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Explicit Hybrid Numerical Method for the Allen-Cahn Type Equations on Curved Surfaces

Yongho Choi[1], Yibao Li[2], Chaeyoung Lee[3], Hyundong Kim[3] and Junseok Kim[3,*]

[1] *Department of Mathematics and Big Data, Daegu University, Gyeongsan-si, Gyeongsangbuk-do 38453, Republic of Korea*
[2] *School of Mathematics and Statistics, Xi'an Jiaotong University, Xi'an 710049, China*
[3] *Department of Mathematics, Korea University, Seoul 02841, Republic of Korea*

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Abstract. We present a simple and fast explicit hybrid numerical scheme for the motion by mean curvature on curved surfaces in three-dimensional (3D) space. We numerically solve the Allen-Cahn (AC) and conservative Allen-Cahn (CAC) equations on a triangular surface mesh. We use the operator splitting method and an explicit hybrid numerical method. For the AC equation, we solve the diffusion term using a discrete Laplace-Beltrami operator on the triangular surface mesh and solve the reaction term using the closed-form solution, which is obtained using the separation of variables. Next, for the CAC equation, we additionally solve the time-space dependent Lagrange multiplier using an explicit scheme. Our numerical scheme is computationally fast and efficient because we use an explicit hybrid numerical scheme. We perform various numerical experiments to demonstrate the robustness and efficiency of the proposed scheme.

AMS subject classifications: 65M06, 65Z05, 68U20

Key words: Allen-Cahn equation, conservative Allen-Cahn equation, Laplace-Beltrami operator, triangular surface mesh, hybrid numerical method, PDE on surface.

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1. Introduction

The Allen-Cahn (AC) equation was first proposed by Allen and Cahn in 1979 [1] as a mathematical model for antiphase domain coarsening in Fe-Al alloys

*Corresponding author.
Email addresses: `yongho_choi@daegu.ac.kr` (Y. Choi), `cfdkim@korea.ac.kr` (J.S. Kim)

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta \phi(\mathbf{x},t), \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{1.1}$$

where $F(\phi) = 0.25(\phi^2 - 1)^2$ and ϵ is the gradient energy coefficient. Here, ϕ is the difference between the concentrations, i.e., $\phi = c_A - c_B$, where c_A and c_B are the mass fractions of components A and B in binary alloys. Therefore, the range of ϕ is $-1 \le \phi \le 1$. It is well known that the AC equation has a property that does not conserve the total mass. The $F(\phi)$ is Ginzburg-Landau double-well potential energy function with minimum values at -1 and 1 [12].

For the motion by mean curvature with conservation of area, the conservative AC (CAC) equation [4, 16] was proposed using the Lagrange multiplier, which depends on not only time but also space, and is given by

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta \phi(\mathbf{x},t) + \beta(t)\sqrt{F(\phi(\mathbf{x},t))}, \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{1.2}$$

where $\Omega \subset \mathbb{R}^d$ is a domain, ϕ is the order parameter, $\sqrt{F(\phi)} = 0.5|\phi^2 - 1|$, ϵ is a constant related to the interfacial thickness, and $\beta(t)$ is given by

$$\beta(t) = \frac{\int_\Omega F'(\phi(\mathbf{x},t))d\mathbf{x}}{\epsilon^2 \sqrt{\int_\Omega F(\phi(\mathbf{x},t))d\mathbf{x}}}. \tag{1.3}$$

It is well known that the non-standard time-space dependent Lagrange multiplier $\beta(t)\sqrt{F(\phi(\mathbf{x},t))}$ has a better area-preserving property than the standard time-only dependent Lagrange multiplier. Further explanation of its derivation can be found in [4].

In this study, we present a simple explicit hybrid numerical scheme for the AC type equations on curved surfaces in 3D space. First, let us consider the surface AC equation [31]

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = -\frac{F'(\phi(\mathbf{x},t))}{\epsilon^2} + \Delta_{\mathcal{S}} \phi(\mathbf{x},t), \quad \mathbf{x} \in \mathcal{S}, \quad t > 0, \tag{1.4}$$

where $\mathcal{S}$ is a surface in $\mathbb{R}^3$. Here, $\Delta_{\mathcal{S}} = \nabla_{\mathcal{S}} \cdot \nabla_{\mathcal{S}}$ is the Laplace-Beltrami operator on $\mathcal{S}$ and $\nabla_{\mathcal{S}}$ is the surface gradient. One of the definitions of surface gradient uses a smooth extension [21]. Let $\mathcal{N}$ be a narrow embedding band around $\mathcal{S}$, i.e., $\mathcal{S} \subset \mathcal{N}$. Let $\phi_E : \mathcal{N} \to \mathbb{R}$ be a smooth extension of $\phi : \mathcal{S} \to \mathbb{R}$. Then, the surface gradient is defined as

$$\nabla_{\mathcal{S}} \phi := \nabla \phi_E - \frac{\nabla \psi}{|\nabla \psi|} \left(\frac{\nabla \psi}{|\nabla \psi|} \right)^T \nabla \phi_E, \tag{1.5}$$

where ψ is a function on $\mathcal{N}$ such that $\mathcal{S} = \{\mathbf{x} \in \mathcal{N} \,|\, \psi(\mathbf{x}) = 0\}$. Here, the gradient is a column vector. More details about the Laplace-Beltrami operator can be found in [21, 31]. The surface AC equation is a gradient flow in $L^2(\mathcal{S})$ for the total energy functional

$$\mathcal{E}(\phi) = \int_{\mathcal{S}} \left(\frac{F(\phi)}{\epsilon^2} + \frac{|\nabla_{\mathcal{S}} \phi|^2}{2} \right) dA. \tag{1.6}$$