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A Positivity-Preserving Second-Order BDF Scheme for the Cahn-Hilliard Equation with Variable Interfacial Parameters

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Abstract. We present and analyze a new second-order finite difference scheme for the Macromolecular Microsphere Composite hydrogel, Time-Dependent Ginzburg-Landau (MMC-TDGL) equation, a Cahn-Hilliard equation with Flory-Huggins-deGennes energy potential. This numerical scheme with unconditional energy stability is based on the Backward Differentiation Formula (BDF) method in time derivation combining with Douglas-Dupont regularization term. In addition, we present a pointwise bound of the numerical solution for the proposed scheme in the theoretical level. For the convergent analysis, we treat three nonlinear logarithmic terms as a whole and deal with all logarithmic terms directly by using the property that the nonlinear error inner product is always non-negative. Moreover, we present the detailed convergent analysis in $\ell^\infty(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$ norm. At last, we use the local Newton approximation and multigrid method to solve the nonlinear numerical scheme, and various numerical results are presented, including the numerical convergence test, positivity-preserving property test, spinodal decomposition, energy dissipation and mass conservation properties.

AMS subject classifications: 35K35, 65M06, 65M12

Key words: Cahn-Hilliard equation, Flory-Huggins energy, deGennes diffusive coefficient, energy stability, positivity preserving, convergence analysis.

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1 Introduction

The Time-Dependent Ginzburg-Landau mesoscopic model for the macromolecular microsphere composite (MMC) hydrogel, called MMC-TDGL equation, was recently proposed in [53] as a new approach to simulating a reticular structure and phase transition process of MMC hydrogel. The MMC-TDGL model accounts for the periodic network structure of MMC through a coarse-grained free energy functional of the Flory-Huggins-deGennes type [53]. The model can describe the growth detail of the well-defined structures intermittent phenomenon with increasing reaction temperature, and many other chemical observable phenomena [32]. The idea is that a conserved field variable represents the concentration of one of the components of the mixture (or sometimes, the difference between the concentration of the two components of a binary mixture). The approach is derived via Boltzmann entropy theorem.

Allen-Cahn and Cahn-Hilliard equations are the prototypical models for gradient flows with the Ginzburg-Landau or Flory-Huggins free energy. In some cases, certain stochastic force term has been added in the model, such as the Cahn-Hilliard-Cook model. This model can simulate the structural evolution of mixtures with polymers and block copolymers [28] and the phase separation of the small molecule systems including binary alloys, fluid mixtures, inorganic glasses [3]. Concerning the computation and analysis of these models, Du et al. had a series of works [14, 15, 27]. Yang et al. presented an invariant energy quadratization (IEQ) approximation [50–52, 55, 56]. Chen et al. used the phase field method to investigate composite materials and presented some numerical methods [4, 21]. Shen et al. designed a few high-order energy stability preserving numerical schemes and provided the corresponding error estimates [38–43]. These works investigated the nucleation by using string method in virtue of stochastic Allen-Cahn and Cahn-Hilliard equations [54]. For the MMC-TDGL equation, Li et al. [33] also have performed some numerical simulations. Also see the related works [2, 17], etc.

The convex splitting approach advanced by Eyre [22] is one of the popular energy stable methods. The idea is that the energy admits a splitting into purely convex and concave parts, that is, $E=E_c-E_e$, where E_c and E_e are both convex. Recently, such an idea has also been applied to a wide class of gradient flows, including either first or second order accurate in both time and space. See the related works for the PFC equation and the modified PFC (MPFC) equation [19, 45, 46, 48]; the epitaxial thin film growth models [5, 8, 11, 26, 37, 44], and the Cahn-Hilliard flow coupled with fluid motion [6, 7, 16, 18, 30, 35, 47], etc. One well-known drawback of the first order convex splitting approach is that an extra dissipation added to ensure unconditionally stability also introduces a significant amount of numerical error [12]. Due to this, second-order energy stable methods have been highly desirable. Recently, a second order convex splitting scheme based on the Crank-Nicolson temporal approximation for solving the MMC-TDGL equation has been proposed in [34], however, its convergence analysis is still a large challenge.

The goal of this paper is to extend the convex-splitting framework to develop a second order in both time and space for the MMC-TDGL equation. While some of the technique