal (PFC) model has been suggested to study the microstructural evolution of two-phase systems on atomic length and diffusive time scales. Elder et al. [5,6] introduce the PFC model to minimize the Swift–Hohenberg free energy functional [7],

$$E(\phi) = \int_{\Omega} \left( \frac{1}{4} \phi^4 + \frac{1}{2} \phi \left( -\epsilon + (1 + \Delta)^2 \right) \phi \right) \, dx,$$  \hspace{1cm} (3)

where $\phi$ is the density field and $\epsilon$ is a positive bifurcation constant with physical significance. For the interested readers, we refer [7] for a detailed physical meaning of the functional. In
particular, \((1 + \Delta)^2\) of free energy is from fitting to an experimental structure factor [6]. The PFC equation arising from \(\mathcal{E}(\phi)\) under the constraint of mass conservation can be written as follows:

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

(4)

where \(\mu\) is the chemical potential defined as \(\mu = \frac{\delta \mathcal{E}}{\delta \phi}\) and \(\frac{\delta \mathcal{E}}{\delta \phi}\) denotes the variational derivative with respect to \(\phi\). Since it is originally modeled to produce the periodic states [5], we assume that the density field \(\phi\) is periodic on \(\Omega\).

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

\[
\mathcal{E}_{DF}^c(\phi) = \int_{\Omega} \left( \frac{1}{4} \phi^4 + \frac{1 - \epsilon}{2} \phi^2 + \frac{1}{2} (\Delta \phi)^2 \right) d\mathbf{x}, \quad \mathcal{E}_{DF}^e(\phi) = \int_{\Omega} |\nabla \phi|^2 d\mathbf{x},
\]

(5)

with \(\epsilon \leq 1\). Here, the diffusion (DF) term is used for the expansive part. Wise et al. [3] propose a first order and unconditionally gradient stable scheme based on the convex splitting (5). Hu et al. [4] propose a second order convex splitting method, which is weakly energy stable.

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

\[
\mathcal{E}_{BF}^c(\phi) = \int_{\Omega} \left( \frac{1}{4} \phi^4 + \frac{1}{2} \phi (1 + \Delta)^2 \phi \right) d\mathbf{x}, \quad \mathcal{E}_{BF}^e(\phi) = \int_{\Omega} \epsilon \phi^2 d\mathbf{x}.
\]

(6)

Here, the bifurcation (BF) term is used for the expansive part. The proposed energy splitting is also applicable to the frameworks of first and second order convex splitting methods [3,4]. Applying these frameworks, we propose the first and second order convex splitting methods and completely prove mass conservation, unique solvability, energy stability, and the order of truncation error for the proposed methods. Moreover, we try to numerically demonstrate that (6) is a good choice in the convex splitting strategy for accurate numerical methods.

REFERENCES