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A second order operator splitting method for Allen–Cahn type equations with nonlinear source terms

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HIGHLIGHTS

- The proposed operator splitting method is second order accurate and stable.
- The method can be easily applicable to wide class of Allen–Cahn type equations with non-linear source terms.
- Simulations for multi-component phase separation and dendrite growth show the feasibility of the method.

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ABSTRACT

Allen–Cahn (AC) type equations with nonlinear source terms have been applied to a wide range of problems, for example, the vector-valued AC equation for phase separation and the phase-field equation for dendritic crystal growth. In contrast to the well developed first and second order methods for the AC equation, not many second order methods are suggested for the AC type equations with nonlinear source terms due to the difficulties in dealing with the nonlinear source term numerically. In this paper, we propose a simple and stable second order operator splitting method. A core idea of the method is to decompose the original equation into three subequations with the free-energy evolution term, the heat evolution term, and a nonlinear source term, respectively. It is important to combine these three subequations in proper order to achieve the second order accuracy and stability. We propose a method with a half-time free-energy evolution solver, a half-time heat evolution solver, a full-time midpoint solver for the nonlinear source term, and a half-time heat evolution solver followed by a final half-time free-energy evolution solver. We numerically demonstrate the second order accuracy of the new numerical method through the simulations of the phase separation and the dendritic crystal growth.

1. Introduction

The Allen–Cahn (AC) equation was originally introduced as a phenomenological model for antiphase domain coarsening in a binary alloy [1]. The AC equation arises from minimization of the Ginzburg–Landau free energy

$$\mathcal{E}(\phi) := \int_{\Omega} \left(\frac{F(\phi)}{\epsilon^2} + \frac{|\nabla \phi|^2}{2} \right) d\mathbf{x},$$

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where Ω is a domain in $\mathbb{R}^d$ ($d = 1, 2, 3$). The quantity $\phi(\mathbf{x}, t)$ is defined as the difference between the concentrations of the two components in a mixture (e.g., $\phi(\mathbf{x}, t) = (m_\alpha - m_\beta)/(m_\alpha + m_\beta)$, where m_α and m_β are the masses of phases α and β). The function $F(\phi) = 0.25(\phi^2 - 1)^2$ is the Helmholtz free-energy density for ϕ, which has a double-well form, and $\epsilon > 0$ is the gradient energy coefficient. The AC equation is the L^2-gradient flow of the free energy $\mathcal{E}(\phi)$:

$$\frac{\partial \phi}{\partial t} = -\text{grad}\, \mathcal{E}(\phi), \tag{1}$$

where the symbol "grad" denotes the gradient in the sense of the Gâteaux derivative. Let the domain of the functional $\mathcal{E}$ be $\mathcal{D} = \{\phi \in H^2(\Omega) \mid \frac{\partial \phi}{\partial \mathbf{n}} = 0 \text{ on } \partial\Omega\}$. For any $\phi,\ \psi \in \mathcal{D}$, we have

$$\begin{aligned}(\text{grad}\, \mathcal{E}(\phi), \psi)_{L^2} &= \frac{\mathrm{d}}{\mathrm{d}\theta} \mathcal{E}(\phi + \theta\psi)\Big|_{\theta=0} = \lim_{\theta \to 0} \frac{1}{\theta}\big(\mathcal{E}(\phi + \theta\psi) - \mathcal{E}(\phi)\big) \\ &= \int_\Omega \left(\frac{F'(\phi)}{\epsilon^2} - \Delta\phi\right) \psi \,\mathrm{d}\mathbf{x} = \left(\frac{F'(\phi)}{\epsilon^2} - \Delta\phi, \psi\right)_{L^2}.\end{aligned}$$

See Ref. [2] for details of the notation and the derivation of the formula. We identify $\text{grad}\, \mathcal{E}(\phi) \equiv F'(\phi)/\epsilon^2 - \Delta\phi$, then Eq. (1) becomes the AC equation

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \underbrace{-\frac{1}{\epsilon^2} F'(\phi(\mathbf{x}, t))}_{\text{Free-energy evolution}} + \underbrace{\Delta\phi(\mathbf{x}, t)}_{\text{Heat evolution}}, \quad \mathbf{x} \in \Omega,\ 0 < t \le T. \tag{2}$$

