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A PRECONDITIONED STEEPEST DESCENT SOLVER FOR THE CAHN-HILLIARD EQUATION WITH VARIABLE MOBILITY

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Abstract. In this paper we provide a detailed analysis of the preconditioned steepest descent (PSD) iteration solver for a convex splitting numerical scheme to the Cahn-Hilliard equation with variable mobility function. In more details, the convex-concave decomposition is applied to the energy functional, which in turn leads to an implicit treatment for the nonlinear term and the surface diffusion term, combined with an explicit update for the expansive concave term. In addition, the mobility function, which is solution-dependent, is explicitly computed, which ensures the elliptic property of the operator associated with the temporal derivative. The unique solvability of the numerical scheme is derived following the standard convexity analysis, and the energy stability analysis could also be carefully established. On the other hand, an efficient implementation of the numerical scheme turns out to be challenging, due to the coupling of the nonlinear term, the surface diffusion part, and a variable-dependent mobility elliptic operator. Since the implicit parts of the numerical scheme are associated with a strictly convex energy, we propose a preconditioned steepest descent iteration solver for the numerical implementation. Such an iteration solver consists of a computation of the search direction (involved with a Poisson-like equation), and a one-parameter optimization over the search direction, in which the Newton's iteration becomes very powerful. In addition, a theoretical analysis is applied to the PSD iteration solver, and a geometric convergence rate is proved for the iteration. A few numerical examples are presented to demonstrate the robustness and efficiency of the PSD solver.

Key words. Cahn-Hilliard equation, variable mobility function, convex splitting numerical scheme, energy stability, preconditioned steepest descent iteration solver, iteration convergence analysis.

1. Introduction

The Allen-Cahn (AC) [1] (non-conserved dynamics) and Cahn-Hilliard (CH) [4] (conserved dynamics) equations are well known gradient flows with respect to a particular free energy. Suppose that $\Omega \subset \mathbb{R}^d$ (with $d = 2$ or $d = 3$) is a bounded open domain. The CH free energy functional is formulated as

$$E(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 - \frac{1}{2}\phi^2 + \frac{\varepsilon^2}{2}|\nabla\phi|^2 \right) d\mathbf{x}, \tag{1}$$

for any phase field function $\phi \in H^1(\Omega)$, where ε is an interface width parameter. This free energy is termed *regular* since it is defined for all $\phi \in H^1(\Omega)$. Other free energies, such as those only defined for $0 \le \phi \le 1$, are possible but will not be considered here. For simplicity, we assume that Ω is a rectangular domain, and periodic boundary conditions for ϕ are enforced. The standard CH equation is the conserved gradient flow with respect to the free energy functional (1):

$$\phi_t = \nabla \cdot \Big(\mathcal{M}(\phi) \nabla \mu \Big), \quad \mu := \delta_\phi E = \phi^3 - \phi - \varepsilon^2 \Delta \phi. \tag{2}$$

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This equation is termed *degenerate* if there are values of ϕ for which $\mathcal{M}(\phi) = 0$. A common choice for the degenerate case is

$$\mathcal{M}(\phi) = \begin{cases} (1+\phi)(1-\phi), & -1 \le \phi \le 1 \\ 0, & |\phi| > 1. \end{cases} \tag{3}$$

Otherwise, the equation is *non-degenerate*. Often times, researchers assume that $\mathcal{M} \equiv 1$, for simplicity. In this paper, we will consider the non-degenerate, non-constant case. In particular, we will assume that, for all ϕ,

$$0 < \mathcal{M}_0 \le \mathcal{M}(\phi) \le \mathcal{M}_1 < \infty. \tag{4}$$

A specific example that we could consider might be the mobility

$$\mathcal{M}(\phi) = \begin{cases} \sqrt{(1+\phi)^2(1-\phi)^2 + \delta^2}, & -1 \le \phi \le 1 \\ \delta, & |\phi| > 1, \end{cases} \tag{5}$$

which is a regularized version of (3). The regularization parameter δ is assumed to be a fixed value, independent on ε. Subsequently, the following energy dissipation law is available, which comes from the gradient structure of (2):

$$\frac{d}{dt} E(\phi(t)) = -\int_\Omega \mathcal{M}(\phi) |\nabla \mu|^2 d\mathbf{x} \le 0. \tag{6}$$

Of course, the usual mass conservative property is valid, i.e., $\int_\Omega \partial_t \phi \, d\mathbf{x} = 0$, which follows from the conservative structure of the equation.

There have been extensive numerical works for the Cahn-Hilliard equation. In particular, energy stability has attracted more and more attentions, since it plays an essential role in the accuracy of long time numerical simulation. The standard convex splitting scheme, pioneered by Eyre's work [16], is a very useful approach to obtain the energy stability at a numerical level. This framework treats the convex part of the chemical potential implicitly and the concave part explicitly. In turn, the unique solvability and energy stability could be theoretically justified by a convexity analysis. An extension to the second order energy stable numerical schemes have also been reported, based on either Crank-Nicolson [12, 15, 24, 25] or BDF-type [10, 43] temporal discretization. Similar ideas have been widely applied to various gradient flows, and both first and second order accurate (in time) algorithms have been developed. See the related works for the phase field crystal (PFC) equation and the modified phase field crystal (MPFC) equation [2, 3, 27, 39, 42]; epitaxial thin film growth models [5, 9, 34, 38]; non-local Cahn-Hilliard-type models [21, 22, 23]; the Cahn-Hilliard-Fluid and related models [6, 7, 13, 14, 20, 26, 41]; *et cetera*. Other than these numerical algorithms, which preserve the energy dissipation in the original phase variable, a few other numerical works have been reported for the reformulated physical system with an introduction of certain auxiliary variables, such as the scalar auxiliary variable (SAV) approach [35, 36, 37]. Some linear numerical schemes with stabilization approach [30, 31, 32, 40] have been reported as well.

Most existing numerical works have been focused on the Cahn-Hilliard flow with a constant mobility function, and the numerical investigation of variable mobility gradient flow turns out to be limited. In addition, the numerical implementation for the variable mobility equation is usually challenging. In this article, we look at a first order accurate in time, energy stable numerical scheme for the Cahn-Hilliard equation, propose a nonlinear iteration solver, and provide a theoretical analysis for the convergence of the solver. For simplicity, we use apply the convex splitting method for the chemical potential, in which the nonlinear term and the surface