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# CONVERGENCE ANALYSIS OF A PRECONDITIONED STEEPEST DESCENT SOLVER FOR THE CAHN-HILLIARD EQUATION WITH LOGARITHMIC POTENTIAL

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**Abstract.** In this paper, we provide a theoretical analysis for a preconditioned steepest descent (PSD) iterative solver that improves the computational time of a finite difference numerical scheme for the Cahn-Hilliard equation with Flory-Huggins energy potential. In the numerical design, a convex splitting approach is applied to the chemical potential such that the logarithmic and the surface diffusion terms are treated implicitly while the expansive concave term is treated with an explicit update. The nonlinear and singular nature of the logarithmic energy potential makes the numerical implementation very challenging. However, the positivity-preserving property for the logarithmic arguments, unconditional energy stability, and optimal rate error estimates have been established in a recent work and it has been shown that successful solvers ensure a similar positivity-preserving property at each iteration stage. Therefore, in this work, we will show that the PSD solver ensures a positivity-preserving property at each iteration stage. The PSD solver consists of first computing a search direction (which requires solving a constant-coefficient Poisson-like equation) and then takes a one-parameter optimization step over the search direction in which the Newton iteration becomes very powerful. A theoretical analysis is applied to the PSD iteration solver and a geometric convergence rate is proved for the iteration. In particular, the strict separation property of the numerical solution, which indicates a uniform distance between the numerical solution and the singular limit values of $\pm 1$ for the phase variable, plays an essential role in the iteration convergence analysis. A few numerical results are presented to demonstrate the robustness and efficiency of the PSD solver.

**Key words.** Cahn-Hilliard equation, logarithmic Flory Huggins energy potential, positivity preserving, energy stability, preconditioned steepest descent iteration solver, iteration convergence analysis.

## 1. Introduction

The Allen-Cahn (AC) [3] (non-conserved dynamics) and Cahn-Hilliard (CH) [7] (conserved dynamics) equations are well known gradient flows with respect to the total free energy given by

$$E(\phi) = \int_\Omega \left( F(\phi) + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x},$$

where $\Omega \subset \mathbb{R}^d$ (with $d = 2$ or $d = 3$) is a bounded domain, $-1 < \phi < 1$ is the variable of interest often representing the concentration of material components in a two-phase system, $\varepsilon$ is a positive constant associated with the diffuse interface width separating the two phases, and $F$ is a given double-well potential. In this work, we consider the Flory-Huggins energy potential. Specifically, for any $\phi \in H^1(\Omega)$ with a point-wise bound, i.e. $-1 < \phi < 1$, the total free energy with Flory-Huggins energy potential is given by

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

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where $\theta_0$ is an additional positive constant associated with the diffuse interface width. The Cahn-Hilliard (CH) equation is then an $H^{-1}$ (conserved) gradient flow of the energy functional (1) and is given by:

$$\partial_t \phi = \nabla \cdot (\mathcal{M}(\phi) \nabla \mu), \tag{2}$$

$$\mu := \delta_\phi E = \ln(1+\phi) - \ln(1-\phi) - \theta_0 \phi - \varepsilon^2 \Delta \phi, \tag{3}$$

where $\mathcal{M}(\phi) > 0$ is a mobility function. Based on the gradient structure of (2), the energy dissipation law is derived as

$$\frac{d}{dt} E(\phi(t)) = -\int_\Omega \mathcal{M}(\phi) |\nabla \mu|^2 d\mathbf{x} \leq 0. \tag{4}$$

For simplicity of presentation, we assume that $\Omega = [0,1]^2$ with periodic boundary conditions but remark that the case with homogeneous Neumann boundary conditions can be analyzed with a similar strategy.

The free energy with the Flory-Huggins logarithmic potential is generally viewed to be more physically realistic than an energy represented by a polynomial expression since the former can be derived from regular or ideal solution theories [25]. On the other hand, the Flory Huggins energy potential posses a computational challenge since it is associated with a singularity as the phase variable approaches $-1$ or 1. Indeed, the system (2) – (3) is only well-defined if a point-wise positivity property is imposed, i.e., $0 < 1-\phi$ and $0 < 1+\phi$, so that the phase variable remains in the interval $(-1, 1)$. See the related works [1, 2, 4, 21, 23, 30, 5, 35, 36, 42, 49, 50], etc.

For the CH equation with a polynomial approximation in the energy potential, a maximum norm bound could be carefully derived, with the help of a global-in-time $H^2$ analysis. However, such an $L^\infty$ bound turns out to be singularly $\varepsilon^{-1}$-dependent, since the surface diffusion estimate has to be used to balance the nonlinear effects; see the related work in [37]. In terms of an $\varepsilon^{-1}$-independent $L^\infty$ bound, the sharpest theoretical analysis in this area could be found in [6], in which a polynomial pattern energy potential is used with a cut-off approach. On the other hand, for the Cahn-Hilliard equation (2) – (3) with a singular Flory-Huggins energy potential (1), an $L^\infty$ bound is automatically satisfied: $-1 < \phi < 1$, so that the PDE is well-defined. Meanwhile, in spite of such an automatic $L^\infty$ bound, a uniform distance between the solution away from the singular limit values will play a more important role, due to the singular nature in the nonlinear analysis. In fact, for the 2-D CH equation (2) – (3), the separation property has also been justified at a theoretical level [2, 23], i.e., a uniform distance between the phase variable and the singular limit values ($-1$ and 1) has been derived, dependent on $\varepsilon$, $\theta_0$ and the initial data. For the 3-D equation, a theoretical proof of the separation property has not been available, while we make such an assumption in this article, to facilitate the numerical iteration analysis.

In addition, the system defined in (1) has a symmetric double-well structure. Notice that $\theta_0 > 0$ is an $O(1)$ constant, and many interesting profiles could be obtained by the scientific computing with such a constant scale; see the detailed numerical simulation results in [11], with $\theta_0 = 3$ and $\theta_0 = 3.5$. A careful calculation reveals that, for $\theta_0 > 1$, this free energy supports a spatially uniform equilibria solution: $\phi \equiv \pm\phi_*$, with $\phi_* \in (0,1)$ satisfying a steady-state equation: $\ln(1+\phi) - \ln(1-\phi) - \theta_0 \phi = 0$. Of course, if the initial data does not have a mass average of $\pm\phi_*$, the PDE solution will not convergence to such a trivial steady-state solution, $\phi \equiv \pm\phi_*$. For the Allen-Cahn (AC) equation, the associated $L^2$ gradient flow, the separation property is satisfied with such a minima value of the double well, i.e., $-\phi_* \leq \phi \leq \phi_*$ at any time, provided that the initial data also satisfied this