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Convergence analysis and numerical implementation of a second order numerical scheme for the three-dimensional phase field crystal equation

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ABSTRACT

In this paper we analyze and implement a second-order-in-time numerical scheme for the three-dimensional phase field crystal (PFC) equation. The numerical scheme was proposed in Hu et al. (2009), with the unique solvability and unconditional energy stability established. However, its convergence analysis remains open. We present a detailed convergence analysis in this article, in which the maximum norm estimate of the numerical solution over grid points plays an essential role. Moreover, we outline the detailed multigrid method to solve the highly nonlinear numerical scheme over a cubic domain, and various three-dimensional numerical results are presented, including the numerical convergence test, complexity test of the multigrid solver and the polycrystal growth simulation.

1. Introduction

Defects, such as vacancies, grain boundaries, and dislocations, are observed in crystalline materials, and a precise and accurate understanding of their formation and evolution is of great interest. The phase field crystal (PFC) model was proposed in [1] as a new approach to simulate crystal dynamics at the atomic scale in space but on diffusive scales in time. This model naturally incorporates elastic and plastic deformations, multiple crystal orientations and defects and has already been used to simulate a wide variety of microstructures, such as epitaxial thin film growth [2], grain growth [3], eutectic solidification [4], and dislocation formation and motion [3,5]. The idea is that the phase variable describes a coarse-grained temporal average of the number density of atoms, and the approach can be related to dynamic density functional theory [6,7]. The method represents a significant advantage over other atomistic methods, such as molecular dynamics methods where the time steps are constrained by atomic-vibration time scales. More detailed descriptions are available in [3,8,9], and the related works for the amplitude expansion approach could be found in [8,10].

Consider the dimensionless energy of the form [1,2,11]:

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

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where $\Omega = (0, L_x) \times (0, L_y) \times (0, L_z) \subset \mathbb{R}^3$, $\phi : \Omega \to \mathbb{R}$ is the atom density field, and $\varepsilon > 0$ is a constant. We assume that ϕ is periodic on Ω. The PFC equation [1,2] is given by the H^{-1} gradient flow associated with the energy (1.1):

$$\begin{aligned} &\phi_t = \nabla \cdot (M(\phi)\nabla\mu), \quad \text{in } \Omega_T = \Omega \times (0, T), \\ &\mu = \delta_\phi E = \phi^3 + (1-\varepsilon)\phi + 2\Delta\phi + \Delta^2\phi, \quad \text{in } \Omega_T, \\ &\phi(x, y, z, 0) = \phi_0(x, y, z), \quad \text{in } \Omega. \end{aligned} \tag{1.2}$$

in which $M(\phi) > 0$ is a mobility and μ is the chemical potential. Periodic boundary conditions are imposed for $\Delta\phi$ and μ.

The PFC equation is a high-order (sixth-order) nonlinear partial differential equation. Regarding the PDE analysis, existence and uniqueness of a global-in-time strong solution and smooth solution for the modified phase field crystal (MPFC) equation – which generalizes the PFC equations and includes a second order temporal derivative $\beta\phi_{tt}$ – has been established in a recent work [12]. In more detail, it was proved that, for any H^m ($m \geq 3$) initial data (for the phase variable ϕ), there is an H^m estimate for the solution at any time $T > 0$, so that a global-in-time strong solution and smooth solution is available, dependent on the regularity of the initial data. Such an analysis could be easily extended to the case with $\beta = 0$, corresponding to the parabolic PFC equation. Therefore, one could always assume the existence and uniqueness of the solution for the PFC equation (1.2), if the initial data has a regularity of at least H^3.

