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Application of locally one-dimensional semi-implicit scheme in phase-field equations

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ABSTRACT

A locally one-dimensional (LOD) semi-implicit scheme is proposed for improving the numerical efficiency in the solving of parabolic partial differential equations in phase-field simulations. With LOD splitting, multi-dimensional parabolic problems can be numerically approximated by treating each of the spatial variables individually in single cycles. Additionally, each spatial variable can be treated in either real or Fourier space, allowing equations to be solved across a range of boundary conditions, including periodic, non-periodic, and even partial periodic. The proposed LOD semi-implicit scheme exhibits noticeable advantages over both explicit and implicit traditional schemes in terms of computational efficiency and accuracy, as demonstrated by two standard numerical tests. It is anticipated that future large-scale phase-field simulations will benefit greatly from the use of this LOD scheme.

1. Introduction

In the past several decades, the phase-field method has been emerged as a powerful tool for simulating the microstructure evolution processes of various materials [1–5]. In particular, the assumption of diffuse interface in the phase-field method allows explicit tracking of interfaces positions to be avoided, a feat that is difficult to achieve with sharp-interface models in two-dimensional (2-D) and three-dimensional (3-D) simulations. Another advantage of the phase-field method lies in its description of the non-equilibrium state in general, which has resulted in its being widely employed throughout the materials community. Application of the phase-field method has recently broadened even further due to the development of phase-field model with finite interface dissipation [6–8]. This model can be used with various kinetic processes at the mesoscopic scale without being restricted to a specific type of transformation, extending its application range from chemical equilibrium to strongly non-equilibrium phase transformations.

In typical phase-field models, a given system is described using a set of field variables. The temporal evolution of these field variables is governed by partial differential equations (PDEs), such as the Ginzburg–Landau [9] and Cahn–Hilliard equations [10]. Because such PDEs are usually nonlinear, they can be only solved numerically. The classical forward-Euler (FE) finite-difference (FD) method is most commonly employed in phase-field simulations, with FE used for time and FD for space, because in most cases, it can be easily coded. In order to guarantee the stability of the numerical solutions obtained with the classical FE–FD method, the time step Δt is constrained by the space step Δx [11]. This extremely limits simulation efficiency, especially when the PDEs have coefficients of different orders of magnitude. Such constraint can be avoided using the implicit FD scheme, but in 2-D and 3-D cases this leads to a large band matrix, which in turn requires researchers with specific skill sets of computer for storage and operation of such matrix.

In order to improve the efficiency and accuracy of phase-field simulations, a number of advanced numerical schemes have been developed to replace the classical FE–FD method. These include the semi-implicit Fourier-spectral (FS) scheme [12,13], which ensures higher accuracy through exponential convergence, and the FFTW (the Faster Fourier Transform in the West) library [14], which operates at a higher efficiency. However, the semi-implicit FS scheme can be only employed with periodic boundary conditions, and thus lacks universal application. Using a more general Legendre or Chebyshev transform instead of a Fourier transform, semi-implicit spectral schemes can accommodate Dirichlet, Neumann, or mixed boundary conditions [2,15,16]. Unfortunately, this also prevents wide application in the phase-field community, as both Legendre and Chebyshev transforms are more complicated than the Fourier transform.

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Consequently, we propose a numerical scheme for phase-field modeling based on so-called locally one-dimensional (LOD) splitting [17] that is both accurate and efficient. LOD is an operator splitting method, that splits multi-dimensional problems into multiple one-dimensional problems. A significant and well-known advantage of such splitting methods in the construction of implicit FD schemes in 2-D and 3-D cases is that large band matrices can be avoided. In fact as early as in 1955, the ADI (alternating direction implicit) method, based on the strategy of operator splitting, was proposed for solving parabolic and elliptic PDEs [18]. More than half a century later, ADI, LOD, and their variants have been widely used to solve parabolic, elliptic, and hyperbolic PDEs. The major difference between LOD and ADI is how the operator is split, for example, the Laplacian. It has been found LOD splitting solves parabolic PDEs in a way that enables each step to be treated in Fourier space with ease, meaning that each spatial variable can be treated in either real or Fourier space depending on the boundary conditions. If the periodic boundary condition is set along the X direction, then the semi-implicit FS scheme can be used for the variable along the X direction. Thus, a scheme that combines LOD splitting with a semi-implicit FS method can solve parabolic PDEs in phase-field simulations with greater computational efficiency and accuracy than traditional scheme.

In next section, we present a numerical scheme for phase-field modeling based on the LOD splitting and semi-implicit methods and discuss different cases, such as constant and variable coefficients in parabolic PDEs. In Section 3, the advanced features of the proposed scheme are demonstrated using two standard numerical tests: the standard Fick's diffusion equation and a phase-field simulation of the coarsening and ripening processes of a Si–As alloy. Finally, a summary of the conclusions is given.

