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A Third Order Accurate in Time, BDF-Type Energy Stable Scheme for the Cahn-Hilliard Equation

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Abstract. In this paper we propose and analyze a backward differentiation formula (BDF) type numerical scheme for the Cahn-Hilliard equation with third order temporal accuracy. The Fourier pseudo-spectral method is used to discretize space. The surface diffusion and the nonlinear chemical potential terms are treated implicitly, while the expansive term is approximated by a third order explicit extrapolation formula for the sake of solvability. In addition, a third order accurate Douglas-Dupont regularization term, in the form of $-A_0\Delta t^2\Delta_N(\phi^{n+1}-\phi^n)$, is added in the numerical scheme. In particular, the energy stability is carefully derived in a modified version, so that a uniform bound for the original energy functional is available, and a theoretical justification of the coefficient A becomes available. As a result of this energy stability analysis, a uniform-in-time L_N^6 bound of the numerical solution is obtained. And also, the optimal rate convergence analysis and error estimate are provided, in the $L^\infty_{\Delta t}(0,T;L_N^2)\cap L^2_{\Delta t}(0,T;H_h^2)$ norm, with the help of the L_N^6 bound for the numerical solution. A few numerical simulation results are presented to demonstrate the efficiency of the numerical scheme and the third order convergence.

AMS subject classifications: 35K30, 35K55, 65L06, 65M12, 65M70, 65T40

Key words: Cahn-Hilliard equation, third order backward differentiation formula, unique solvability, energy stability, discrete L_N^6 estimate, optimal rate convergence analysis.

1. Introduction

The Allen-Cahn (AC) [1] (non-conserved dynamics) and Cahn-Hilliard (CH) [4]

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(conserved dynamics) equations, are some of the best known gradient flow models. They result from the same or similar models for the free energy density and only differ in whether they are conserved or non-conserved flows. The CH equation model spinodal decomposition and phase separation in a binary alloy or fluid. Over a bounded domain $\Omega \subset \mathbb{R}^d$ (with $d = 2$ or $d = 3$), the Cahn-Hilliard energy functional is given by [4]

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

for any $\phi \in H^1(\Omega)$, where ε is a constant associated with the interface width. The CH equation is precisely the H^{-1} (conserved) gradient flow of the energy functional (1.1)

$$\phi_t = \Delta\mu, \quad \mu := \delta_\phi E = \phi^3 - \phi - \varepsilon^2 \Delta\phi. \tag{1.2}$$

Variations of the model may use non-constant mobilities or other free energy densities. For simplicity of presentation, we assume periodic boundary condition in this article, although an extension to other type boundary conditions, such as the homogeneous Neumann one, will be straightforward. Due to the gradient structure of (1.2), the following energy dissipation law holds:

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

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 periodic Neumann boundary conditions for μ. This property can be re-expressed as $(u(\,\cdot\,,t),1) = (u_0,1)$, for all $t \geq 0$.

The Cahn-Hilliard equation is a very important model 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, etc. The scientific challenge of the CH equation model is obvious, due to its fourth-order, nonlinear parabolic-type nature.

The energy stability of a numerical scheme has been a very important issue, since it plays an essential role in the accuracy of long time numerical simulation. There have been extensive existing numerical works with energy stability, in particular for first order and second order accurate (in time) schemes. Among the second order energy stable numerical schemes, the temporal discretization has been focused on either the Crank-Nicolson approximation [7, 17–20, 26–30] or the second order backward differentiation formula (BDF) one [13, 47]. Other than these numerical algorithms for the Cahn-Hilliard model, 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