DOCTORAL THESIS

Numerical analysis and simulations for phase-field equations

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Abstract

Research on interfacial phenomena has a long history, which has attracted tremendous interest in recent years. One of the most successful tools is the phase-field approach. As phase-field models usually involve very complex dynamics and it is nontrivial to obtain analytical solutions, numerical methods have played an important role in various simulations. This thesis is mainly devoted to developing accurate, efficient and robust numerical methods and the related numerical analysis for three representative phase-field models, namely the Allen-Cahn equation, the Cahn-Hilliard equation and the thin film models.

The first part of this thesis is mainly concentrated on the stability analysis for these three models, with particular attention to the Allen-Chan equation. We have established three stability criterion, i.e., nonlinear energy stability, L^∞-stability and L^2-stability.

As shared by most phase-field models, one of the intrinsic properties of the Allen-Cahn and the Cahn-Hilliard equations is that they satisfy a nonlinear stability relationship, usually expressed as a time-decreasing free energy functional. We have studied several stabilized temporal discretization for both the Allen-Cahn and the Cahn-Hilliard equations so that the relevant nonlinear energy stability can be preserved. The corresponding temporal discretization schemes are linear and are of second-order accuracy. We also apply multi-step implicit-explicit methods to approximate the Allen-Cahn equation. We demonstrate that by suitably choosing the parameters in multi-step implicit-explicit methods the nonlinear energy stability can be preserved.

Apart from studying the energy stability for the Allen-Cahn equation, we also establish the numerical maximum principle for some fully discretized schemes. We further extend our analysis technique to the fractional-in-space Allen-Cahn equation. A more general Allen-Cahn-type equation with a nonlinear degenerate mobility and a logarithmic free energy is also considered.

The third stability under investigation is the L^2-stability. We prove that the continuum Allen-Cahn equation satisfies a uniform L^p-stability. Furthermore, we show that both semi-discretized Fourier Galerkin and Fourier collocation methods can inherit this stability for $p = 2$, i.e., L^2-stability. Based on the established L^2-stability, we accomplish the spectral convergence estimate for the Fourier Galerkin methods. We adopt the second-order Strang splitting schemes in the temporal direction with Fourier collocation methods to demonstrate the uniform L^2-stability in the fully discretized scheme.

Another contribution of this thesis is to propose a p-adaptive spectral deferred correction methods for the long time simulations for all three models. We develop a high-order accurate and energy stable scheme to simulate the phase-field models by combining the semi-implicit spectral deferred correction method and first-order stabilized semi-implicit schemes. It is found that the accuracy improvement may affect the overall energy stability. To compromise the accuracy and stability, a local p-adaptive strategy is proposed to enhance the accuracy by sacrificing some local energy stability in an acceptable level. Numerical results demonstrate the high effectiveness of our proposed numerical strategy.

Keywords: Phase-field models, Allen-Cahn equations, Cahn-Hilliard equations, thin film models, nonlinear energy stability, maximum principle, L^2-stability, adaptive simulations, stabilized semi-implicit schemes, finite difference, Fourier spectral methods, spectral deferred correction methods, convex splitting.

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