2. A locally one-dimensional semi-implicit scheme

In a typical phase-field model, there are two types of parabolic PDEs, which can be represented by the following formulae, provided here in a 2-D scheme for simplicity:

$$\frac{\partial u(x,y,t)}{\partial t} = a\nabla^2 u + f, \tag{1}$$

and

$$\frac{\partial u(x,y,t)}{\partial t} = \nabla(a\nabla u) + f, \tag{2}$$

where $t \in [0, +\infty]$ and $(x, y) \in \Omega$. Ω is a bounded rectangular region in $\Re^2$ with a boundary of $\partial\Omega$. The unknown $u(x, y, t)$ can be replaced by either the phase-field or concentration variable. $a(u)$ is a positive coefficient and $f(u)$ represents the remaining source term.

In a general case, we can assume that $\Omega = [0, 1] \times [0, 1]$. The system has a Dirichlet condition along the X direction with a periodic condition along the Y direction. The initial and boundary conditions are then expressed as

$$\begin{aligned} &I.C. \quad u(x,y,0) = u_0(x,y), \\ &B.C. \quad u(0,y,t) = u_l(y), \quad u(1,y,t) = u_r(y) \\ &\qquad u(x,0,t) = u(x,1,t), \end{aligned} \tag{3}$$

where $u_0(x, y)$, $u_l(y)$, and $u_r(y)$ are the given functions. The rectangular region Ω can be divided into $(N_x+2)(N_y+2)$ points. (N_x+2) (or (N_y+2)) and Δx (or Δy) are the number of grids and the space step along the X (or Y) directions. The time step is labeled as Δt. In addition, $R = \Delta t/(\Delta x)^2$, $t^k = k\Delta t$, $u_{i,j} = u(i\Delta x, j\Delta y, t)$ and $u^k_{i,j} = u(i\Delta x, j\Delta y, k\Delta t)$ will be used in this paper.

To clearly demonstrate the proposed numerical scheme, we start the simplest case for Eqs. (1) and (2): that is, when the coefficient a is a constant. In fact, in this case, Eq. (2) is reduced to Eq. (1).

2.1. The locally one-dimensional splitting

With LOD splitting, spatial variables in the multi-dimensional parabolic problems can be individually treated in single cycles [19]. Its contractivity, [20] and unconditional convergence [21] in solving parabolic initial–boundary value problems have been proven mathematically. By means of LOD splitting, we can begin by using the following symmetry fractional step procedures:

$$\frac{1}{2}\frac{\partial u}{\partial t} = a\frac{\partial^2}{\partial x^2}u + \frac{1}{2}f, \quad t \in [t^k, t^{k+1/2}] \tag{4}$$

and

$$\frac{1}{2}\frac{\partial u}{\partial t} = a\frac{\partial^2}{\partial y^2}u + \frac{1}{2}f \quad t \in [t^{k+1/2}, t^{k+1}]. \tag{5}$$

Due to the different boundary conditions along the X and Y directions, Eqs. (4) and (5) can be treated differently. Thus, for Eq. (4), we employ the FD approximation directly on its right-hand side, as such:

$$\frac{1}{2}\frac{\partial u_{i,j}}{\partial t} = \frac{a}{(\Delta x)^2}(u_{i+1,j} + u_{i-1,j} - 2u_{i,j}) + \frac{1}{2}f_{i,j}. \tag{6}$$

Due to the periodic boundary condition along the Y direction, Eq. (5) can be treated in Fourier space, such that

$$\frac{1}{2}\frac{\partial \widetilde{u}_{i,j}}{\partial t} = -ag_j^2 \cdot \widetilde{u}_{i,j} + \frac{1}{2}\widetilde{f}_{i,j}. \tag{7}$$

where $\widetilde{u}_{i,j}$ and $\widetilde{f}(u_{i,j})$ represent the one-dimensional Fourier transforms (for variable y) of $u_{i,j}$ and $f(u_{i,j})$, respectively. g_j is a one-dimensional vector in the corresponding Fourier space.

Let I represent the imaginary unit, and the definition of above-mentioned Fourier transform and its inverse transform can then be given by

$$\widetilde{u}_{i,j}(x, g_j) = \int_{-\infty}^{+\infty} u_{i,j}(x,y)e^{-2\pi I\cdot g_j\cdot y}dy, \tag{8}$$

and

$$u_{i,j}(x,y) = \int_{-\infty}^{+\infty} \widetilde{u}_{i,j}(x,g_j)e^{-2\pi I\cdot g_j\cdot y}dg_j. \tag{9}$$

Though periodic boundary conditions can also be dealt with using the FD treatment, using LOD splitting allows us to apply the FS method in the direction with the periodic boundary condition, which improves both computational accuracy and efficiency to a considerable degree.

2.2. The semi-implicit method

As described above, through LOD splitting, the multi-dimensional problem has been transformed into multiple one-dimensional problems. Subsequently, implicit treatment is still needed to eliminate the limitation of the constraint between time and space steps and thus improve computational efficiency. Commonly used implicit methods include the backward-Euler (BE) and the Crank–Nicolson (CN) methods. The CN method, which provides the second-order convergence in time, is the equal weight combination of both the FE and BE methods, which only provide the first-order convergence. Thus, we will construct CN formats for iteration as far as possible.

Unfortunately, completely implicit methods are usually nonlinear and thus unsolvable due to the nonlinearity of the source term $f(u)$. To obtain a solvable scheme, implicit method can be adapted into a semi-implicit one. This strategy is generally achieved by treating the source term as a constant in the single cycles $t \in [t^k, t^{k+1}]$.