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A Second Order Accurate in Time, Energy Stable Finite Element Scheme for the Flory-Huggins-Cahn-Hilliard Equation

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Abstract. In this paper, we propose and analyze a second order accurate in time, mass lumped mixed finite element scheme for the Cahn-Hilliard equation with a logarithmic Flory-Huggins energy potential. The standard backward differentiation formula (BDF) stencil is applied in the temporal discretization. In the chemical potential approximation, both the logarithmic singular terms and the surface diffusion term are treated implicitly, while the expansive term is explicitly updated via a second-order Adams-Bashforth extrapolation formula, following the idea of the convex-concave decomposition of the energy functional. In addition, an artificial Douglas-Dupont regularization term is added to ensure the energy dissipativity. In the spatial discretization, the mass lumped finite element method is adopted. We provide a theoretical justification of the unique solvability of the mass lumped finite element scheme, using a piecewise linear element. In particular, the positivity is always preserved for the logarithmic arguments in the sense that the phase variable is always located between -1 and 1. In fact, the singular nature of the implicit terms and the mass lumped approach play an essential role in the positivity preservation in the discrete setting. Subsequently, an unconditional energy stability is proven for the proposed numerical scheme. In addition, the convergence analysis and error estimate of the numerical scheme are also presented. Two numerical experiments are carried out to verify the theoretical properties.

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1 Introduction

The Cahn-Hilliard equation plays an important role in materials science and biological applications. It was constructed by Cahn and Hilliard [9] as a conserved gradient flow with respect to the free energy of an isothermal, isotropic fluid. Usually, the evolution of the system is driven by the gradient of the singular Flory-Huggins free energy and describes phase separation processes with respect to the concentration ϕ. Phase separation can be observed, e.g., when a binary alloy is cooled down sufficiently. One then may observe spinodal decomposition, whereby the material quickly becomes inhomogeneous, forming a fine-grained structure in which each of the two phases appears in a more or less alternating pattern. In the second stage, which is called coarsening, and which occurs at a slower time scale, the average size of phases in the microstructure grows with time. Such phenomena play an essential role in the structural and mechanical properties of the material [4, 17, 38]. The equation is flexible, allowing several variants–based on the choices of mobility and free energy density–which are relevant in different contexts and for disparate physical and biological processes in which phase separation and coarsening/clustering processes can be observed (see [34, 37]).

There have been a lot of theoretical analyses and numerical approximations for these gradient flows in the two-phase case. The existence of solutions and attractors to the Cahn-Hilliard equation with degenerate mobility and logarithmic nonlinearities has been proved in [24,36,44,45]. For the time integration, several numerical techniques have been applied to design the energy dissipative schemes for gradient flows [2,5,6,10,15,29,54], including convex splitting [25,55,57], stabilization [29,49], auxiliary variable approaches [1] (such as invariant energy quadrature method [60, 64] and scalar auxiliary variable version [16,46–48]). In particular, the convex splitting method has been widely used to solve various phase field equations by virtue of its theoretical advantages [11, 13, 26, 30, 31, 50, 52]. Meanwhile, the IEQ and SAV approaches can be used to design linear and energy stable numerical schemes, which can improve the computational efficiency of many relatively complex problems [41, 43, 48, 51, 56, 61], and have been rapidly developed in recent years. And also, the stabilization method turns out to be a useful tool to extend the above methods to a higher-order accuracy of time [28, 29, 48, 58, 59]. These numerical techniques possess two main features: mass conservation and energy dissipativity (conditionally/unconditionally).

Meanwhile, most above-mentioned works have been focused on the physical model with a polynomial approximation in the energy potential expansion. For the Cahn-Hilliard equation with the original Flory-Huggins logarithmic energy potential, a the-