The main difficulty when developing a numerical method for solving Eq. (2) is that the free-energy evolution term $F'(\phi)$ yields a severe stability restriction on the time step. In order to deal with this restriction, Eyre [3,4] proposed a semi-implicit method, which is first order accurate in time and unconditionally gradient stable, and Eyre's method was used to solve Eq. (2) in Ref. [5]. Many researchers employed first and second order stabilized semi-implicit methods for solving Eq. (2) [6–9], in which the heat evolution term $\Delta\phi$ is treated implicitly and the free-energy evolution term $F'(\phi)$ is treated explicitly to avoid the expensive process of solving nonlinear equations at each time step with an extra stabilizing term added to alleviate the stability constraint while maintaining accuracy and simplicity.

Alternative methods implemented for the AC equation are first and second order operator splitting methods [8,10,11], which become the base of our proposed method for more general form of AC type equations. Operator splitting schemes have been and continue to be used for many types of evolution equations [12–14]. It is easy to construct a first order solution $A(t^{n+1})$ of time evolution equation

$$\frac{\partial A}{\partial t} = f_1(A) + f_2(A)$$

by computing $A(t^n + \Delta t) \approx \left(\mathcal{S}_1^{\Delta t} \mathcal{S}_2^{\Delta t}\right) A(t^n)$ where $\mathcal{S}_1^{\Delta t}$ and $\mathcal{S}_2^{\Delta t}$ are the solution operators for $\frac{\partial A}{\partial t} = f_1(A)$ and $\frac{\partial A}{\partial t} = f_2(A)$, respectively. Then a second order scheme can be derived simply by symmetrizing the first order scheme:

$$A(t^n + \Delta t) \approx \left(\mathcal{S}_1^{\Delta t/2} \mathcal{S}_2^{\Delta t} \mathcal{S}_1^{\Delta t/2}\right) A(t^n).$$

The basic idea of the operator splitting methods for AC equation is to decompose the original equation into heat and free-energy evolution subequations at each time step, in which the free-energy evolution subequation has a closed-form solution. The first and the second order operator splitting methods in Refs. [8,10,11] are unconditionally stable thanks to the unconditional stability of each substep. The derivation and numerical properties of the higher order operator splitting method for AC equation will appear in Ref. [15].

Our main concern in this paper is the AC type equations with a nonlinear source term in the form of

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \underbrace{-\frac{1}{\epsilon^2} F'(\phi(\mathbf{x}, t))}_{\text{Free-energy evolution}} + \underbrace{\Delta\phi(\mathbf{x}, t)}_{\text{Heat evolution}} + \underbrace{S(\phi(\mathbf{x}, t))}_{\text{Nonlinear source}}. \tag{3}$$

This type of equations have been applied to a wide range of problems such as phase transitions [1], crystal growth [16–19], grain growth [20–24], image analysis [25–28], motion by mean curvature [29–33], two-phase fluid flows [34], and vesicle membranes [35,36]. Since available analytical solutions for these equations are limited, numerical methods are important tools for understanding dynamics of the equations. In contrast to the well developed first and second order methods for the AC equation, only first order methods are suggested for the AC type equations with nonlinear source terms due to the difficulties in dealing with the nonlinear source term numerically [17,19,21,23,25–28,35,37,38].

In this paper, we propose a second order operator splitting method for solving the AC type equations with nonlinear source terms. Our method is a generalization of the second order operator schemes for three subequations with the free-energy evolution term, the heat evolution term, and a nonlinear source term, respectively. It is important to combine these

three subequations in proper order to achieve the second order accuracy and stability. It is also worth noting that the free-energy and heat evolution subequations can be solved in semi-analytic form as in the method for the AC equation [11]. Our proposed scheme combines with a half-time free-energy evolution solver, a half-time heat evolution solver, a full-time midpoint solver for the nonlinear source term, and a half-time heat evolution solver followed by a final half-time free-energy evolution solver.

