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High-order and mass conservative methods for the conservative Allen–Cahn equation

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ABSTRACT

The conservative Allen–Cahn (AC) equation has been studied analytically and numerically. Our mathematical analysis and numerical experiment, however, show that previous numerical methods are not second-order accurate in time and/or do not conserve the initial mass. The aim of this paper is to propose high-order and mass conservative methods for solving the conservative AC equation. In the methods, we discretize the conservative AC equation by using a Fourier spectral method in space and first-, second-, and third-order implicit–explicit Runge–Kutta schemes in time. We show that the methods inherit the mass conservation. Numerical experiments are presented demonstrating the accuracy and efficiency of proposed methods.

1. Introduction

The Allen–Cahn (AC) equation was originally introduced as a phenomenological model for antiphase domain coarsening in a binary alloy [1]:

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta\phi(\mathbf{x},t), \quad \mathbf{x} \in \Omega,\ 0 < t \le T, \tag{1}$$

where Ω is a domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$. Let $\phi(\mathbf{x},t) = (m_\alpha - m_\beta)/(m_\alpha + m_\beta)$ be the difference between the concentrations of the two components in a mixture, where m_α and m_β are the masses of phases α and β. The function $F(\phi) = 0.25(1-\phi^2)^2$ 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 and its various modified forms have been applied to a wide range of problems, such as phase transitions [1], image segmentation and image inpainting [2–4], motion by mean curvature [5–11], two-phase fluid flows [12], crystal growth [13,14], and grain growth [15–19].

Since the classical AC equation (1) does not conserve the initial volume, Rubinstein and Sternberg [20] added a Lagrange multiplier $\beta(t)$ to Eq. (1) in order to impose the conservation of volume:

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta\phi(\mathbf{x},t) + \beta(t), \tag{2}$$

where $\beta(t) = \int_\Omega F'(\phi(\mathbf{x},t))d\mathbf{x}/(\epsilon^2 \int_\Omega d\mathbf{x})$. This equation has been studied analytically and numerically [12,21–29]. However, it has a drawback of maintaining small geometric features since the Lagrange multiplier is only dependent on t.

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Recently, Brassel and Bretin [30] introduced the following conservative AC equation and they observed that it has better volume-preserving properties than Eq. (2) (Eq. (3) shows an $O(\epsilon^2)$ error for the conservation of volume, whereas Eq. (2) shows an $O(\epsilon)$ error):

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta\phi(\mathbf{x},t) + \beta(t)\sqrt{F(\phi(\mathbf{x},t))}, \tag{3}$$

where $\beta(t) = \int_\Omega F'(\phi(\mathbf{x},t))d\mathbf{x}/(\epsilon^2 \int_\Omega \sqrt{F(\phi(\mathbf{x},t))}d\mathbf{x})$.

Kim et al. [31] proposed a practically unconditionally stable hybrid scheme for solving Eq. (3). The method conserves the initial mass exactly, but is only first-order accurate in time. Zhai et al. [32,33] proposed several methods, including Crank–Nicolson and operator splitting, for solving Eq. (3) and its fractional-in-space version. However, these methods are not second-order accurate in time and/or do not conserve the initial mass (we will discuss this in more detail in Section 2). To the best of our knowledge, there is no method which can achieve high-order time accuracy and keep the mass conservation. The aim of this paper is to propose high-order and mass conservative methods for solving Eq. (3). In the methods, we discretize Eq. (3) by using a Fourier spectral method in space and first-, second-, and third-order implicit–explicit (IMEX) Runge–Kutta schemes [34] in time. We show that the methods inherit the mass conservation.

This paper is organized as follows. In Section 2, we review previous numerical methods for solving Eq. (3). In Section 3, we construct high-order and mass conservative methods for solving Eq. (3). Numerical experiments showing the accuracy and efficiency of proposed methods are presented in Section 4. Finally, conclusions are drawn in Section 5.

2. Review on previous numerical methods

In this section, we review previous numerical methods for solving the conservative AC equation (3). For simplicity and clarity of exposition, we consider Eq. (3) in one-dimensional space $\Omega = (0, L)$ with a homogeneous Neumann boundary condition:

$$\frac{\partial \phi(x,t)}{\partial t} = -\frac{F'(\phi(x,t))}{\epsilon^2} + \frac{\partial^2 \phi(x,t)}{\partial x^2} + \beta(t)\sqrt{F(\phi(x,t))}, \tag{4}$$

where $\beta(t) = \int_\Omega F'(\phi(x,t))dx/(\epsilon^2 \int_\Omega \sqrt{F(\phi(x,t))}dx)$. Let M be a positive integer, $h = L/M$ be the space step size, and Δt be the time step size. Let ϕ_m^n be an approximation of $\phi(x_m, t^n)$, where $x_m = (m - 1/2)h$ for $m = 1, \ldots, M$ and $t^n = n\Delta t$. The discrete cosine transform and its inverse transform are

$$\widehat{\phi}_k = \omega_k \sum_{m=1}^{M} \phi_m \cos(x_m \xi_k) \tag{5}$$

and

$$\phi_m = \sum_{k=1}^{M} \omega_k \widehat{\phi}_k \cos(x_m \xi_k), \tag{6}$$

where $\omega_1 = 1/\sqrt{M}$, $\omega_k = \sqrt{2/M}$ for $2 \le k \le M$, and $\xi_k = \pi(k-1)/L$.

Zhai et al. [32] proposed Crank–Nicolson (CN) method and operator splitting (OS) method to achieve second-order time accuracy. However, these methods have drawbacks. It is well-known that the CN method is second-order accurate in time, but the authors observed that the CN method cannot keep the mass conservation and, for the OS method, the authors split Eq. (4) into three subequations as follows:

$$\frac{\partial \phi(x,t)}{\partial t} = \frac{\partial^2 \phi(x,t)}{\partial x^2}, \tag{7}$$

$$\frac{\partial \phi(x,t)}{\partial t} = -\frac{F'(\phi(x,t))}{\epsilon^2}, \tag{8}$$

$$\frac{\partial \phi(x,t)}{\partial t} = \beta(t)\sqrt{F(\phi(x,t))}. \tag{9}$$

Eq. (7) was solved using the CN method

$$\frac{\phi_m^{(1)} - \phi_m^n}{\Delta t} = \frac{1}{2}\left(\frac{\partial^2 \phi_m^{(1)}}{\partial x^2} + \frac{\partial^2 \phi_m^n}{\partial x^2}\right), \quad \text{i.e., } \phi_m^{(1)} = \mathcal{C}^{-1}\left[\frac{1 - \frac{\Delta t}{2}\xi_k^2}{1 + \frac{\Delta t}{2}\xi_k^2}\mathcal{C}[\phi_m^n]\right], \tag{10}$$

where $\mathcal{C}$ denotes the discrete cosine transform and $\mathcal{C}^{-1}$ its inverse transform. Eq. (8) can be solved analytically in the physical space and the solution $\phi_m^{(2)}$ is given as follows [35,36]:

$$\phi_m^{(2)} = \frac{\phi_m^{(1)}}{\sqrt{e^{\frac{-2\Delta t}{\epsilon^2}} + \left(\phi_m^{(1)}\right)^2 \left(1 - e^{\frac{-2\Delta t}{\epsilon^2}}\right)}}. \tag{11}$$