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Convex Splitting Runge–Kutta methods for phase-field models

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ABSTRACT

In this paper, we present the Convex Splitting Runge–Kutta (CSRK) methods which provide a simple unified framework to solve phase-field models such as the Allen–Cahn, Cahn–Hilliard, and phase-field crystal equations. The core idea of the CSRK methods is the combination of convex splitting methods and multi-stage implicit–explicit Runge–Kutta methods. Our CSRK methods are high-order accurate in time and we investigate the energy stability numerically. We present numerical experiments to show the accuracy and efficiency of the proposed methods up to the third-order accuracy.

1. Introduction

Phase-field models have emerged as a powerful computational approach for modeling and predicting mesoscale morphological and microstructure evolution in materials. The most popular models are the Allen–Cahn (AC) [1] and Cahn–Hilliard (CH) [2] equations with non-conserved or conserved order parameters ϕ that vary continuously over thin interfacial layers and are mostly uniform in the bulk phases [3]. The equations are derived from the Ginzburg–Landau free energy:

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

where Ω is a domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$, $\Psi(\phi)$ is the bulk free energy with two minima corresponding to the two phases, and $\epsilon > 0$ is a parameter related to the interfacial thickness. The AC and CH equations are the gradient flow for (1) under the L^2 and H^{-1} inner product, respectively. The equations have previously been applied to a wide range of physical problems [4].

The most significant difficulties in solving phase-field models are their nonlinear and high-order derivative terms, since they cause a severe restriction on the time step size for stability. In order to overcome this problem, the authors in [5,6] proposed the first-order convex splitting method. In the method, $\mathcal{E}(\phi)$ is split appropriately into a contractive part and an expansive part:

$$\mathcal{E}(\phi) = \int_{\Omega} \left(\Psi_c(\phi) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x} - \int_{\Omega} \Psi_e(\phi)\, d\mathbf{x} = \mathcal{E}_c(\phi) - \mathcal{E}_e(\phi), \tag{2}$$

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where both $\mathcal{E}_c(\phi)$ and $\mathcal{E}_e(\phi)$ are convex. Also, $\mathcal{E}_c(\phi)$ is treated implicitly, whereas $\mathcal{E}_e(\phi)$ is treated explicitly. The first-order method has been proven to be unconditionally energy stable, which means that $\mathcal{E}(\phi)$ is non-increasing in time for any time step. Since the method is only first-order accurate in time, a number of second-order methods have been proposed considering the energy stability. For example, the schemes in [7–9] are based on the convex splitting and multi-step discretization and the schemes in [10,11] are based on the Crank–Nicolson type scheme with convex splitting and stabilization. Many other attempts have also been made to achieve high-order accuracy without using a convex splitting scheme [12–19]. However, only a limited number of high-order methods guarantee energy stability [18].

In this paper, we present the Convex Splitting Runge–Kutta (CSRK) methods in order to provide a simple unified framework to solve phase-field models with high-order time accuracy. The core idea of the methods is to couple convex splitting methods described in Section 2 with the multi-stage implicit–explicit Runge–Kutta (IMEX-RK) methods described in Section 3. In Section 4.1, it is numerically shown that the convexity of splitting is crucial to ensure the energy stability of the CSRK methods. We investigate the order of accuracy and stability of the CSRK methods depending on the IMEX-RK tables described in Sections 4.2 and 4.3. In Section 5, we numerically demonstrate the order of accuracy with typical spinodal decomposition examples. We also simulate further complex examples to show the applicability and feasibility of the proposed method. Finally, conclusions are drawn in Section 6. We briefly introduce the derivation of order conditions in Appendix A and provide some specific examples in Appendix B. It is worth to note that spectral methods similar to those in [16,9] are used for spatial discretization in our numerical computations.

2. First-order convex splitting method

Phase-field models such as the AC and CH equations are characterized by a bulk free energy $\Psi(\phi)$ and an interfacial energy $\frac{\epsilon^2}{2}|\nabla\phi|^2$. Time discretization methods have to deal with the nonlinear term $\Psi'(\phi)$ which yields a severe stability restriction on the time step. This stability issue has motivated a large number of studies in which schemes are developed that are provably energy stable.

In this section, we briefly review the convex splitting method, which is a successful attempt to overcome the stability restriction. For simplicity, we consider the AC or CH equation as follows:

$$\frac{\partial\phi}{\partial t} = \mathcal{L}\left(\Psi'(\phi) - \epsilon^2\Delta\phi\right), \tag{3}$$

where $\mathcal{L} = -1$ for AC or $\mathcal{L} = \Delta$ for CH. With the energy splitting (2), the first-order convex splitting method is

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \mathcal{L}\left(\Psi_c'(\phi^{n+1}) - \epsilon^2\Delta\phi^{n+1} - \Psi_e'(\phi^n)\right). \tag{4}$$

Considering a typical polynomial energy $\Psi(\phi) = \frac{1}{4}(\phi^2-1)^2$, nonlinear convex splitting can be given as follows:

$$\Psi_c(\phi) = \frac{1}{4}\phi^4 + \frac{1}{4}, \qquad \Psi_e(\phi) = \frac{1}{2}\phi^2. \tag{5}$$

Applying the nonlinear convex splitting (5), we have

$$\frac{\phi^{n+1}-\phi^n}{\Delta t} = \mathcal{L}\left(\left(\phi^{n+1}\right)^3 - \epsilon^2\Delta\phi^{n+1} - \phi^n\right). \tag{6}$$

In order to treat the nonlinearity of ϕ^3, we consider a Newton-type iterative method. Using the mth Newton's iteration $\phi^{n,m}$ of ϕ^{n+1}, we linearize the nonlinear term $\left(\phi^{n+1}\right)^3$ as follows,

$$\left(\phi^{n+1}\right)^3 \approx \left(\phi^{n,m}\right)^3 + 3\left(\phi^{n,m}\right)^2\left(\phi^{n+1}-\phi^{n,m}\right) \tag{7}$$

for $m = 0, 1, \ldots$. We then get

$$\frac{\phi^{n,m+1}-\phi^n}{\Delta t} = \mathcal{L}\left(3\left(\phi^{n,m}\right)^2\phi^{n,m+1} - 2\left(\phi^{n,m}\right)^3 - \epsilon^2\Delta\phi^{n,m+1} - \phi^n\right) \tag{8}$$

with an initial estimate $\phi^{n,0} = \phi^n$. We then set $\phi^{n+1} = \phi^{n,m+1}$ if a relative l_2-norm of the consecutive error $\frac{\left\|\phi^{n,m+1}-\phi^{n,m}\right\|}{\|\phi^{n,m}\|}$ is less than a given tolerance *tol*.

The nonlinear convex splitting (5) preserves the convexity of $\Psi_c(\phi)$ and $\Psi_e(\phi)$, regardless of the value of ϕ, whereas the splitting is computationally expensive due to the nonlinear iterative steps. Fig. 1 shows the number of m-iterations averaged over the simulation times $T_f = 156.25$ and $T_f = 156.25\cdot\epsilon^2$ as a function of Δt and $\Delta\tau = \Delta t/\epsilon^2$ for the AC and CH equations with zero Neumann boundary condition, respectively. Here, an initial condition on a domain $\Omega = [0, 1]$ is $\phi(x, 0) = 0.001\cdot\text{rand}(x)$, where rand$(x)$ is a random number between -1 and 1, and $\epsilon = 0.01$, $\Delta x = 1/128$, $\Delta t = T_f/2^{12}, T_f/2^{11}, \ldots, T_f/2^3$, and $tol = 10^{-10}$.