This paper is organized as follows. In Section 2, we review the second order operator splitting methods for the AC equation. In Section 3, we briefly review a derivation of the vector-valued AC equation and propose a second order operator splitting method with the numerical experiment for phase separation. In Section 4, we also propose a second order operator splitting method for the phase-field equation for dendritic crystal growth and present the numerical experiment. Finally, conclusions are drawn in Section 5.

2. Review of the second order operator splitting methods for the Allen–Cahn equation

We consider the AC equation (2) in two-dimensional space $\Omega = (0, L_1) \times (0, L_2)$. For simplicity of notation, we define the "*free-energy evolution operator*" $\mathcal{F}^{\Delta t}$ as follows:

$$\mathcal{F}^{\Delta t}(\phi(t^n)) := \phi(t^n + \Delta t),$$

where $\phi(t^n + \Delta t)$ is a solution of the first order differential equation

$$\frac{\partial \phi}{\partial t} = -\frac{F'(\phi)}{\epsilon^2}$$

with an initial condition $\phi(t^n)$. For given $F'(\phi) = \phi^3 - \phi$, we have an analytical formula (see Refs. [8,10,11]) for the evolution operator $\mathcal{F}^{\Delta t}$ in the physical space

$$\mathcal{F}^{\Delta t}(\phi) = \frac{\phi}{\sqrt{\phi^2 + (1-\phi^2)\mathrm{e}^{-\frac{2\Delta t}{\epsilon^2}}}} \quad \text{for } \epsilon = \text{constant}. \tag{4}$$

Here it is worth to note that $|\mathcal{F}^{\Delta t}(\phi)|$ is bounded by $\max(1, |\phi|)$ since

$$\begin{aligned} |\mathcal{F}^{\Delta t}(\phi)| &\le \frac{|\phi|}{\sqrt{\phi^2}} = 1, \quad \text{for } |\phi| \le 1 \\ |\mathcal{F}^{\Delta t}(\phi)| &\le \frac{|\phi|}{\sqrt{\phi^2 + (1-\phi^2)}} = |\phi|, \quad \text{for } |\phi| \ge 1. \end{aligned} \tag{5}$$

On the other hand, for any fixed Δt, $|\mathcal{F}^{\Delta t}(\phi)|$ is also bounded by some constant $B(\Delta t)$ regardless of size of $|\phi|$,

$$|\mathcal{F}^{\Delta t}(\phi)| \le \frac{|\phi|}{\sqrt{\phi^2\left(1 - \mathrm{e}^{-\frac{2\Delta t}{\epsilon^2}}\right)}} = \frac{1}{\sqrt{1 - \mathrm{e}^{-\frac{2\Delta t}{\epsilon^2}}}} = B(\Delta t). \tag{6}$$

We also define the "*heat evolution operator*" $\mathcal{H}^{\Delta t}$ as follows:

$$\mathcal{H}^{\Delta t}(\phi(t^n)) := \phi(t^n + \Delta t),$$

where $\phi(t^n + \Delta t)$ is a solution of the first order differential equation

$$\frac{\partial \phi}{\partial t} = \Delta \phi$$

with an initial condition $\phi(t^n)$. In this paper, we employ the discrete cosine transform [39] to solve the AC equation with the zero Neumann boundary condition: for $k_1 = 0, \ldots, N_1 - 1$ and $k_2 = 0, \ldots, N_2 - 1$,

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

where $\phi_{l_1 l_2} = \phi\left(\frac{L_1}{N_1}\left(l_1 + \frac{1}{2}\right), \frac{L_2}{N_2}\left(l_2 + \frac{1}{2}\right)\right)$ and $\alpha_0 = \sqrt{1/N_1}$, $\beta_0 = \sqrt{1/N_2}$, $\alpha_{k_1} = \sqrt{2/N_1}$, $\beta_{k_2} = \sqrt{2/N_2}$ for $k_1, k_2 \ge 1$. (Here we slightly abuse the notation ϕ which itself depends continuously on time and space. The subscripts l_1, l_2 are used for spatial discretization, thus $\phi_{l_1 l_2}$ denotes a time dependent function. We later use superscript n to denote time discretization of ϕ.) Then, we have a semi-analytical formula for the evolution operator $\mathcal{H}^{\Delta t}$ in the discrete cosine space

