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An Energy Stable Second-Order Accurate Scheme for Microphase Separation of Periodic Diblock Copolymers

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Abstract. A linear, unconditionally energy stable, and second-order accurate numerical scheme for the Ohta-Kawasaki equation modeling the diblock copolymer dynamics is proposed. The temporal discretisation is based on the Crank-Nicolson temporal discretisation and extrapolation. To suppress the dominance of nonlinear term, a proper stabilising parameter is used. All nonlinear parts are linearised by using the extrapolation from the information at preceding time levels. To solve the resulting linear system, an efficient linear multigrid algorithm is used. The unconditionally energy stability, mass conservation, and unique solvability of the scheme are analytically proved. In two-dimensional case, we run convergence and stability tests, and consider pattern formations for various average concentrations. Pattern formations in three-dimensional space are also studied.

AMS subject classifications: 35K35, 35Q35, 65M12

Key words: Unconditional energy stability, second-order accuracy, Ohta-Kawasaki model, finite difference method.

1. Introduction

A diblock copolymer generally consists of two different monomer types A and B. If temperature decreases below a critical value, these monomers become incompatible and melt. The separation phase usually generates periodic structures such as lamellae, cylinders, spheres and so on [3]. Such a self-assembly property is widely used in nanoscale patterning [7] and was studied through experiments [4,21,23], mathematical modeling [2,5,16], and numerical computations [1,19,20]. From a mesoscopic point of view, the phase separation is caused by emerging A- and B-rich regions and leads to variation of density field. The Ohta-Kawasaki model [33] used to describe the microphase separation patterns has the form

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$$\phi(\mathbf{x},t) = \Delta\mu(\mathbf{x},t) - \alpha\big(\phi(\mathbf{x},t) - \bar{\phi}\big),$$
$$\mu(\mathbf{x},t) = f\big(\phi(\mathbf{x},t)\big) - \epsilon^2\Delta\phi(\mathbf{x},t),$$

and is considered in a domain $\Omega \subset \mathbb{R}^d$, where $d = 1,2,3$ is the space dimension, $\phi = \rho_A - \rho_B$ the difference between the local volume fractions of monomer A and monomer B, which has the value located in [-1,1], μ the chemical potential, $\bar{\phi} = \int_\Omega \phi(\mathbf{x},0)d\mathbf{x}/\int_\Omega d\mathbf{x}$ is the average concentration, f the first derivative of the following Helmholtz free energy functional $F(\phi) = 0.25(\phi^2-1)^2$, ϵ is a non-negative parameter related to the interfacial energy, and a positive parameter α is inversely proportional to the square of the total chain length of the copolymer. Note that if $\alpha = 0$, then the Ohta-Kawasaki model changes to the classical Cahn-Hilliard (CH) model with the properties of energy dissipation and mass conservation. For physical and mathematical derivations of the CH model the reader can consult [26]. The CH model has extensive applications in the phase separation of mixing alloys [6,36], fluid dynamics [22,24], tumor growth [38,39], topology optimization [31], etc. Since the CH model is a nonlinear and fourth-order partial differential equation, it is hard to find its analytical solution. In the numerically study of the CH dynamics, the first-order convex splitting scheme [15] and first-order stabilisation scheme [34] are a popular tool. Shin *et al.* [35] proposed an efficient parallel multigrid algorithm for the CH equation. Chen and Xu [8] developed a time splitting spectral element method for the CH equation. Hofmann *et al.* [17] introduced an efficient immersed interface method for treating the CH equation in arbitrary domains. Luo *et al.* [30] developed efficient adaptive time step algorithms for the CH equation. Recently, with the increasing requirements of high-order accuracy, many researchers studies various high-order energy stable schemes for the CH model. For example, the temporal discretisations based on the Crank-Nicolson scheme [9,29] or BDF2 scheme [10,41], fourth-order compact difference schemes [11,27], etc. If $\alpha > 0$, the nonlocal CH equation becomes the Ohta-Kawasaki model. Note that the Ohta-Kawasaki model also has the basic properties of energy dissipation and mass conservation. The total energy $\mathscr{E}(\phi)$ in the Ohta-Kawasaki model can be divided into short-range energy $\mathscr{E}_s(\phi)$ and long-range energy $\mathscr{E}_l(\phi)$, which are defined by

$$\mathscr{E}_s(\phi) = \int_\Omega \left(F(\phi) + \frac{\epsilon^2}{2}|\nabla\phi|^2 \right) d\mathbf{x},$$
$$\mathscr{E}_l(\phi) = \frac{\alpha}{2}\int_\Omega\int_\Omega G(\mathbf{x}-\mathbf{y})\big(\phi(\mathbf{x}) - \bar{\phi}\big)\big(\phi(\mathbf{y}) - \bar{\phi}\big)d\mathbf{y}d\mathbf{x},$$

where G is a Green's function. Note that if there is a variable v and $-\Delta v = \phi - \bar{\phi}$, then taking the periodic boundary condition, the long-range energy can be rewritten to be [13]

$$\mathscr{E}_l(\phi) = \frac{\alpha}{2}\int_\Omega \Delta_{\mathbf{x}} v(\mathbf{x}) \left[\int_\Omega \Delta_{\mathbf{y}} G(\mathbf{x}-\mathbf{y})\, v(\mathbf{y}) \right] d\mathbf{x} = \frac{\alpha}{2}\int_\Omega |\nabla v\mathbf{x}|^2 d\mathbf{x}.$$

Combining the short-range and long-range energy together, we have the following total energy functional: