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A semi-analytical Fourier spectral method for the Allen–Cahn equation

Hyun Geun Lee [a], June-Yub Lee [b,*]

[a] Institute of Mathematical Sciences, Ewha Womans University, Seoul 120-750, Republic of Korea
[b] Department of Mathematics, Ewha Womans University, Seoul 120-750, Republic of Korea

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ABSTRACT

In recent years, Fourier spectral methods have been widely used as a powerful tool for solving phase-field equations. To improve its effectiveness, many researchers have employed stabilized semi-implicit Fourier spectral (SIFS) methods which allow a much larger time step than a usual explicit scheme. Our mathematical analysis and numerical experiments, however, suggest that an effective time step is smaller than a time step specified in the SIFS schemes. In consequence, the SIFS scheme is inaccurate for a considerably large time step and may lead to incorrect morphologies in phase separation processes. In order to remove the time step constraint and guarantee the accuracy in time for a sufficiently large time step, we present a first and a second order semi-analytical Fourier spectral (SAFS) methods for solving the Allen–Cahn equation. The core idea of the methods is to decompose the original equation into linear and nonlinear subequations, which have closed-form solutions in the Fourier and physical spaces, respectively. Both the first and the second order methods are unconditionally stable and numerical experiments demonstrate that our proposed methods are more accurate than the stabilized semi-implicit Fourier spectral method.

1. Introduction

The phase-field method has recently emerged as a powerful computational approach for modeling and predicting mesoscale morphological and microstructure evolution in materials. This method replaces sharp interfaces by thin but nonzero thickness transition regions where the interfacial forces are smoothly distributed [1]. The basic idea is to introduce conserved or non-conserved order parameters ϕ that vary continuously over thin interfacial layers and are mostly uniform in the bulk phases. The temporal and spatial evolution of the order parameters is governed by the Cahn–Hilliard equation [2–10] or the Allen–Cahn (AC) equation [11–15]. The most significant computational advantage of the phase-field method is that an explicit tracking of the interface is unnecessary.

Numerous numerical algorithms have been developed to improve the accuracy and numerical stability of the phase-field method. There are two types of approaches to achieve high spatial accuracy. One is the adaptive mesh refinement method [16–18] in which additional grid points are placed in regions where the order parameters have large gradients, and the other is the Fourier spectral method [19–30] which uses a spectral representation of a continuous spatial profile of the order parameter. The Fourier spectral method is good for evaluating spatial derivatives since the differential operators are

* Corresponding author.
E-mail address: jyllee@ewha.ac.kr (J.-Y. Lee).

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represented in the transform space by diagonal matrices that are trivially inverted. Here, we focus on the Fourier spectral method.

To improve the effectiveness of the Fourier spectral method, many researchers have employed stabilized semi-implicit schemes [21,23,24,26,28–30] for the time variable, in which the principal elliptic operator is treated implicitly to reduce the associated stability constraint, while the nonlinear term is still treated explicitly to avoid the expensive process of solving nonlinear equations at each time step [19]. And an extra stabilizing term is added to improve the stability while preserving the simplicity. Stabilized semi-implicit schemes alleviate the time step restriction of explicit schemes, i.e., enable us to use a considerably large time step. But, we observed, through both mathematical analysis and numerical examples, that if we use a large time step, then an effective time step becomes smaller than a time step specified in the stabilized semi-implicit scheme. (Cheng and Rutenberg [31] also pointed out this problem.) In consequence, the stabilized semi-implicit scheme is inaccurate, leading to incorrect morphologies in phase separation processes.

To allow the use of a sufficiently large time step with neither loss of accuracy nor technical difficulty, we present a first and a second order (in time) semi-analytical Fourier spectral methods for solving the AC equation. A core idea of this method is to decompose the original equation into linear and nonlinear subequations, which have closed-form solutions in the Fourier and physical spaces, respectively. In particular, our method requires no additional computational cost and is unconditionally stable in the sense that the solution remains to be bounded for all time regardless of the time step size. It can be used to solve various modified forms of the AC equation such as crystal growth [32,33], grain growth [34–36], and image analysis [37–44].

