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A second order operator splitting method for Allen–Cahn type equations with nonlinear source terms

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HIGHLIGHTS

- The proposed operator splitting method is second order accurate and stable.
- The method can be easily applicable to wide class of Allen–Cahn type equations with non-linear source terms.
- Simulations for multi-component phase separation and dendrite growth show the feasibility of the method.

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ABSTRACT

Allen–Cahn (AC) type equations with nonlinear source terms have been applied to a wide range of problems, for example, the vector-valued AC equation for phase separation and the phase-field equation for dendritic crystal growth. In contrast to the well developed first and second order methods for the AC equation, not many second order methods are suggested for the AC type equations with nonlinear source terms due to the difficulties in dealing with the nonlinear source term numerically. In this paper, we propose a simple and stable second order operator splitting method. A core idea of the method is to decompose the original equation into three subequations with the free-energy evolution term, the heat evolution term, and a nonlinear source term, respectively. It is important to combine these three subequations in proper order to achieve the second order accuracy and stability. We propose a method with a half-time free-energy evolution solver, a half-time heat evolution solver, a full-time midpoint solver for the nonlinear source term, and a half-time heat evolution solver followed by a final half-time free-energy evolution solver. We numerically demonstrate the second order accuracy of the new numerical method through the simulations of the phase separation and the dendritic crystal growth.

1. Introduction

The Allen–Cahn (AC) equation was originally introduced as a phenomenological model for antiphase domain coarsening in a binary alloy [1]. The AC equation arises from minimization of the Ginzburg–Landau free energy

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

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where Ω is a domain in $\mathbb{R}^d$ ($d = 1, 2, 3$). The quantity $\phi(\mathbf{x}, t)$ is defined as the difference between the concentrations of the two components in a mixture (e.g., $\phi(\mathbf{x}, t) = (m_\alpha - m_\beta)/(m_\alpha + m_\beta)$, where m_α and m_β are the masses of phases α and β). The function $F(\phi) = 0.25(\phi^2 - 1)^2$ is the Helmholtz free-energy density for ϕ, which has a double-well form, and $\epsilon > 0$ is the gradient energy coefficient. The AC equation is the L^2-gradient flow of the free energy $\mathcal{E}(\phi)$:

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

where the symbol "grad" denotes the gradient in the sense of the Gâteaux derivative. Let the domain of the functional $\mathcal{E}$ be $\mathcal{D} = \{\phi \in H^2(\Omega) \mid \frac{\partial \phi}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega\}$. For any $\phi,\ \psi \in \mathcal{D}$, we have

$$\begin{aligned}(\text{grad}\, \mathcal{E}(\phi), \psi)_{L^2} &= \frac{\mathrm{d}}{\mathrm{d}\theta} \mathcal{E}(\phi + \theta\psi)\Big|_{\theta=0} = \lim_{\theta \to 0} \frac{1}{\theta}\big(\mathcal{E}(\phi + \theta\psi) - \mathcal{E}(\phi)\big) \\ &= \int_\Omega \left(\frac{F'(\phi)}{\epsilon^2} - \Delta\phi\right) \psi \,\mathrm{d}\mathbf{x} = \left(\frac{F'(\phi)}{\epsilon^2} - \Delta\phi, \psi\right)_{L^2}.\end{aligned}$$

See Ref. [2] for details of the notation and the derivation of the formula. We identify $\text{grad}\, \mathcal{E}(\phi) \equiv F'(\phi)/\epsilon^2 - \Delta\phi$, then Eq. (1) becomes the AC equation

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \underbrace{-\frac{1}{\epsilon^2} F'(\phi(\mathbf{x}, t))}_{\text{Free-energy evolution}} + \underbrace{\Delta\phi(\mathbf{x}, t)}_{\text{Heat evolution}}, \quad \mathbf{x} \in \Omega,\ 0 < t \le T. \tag{2}$$

The main difficulty when developing a numerical method for solving Eq. (2) is that the free-energy evolution term $F'(\phi)$ yields a severe stability restriction on the time step. In order to deal with this restriction, Eyre [3,4] proposed a semi-implicit method, which is first order accurate in time and unconditionally gradient stable, and Eyre's method was used to solve Eq. (2) in Ref. [5]. Many researchers employed first and second order stabilized semi-implicit methods for solving Eq. (2) [6–9], in which the heat evolution term $\Delta\phi$ is treated implicitly and the free-energy evolution term $F'(\phi)$ is treated explicitly to avoid the expensive process of solving nonlinear equations at each time step with an extra stabilizing term added to alleviate the stability constraint while maintaining accuracy and simplicity.

Alternative methods implemented for the AC equation are first and second order operator splitting methods [8,10,11], which become the base of our proposed method for more general form of AC type equations. Operator splitting schemes have been and continue to be used for many types of evolution equations [12–14]. 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 $A(t^n + \Delta t) \approx \left(\mathcal{S}_1^{\Delta t} \mathcal{S}_2^{\Delta t}\right) A(t^n)$ where $\mathcal{S}_1^{\Delta t}$ and $\mathcal{S}_2^{\Delta t}$ are the solution 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:

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

The basic idea of the operator splitting methods for AC equation is to decompose the original equation into heat and free-energy evolution subequations at each time step, in which the free-energy evolution subequation has a closed-form solution. The first and the second order operator splitting methods in Refs. [8,10,11] are unconditionally stable thanks to the unconditional stability of each substep. The derivation and numerical properties of the higher order operator splitting method for AC equation will appear in Ref. [15].

Our main concern in this paper is the AC type equations with a nonlinear source term in the form of

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \underbrace{-\frac{1}{\epsilon^2} F'(\phi(\mathbf{x}, t))}_{\text{Free-energy evolution}} + \underbrace{\Delta\phi(\mathbf{x}, t)}_{\text{Heat evolution}} + \underbrace{S(\phi(\mathbf{x}, t))}_{\text{Nonlinear source}}. \tag{3}$$

This type of equations have been applied to a wide range of problems such as phase transitions [1], crystal growth [16–19], grain growth [20–24], image analysis [25–28], motion by mean curvature [29–33], two-phase fluid flows [34], and vesicle membranes [35,36]. Since available analytical solutions for these equations are limited, numerical methods are important tools for understanding dynamics of the equations. In contrast to the well developed first and second order methods for the AC equation, only first order methods are suggested for the AC type equations with nonlinear source terms due to the difficulties in dealing with the nonlinear source term numerically [17,19,21,23,25–28,35,37,38].

In this paper, we propose a second order operator splitting method for solving the AC type equations with nonlinear source terms. Our method is a generalization of the second order operator schemes for three subequations with the free-energy evolution term, the heat evolution term, and a nonlinear source term, respectively. It is important to combine these