There have been some related works to develop numerical schemes for the PFC equation. Cheng and Warren [13] introduced a linearized spectral scheme, similar to one for the Cahn–Hilliard equation analyzed in [14]. This scheme is not expected to be provably unconditionally energy stable. The finite element PFC method of Backofen et al. [6] employs what is essentially a standard backward Euler scheme, but where the nonlinear term ϕ^3 in the chemical potential is linearized via $(\phi^{k+1})^3 \approx 3(\phi^k)^2\phi^{k+1} - 2(\phi^k)^3$. Both energy stability and solvability are issues for this scheme, because the term $2\Delta\phi$ is implicit in the chemical potential. Tegze et al. [15] developed a semi-implicit spectral scheme for the binary PFC equations that is not expected to unconditionally stable. Also see other related numerical works [16–19] in recent years.

The energy stability of a numerical scheme has always been a very important issue, since it plays an essential role in the accuracy of long time numerical simulation. The standard convex splitting scheme, originated from Eyre's work [20], has been a well-known approach to achieve numerical energy stability. In this framework, the convex part of the chemical potential is treated implicitly, while the concave part is updated explicitly. A careful analysis leads to the unique solvability and unconditional energy stability of the numerical scheme, unconditionally with respect to the time and space step sizes. Such an idea has been applied to a wide class of gradient flows in recent years, and both first and second order accurate in time algorithms have been developed. See the related works for the PFC equation and the modified PFC (MPFC) equation [12,21–27].

On the other hand, a well-known drawback of the first order convex splitting approach is that an extra dissipation has been added to ensure unconditional stability; in turn, the first order numerical approach introduces a significant amount of numerical error [28]. For this reason, second-order energy stable methods have been highly desirable.

There have been other related works of "energy stable" schemes for the certain gradient flows in recent years. For example, an alternate variable is used in [29], denoted as a second order approximation to $v = \phi^2 - 1$ in the Cahn–Hilliard model. A linearized, second order accurate scheme is derived as the outcome of this idea, and the stability is established for a modified energy. A similar idea has been applied to the PFC model in a more recent article [30]. However, such an energy stability is applied to a pair of numerical variables (ϕ, v), and an H^2 stability for the original physical variable ϕ has not been justified. As a result, the convergence analysis is not available for this numerical approach. Similar methodology has been reported in the invariant energy quadratization (IEQ) approach [31–33], etc.

In comparison, a second order numerical scheme was proposed and studied for the PFC equation in [21]. By a careful choice of the second order temporal approximations to each term in the chemical potential, the unique solvability and unconditional energy were justified at a theoretical level, with the centered difference discretization taken in space. In particular, this energy stability is derived with respect to the original energy functional, combined with an auxiliary, non-negative correction term, so that a uniform in time H^2 bound is available for the numerical solution. Meanwhile, a detailed convergence analysis has not been theoretically reported for the proposed second order scheme, although the full convergence order was extensively demonstrated in the numerical experiments. The key difficulty in the convergence analysis is associated with the maximum norm bound estimate for the numerical solution, and such a bound plays an essential role in the theoretical convergence derivation. In more details, the unconditional energy stability indicates a uniform in time H^2 bound of the numerical solution at a discrete level. Although the Sobolev embedding from H^2 to L^∞ is straightforward in three-dimensional space, a direct estimate for the corresponding grid function is not directly available. In two-dimensional space, such a discrete Sobolev embedding has been proved in the earlier works [21,27], using complicated calculations of the difference operators. However, as stated in Remark 12 of [21], *"the proof presented in* [27] *does not automatically extend to three dimensions. This is because a discrete Sobolev inequality is used to translate energy stability into point-wise stability, and the inequality fails in three dimensions. We are currently studying the three dimensional case in further detail"*.

In this paper, we provide a detailed convergence analysis for the fully discrete scheme formulated in [21], which is shown to be second order accurate in both time and space. In particular, the maximum norm estimate of the three-dimensional numerical solution is accomplished via a discrete Fourier transformation over a uniform numerical grid, so that the discrete Parseval equality is valid. And also, the equivalence between the discrete and continuous H^2 norms for the numerical grid function and its continuous version, respectively, can be established. In turn, the discrete Sobolev inequality is obtained from its continuous version. Such an ℓ^∞ bound of the discrete numerical solution is crucial, so that the convergence analysis

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