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Efficient Energy Stable Schemes with Spectral Discretization in Space for Anisotropic Cahn-Hilliard Systems

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Abstract. We develop in this paper efficient and robust numerical methods for solving anisotropic Cahn-Hilliard systems. We construct energy stable schemes for the time discretization of the highly nonlinear anisotropic Cahn-Hilliard systems by using a stabilization technique. At each time step, these schemes lead to a sequence of linear coupled elliptic equations with constant coefficients that can be efficiently solved by using a spectral-Galerkin method. We present numerical results that are consistent with earlier work on this topic, and also carry out various simulations, such as the linear bi-Laplacian regularization and the nonlinear Willmore regularization, to demonstrate the efficiency and robustness of the new schemes.

AMS subject classifications: 65N35, 65M12, 35K55

Key words: Spectral-Galerkin, phase-field, anisotropic, Cahn-Hilliard, stabilization, coupled elliptic equations.

1 Introduction

The phase-field method has been frequently used in the study of the dynamics of heterogeneous materials, such as crystal growth, phase separations in binary mixtures, and multi-phase fluid flows. Its ubiquitous advantage over the sharp-interface approach is that there is no need to track the interface explicitly. Usual phase-field approaches often lead to a second-order Allen-Cahn equations [1] or a fourth-order Cahn-Hilliard equation [3]. It is usually more challenging to solve the Cahn-Hilliard equation than the Allen-Cahn equation due to its high-order nature and its stiffness caused by small parameters in the physical system.

We consider in this paper a classical problem in materials science, namely, determining the equilibrium shape of a solid crystal in its own liquid matrix. When anisotropy

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of the micro-mechanical system is sufficiently strong, the surface energy function, $f(\phi)$, may become too large or singular on certain orientations. Thus, these orientations may be missing in the equilibrium shape (or Wulff shape) in order to achieve a well-defined energy for the system. Consequently, the equilibrium interface will not be a smooth curve, but present facets and corners with slope discontinuities (cf. [17]). Fundamentally, the gradient energy density loses its convexity (see a proof in the Appendix of [20]) when the so-called 'surface stiffness' changes its sign (cf. [10] for the sharp interface approach on the same topic). In this case, the corresponding Cahn-Hilliard equation is intrinsically of a backward parabolic type. Thus it is an ill-posed problem and requires regularizations. The linear bi-Laplacian regularization and the nonlinear Willmore regularization (cf. [6, 7, 11]) will be considered in this paper. While the former is easier to deal with numerically, its asymptotic results does not match the correct physics. The latter is more physically consistent, with sharp corners of the Wulff shape replaced by rounded corners while major parts of edges remains unchanged, but its free energy is also much more complicated. Both regularizations lead to a sixth-order Cahn-Hilliard type equations which present significant challenges for developing efficient and accurate numerical schemes. There are two main difficulties: (i) the presence of a small parameter ϵ, representing the interfacial width, which makes the (time continuous) discretized system very stiff; and (ii) the high-order spatial derivatives, which make the spatially discretized system very difficult to solve.

In [8], the authors used a second-order central difference discretization in space for solving the anisotropic Cahn-Hilliard equation. A convexification technique was employed so that the regularization was not needed. However, it used an explicit time discretization, resulting in severe time step restrictions. In the recent work [18, 20], the authors solved the regularized anisotropic Cahn-Hilliard system with an adaptive nonlinear multigrid finite difference method.

We propose to solve the regularized anisotropic Cahn-Hilliard systems with a stabilized time discretization that allows large time steps and a spectral discretization in space. Unlike in [18,20], our numerical schemes do not lead to a nonlinear system at each time step, instead, only a system of three coupled linear elliptic equations with constant coefficients that can be efficiently solved by a suitable spectral method.

The paper is organized as follows: in Section 2, we describe the governing PDE system for the anisotropic crystal growth. The main idea of the paper is given in Section 3, where we propose our time discretizations and spectral methods for the system. Numerical tests and simulations are given in Section 4. We conclude with a few remarks in the last section.

2 Phase-field models for anisotropic systems

Let $\Omega \subset \mathbb{R}^d$ ($d = 2,3$), and $\phi(\mathbf{x})$ be an order parameter that takes the values ± 1 in the two phases with a smooth transitional layer of thickness ϵ. We consider the following free