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A conservative Allen–Cahn equation with a space–time dependent Lagrange multiplier

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ABSTRACT

We present a new numerical scheme for solving a conservative Allen–Cahn equation with a space–time dependent Lagrange multiplier. Since the well-known classical Allen–Cahn equation does not have mass conservation property, Rubinstein and Sternberg introduced a nonlocal Allen–Cahn equation with a time dependent Lagrange multiplier to enforce conservation of mass. However, with their model it is difficult to keep small features since they dissolve into the bulk region. One of the reasons for this is that mass conservation is realized by a global correction using the time-dependent Lagrange multiplier. To resolve the problem, we use a space–time dependent Lagrange multiplier to preserve the volume of the system and propose a practically unconditionally stable hybrid scheme to solve the model. The numerical results indicate a potential usefulness of our proposed numerical scheme for accurately calculating geometric features of interfaces.

1. Introduction

The Allen–Cahn (AC) equation (Allen & Cahn, 1979) was introduced originally as a phenomenological model for antiphase domain coarsening in a binary alloy:

$$\frac{\partial \phi}{\partial t}(\mathbf{x},t) = -M\left(\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} - \Delta\phi(\mathbf{x},t)\right), \quad \mathbf{x}\in\Omega, \quad t>0, \tag{1}$$

$$\mathbf{n}\cdot\nabla\phi(\mathbf{x},t) = 0, \quad \mathbf{x}\in\partial\Omega. \tag{2}$$

Here Ω, t, M, and $\mathbf{n}$ denote a bounded domain, time, a positive kinetic coefficient, and the unit outer normal vector on the domain boundary, respectively. $F(\phi) = 0.5\phi^2(1-\phi)^2$ is a double-well potential and ϵ is the gradient energy coefficient related to the interfacial energy. The quantity $\phi(\mathbf{x},t)\in[0,1]$ is an order parameter, which is one of the concentrations of the two components in a binary mixture. For example, $\phi = 1$ in the one phase and $\phi = 0$ in the other phase. The interface between two phases is defined by $\Gamma = \{\mathbf{x}\in\Omega|\phi(\mathbf{x},t) = 0.5\}$. Allen and Cahn (1979) also showed that the normal velocity v on a single closed interface Γ is governed by its mean curvature

$$v(\mathbf{x},t) = \kappa(\mathbf{x},t), \quad \mathbf{x}\in\Gamma, \tag{3}$$

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where $\kappa(\mathbf{x},t)$ is the mean curvature of the interface Γ. This dynamical property has been studied in Ma, Jiang, and Xiang (2009), Brassel and Bretin (2011), Ren and Wei (2009), Ward and Wetton (2001). Fig. 1(a) and (b) show the temporal evolutions of curves with the classical AC and the conservative AC equations in two dimensions, respectively. The dashed lines are the initial curves and the solid lines are the evolutions of interfaces. The directions of evolutions are indicated by arrows. We observe that the classical AC does not conserve its initial mass, whereas the conservative AC equation does. We can check that the AC type dynamics does not preserve the volume fractions, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \phi\,\mathrm{d}\mathbf{x} = \int_\Omega \phi_t\,\mathrm{d}\mathbf{x} = \int_\Omega M\left(-\frac{F'(\phi)}{\epsilon^2}+\Delta\phi\right)\mathrm{d}\mathbf{x} = -\int_\Omega \frac{MF'(\phi)}{\epsilon^2}\,\mathrm{d}\mathbf{x} + \int_{\partial\Omega} M\mathbf{n}\cdot\nabla\phi\,\mathrm{d}s = -\int_\Omega \frac{MF'(\phi)}{\epsilon^2}\,\mathrm{d}\mathbf{x},$$

which is not always zero. Here, we set $M = 1$ for simplicity. To preserve the volume, Rubinstein and Sternberg (1992) introduced a Lagrange multiplier $\beta(t)$ into the AC model

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

Here $\beta(t)$ must satisfy $\beta(t) = \int_\Omega F'(\phi(\mathbf{x},t))\,\mathrm{d}\mathbf{x}/(\epsilon^2\int_\Omega\,\mathrm{d}\mathbf{x})$ to keep the mass conservation, and this formulation has been widely used (Bates & Jin, 2013; Yang, Feng, Liu, & Shen, 2006; Zhang & Tang, 2007). The normal velocity v on a single closed interface Γ is given by the volume-preserving mean curvature flow:

$$v(\mathbf{x},t) = \kappa(\mathbf{x},t) - \frac{1}{|\Gamma|}\int_\Gamma \kappa\,\mathrm{d}s, \quad \mathbf{x}\in\Gamma, \tag{5}$$

where $|\Gamma|$ is the total curve length in two-dimensional space and the total area in three-dimensional space. Rubinstein and Sternberg's model has been studied analytically and numerically (Beneš, Yazaki, & Kimura, 2011; Brassel & Bretin, 2011; Bronsard & Stoth, 1997; Ward, 1996; Xia, Xu, & Shu, 2009; Yue, Zhou, & Feng, 2007;). However, it has a drawback on preserving small features since the Lagrange multiplier is only a function of time variable. For example, there is a critical radius of drop which eventually disappears below the radius. This phenomenon is observed in the frame of the Cahn–Hilliard model (Yue et al., 2007).

The main purpose of this article is to propose a practically unconditionally stable numerical scheme for the conservative AC equation with a space–time dependent Lagrange multiplier. The scheme is based on the recently developed hybrid scheme for the AC equation (Li, Lee, Jeong, & Kim, 2010) with an exact mass-conserving update at each time step.

The paper is organized as follows. In Section 2, we present the conservative AC equation with a space–time dependent Lagrange multiplier. A numerical algorithm using an operator splitting method is described in Section 3. Several numerical results demonstrating the accuracy and robustness of the proposed scheme are described in Section 4. Conclusions are made in Section 5.

2. Conservative Allen–Cahn equation

The authors in Brassel and Bretin (2011) proposed the following conservative AC equation which guarantees to preserve small geometric features:

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta\phi(\mathbf{x},t) + \beta(t)\sqrt{2F(\phi(\mathbf{x},t))}, \tag{6}$$

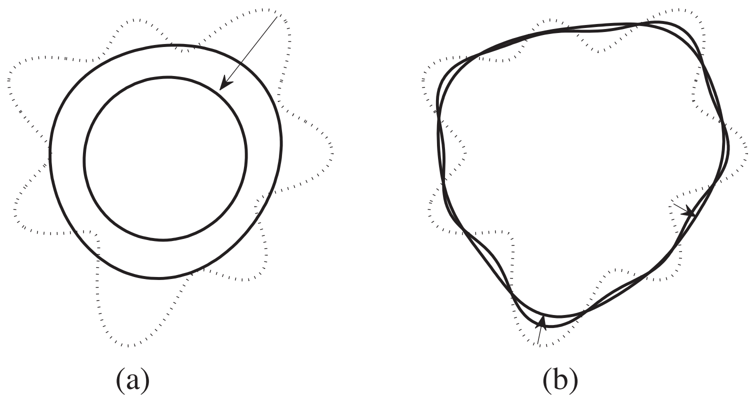

Fig. 1. Temporal evolutions of arbitrary curves with (a) the AC equation and (b) the conservative AC equation. The dashed lines are the initial curves and directions of evolutions are indicated by arrows.