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Linear, first and second-order, unconditionally energy stable numerical schemes for the phase field model of homopolymer blends

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ABSTRACT

In this paper, we develop a series of efficient numerical schemes to solve the phase field model for homopolymer blends. The governing system is derived from the energetic variational approach of a total free energy, that consists of a nonlinear logarithmic Flory–Huggins potential, and a gradient entropy with a concentration-dependent de-Gennes type coefficient. The main challenging issue to solve this kind of models numerically is about the time marching problem, i.e., how to develop suitable temporal discretizations for the nonlinear terms in order to preserve the energy stability at the discrete level. We solve this issue in this paper, by developing the first and second order temporal approximation schemes based on the "Invariant Energy Quadratization" method, where all nonlinear terms are treated semi-explicitly. Consequently, the resulting numerical schemes lead to a symmetric positive definite linear system to be solved at each time step. The unconditional energy stabilities are further proved. Various numerical simulations of 2D and 3D are presented to demonstrate the stability and the accuracy of the proposed schemes.

1. Introduction

In this paper, we aim to develop some efficient and effective numerical schemes to solve a phase field model for homopolymer blends (PF-HB) (cf. [1,4,6,9]). The evolution PDE system is resulted from the energetic variation of the action functional of the total free energy in the H^{-1} Sobolev space, i.e., the Cahn–Hilliard (CH) equation. The total free energy consists of a logarithmic Flory–Huggins (F–H) type potential, and a gradient entropy with a concentration-dependent de-Gennes type coefficient [9], that is quite similar to the classical CH system [4], in which the free energy consists of the Ginzburg–Landau double well potential, and the gradient entropy with the constant coefficient. This PF-HB model is also referred as the Cahn–Hilliard–Cook model, or the Stochastic-Cahn–Hilliard equation when the PDE system is equipped with an imposed external thermal noise (stochastic term, or called as Cook-noise [6]).

It is well known that the CH system is one of typical systems of the phase field model with a long history dated back to one century ago (cf. the classical literatures of Rayleigh [30] and Van der Waals [33]). Due to the energetic variational approach applied in the modeling procedure, the exact solutions to the phase field model lead to a decreasing-in-time energy functional. A significant goal in the numerical simulation of the model is the development of algorithms that can

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verify this property at the discrete level irrespectively of the coarseness of the discretization (in what follows, algorithms of this type will be called unconditionally energy stable or thermodynamically consistent). The unconditionally energy stable scheme is not only critical to capture the correct long time dynamics of the coarse-graining (macroscopic) process, but also can provide flexibility for dealing with stiffness issues. We also remark that the "unconditional" here means the schemes have no constraints for the time step, however, large time step size will definitely induce large errors in practice.

The main challenging issue to solve a variety of phase field models numerically is about the time marching problem, i.e., to design suitable approaches to discretize the nonlinear terms while preserving the energy stability. For the classical CH equation, the only nonlinear term is the cubic polynomial term that is induced from the double well potential. The popular numerical techniques to discretize such terms mainly include the nonlinear convex splitting approach and the linear stabilization approach (cf. [13,15,20,25,28,31,38] and the references therein). However, the PF-HB model is far more complicated than the classical CH equation since the system has very special nonlinear complexities, where one is the gradient entropy that is accompanied with a non-constant coefficient, and the other is the logarithmic type bulk potential. To the best of the author's knowledge, there does not exist any numerical scheme with provable unconditional energy stabilities for the PF-HB model so far. Moreover, we emphasize that the two prevalent methods mentioned above are actually not applicable for the PF-HB model (cf. the detailed discussions in section 3).

Therefore, in this paper, in order to develop efficient, unconditionally energy stable numerical schemes to solve the PF-HB model, instead of designing special linear stabilizers or constructing convex–concave combinations for nonlinear functionals, we adopt the so-called *Invariant Energy Quadratization* (IEQ) method, which is a novel approach and had been successfully applied for the polynomial type potentials for other phase field models in the author's work (cf. [19,35,37]). The essential idea of the IEQ method is to transform the free energy into a quadratic form (since the nonlinear potential is usually bounded from below) of a set of new variables via a change of variables. The new, equivalent system still retains the similar energy dissipation law in terms of the new variables. For the time-continuous case, the energy law of the new reformulated system is equivalent to the energy law of the original system. One great advantage of such a reformulation is that all nonlinear terms can be treated semi-explicitly accordingly, which in turn produces a linear system. Moreover, the resulted linear operator of the system is symmetric positive definite, thus it can be solved by many available efficient linear solvers, e.g., CG, GMRES, or other Krylov subspace methods.

Based on this new approach, we develop some efficient schemes which are *accurate* (ready for second or even higher order in time), *easy-to-implement* (linear), and *unconditionally energy stable* (with a discrete energy dissipation law) to solve the PF-HB model numerically. We rigorously prove the unconditionally energy stabilities for proposed schemes, including the first order backward Euler, the second order Adam–Bashforth, the second order Crank–Nicolson schemes. Through various classical benchmark 2D and 3D simulations, we demonstrate the stability and the accuracy of the proposed schemes as well. To the best of the author's knowledge, the proposed schemes are the first linear and unconditionally energy stable schemes for the PF-HB model.

The rest of the paper is organized as follows. In Section 2, we present the whole model and give the PDE energy law. In Section 3, we develop the numerical schemes and prove the well-posedness of the linear system, as well as the unconditional energy stabilities. In Section 4, we present various 2D and 3D numerical simulations to validate our numerical schemes. Finally, some concluding remarks are presented in Section 5.

2. Model equations

We now give a brief introduction to the PF-HB model that considers a symmetric homopolymer blend consisting of molecules of type I and II. The average volume fraction of the I-component in the system is ϕ_0. The state of the system is described by the local volume fraction of the component I, $\phi(\boldsymbol{x}, t)$, at all points $\boldsymbol{x} \in \Omega^d, d = 2, 3$ and at time t. The phenomenological mesoscopic dynamic equation that relates a temporal change of $\phi(\boldsymbol{x}, t)$ to a local current of the I component, $J_I(\boldsymbol{x})$, is governed by the following PF-HB equation (cf. [1,4,9]):

$$\phi_t = -\nabla \cdot J_I(\boldsymbol{x}). \tag{2.1}$$

The transport in the system (2.1) follows the difference of the chemical potential. Here, we assume a linear relation between the local current and the gradient of the local chemical potential difference $\rho(\boldsymbol{x}, t)$ [2]. Thus, the flux J_I is given by

$$J_I(\boldsymbol{x}, t) = -\lambda \nabla \rho(\boldsymbol{x}, t), \tag{2.2}$$

where λ is the Onsager mobility coefficient, and the local chemical potential difference $\rho(x, t)$ is the functional derivative of a coarse-grained free energy functional $\mathbb{E}(\phi)$, i.e.,

$$\rho(x, t) = \frac{\delta \mathbb{E}(\phi)}{\delta \phi}, \tag{2.3}$$

with

$$\mathbb{E}(\phi) = \int_{\Omega} \Big(\frac{\nu \alpha^2}{36} \kappa(\phi) |\nabla \phi|^2 + \mathbb{F}(\phi) \Big) d\boldsymbol{x}, \tag{2.4}$$