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A finite difference method for a conservative Allen–Cahn equation on non-flat surfaces

Junseok Kim, Darae Jeong, Seong-Deog Yang, Yongho Choi *

Department of Mathematics, Korea University, Seoul 02841, Republic of Korea

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ABSTRACT

We present an efficient numerical scheme for the conservative Allen–Cahn (CAC) equation on various surfaces embedded in a narrow band domain in the three-dimensional space. We apply a quasi-Neumann boundary condition on the narrow band domain boundary using the closest point method. This boundary treatment allows us to use the standard Cartesian Laplacian operator instead of the Laplace–Beltrami operator. We apply a hybrid operator splitting method for solving the CAC equation. First, we use an explicit Euler method to solve the diffusion term. Second, we solve the nonlinear term by using a closed-form solution. Third, we apply a space–time-dependent Lagrange multiplier to conserve the total quantity. The overall scheme is explicit in time and does not need iterative steps; therefore, it is fast. A series of numerical experiments demonstrate the accuracy and efficiency of the proposed hybrid scheme.

1. Introduction

The Allen–Cahn (AC) equation is a second-order nonlinear parabolic partial differential equation, which was originally proposed by Allen and Cahn [1] to describe the phase separation in binary alloys. The classical AC equation is

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

The AC equation has been used to model many phenomena such as crystal growth [2,3], image inpainting [4,5], image segmentation [6,7], and tumor growth [8] on flat surfaces. Moreover, it has been studied on non-flat surfaces [9]. Although the conservative Allen–Cahn (CAC) equation has been solved and studied on flat surfaces [10–13], to the best of authors' knowledge, there is no research work that has attempted to solve this equation on non-flat surfaces.

Therefore, the main purpose of this study is to develop a fast and computationally efficient finite difference method for the CAC equation on non-flat surfaces in three-dimensional space. The problem for partial differential equations on the surfaces has been studied in various fields such as image processing [14,15] and biological modeling [15–17]. Therefore, solving the CAC equation on surfaces is an important issues, both in the geometrical and numerical sense. We employ a hybrid explicit numerical method, which is based on an operator splitting method and we solve the resulting discrete

* Corresponding author.
E-mail addresses: cfdkim@korea.ac.kr (J. Kim), poohyongho@korea.ac.kr (Y. Choi).
URL: http://math.korea.ac.kr/~cfdkim/ (J. Kim).

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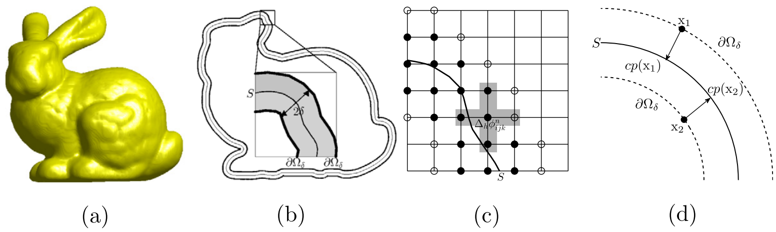

Fig. 1. (a) Bunny surface, (b) slice data of the band domain, (c) part of the bunny's ear in (b), definition of the Laplacian using the points on the shaded region, (d) closest points $cp(\mathbf{x}_1)$ and $cp(\mathbf{x}_2)$ for boundary points $\mathbf{x}_1$ and $\mathbf{x}_2$.

equations on a narrow band domain. We use the idea of the closest point method [18] to define the boundary condition. The numerical results demonstrated that the proposed algorithm is accurate and efficient.

The rest of the paper is structured as follows. In Section 2, we describe the governing equation, i.e., the CAC equation on a narrow band domain. In Section 3, we provide the numerical scheme and algorithm. We present the various numerical results in Section 4. Finally, in Section 5, we provide the conclusion.

2. The conservative Allen–Cahn equation

In this section, we describe the CAC equation [13]

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

where $\phi(\mathbf{x},t)$ is the order parameter, $\sqrt{F(\phi)} = 0.5|\phi^2 - 1|$, ϵ is the thickness of the transition layer, and β is the Lagrange multiplier used for conserving the total mass. Let S be a smooth surface in $\mathbb{R}^3$ and Ω_δ be a neighborhood of S which is defined as $\Omega_\delta = \{\mathbf{y}|\mathbf{x} \in S, \mathbf{y} = \mathbf{x} + \theta\mathbf{n}(\mathbf{x})$ for $|\theta| < \delta\}$ where $\mathbf{n}$ is a unit normal vector on surface S and δ is a positive constant.

