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Unconditional Energy Stable Runge-Kutta Schemes for a Phase Field Model for Diblock Copolymers

Lizhen Chen and Bo Ren*

Beijing Computational Science Research Center, Beijing 100193, P.R. China.

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Abstract. A high-accuracy and unconditional energy stable numerical scheme for a phase field model for diblock copolymers (PF-BCP model) is developed. The PF-BCP model is reformulated into an equivalent model, which based on scaler auxiliary variable (SAV) formulation. After that a stable Runge-Kutta (RK) method and a Fourier-spectral method are applied to the SAV-reformulated PF-BCP model to discretize on the temporal and spatial dimensions respectively. The fully discretized numerical scheme is computed by fixed-point iterations. Meanwhile, the unconditional energy decay property is proved rigorously. Finally, we present the results of numerical experiments to show the accuracy and efficiency of the RK scheme used and discuss the influence of physical parameters and initial conditions on the phase separation in the simulation of the PF-BCP model. In addition, the energy decay property of the numerical solutions is verified.

AMS subject classifications: 65M10, 78A48

Key words: Phase field model, diblock copolymer, auxiliary variable method, Runge-Kutta method.

1. Introduction

The diblock copolymer model (DC model) is the system for a copolymer composed of two different monomers blocks A and B. The copolymer is formed by a linear-chain molecule of sub-chains of two different monomers blocks linked together at molecular scale characterized by fluid-like disorder. Due to incompatibility between two monomer blocks, they repulse each other, then tend to separate from mixture into pure blocks with free interfaces' occurring and deforming between two blocks. Finally, periodic structure is formed in diblock copolymer such as lamellar or cylindrical structures, which illustrates specific nano-materials.

To describe a complex system with fluid-like disorder composed of multiple components with free interfaces between them, we encounter challenges in matching boundary conditions on the interfaces in the Lagrangian framework. As a solution, the system is described

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[*] Corresponding author. *Email addresses:* `lzchen@csrc.ac.cn` (L. Chen), `renbo_mech@csrc.ac.cn` (B. Ren)

by a phase field in the Eulerian framework, where the interface can be identified by field variable. The phase field model has been widely recognized as an effective approach to accurately depict such systems [6].

Firstly, we give some mathematical notions. For any functions f, g defined on a domain Ω, we write

$$(f,g) := \int_\Omega f(\mathbf{x})g(\mathbf{x})d\mathbf{x}$$

for the L^2 inner product of f, g. Besides, let $\|f\| := \sqrt{(f,f)}$ be the L^2—norm of f and

$$\bar{f} := \frac{1}{|\Omega|}\int_\Omega f(\mathbf{x})d\mathbf{x}$$

the mean value of f.

The DC model is accurately described by the phase field for diblock copolymers (PF-BCP) in mean field theory. In the PF-BCP model, the phase field variable denoted by $\phi(\mathbf{x},t)$ is introduced in the domain Ω. This variable represents the difference in the fraction of mass between the two monomer blocks — i.e. N_A and N_B respectively denote the masses of monomer blocks A and B at the position $\mathbf{x}$, and the phase field variable $\phi(\mathbf{x},t)$ is defined by

$$\phi(\mathbf{x},t) := (N_A - N_B)/(N_A + N_B).$$

The phase field ϕ is a scalar variable representing the phase or state of the system. It takes values in the interval $[-1,1]$. The evolution of the PF-BCP model is to minimize the total free energy. The mixture state tends to separate and evolve into distinct pure A-monomer and pure B-monomer states with a specified infinitesimal interface between them. Over time, the PF-BCP system reaches a stable configuration where the separated phases coexist.

In the process of the DC model evolution, the total mass of the two monomers is conserved, resulting in the mass conservation property of the phase field. This can be expressed as

$$\frac{d}{dt}\int_\Omega \phi d\mathbf{x} = 0.$$

The evolution equation of the PF-BCP model is derived from the constrained gradient flow of the total free energy functional $E(\phi)$ in the space H^{-1}, as described in [4]. The total free energy $E(\phi)$ is a functional of the Cahn-Hilliard type energy endowed with an additional nonlocal term and is defined as

$$E(\phi) = \int_\Omega \left(\frac{\varepsilon^2}{2}|\nabla\phi|^2 + F(\phi) + \frac{\alpha}{2}|\nabla\psi|^2\right) d\mathbf{x},$$

where

$$F(\phi) = \frac{(\phi^2-1)^2}{4}, \quad \psi = -\Delta^{-1}(\phi - \bar{\phi}).$$