$$\mathcal{H}^{\Delta t}(\phi) = \mathcal{C}^{-1}\left[\mathrm{e}^{A_{k_1 k_2}\Delta t}\mathcal{C}\left[\phi\right]\right], \tag{7}$$

where $A_{k_1 k_2} = -\pi^2\left[\left(\frac{k_1}{L_1}\right)^2 + \left(\frac{k_2}{L_2}\right)^2\right]$ and $\mathcal{C}$ denotes the discrete cosine transform.

In Ref. [11], Lee and Lee proposed a second order semi-analytical method based on operator splitting scheme for the AC equation:

$$\phi^{n+1} = \left(\mathcal{H}^{\Delta t/2}\mathcal{F}^{\Delta t}\mathcal{H}^{\Delta t/2}\right)\phi^n, \tag{8}$$

where ϕ^n and ϕ^{n+1} are numerical approximations of $\phi(t^n)$ and $\phi(t^n + \Delta t)$, respectively. It is easy to show that the Lee and Lee's method is unconditionally stable (in the sense that the solution remains to be bounded by 1 for all time). Let $\phi^* = \mathcal{H}^{\Delta t/2}(\phi^n)$ and $\phi^{**} = \mathcal{F}^{\Delta t}(\phi^*)$. A function defined as a cosine series

$$\psi^{\Delta t/2}(x_1, x_2) := \sum_{k_1=0}^{N_1-1}\sum_{k_2=0}^{N_2-1} \mathrm{e}^{A_{k_1k_2}\Delta t/2}\widehat{\psi^0}_{k_1k_2}\cos\left(\frac{\pi}{N_1}k_1x_1\right)\cos\left(\frac{\pi}{N_2}k_2x_2\right)$$

is a solution of the heat equation with an initial condition $\psi^0(x_1, x_2)$ thus satisfies the maximum principle, $\max_{x_1,x_2}|\psi^{\Delta t/2}(x_1, x_2)| \le \max_{x_1,x_2}|\psi^0(x_1, x_2)|$. Therefore,

$$\max_{l_1,l_2}|\phi^*_{l_1l_2}| = \max_{x_1,x_2}|\phi^*(x_1, x_2)| \le \max_{x_1,x_2}|\phi^n(x_1, x_2)| = \max_{l_1,l_2}|\phi^n_{l_1l_2}|.$$

Next, if we assume that $|\phi^*_{l_1l_2}| \le 1$ for each l_1, l_2 (which is a natural consequence of the assumption $|\phi^n_{l_1l_2}| \le 1$), we have

$$|\phi^{**}_{l_1l_2}| = |\mathcal{F}^{\Delta t}(\phi^*_{l_1l_2})| = \frac{|\phi^*_{l_1l_2}|}{\sqrt{(\phi^*_{l_1l_2})^2 + \left(1 - (\phi^*_{l_1l_2})^2\right)\mathrm{e}^{\frac{-2\Delta t}{\epsilon^2}}}} \le 1.$$

Finally, it can also be shown that $\max_{l_1,l_2}|\phi^{n+1}_{l_1l_2}| \le \max_{l_1,l_2}|\phi^{**}_{l_1l_2}|$. Therefore, the Lee and Lee's method is unconditionally stable regardless of time step size in the sense that $\max_{l_1,l_2}|\phi^{n+1}_{l_1l_2}| \le 1$ for given $\max_{l_1,l_2}|\phi^n_{l_1l_2}| \le 1$.

When solving the AC equation using the operator splitting method in the type of (8), the numerical results are almost not affected by the order of operator evaluation. The desired order of accuracy is achieved regardless of operator evaluation order since both $\mathcal{F}^{\Delta t}$ and $\mathcal{H}^{\Delta t}$ have semi-analytic formulas satisfying semigroup properties and the stability is guaranteed since both $|\mathcal{F}^{\Delta t}(\phi)|$ and $|\mathcal{H}^{\Delta t}(\phi)|$ are bounded by 1 for $|\phi| \le 1$. However, in the case of AC type equations with nonlinear source terms, the accuracy and stability of numerical results are affected by the order of operator evaluations. Therefore, when one wants to develop a high order time discretization method for solving such type equations, it needs to consider the proper order of operator evaluations.