We describe how to find the boundary points by using the closest point method. In the numerical simulation section, we will show a test that solves the CAC equation on the bunny. We will explain how to define the Laplacian and boundary condition by using that example. To help the reader understand the idea, we will explain how the algorithm works in two-dimensional space. Fig. 1(a) shows the surface of the bunny, and we define surface S, boundary $\partial\Omega_\delta$, band width 2δ, and band domain Ω_δ, which is denoted by the shaded region in Fig. 1(b). When we calculate $\Delta_h \phi^n_{ijk}$, the boundary values at the empty circles shown in Fig. 1(c) are needed. For each point $\mathbf{x} \in \partial\Omega_\delta$, using a trilinear interpolation, we define the closest point function $\text{cp} : \partial\Omega_\delta \to S$, which assigns the value of the closest point $\text{cp}(\mathbf{x},t)$, as shown in Fig. 1(d). Therefore, we define the boundary condition as

$$\phi(\mathbf{x},t) = \phi(\text{cp}(\mathbf{x}),t) \quad \text{on } \partial\Omega_\delta. \tag{3}$$

In the next section, we describe how to solve the CAC equation on the narrow band domain.

3. Numerical solution

In this section, we represent the numerical schemes for the CAC equation on the narrow band domain, Ω_δ. The CAC equation is discretized on the three-dimensional domain $\Omega = (a,b) \times (c,d) \times (e,f)$. The uniform spatial step size is $h = (b-a)/N_x = (d-c)/N_y = (f-e)/N_z$, where N_x, N_y, and N_z are the number of cells in the x-, y-, and z-directions, respectively. Discrete domain Ω^h is defined as $\Omega^h = \{\mathbf{x}_{ijk} = (x_i, y_j, z_k) = (a+hi, c+hj, e+hk) \big| 0 \le i \le N_x,\ 0 \le j \le N_y,\ 0 \le k \le N_z\}$, and $\Omega^h_\delta = \{\mathbf{x}_{ijk} \big| |\psi_{ijk}(\mathbf{x}_{ijk})| < \delta\}$ is the discrete narrow band domain, where ψ is a signed distance function. The narrow band domain must contain the stencil as in Fig. 1(c); therefore, we should take $\delta \ge \sqrt{3}h$. Let the boundary points be defined as $\partial\Omega^h_\delta = \{\mathbf{x}_{ijk} \big| I_{ijk}|\nabla_h I_{ijk}| \ne 0\}$, where $\nabla_h I_{ijk} = (I_{i+1,jk} - I_{i-1,jk}, I_{i,j+1,k} - I_{i,j-1,k}, I_{ij,k+1} - I_{ij,k-1})/(2h)$. Here, $I_{ijk} = 0$ if $\mathbf{x}_{ijk} \in \Omega^h_\delta$; otherwise, $I_{ijk} = 1$.

Let ϕ^n_{ijk} be the approximations of $\phi(\mathbf{x}_{ijk}, n\Delta t)$, where $\Delta t = T/N_t$ is the time step, T is the final time, and N_t is the total number of time steps. In Ω^h_δ, we define a discrete L^2-norm error as $\|\phi\|_{L^2} = \sqrt{\frac{1}{\#\Omega^h_\delta}\sum_{\mathbf{x}_{ijk}\in\Omega^h_\delta} \phi^2_{ijk}}$, where $\#\Omega^h_\delta$ is the number of points on the band. We consider the discretization of the CAC Eq. (2). First, we solve the AC equation which is obtained by using an operator splitting method. We solve the diffusion term on the narrow band domain Ω^h_δ by using an explicit Euler method with the boundary condition $\phi^n_{ijk} = \phi^n(\text{cp}(\mathbf{x}_{ijk}))$ on $\partial\Omega^h_\delta$:

$$\frac{\phi^*_{ijk} - \phi^n_{ijk}}{\Delta t} = \Delta_h \phi^n_{ijk}. \tag{4}$$

Here, we use the standard Laplacian $\Delta_h \phi_{ijk} = (\phi_{i+1,jk} + \phi_{i-1,jk} + \phi_{i,j+1,k} + \phi_{i,j-1,k} + \phi_{ij,k+1} + \phi_{ij,k-1} - 6\phi_{ijk})/h^2$.