Stabilized Crank-Nicolson/Adams-Bashforth Schemes for Phase Field Models

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Abstract. In this paper, stabilized Crank-Nicolson/Adams-Bashforth schemes are presented for the Allen-Cahn and Cahn-Hilliard equations. It is shown that the proposed time discretization schemes are either unconditionally energy stable, or conditionally energy stable under some reasonable stability conditions. Optimal error estimates for the semi-discrete schemes and fully-discrete schemes will be derived. Numerical experiments are carried out to demonstrate the theoretical results.

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Key words: Allen-Cahn equation, Cahn-Hilliard equation, Crank-Nicolson scheme, Adams-Bashforth scheme, implicit-explicit method, error estimates.

1. Introduction

In this paper, we consider numerical approximations for the Allen-Cahn equation

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta u - \frac{1}{\epsilon^2} f(u), & (x,t) \in \Omega \times (0,T], \\ \frac{\partial u}{\partial n} = 0, & (x,t) \in \partial \Omega \times (0,T], \\ u|_{t=0} = u_0(x), & x \in \Omega; \end{cases}$$
(1.1)

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and the Cahn-Hilliard equation

$$\begin{cases} \frac{\partial u}{\partial t} = \Delta \left(-\Delta u + \frac{1}{\epsilon^2} f(u) \right), & (x,t) \in \Omega \times (0,T], \\ \frac{\partial u}{\partial n}|_{\partial \Omega} = 0, & \frac{\partial \left(\Delta u - \frac{1}{\epsilon} f(u) \right)}{\partial n} = 0, & (x,t) \in \partial \Omega \times (0,T], \\ u|_{t=0} = u_0(x), & x \in \Omega. \end{cases}$$
(1.2)

In the above equations, u = u(x, t) represents the concentration of one of the two metallic components of the alloy and the parameter ϵ represents the interfacial width, which is small compared to the characteristic length of the laboratory scale. In addition, $u_0 : \Omega \rightarrow \mathscr{R}$ is a given initial function, Ω is a bounded domain in \mathscr{R}^d (d = 2, 3), $\partial \Omega$ denotes its boundary, n is the outward normal, T is a given time, and f(u) = F'(u) for a given energy potential F(u). The homogeneous Neumann boundary condition implies that no mass loss occurs across the boundary walls. An important feature of the Allen-Cahn and Cahn-Hilliard equations is that they can be viewed as the gradient flow of the Liapunov energy function

$$E(u) = \int_{\Omega} \left(\frac{1}{2} |\nabla u|^2 + \frac{1}{\epsilon^2} F(u) \right) dx \tag{1.3}$$

in L^2 -space and H^{-1} -space, respectively. By taking the inner product of Eq. (1.1) with $\Delta u + (1/\epsilon^2)f(u)$, the following energy law for Eq. (1.1) can be obtained:

$$\frac{\partial E(u(t))}{\partial t} = -\int_{\Omega} \left| -\Delta u + \frac{1}{\epsilon^2} f(u) \right|^2 dx .$$
 (1.4)

Similarly, the energy law for Eq. (1.2) is given by

$$\frac{\partial E(u(t))}{\partial t} = -\int_{\Omega} \left| \nabla (-\Delta u + \frac{1}{\epsilon^2} f(u)) \right|^2 dx .$$
 (1.5)

Eqs. (1.4) and (1.5) indicate that the free energy decreases monotonically with time. The Allen-Cahn equation was originally introduced to describe the motion of anti-phase boundaries in crystalline solids [1], and the Cahn-Hilliard equation was introduced to describe the complicated phase separation and coarsening phenomena in a solid [7]. The two boundary conditions also imply that the mixture cannot pass through the boundary walls. The Allen-Cahn and Cahn-Hilliard equations have been employed in many complicated moving interface problems in materials science and fluid dynamics — e.g. see [3–5, 8, 11, 23]). As the numerical simulations have been very useful, it is very important to develop accurate and efficient numerical schemes for these phase field models. Note that an essential feature of Eqs. (1.1) and (1.2) is that they must satisfy the energy laws (1.4) and (1.5) respectively, so it is worthwhile to design efficient and accurate numerical schemes that satisfy similar energy decay properties.