Before we close this section, we just want to mention that there exists another second order unconditionally stable operator splitting method by Yang [8] for the AC equation:

$$\phi^{n+1} = \left(\mathcal{F}^{\Delta t/2}\mathcal{H}^{\Delta t}_{\mathrm{CN}}\mathcal{F}^{\Delta t/2}\right)\phi^n,$$

where the heat evolution operator $\mathcal{H}^{\Delta t}_{\mathrm{CN}}$ using standard second order Crank–Nicolson is defined as

$$\mathcal{H}^{\Delta t}_{\mathrm{CN}}(\phi) = \mathcal{C}^{-1}\left[\frac{\left(1 + \Delta t A_{k_1k_2}/2\right)\mathcal{C}[\phi]}{1 - \Delta t A_{k_1k_2}/2}\right].$$

It is worth noting that the method consists of two symmetrized half steps of free-energy evolution operator $\mathcal{F}^{\Delta t/2}$ and a second order full step of heat evolution operator $\mathcal{H}^{\Delta t}_{\mathrm{CN}}$ in between.

3. A vector-valued Allen–Cahn equation

Our first example for the AC type equations with nonlinear source terms is the vector-valued AC equation. The equation was introduced in Garcke et al. [40] and has been extensively used [27,37,38,41], which allows one to consider an arbitrary number of components to the order parameter. In this section, we give some basic information about the vector-valued AC equation and propose a second order operator splitting method for the equation. Numerical experiments finally illustrate the accuracy and stability of the proposed method.

We consider the evolution of multi-component systems on a polygonal (polyhedral) domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$. Let $\mathbf{c} = (c_1, \ldots, c_N)$ be a vector-valued phase-field. The components $\{c_i\}_{i=1}^N$ represent mole fractions of different components in the system. Clearly the total mole fractions must sum to 1,

$$c_1 + \cdots + c_N = 1, \tag{9}$$

hence admissible states will belong to the Gibbs N-simplex

$$G := \left\{\mathbf{c} \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^N c_i = 1,\ 0 \le c_i \le 1\right\}.$$

Without loss of generality, we postulate that the free energy can be written as follows:

$$\mathcal{E}(\mathbf{c}) := \int_\Omega \left(\frac{F(\mathbf{c})}{\epsilon^2} + \frac{1}{2}\sum_{i=1}^{N} |\nabla c_i|^2 \right) \mathrm{d}\mathbf{x},$$

where $F(\mathbf{c}) = 0.25\sum_{i=1}^{N} c_i^2(1-c_i)^2$. The natural boundary condition for the vector-valued AC equation is the zero Neumann boundary condition:

$$\nabla c_i \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega \text{ for } i = 1, \ldots, N, \tag{10}$$

where $\mathbf{n}$ is the unit normal vector to $\partial\Omega$.

Now we review a derivation of the vector-valued AC equation as a gradient flow under the additional constraint (9), which has to hold everywhere at any time. It is natural to seek a law of evolution in the form

$$\frac{\partial \mathbf{c}}{\partial t} = -\text{grad}\, \mathcal{E}(\mathbf{c}). \tag{11}$$

In order to ensure the constraint (9), we use (see Ref. [40]) a variable Lagrange multiplier $\beta(\mathbf{c}) := (-1/N)\sum_{i=1}^{N} f(c_i)$ where $f(c) = c(c-0.5)(c-1)$ for the previously given $F(\mathbf{c})$ and $\mathbf{f}(\mathbf{c}) = (f(c_1), \ldots, f(c_N)) := \frac{\partial F}{\partial \mathbf{c}} = \left(\frac{\partial F}{\partial c_1}, \ldots, \frac{\partial F}{\partial c_N} \right)$. Choosing a general smooth vector-valued function $\boldsymbol{\xi} \in \mathbb{R}^N$ and setting $\mathbf{d} := (d_1, \ldots, d_N) = \boldsymbol{\xi} - \frac{1}{N}\sum_{i=1}^{N} \xi_i \mathbf{1}$ where $\mathbf{1} = (1, \ldots, 1) \in \mathbb{R}^N$, then $\sum_{i=1}^{N} d_i = 0$ and we have the following equation for the evaluation of grad $\mathcal{E}(\mathbf{c})$:

$$\begin{aligned}
(\text{grad}\, \mathcal{E}(\mathbf{c}), \mathbf{d})_{L^2} &= \frac{\mathrm{d}}{\mathrm{d}\eta} \mathcal{E}(\mathbf{c} + \eta\mathbf{d}) \Big|_{\eta=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}\eta} \int_\Omega \sum_{i=1}^{N} \left(\frac{1}{4\epsilon^2}(c_i + \eta d_i)^2(1 - (c_i + \eta d_i))^2 + \frac{1}{2}|\nabla(c_i + \eta d_i)|^2 \right) \mathrm{d}\mathbf{x} \Big|_{\eta=0} \\
&= \int_\Omega \left[\frac{1}{\epsilon^2} \left(\mathbf{f}(\mathbf{c}) \cdot \boldsymbol{\xi} - \mathbf{f}(\mathbf{c}) \cdot \frac{1}{N}\sum_{i=1}^{N} \xi_i \mathbf{1} \right) + \sum_{i=1}^{N} \nabla \left(\xi_i - \frac{1}{N}\sum_{j=1}^{N} \xi_j \right) \cdot \nabla c_i \right] \mathrm{d}\mathbf{x} \\
&= \int_\Omega \left[\frac{\mathbf{f}(\mathbf{c}) + \beta(\mathbf{c})\mathbf{1}}{\epsilon^2} - \Delta\mathbf{c} \right] \cdot \boldsymbol{\xi} \mathrm{d}\mathbf{x} \\
&= \int_\Omega \left[\frac{\mathbf{f}(\mathbf{c}) + \beta(\mathbf{c})\mathbf{1}}{\epsilon^2} - \Delta\mathbf{c} \right] \cdot \mathbf{d}\, \mathrm{d}\mathbf{x} = \left(\frac{\mathbf{f}(\mathbf{c}) + \beta(\mathbf{c})\mathbf{1}}{\epsilon^2} - \Delta\mathbf{c}, \mathbf{d} \right)_{L^2},
\end{aligned}$$

where we have used the boundary condition (10). We identify grad $\mathcal{E}(\mathbf{c}) = \left(\mathbf{f}(\mathbf{c}) + \beta(\mathbf{c})\mathbf{1}\right)/\epsilon^2 - \Delta\mathbf{c}$, then Eq. (11) becomes the vector-valued AC equation

$$\frac{\partial \mathbf{c}}{\partial t} = -\frac{\mathbf{f}(\mathbf{c})}{\epsilon^2} + \Delta\mathbf{c} - \frac{\beta(\mathbf{c})}{\epsilon^2}\mathbf{1}. \tag{12}$$

Before we present our method, let us define the following notations:

$$\mathcal{F}^{\Delta t}(\mathbf{c}) = (\mathcal{F}^{\Delta t}(c_1), \ldots, \mathcal{F}^{\Delta t}(c_N)) \quad \text{and} \quad \mathcal{H}^{\Delta t}(\mathbf{c}) = (\mathcal{H}^{\Delta t}(c_1), \ldots, \mathcal{H}^{\Delta t}(c_N)),$$

where $\mathcal{F}^{\Delta t}(c_i)$ is defined as in (13) but maps $c_i \in [0, 1]$ to $\mathcal{F}^{\Delta t}(c_i) \in [0, 1]$ and $\mathcal{H}^{\Delta t}(c_i)$ is defined in (7). Here the evolution operator $\mathcal{F}^{\Delta t}(c_i)$ whose range is [0, 1] can be written explicitly as follows [38]:

$$\mathcal{F}^{\Delta t}(c_i) = \frac{1}{2} + \frac{2c_i - 1}{2\sqrt{(2c_i - 1)^2 + (1 - (2c_i - 1)^2)\mathrm{e}^{-\frac{\Delta t}{2\epsilon^2}}}}. \tag{13}$$

