Unconditionally Energy Stable Cahn-Hilliard Solvers with Adaptive Free Energy Potentials

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Abstract

The Cahn-Hilliard equation is a cornerstone of nonequilibrium thermodynamics, modeling diffusion-driven phase separation, coarsening, and interfacial dynamics in binary mixtures [1, 2]. It captures the fundamental physics of mass conservation and free energy minimization, with wide-ranging applications in materials science, soft matter physics, and condensed matter systems such as alloys, polymer blends [3], pattern formation in multiphase flows [4], binary fluids[5, 6], and tumor growth dynamics [7]. Due to the equation's strong nonlinearity and stiffness, analytical solutions are rarely attainable, necessitating accurate and stable numerical methods. The choice of free energy potential significantly influences both physical fidelity and numerical stability. In this study, we develop an adaptive free energy approach that switches pointwise between the Flory-Huggins logarithmic potential, which preserves thermodynamic realism, and a polynomial approximation, which prevents singularities near phase limits. The switching ensures physical consistency within the bounded range of the order parameter. Time integration is performed using Eyre's convex-concave splitting scheme combined with first- and second-order backward differentiation formulas, guaranteeing unconditional energy stability, while Fourier cosine spectral discretization with Neumann boundary conditions ensures mass conservation and monotonic energy dissipation. The proposed framework enables stable and physically consistent simulations of phase separation and morphological evolution, offering valuable insights into pattern formation, interfacial motion, and coarsening kinetics that are crucial for understanding microstructure development and nanoscale self-organization in advanced materials.

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