

A Linear Doubly Stabilized Crank-Nicolson Scheme for the Allen–Cahn Equation with a General Mobility

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Abstract. In this paper, a linear second order numerical scheme is developed and investigated for the Allen–Cahn equation with a general positive mobility. In particular, our fully discrete scheme is mainly constructed based on the Crank-Nicolson formula for temporal discretization and the central finite difference method for spatial approximation, and two extra stabilizing terms are also introduced for the purpose of improving numerical stability. The proposed scheme is shown to unconditionally preserve the maximum bound principle (MBP) under mild restrictions on the stabilization parameters, which is of practical importance for achieving good accuracy and stability simultaneously. With the help of uniform boundedness of the numerical solutions due to MBP, we then successfully derive H^1 -norm and L^∞ -norm error estimates for the Allen–Cahn equation with a constant and a variable mobility, respectively. Moreover, the energy stability of the proposed scheme is also obtained in the sense that the discrete free energy is uniformly bounded by the one at the initial time plus a constant. Finally, some numerical experiments are carried out to verify the theoretical results and illustrate the performance of the proposed scheme with a time adaptive strategy.

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1 Introduction

In this paper, we study numerical solution of the following Allen–Cahn equation with a

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general mobility $M(\phi) \geq M_0 > 0$:

$$\begin{cases} \frac{\partial \phi}{\partial t} = -M(\phi)(-\varepsilon^2 \Delta \phi + F'(\phi)), & (\mathbf{x}, t) \in \Omega \times (0, T], \\ \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), & \mathbf{x} \in \Omega, \end{cases} \quad (1.1)$$

which often arises from modeling of phase transitions and interfacial dynamics in materials science. Here, Ω is a bounded Lipschitz domain in \mathbb{R}^d ($d = 1, 2, 3$), $T > 0$ is the terminal time, $\phi(\mathbf{x}, t)$ is the unknown phase function, the positive parameter ε is called the diffuse interface width parameter, and $F(\phi) = \frac{1}{4}(1 - \phi^2)^2$ is the double-well potential function. We also assume that the problem is subject to suitable boundary conditions such as the homogeneous Neumann, the periodic, or the homogeneous Dirichlet boundary condition. The Allen–Cahn equation (1.1) can be viewed as the L^2 gradient flow of the energy

$$E(\phi) = \int_{\Omega} \left(\frac{\varepsilon^2}{2} |\nabla \phi|^2 + F(\phi) \right) d\mathbf{x}, \quad (1.2)$$

which leads to the dissipation of the free energy $E(\phi)$ over time, that is

$$\frac{d}{dt} E(\phi) = - \int_{\Omega} M(\phi) \mu^2 d\mathbf{x} \leq 0. \quad (1.3)$$

Another intrinsic property of the Allen–Cahn equation (1.1) is the maximum bound principle (MBP), i.e., if $|\phi(\mathbf{x}, 0)| \leq 1$ for all $\mathbf{x} \in \Omega$ then $|\phi(\mathbf{x}, t)| \leq 1$ for all $\mathbf{x} \in \Omega$ and $t \geq 0$, and one can refer to [33] for more discussions. To numerically investigate the Allen–Cahn equation (1.1), it is essentially important for the numerical schemes to preserve these physical properties in the discrete level, particularly the preservation of MBP, otherwise it could encounter the negativity of the mobility $M(\phi)$ which may lead to failing of the numerical schemes.

Over the past few decades, a great deal of works [9, 33, 36, 40, 41] has been devoted to developing structure-preserving time-stepping schemes for the Allen–Cahn equation, particularly for the models with constant mobility. Among the existing works, first order (in time) linear stabilized semi-implicit schemes combined with the central finite difference method for spatial discretization were proposed for the Allen–Cahn equation (1.1) in [36] and the generalized case with a advection term in [33]. These proposed schemes unconditionally preserve the discrete MBP in both cases and the energy stability in the constant mobility case. A nonlinear second-order Crank-Nicolson scheme for the space-fractional Allen–Cahn equation was developed in [17], in which the convex splitting approach was taken to deal with the nonlinear term. This scheme was proved to conditionally preserve the discrete MBP and the discrete energy dissipation law, and some corresponding error estimates were also obtained. A nonlinear two-step second-order backward differentiation formula (BDF2) scheme with nonuniform grids for the Allen–Cahn equation was studied in [29], in which the nonlinear term was treated fully implicitly. The MBP preservation and energy stability of the developed scheme were obtained under some