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Second-Order Linear Stabilized Semi-Implicit Crank-Nicolson Scheme for the Cahn-Hilliard Model with Dynamic Boundary Conditions

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Abstract. We propose a kind of second-order stabilized Crank-Nicolson scheme which can be applied to three types of Cahn-Hilliard model with dynamic boundary conditions. We give the corresponding proof of stability and convergence theoretically which takes the reaction rate dependent dynamic boundary conditions as an example. We verify the effectiveness and universality of our proposed scheme by conducting some typical numerical simulations and comparing with the literature works. It's found that second-order scheme takes much less CPU time than the first-order scheme to reach the same final time.

AMS subject classifications: 65M12, 65N12, 65Z05

Key words: Cahn-Hilliard equation, dynamic boundary conditions, reaction rate, second-order Crank-Nicolson formula, energy stability, convergence analysis.

1 Introduction

As pointed out in [33], the evolution range of Cahn-Hilliard equation is quite wide which can describe the important qualitative characteristics of many systems undergoing phase separation at different time stages, such as the phase separation, the process of nucleation, coarsening in heterogeneous systems [4, 5, 33] and extension of coupling classical

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phase-field model with magnetic field [1,53]. Cahn-Hilliard equation is a representative of the so-called diffusion interface model which describes the evolution of free interface during phase transition [44]. Different from the classical sharp-interface formulation, this approach has several advantages. For instance, it can avoid evolution of complex geometries and topological changes of the interface [12], and explicit tracking of the interface.

The standard Cahn-Hilliard equation can be written as follows,

$$\begin{cases} \phi_t = \Delta\mu, & (\mathbf{x},t)\in\Omega\times(0,T), \\ \mu = -\varepsilon\Delta\phi + \dfrac{1}{\varepsilon}F'(\phi), & (\mathbf{x},t)\in\Omega\times(0,T), \end{cases} \tag{1.1}$$

where μ denotes the chemical potential, the parameter $\varepsilon>0$ means the thickness of the interface and $\Omega\subseteq\mathbb{R}^d\,(d=2,3)$ denotes a bounded domain whose boundary $\Gamma=\partial\Omega$ with the unit outward normal vector $\mathbf{n}$. The function ϕ has different interpretations depending on the physical environment, such as volume fraction, mass fraction or mole fraction [12,33]. In general, it represents the concentration of two components by rescaling, therefore the value of ϕ shall be taken in the physical interval $[-1,1]$ with the $\phi=\pm1$ corresponding to the pure phase of the materials, which are separated by an interfacial region whose thickness is proportional to ε.

The Cahn-Hilliard equation can be alternatively viewed as the gradient flow of the Ginzburg-Landau type energy functional

$$E^{bulk}(\phi) = \int_\Omega \left\{ \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}F(\phi) \right\} dx,$$

in H^{-1}. The energy functional E^{bulk} consists of two parts: the hydrophilic (gradient term) and hydrophobic (double-well term) tendency of the phase-field variable ϕ. $F(x)$ is a given double-well potential and $f(x)=F'(x)$ as below

$$F(x) = \frac{1}{4}(x^2-1)^2, \quad f(x) = x^3 - x, \quad x\in\mathbb{R}. \tag{1.2}$$

Since (1.1) is a fourth order parabolic equation for variable ϕ, suitable initial and boundary conditions should be taken to form a well-posed problem. The classical setting is homogeneous Neumann condition:

$$\begin{cases} \partial_{\mathbf{n}}\mu = 0, & (\mathbf{x},t)\in\Gamma\times(0,T), \\ \partial_{\mathbf{n}}\phi = 0, & (\mathbf{x},t)\in\Gamma\times(0,T), \end{cases}$$

where $\partial_{\mathbf{n}}$ represents the outward normal derivative on Γ. The energetic variational approach reveals that the Cahn–Hilliard equation together with the classical boundary conditions naturally fulfills two important physical constraints, the mass conservation

$$\int_\Omega \phi(t)dx = \int_\Omega \phi(0)dx, \quad \forall t\in[0,T],$$