This paper is organized as follows. In Section 2, we present a first order semi-analytical Fourier spectral method for the AC equation and prove the unconditional stability of this method. We present numerical experiments of the first order stabilized semi-implicit and semi-analytical schemes in Section 3. In Section 4, we introduce the second order stabilized semi-implicit and semi-analytical schemes, and present numerical experiments of both schemes. Conclusions are drawn in Section 5.

2. A semi-analytical Fourier spectral method

We consider the AC equation in two-dimensional space:

$$\frac{\partial \phi(\mathbf{x},t)}{\partial t} = \frac{\phi(\mathbf{x},t) - \phi^3(\mathbf{x},t)}{\epsilon^2} + \Delta\phi(\mathbf{x},t), \quad \mathbf{x} \in \Omega,\ 0 < t \le T, \tag{1}$$

where $\mathbf{x} = (x_1, x_2)$ is a point inside a rectangular domain $\Omega = (0, L_1) \times (0, L_2)$. The boundary condition is the zero Neumann boundary condition:

$$\nabla\phi \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega, \tag{2}$$

where $\mathbf{n}$ is the unit normal vector to $\partial\Omega$. Instead of using a finite difference approximation, we propose using a Fourier spectral approximation to the AC equation. To solve the AC equation with the boundary condition (2), we employ the discrete cosine transform [45]: for $k_1 = 0, \ldots, N_1 - 1$ and $k_2 = 0, \ldots, N_2 - 1$,

$$\widehat{\phi}_{k_1k_2} = \alpha_{k_1}\beta_{k_2} \sum_{l_1=0}^{N_1-1} \sum_{l_2=0}^{N_2-1} \phi_{l_1l_2} \cos\left[\frac{\pi}{N_1} k_1 \left(l_1 + \frac{1}{2}\right)\right] \cos\left[\frac{\pi}{N_2} k_2 \left(l_2 + \frac{1}{2}\right)\right],$$

where $\alpha_0 = \sqrt{1/N_1}$, $\beta_0 = \sqrt{1/N_2}$, $\alpha_{k_1} = \sqrt{2/N_1}$, $\beta_{k_2} = \sqrt{2/N_2}$ if $k_1, k_2 \ge 1$, and $\phi_{l_1l_2} = \phi\left(\frac{L_1}{N_1}\left(l_1 + \frac{1}{2}\right), \frac{L_2}{N_2}\left(l_2 + \frac{1}{2}\right)\right)$. Then, Eq. (1) can be transformed into a set of ordinary differential equations in the cosine space:

$$\frac{\partial \widehat{\phi}_{k_1k_2}}{\partial t} = \frac{\widehat{\phi}_{k_1k_2} - \widehat{\phi^3}_{k_1k_2}}{\epsilon^2} + A_{k_1k_2}\widehat{\phi}_{k_1k_2}, \tag{3}$$

where $A_{k_1k_2} = -\pi^2\left[\left(\frac{k_1}{L_1}\right)^2 + \left(\frac{k_2}{L_2}\right)^2\right]$.

An Explicit Fourier Spectral (ExFS) method is to approximate (3) by

$$\widehat{\phi}^{n+1}_{k_1k_2} = \widehat{\phi}^{n}_{k_1k_2} + \Delta t\left(\frac{\widehat{\phi}^{n}_{k_1k_2} - \widehat{(\phi^n)^3}_{k_1k_2}}{\epsilon^2} + A_{k_1k_2}\widehat{\phi}^{n}_{k_1k_2}\right). \tag{4}$$

This method offers excellent spatial accuracy, but it is only first order accurate in time and suffers from the severe time step restriction for stability. To overcome this problem, many researchers have used the first order stabilized Semi-Implicit Fourier Spectral (SIFS) method [26,28,29]:

$$\left(1 - \Delta t A_{k_1k_2} + \frac{S\Delta t}{\epsilon^2}\right)\widehat{\phi}^{n+1}_{k_1k_2} = \widehat{\phi}^{n}_{k_1k_2} + \Delta t\frac{(S+1)\widehat{\phi}^{n}_{k_1k_2} - \widehat{(\phi^n)^3}_{k_1k_2}}{\epsilon^2}, \tag{5}$$