A SECOND-ORDER CONVEX SPLITTING SCHEME FOR A CAHN-HILLIARD EQUATION WITH VARIABLE INTERFACIAL PARAMETERS*

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Abstract

In this paper, the MMC-TDGL equation, a stochastic Cahn-Hilliard equation with a variable interfacial parameter, is solved numerically by using a convex splitting scheme which is second-order in time for the non-stochastic part in combination with the Crank-Nicolson and the Adams-Bashforth methods. For the non-stochastic case, the unconditional energy stability is obtained in the sense that a modified energy is non-increasing. The scheme in the stochastic version is then obtained by adding the discretized stochastic term. Numerical experiments are carried out to verify the second-order convergence rate for the non-stochastic case, and to show the long-time stochastic evolutions using larger time steps.

Mathematics subject classification: 65M06, 65M12, 65Z05.
Key words: Cahn-Hilliard equation, Second-order accuracy, Convex splitting, Energy stability.

1. Introduction

In this work, we consider a two-dimensional stochastic Cahn-Hilliard equation of the form

$$\frac{\partial \phi}{\partial t} = D\Delta \frac{\delta U(\phi)}{\delta \phi} + \varepsilon \xi(\boldsymbol{r}, t), \quad \boldsymbol{r} \in \Omega,\ t \in (0, T], \tag{1.1}$$

where $\Omega = (0, L_x) \times (0, L_y)$ and $\phi = \phi(\boldsymbol{r}, t)$ is the unknown function subject to the periodic boundary condition. $U(\phi)$ is the Ginzburg-Landau type energy functional of the form

$$U(\phi) = \int_\Omega \left(F(\phi) + \kappa(\phi)|\nabla \phi|^2 \right) \mathrm{d}\boldsymbol{r}, \tag{1.2}$$

where $F(\phi)$ is a potential and $\kappa(\phi)$ is the interfacial parameter weighting the gradient energy. The constant $D > 0$ is a diffusion coefficient, and the function $\xi(\boldsymbol{r}, t)$ is a stochastic term representing a kind of noise whose strength is scaled by $\varepsilon > 0$.

In the field of small molecules or polymer mixture systems, the phase transition process has attracted many theoretical and experimental studies [5, 14, 44]. Cahn-Hilliard dynamics, namely (1.1) with $\varepsilon = 0$, proposed by Cahn and Hilliard [4], turns out to be one of the most suitable models for simulating phase transitions of a uniform thermodynamic system [15]. Here, ϕ represents the concentration of one of the components of the mixture (or sometimes, the difference between the concentrations of the two components of a binary mixture [13]). To consider the random disturbance in the system, the stochastic term $\xi(\boldsymbol{r}, t)$ is added into the equation by Cook [7]. In physics, the stochastic term ξ, treated as random force, reflects the thermal disturbance caused by the chaos motion of molecules, and is required to satisfy the fluctuation-dissipation theorem [5, 19]

$$\mathbb{E}[\xi(\boldsymbol{r}_1, t_1)\xi(\boldsymbol{r}_2, t_2)] = -2D\Delta\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)\delta(t_1 - t_2), \tag{1.3}$$

where $\mathbb{E}$ represents the mathematical expectation operator. The Laplacian in (1.3) expresses the conservation law for the field [17]. A random force component which piles up matter at one site must be exactly balanced by force contributions at neighboring sites which deplete those sites of matter.

In mathematics, the analytical and numerical studies on the stochastic Cahn-Hilliard equation (1.1), also called Cahn-Hilliard-Cook equation, have been investigated by many authors. The existence and regularity of the solutions are proved under some certain conditions [8, 31]. One of the applications of the stochastic Cahn-Hilliard equations is the nucleation and phase transition of the polymer mixtures. In [3], the nucleation is explained by the stochastically driven exit in the limit of small noise intensity from the domain of attraction of an asymptotically stable homogeneous equilibrium state for the associated deterministic model. The process of nucleation by formal arguments using two spatial scales and two temporal scales is described in [2]. In addition, the numerical simulation of the phase transition attracts many attentions. In [17], a class of finite difference schemes are presented and compared with each other for simulating the nucleation in one-, two- and three-dimensional cases. Mesforush et al present the error estimates of the finite element approximations to the Cahn-Hilliard-Cook equation and its linearized version [20, 21]. Spinodal decomposition of binary alloys is studied via Monte-Carlo simulation in [29], considering a two-dimensional system at critical concentration. The so-called string method is adopted to calculate the minimal energy path connecting two metastable states in both one- and two-dimensional cases in [25, 47].

The form of the potential $F(\phi)$ depends on the considered systems. For the phase separation of the small molecules or atomic systems consisting of two components, $F(\phi)$ is usually chosen as a quartic double-well potential function

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2, \tag{1.4}$$

where ϕ represents the difference between the concentrations of the two components, and the coefficient $\kappa(\phi)$ is often considered as a positive constant. For the studies of spinodal decomposition in polymer blends, Flory and Huggins developed a lattice theory and gave the Flory-Huggins free energy [11]

$$F(\phi) = \frac{\phi}{N_{\mathrm{A}}}\ln\phi + \frac{1-\phi}{N_{\mathrm{B}}}\ln(1-\phi) + \chi\phi(1-\phi), \tag{1.5}$$

where ϕ is the concentration of the polymer A, N_{A} and N_{B} represent the degree of polymerization of the polymer A and B, respectively, and χ is the Huggins interaction parameter. It is noted in [14] that the gradient energy contribution for the polymer mixtures should be weighted