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Efficient energy stable schemes for isotropic and strongly anisotropic Cahn–Hilliard systems with the Willmore regularization

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ABSTRACT

We develop efficient energy stable numerical methods for solving isotropic and strongly anisotropic Cahn–Hilliard systems with the Willmore regularization. The scheme, which involves adaptive mesh refinement and a nonlinear multigrid finite difference method, is constructed based on a convex splitting approach. We prove that, for the isotropic Cahn–Hilliard system with the Willmore regularization, the total free energy of the system is non-increasing for any time step and mesh sizes. A straightforward modification of the scheme is then used to solve the regularized strongly anisotropic Cahn–Hilliard system, and it is numerically verified that the discrete energy of the anisotropic system is also non-increasing, and can be efficiently solved by using the modified stable method. We present numerical results in both two and three dimensions that are in good agreement with those in earlier work on the topics. Numerical simulations are presented to demonstrate the accuracy and efficiency of the proposed methods.

1. Introduction

Phase field methods have been widely used to study the dynamics of different material phases via order parameters, such as phase transformations in binary alloys, e.g., [22,19,20]; epitaxial thin film growth, e.g., [15,44,26,35,34,46]; crystal faceting, e.g., [36,27,28,7]; multiphase fluid flow, e.g., [23,2,3,12]; and solid tumor growth, e.g., [43,42,13,11], just to name a few. The methods are capable of describing the evolution of complex, morphology-changing surfaces and can provide a general framework to consider more physical effects. The well-studied second order Allen–Cahn [1] and fourth order Cahn–Hilliard models [8] are sub-classes of phase field models, which are of interest in materials science.

Crystalline anisotropy is a critical contributing factor to the equilibria and dynamic macroscopic shapes of heterogeneous materials. In the absence of anisotropy, the microscopic shape is rotationally symmetric. Anisotropy breaks this symmetry as certain directions are endowed with higher energy. For sufficiently strong anisotropy, the double-well surface density function may become negative. At equilibrium, the system responds by removing these orientations (termed

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missing orientations) in the shape of the crystal (Wulff shape) driven by minimizing the total surface energy of the system. As a result, the equilibrium interface is no longer a smooth curve, but presents sharp corners or facets with slope discontinuities [33]. In three dimensions, the onset of missing orientations occurs at a convex-to-concave transition in a polar plot of the reciprocal of the surface free energy (γ) [29], which is equivalent to show that the normal to the $1/\gamma$-plot is proportional to the ξ vector in [9]. The anisotropic phase field model becomes ill-posed when the gradient energy is non-convex, which is equivalent with the sign change of the surface stiffness [33,41]. To overcome ill-posedness and loss of smoothness of the anisotropic Cahn–Hilliard model, a higher order derivative regularization is added to the surface energy [14,6]. For example, a Laplacian-squared regularization is used in [41,10], and a nonlinear Willmore regularization is considered in [35,10,27,28]. Recently, some theoretical studies of the regularized Cahn–Hilliard equation have been conducted. For instance, well-posedness for the isotropic Cahn–Hilliard equation with Willmore regularization was shown in [25], and the proof of existence and uniqueness of the solution to the strongly anisotropic Cahn–Hilliard equation with Willmore regularization was obtained in [24]. For both regularizations, the resulting Cahn–Hilliard-type equations are sixth order in space, which bring significant challenges in the development of efficient and accurate numerical schemes.

Eggleston et al. [16] used a convexification technique for the strongly anisotropic Cahn–Hilliard system and performed one-sided difference approximation to treat the corners to maintain the stability of the numerical method. The simulation results showed excellent agreement with sharp interface equilibrium shapes. However, the use of explicit time discretization leaded to severe time step restrictions. Torabi et al. [35] implemented finite difference in space and a Crank–Nicholson scheme to discretize in time. Recently, a stabilized time discretization and spectral discretization in space were used to solve the regularized anisotropic Cahn–Hilliard equation in [10]. This scheme is unconditionally energy stable.

As a first step towards the development of a scheme for the anisotropic system, we first develop an energy stable time discretization scheme based on a convex splitting approach for the isotropic Cahn–Hilliard–Willmore system, and prove that it is unconditionally energy stable. For the spatial discretization, we use centered finite difference method with a dynamic, block-structured Cartesian mesh refinement. An adaptive nonlinear multigrid method is used to solve the resulting nonlinear system at each time step [41,43,42,13]. We note that the convex splitting we use here is different from that used in [18] which was intended for the functionalized Cahn–Hilliard equation but can also be used for the isotropic Cahn–Hilliard–Willmore equation. However, we encountered difficulty in implementing the nonlinear multigrid method using the scheme in [18] for the isotropic Cahn–Hilliard–Willmore equation.

We then extend this scheme to the strongly anisotropic Cahn–Hilliard system with the Willmore regularization. We present numerical results in 2D and 3D to show that the scheme is still energy stable with arbitrary time steps, although we are not able to prove this analytically.

This paper is organized as follows. In Section 2, we describe the isotropic Cahn–Hilliard and strongly anisotropic Cahn–Hilliard systems with the Willmore regularization. In Section 3, we proposed energy stable numerical methods based on a convex splitting approach for solving the model systems. Two and three dimensional numerical simulations and a summary are presented in Section 4.

2. Diffuse interface anisotropy

Here, we consider a boundary domain $\Omega \subset \mathbb{R}^d$ with $d = 2, 3$. Let $\phi : \Omega \to \mathbb{R}$ be an order parameter; $\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|}$ is the unit normal vector, and $\mathbf{P} = \mathbf{I} - \mathbf{n} \otimes \mathbf{n}$, where $\mathbf{I}$ is the identity matrix. We consider an anisotropic surface energy [35] as

$$E(\phi) = \int_\Omega \frac{\gamma(\mathbf{n})}{\epsilon}\Big(f(\phi) + \frac{\epsilon^2}{2}|\nabla\phi|^2\Big)d\mathbf{x}, \tag{1}$$

where ϵ is a small parameter that measures the thickness of the interface transition layer, $f(\phi) = \frac{1}{4}\phi^2(1-\phi)^2$ is a double well potential, $\gamma(\mathbf{n})$ is an interfacial energy function describing the property of the anisotropy. Note that the interface thickness is independent of orientation. This is a natural formulation if we interpret the term $\frac{1}{\epsilon}(f(\phi) + \frac{\epsilon^2}{2}|\nabla\phi|^2)$ as the approximation of the surface delta function. The corresponding evolution equations are as follows:

$$\frac{\partial\phi}{\partial t} = \frac{1}{\epsilon}\nabla\cdot(M(\phi)\nabla\mu), \tag{2}$$

$$\mu = \frac{1}{\epsilon}(\gamma(\mathbf{n})f'(\phi) - \epsilon^2\nabla\cdot\mathbf{m}), \tag{3}$$

with

$$\mathbf{m} = \gamma(\mathbf{n})\nabla\phi + \mathbf{P}\nabla_n\gamma(\mathbf{n})\Big(\frac{f(\phi)}{\epsilon^2|\nabla\phi|} + \frac{1}{2}|\nabla\phi|\Big). \tag{4}$$

Following [35], we use the asymptotic result that near interface $f(\phi) \sim (\epsilon^2/2)|\nabla\phi|^2$, to yield the approximation

$$\mathbf{m} \sim \gamma(\mathbf{n})\nabla\phi + |\nabla\phi|\mathbf{P}\nabla_n\gamma(\mathbf{n}). \tag{5}$$