A Second-Order Energy Stable BDF Numerical Scheme for the Cahn-Hilliard Equation

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Abstract. In this paper we present a second order accurate (in time) energy stable numerical scheme for the Cahn-Hilliard (CH) equation, with a mixed finite element approximation in space. Instead of the standard second order Crank-Nicolson methodology, we apply the implicit backward differentiation formula (BDF) concept to derive second order temporal accuracy, but modified so that the concave diffusion term is treated explicitly. This explicit treatment for the concave part of the chemical potential ensures the unique solvability of the scheme without sacrificing energy stability. An additional term $A\tau\Delta(u^{k+1}-u^k)$ is added, which represents a second order Douglas-Dupont-type regularization, and a careful calculation shows that energy stability is guaranteed, provided the mild condition $A \geq \frac{1}{16}$ is enforced. In turn, a uniform in time H^1 bound of the numerical solution becomes available. As a result, we are able to establish an $\ell^\infty(0,T;L^2)$ convergence analysis for the proposed fully discrete scheme, with full $\mathcal{O}(\tau^2+h^2)$ accuracy. This convergence turns out to be unconditional; no scaling law is needed between the time step size τ and the spatial grid size h. A few numerical experiments are presented to conclude the article.

1 Introduction

The Allen-Cahn (AC) [1] (non-conserved dynamics) and Cahn-Hilliard (CH) [7] (conserved dynamics) equations, which model spinodal decomposition in a binary alloy, are

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perhaps the most well-known of the gradient flow-type PDEs. In deriving the CH equation, we consider a bounded domain $\Omega \subset \mathbb{R}^d$ (with $d=2$ or $d=3$). For any $u \in H^1(\Omega)$, the CH energy functional is given by

$$E(u) = \int_\Omega \left(\frac{1}{4}u^4 - \frac{1}{2}u^2 + \frac{\varepsilon^2}{2}|\nabla u|^2 \right) d\mathbf{x}, \tag{1.1}$$

where ε is a positive constant that dictates the interface width. (See [7] for a detailed derivation.) The CH equation is precisely the H^{-1} (conserved) gradient flow of the energy functional (1.1):

$$\begin{cases} u_t = \Delta w, & \text{in} \quad \Omega \times (0,T), \\ w := \delta_\phi E = u^3 - u - \varepsilon^2 \Delta u, & \text{in} \quad \Omega \times (0,T), \\ \partial_n u = \partial_n w = 0, & \text{on} \quad \partial\Omega \times (0,T), \\ u(\cdot,0) = u_0, & \text{in} \quad \Omega, \end{cases} \tag{1.2}$$

where $T > 0$ is the final time, which may be infinite; $\partial_n u := \mathbf{n} \cdot \nabla u$; and $\mathbf{n}$ the unit normal vector on the boundary. Due to the gradient structure of (1.2), the following energy dissipation law holds:

$$\frac{d}{dt}E(u(t)) = -\int_\Omega |\nabla w|^2 d\mathbf{x}. \tag{1.3}$$

In integral form, the energy decay may be expressed as

$$E(u(t_1)) + \int_{t_0}^{t_1} \int_\Omega |\nabla w(t)|^2 d\mathbf{x} dt = E(u(t_0)). \tag{1.4}$$

Furthermore, the equation is mass conservative, $\int_\Omega \partial_t u \, d\mathbf{x} = 0$, which follows from the conservative structure of the equation together with the homogeneous Neumann boundary conditions for w. This property can be re-expressed as $(u(\cdot,t),1) = (u_0,1)$, for all $t \geq 0$.

The Cahn-Hilliard equation is one of the most important models in mathematical physics. It is often paired with equations that describe important physical behavior of a given physical system, typically through nonlinear coupling terms. Examples of such coupled models include the Cahn-Hilliard-Navier-Stokes (CHNS) equation for two-phase, immiscible flow; the Cahn-Larché model of binary solid state diffusion for elastic misfit; the Cahn-Hilliard-Hele-Shaw (CHHS) equation for spinodal decomposition of a binary fluid in a Hele-Shaw cell; et cetera. The numerical and PDE analyses for the CH equation are quite challenging, since the equation is a fourth-order, nonlinear parabolic-type PDE. There have been many existing numerical works, in particular for first order accurate (in time) schemes.

Meanwhile, second order accurate (in time) numerical schemes have also attracted a great deal of attention in recent years, due to the great advantage over their first order counterparts in terms of numerical efficiency and accuracy. However, the analysis for the second order schemes is significantly more difficult than that for the first order ones,