A Modified Crank-Nicolson Numerical Scheme for the Flory-Huggins Cahn-Hilliard Model

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Abstract. In this paper we propose and analyze a second order accurate numerical scheme for the Cahn-Hilliard equation with logarithmic Flory Huggins energy potential. A modified Crank-Nicolson approximation is applied to the logarithmic nonlinear term, while the expansive term is updated by an explicit second order Adams-Bashforth extrapolation, and an alternate temporal stencil is used for the surface diffusion term. A nonlinear artificial regularization term is added in the numerical scheme, which ensures the positivity-preserving property, i.e., the numerical value of the phase variable is always between -1 and 1 at a point-wise level. Furthermore, an unconditional energy stability of the numerical scheme is derived, leveraging the special form of the logarithmic approximation term. In addition, an optimal rate convergence estimate is provided for the proposed numerical scheme, with the help of linearized stability analysis. A few numerical results, including both the constant-mobility and solution-dependent mobility flows, are presented to validate the robustness of the proposed numerical scheme.

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1 Introduction

The Allen-Cahn (AC) [3] and Cahn-Hilliard (CH) [9] equations are fundamental gradient flow models in the description of phase transitions. For any $\phi \in H^1(\Omega)$, the Cahn-Hilliard-Flory-Huggins energy functional is formulated as

$$E(\phi) = \int_\Omega \left((1+\phi)\ln(1+\phi) + (1-\phi)\ln(1-\phi) - \frac{\theta_0}{2}\phi^2 + \frac{\varepsilon^2}{2}|\nabla\phi|^2 \right) d\mathbf{x}, \qquad (1.1)$$

where $\Omega \subset \mathbb{R}^d$ ($d=2$ or $d=3$) is a bounded domain and the point-wise bound $-1 \leq \phi \leq 1$ is assumed for phase field variable ϕ. The physical parameters $\varepsilon > 0$ and $\theta_0 > 0$ are associated with the diffuse interface width and the temperature, respectively. The CH equation is an H^{-1}-like conserved gradient flow of the energy functional (1.1):

$$\partial_t \phi = \nabla \cdot (\mathcal{M}(\phi)\nabla\mu), \qquad (1.2)$$

$$\mu := \delta_\phi E = \ln(1+\phi) - \ln(1-\phi) - \theta_0\phi - \varepsilon^2\Delta\phi, \qquad (1.3)$$

where $\mathcal{M}(\phi) > 0$ stands for the mobility function. As a consequence, the gradient structure indicates an energy dissipation law: $\frac{d}{dt}E(\phi(t)) = -\int_\Omega \mathcal{M}(\phi)|\nabla\mu|^2 d\mathbf{x} \leq 0$. See the related references [8, 19, 23, 28]. In this article, we assume that $\Omega = (0,1)^3$, and consider periodic boundary conditions, for simplicity of presentation. An extension of our results for the model with homogeneous Neumann boundary conditions is straightforward.

Of course, the most visible difficulty for the Cahn-Hilliard equation (1.2) with logarithmic Flory Huggins energy potential is associated with the singularity in its derivative as the value of ϕ approaches -1 or 1. In fact, the positivity property, i.e., $0 < 1-\phi$ and $0 < 1+\phi$, has been established at the PDE analysis level in [2, 20, 28, 53]. As a further development, a separation property has also been justified for the 1-D and 2-D equations at a theoretical level. This property guarantees that a uniform distance exists between the value of the phase variable and the singular limit values. Such a distance only depends on ε, θ_0 and the initial data. See also the related works [1, 4, 18, 28, 33, 34, 52], et cetera. The free energy with the logarithmic pattern is considered in many cases to be more physically realistic than the regularly use polynomial version [23].

Regarding numerical approximation of the Cahn-Hilliard equation (1.2) with the Flory-Huggins energy (1.1), there have been extensive works [29, 41–43, 47, 54–56, 58, 61, 65], et cetera. Among the existing works, it is worth mentioning the pioneering work [19], which addresses the issue of the positivity-preserving property (for $1+\phi$ and $1-\phi$) when the implicit Euler scheme is applied and analyzed. Meanwhile, a time step constraint, $\Delta t \leq \frac{4\varepsilon^2}{\theta_0^2}$, must be assumed, which comes from the implicit treatment of the expansive term. An extension to the multi-component Cahn-Hilliard flow has also been reported in [7].

A more recent work [13] has overcome the time step restriction, making use of the convex-concave decomposition approach. The positivity-preserving property, unique