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Efficient and Energy Stable Scheme for an Anisotropic Phase-field Dendritic Crystal Growth Model Using the Scalar Auxiliary Variable (SAV) Approach

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Dedicated to Professor Jie Shen on the Occasion of his 60th Birthday

Abstract. The phase-field dendritic crystal growth model is a highly nonlinear system that couples the anisotropic Allen-Cahn type equation and the heat equation. By combining the recently developed SAV (Scalar Auxiliary Variable) method with the linear stabilization approach, as well as a special decoupling technique, we arrive at a totally decoupled, linear, and unconditionally energy stable scheme for solving the dendritic model. We prove its unconditional energy stability rigorously and present various numerical simulations to demonstrate the stability and accuracy.

AMS subject classifications: 65M12, 65M70, 65Z05

Key words: Phase-field, dendritic, stabilized-SAV method, anisotropy, Allen-Cahn, decoupled.

1 Introduction

The use of the phase-field method for investigating the process of dendritic crystal growth can be attributed to the pioneering modeling work by Halperin, Kobayashi, and Collins et. al. in [1–3], and see also the subsequent modeling/simulations in [4–15]. In a typical phase-field dendritic crystal system, an order parameter (called phase-field variable) is usually introduced to define the physical state (liquid or solid) at each point and the total free energy incorporates a specific form of the conformational entropy with anisotropic spatial gradients. The system usually consists of two coupled nonlinear, second-order equations: the Allen-Cahn type equation with a gradient-dependent anisotropic coefficient, and the heat transfer equation.

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In this paper, we consider numerical approximations for a phase-field dendritic crystal growth model which was proposed by Karma and Rappel in [12]. It is well known that the main objective of algorithm design for phase-field related models is to construct efficient and easy-to-implement numerical schemes that can verify a discrete energy law. For the particular dendritic model proposed in [12], the associated difficulties to this aim lie on how to discretize three nonlinear terms, including the anisotropic coefficient, the cubic polynomial term, as well as the heat transfer term. Simple explicit treatment for these nonlinear terms will induce large spatial oscillations that may cause the computations easily blow up or loss of accuracy (shown in Figure 2, Figure 4, and Figure 5(b)).

We recall there exist plenty of time discretization methods that had been proved to be effective for solving the phase field models, see [15–38]. However, for this particular model considered in this paper, most of the available schemes are either nonlinear which need some efficient iterative solvers, and/or do not preserve energy stability at all (cf. [7, 39–44] and the references therein). Therefore, in this paper, by combining the recently developed SAV (Scalar Auxiliary Variable) method with the linear stabilization approach, as well as a special decoupling technique, we arrive at a fully-decoupled, stabilized-SAV scheme. The novelty of this scheme is that two linear stabilization terms are added in the SAV scheme, where one is used to remove the oscillations caused by the anisotropic coefficient, and the other is added to the latent heat transfer term in order to realize the decoupling. At each time step, one can only solve an elliptic system for the phase function, and a linear elliptic equation for the temperature. We then prove that the unconditionally energy stability of the scheme and present numerous numerical examples to illustrate its accuracy and stability numerically.

The rest of the paper is organized as follows. In Section 2, we give a brief introduction of the governing PDE system for the phase-field anisotropic dendritic crystal growth model. In Section 3, we develop the scheme for solving the model, and rigorously prove the unconditional energy stability. Various numerical experiments are given in Section 4 to demonstrate the accuracy and efficiency of the proposed numerical scheme. Finally, some concluding remarks are given in Section 5.

2 Model equations

We give a brief description of the anisotropic phase-field dendritic crystal growth model proposed in [12]. Let Ω be a smooth, open, bounded, connected domain in $\mathbb{R}^d$ with $d=2,3$. A scalar phase-field function $\phi(\boldsymbol{x},t)$ is introduced to label the liquid and solid phase, where $\phi=1$ for the solid and $\phi=-1$ for the fluid. These two regions are connected by a smooth transitional layer with the thickness ϵ. The total free energy is postulated as follows,

$$E(\phi,T)=\int_\Omega\Big(\frac{1}{2}|\kappa(\nabla\phi)\nabla\phi|^2+\frac{\lambda}{2\epsilon K}T^2+\frac{1}{4\epsilon^2}F(\phi)\Big)d\boldsymbol{x}, \tag{2.1}$$