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An adaptive time-stepping strategy for solving the phase field crystal model

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ABSTRACT

In this work, we will propose an adaptive time step method for simulating the dynamics of the phase field crystal (PFC) model. The numerical simulation of the PFC model needs long time to reach steady state, and then large time-stepping method is necessary. Unconditionally energy stable schemes are used to solve the PFC model. The time steps are adaptively determined based on the time derivative of the corresponding energy. It is found that the use of the proposed time step adaptivity cannot only resolve the steady state solution, but also the dynamical development of the solution efficiently and accurately. The numerical experiments demonstrate that the CPU time is significantly saved for long time simulations.

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1. Introduction

The phase field crystal (PFC) model was recently proposed in [4,5] to study the nonequilibrium microstructure formation by introducing a free energy functional of the local-time-averaged density field. It is a conservative form of the familiar, nonconserved, Swift–Hohenberg (SH) equation [17]. This model addresses the crystal formation at the atomic scale in space but on a coarse-grained diffusive time scale, which is a significant advantage over other atomistic methods where the time steps are constrained by atomic-vibration time scales. The model can account for elastic and plastic deformations, multiple crystal orientations, and many other observable phenomena, see, e.g., [12], for a recent review.

Consider a dimensionless energy of the form [4,17]

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

where the domain $\Omega \subset R^D$, $\phi : \Omega \to R$ is the density field, ϵ is a constant assumed to be less than 1, and ∇ and Δ are the gradient and Laplacian operators, respectively. Suppose that $\Omega = (0, L_x) \times (0, L_y)$ and that ϕ and $\Delta\phi$ are periodic on Ω.

We consider two types of gradient dynamics on Ω:

(i) Nonconserved dynamics (SH)

$$\partial_t \phi = -M(\phi)\mu \tag{1.2}$$

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where $M(\phi) > 0$ is a mobility, μ is the chemical potential defined as

$$\mu := \delta_\phi E = \phi^3 + (1-\epsilon)\phi + 2\Delta\phi + \Delta^2\phi, \tag{1.3}$$

and $\delta_\phi E$ denotes the variational derivative with respect to ϕ, and

(ii) Conserved dynamics (PFC)

$$\partial_t \phi = \nabla \cdot (M(\phi)\nabla\mu). \tag{1.4}$$

Because the dynamical equations are of gradient type, it is easy to see that the energy (1.1) is nonincreasing in time along the solution trajectories of either (1.2) or (1.4). Eq. (1.2) is referred to as the Swift–Hohenberg (SH) equation and is fourth-order in space. Eq. (1.4) is the phase field crystal (PFC) equation and is sixth-order in space.

The SH equation and the PFC equation are high order nonlinear partial differential equations. They cannot generally be solved analytically. Therefore, efficient numerical algorithms are essential in the computer simulations. The standard explicit Euler scheme is known to be unstable for the time step Δt above the threshold fixed by the lattice spacing Δx; more precisely, Δt should be proportional to $(\Delta t)^4$ for the SH equation and $(\Delta t)^6$ for the PFC equation. It is very time-consuming for long time simulations. In [1], a backward Euler scheme was presented with the linearized discretization $3(\phi^k)^2\phi^{k+1} - 2(\phi^k)^3$ for the nonlinear term ϕ^3. Although the stability analysis was not given, it was claimed that relatively large time steps can be achieved. A linear splitting scheme was proposed in [2] for the PFC equation. Three parameters are involved to control the degree of the splitting. By applying the standard Fourier stability analysis, the constraints on these parameters are obtained which help to yield an unconditionally stable difference scheme. Similar schemes have been used for the numerical simulations of a nonlinear epitaxial growth model [13], and the Cahn–Hilliard (CH) and Allan–Cahn (AC) equations [19]. All these schemes are linearized difference schemes. The unique solvability and convergence of the numerical solution can be achieved. However, the energy stability has not been considered, which attracts more attentions from the application point of view for the SH and PFC equations.

Eyre [7] exploited a convex splitting of the energy functional method to study the unconditionally energy stable time discretization of the Cahn–Hilliard equation. This method has been extensively used for a variety of gradient flow problems, see e.g., [15,20–22] and their reference therein. Recently, a one-step first order nonlinear difference scheme has been presented in [23] for the PFC equation. The unconditionally energy stability $E(\phi^{k+1}) \leqslant E(\phi^k)$ was proved by the convex splitting of the energy functional. Under the same theoretical framework, a second order nonlinear scheme was proposed in [9]. In stead of the unconditionally energy stability, an unconditionally weak energy stability $E(\phi^{k+1}) \leqslant E(\phi^0)$ was proved. The unconditionally unique solvability and discrete mass conservation were also given in [9,23]. An alternate approach to these energy stable nonlinear convex splitting schemes for the SH and PFC equations is the conditionally energy stable linear splitting scheme as was suggested in [24] for a molecular beam epitaxial (MBE) equation and in [8] for the CH equation. This would involve the splitting parameters which should be chosen sufficiently large to ensure the energy stability. However, these parameters depend on the unknown solutions as shown in [8,9,24].

In this paper, we will first present the energy identity results for the SH and PFC equations which reveal the energy dissipation property. A first order and a second order nonlinear one-step difference schemes will be employed. The unconditionally energy stability can be derived by using the discrete Green's formula and Cauchy–Schwartz inequality for the first order scheme, which is a different approach of the analysis as that in [23]. For the proposed second order scheme, it uses a special combination of the nonlinear term, which has been used to construct unconditionally energy stable schemes for the CH equation in [3,6]. It will be shown that with this approach, not only the decay properties are preserved for the discrete energy, the discrete energy identities can also hold for the SH and PFC equations. These energy stable schemes allow large time steps, and therefore are very useful for long time simulations. To further improve the efficiency of our method, we are going to propose an adaptive time-stepping strategy. Adaptive time stepping has been well studied for solving initial value problems in ODEs. Söderlind [16] reviewed some time step control methods for local time adaptivity based on linear feedback theory. In [11], two adaptive time methods are compared with constant time steps for coupled flow and deformation models. In their work, the pore pressure method is an inexpensive adaptive method whose behavior closely follows the physics of the problem, while the local error method is more time-consuming at each time step because feedback steps may be involved. In [18], a locally varying time step method was developed for solving hyperbolic conservative PDEs. At the same time level, the large time step is adopted in the domain with smooth solutions, while the small time step is taken in the region with nearly singular solutions. In this work, our adaptive time-stepping technique will be developed based on the energy variation which is an important physical quantity in the SH and PFC model. This adaptive time-stepping strategy was introduced in [14] and was also successfully applied in the simulations of the Cahn–Hilliard equation in [25]. The small time steps will be adopted when the energy has a quick decay and large time steps will be used when the energy decays slowly. It can be observed in the numerical simulations that this adaptive time-stepping strategy can greatly save the CPU time without losing the accuracy.

This paper is organized as follows. In Section 2, we construct two unconditionally energy stable implicit finite difference schemes for solving the SH and PFC equations. An adaptive time-stepping technique is proposed in Section 3, where the adaptive time step is determined based on the variation of the energy. Numerical experiments are presented in Section 4, and some concluding remarks are given in the final section.

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