We also define the "*nonlinear constraint evolution operator*" $\mathcal{N}_\beta^{\Delta t}$ as follows:

$$\mathcal{N}_\beta^{\Delta t}(\mathbf{c}(t^n)) := \mathbf{c}(t^n + \Delta t),$$

where $\mathbf{c}(t^n + \Delta t)$ is a solution of the first order nonlinear differential equation

$$\frac{\partial \mathbf{c}}{\partial t} = -\frac{\beta(\mathbf{c})}{\epsilon^2}\mathbf{1}$$

with an initial condition $\mathbf{c}(t^n)$ and the variable Lagrange multiplier $\beta(\mathbf{c}(t))$. Since there is no analytic form of the solution for this nonlinear evolution equation, we define a numerical approximation of the evolution operator $\mathcal{N}_{\beta_m}^{\Delta t}$ based on the Euler method,

$$\mathcal{N}_{\beta_m}^{\Delta t}(\mathbf{c}(t^n)) = \mathbf{c}(t^n) - \frac{\beta(\mathbf{c}(t^m))\Delta t}{\epsilon^2}\mathbf{1}. \tag{14}$$

Note that $\mathcal{N}_{\beta_n}^{\Delta t}(\mathbf{c}^n)$ is a first order forward Euler approximation, $\mathcal{N}_{\beta_{n+1}}^{\Delta t}(\mathbf{c}^n)$ is a backward Euler approximation, and $\mathcal{N}_{\beta_{n+\frac{1}{2}}}^{\Delta t}(\mathbf{c}^n)$ is a second order mid-point approximation of $\mathbf{c}(t^n + \Delta t)$.

A first order stable operator splitting method for Eq. (12) is

$$\mathbf{c}^{n+1} = \left(\mathcal{F}^{\Delta t}\mathcal{H}^{\Delta t}\mathcal{N}_{\beta_n}^{\Delta t}\right)\mathbf{c}^n. \tag{15}$$

This is an operator splitting method combining two semi-analytic evolution operators and a first order approximation of the nonlinear evolution operator. Note that the free-energy evolution operator $\mathcal{F}^{\Delta t}$ makes the result to be bounded by $B(\Delta t)$ as in (6) regardless of size of $\left|\mathbf{c}^* = \left(\mathcal{H}^{\Delta t}\mathcal{N}_{\beta_n}^{\Delta t}\right)\mathbf{c}^n\right|$,

$$\max_{\mathbf{x}\in\Omega}\left|\mathcal{F}^{\Delta t}\left(c_i^*(\mathbf{x})\right) - \frac{1}{2}\right| \le B(\Delta t) := \frac{1}{2}\left(1 - \mathrm{e}^{-\Delta t/2\epsilon^2}\right)^{-1/2} \tag{16}$$

for each i. This provides a reasonably good bound for a larger time step Δt and $\lim_{\Delta t\to\infty}\left|\mathcal{F}^{\Delta t}\left(c_i^*(\mathbf{x})\right) - 1/2\right| = 1/2$. As Δt approaches to 0, $B(\Delta t)$ is no longer useful to get a tight bound and we may apply another inequality,

$$\left|\mathcal{F}^{\Delta t}\left(c_i^*(\mathbf{x})\right) - \frac{1}{2}\right| \le \max\left(\frac{1}{2}, \left|c_i^*(\mathbf{x}) - \frac{1}{2}\right|\right) \tag{17}$$

where $|c_i^* - c_i^n|$ is linearly bounded by smaller time step Δt. Instead of developing a tighter bound for the solution $c_i^{T/\Delta t}$ at any given time T, we just want to conclude this argument with a comment that $\left|\mathcal{F}^{\Delta t}\left(c_i^*(\mathbf{x})\right) - 1/2\right|$ is always bounded by $B(\Delta t)$ for any fixed Δt. For this reason, it is important to evaluate $\mathcal{F}^{\Delta t}$ at the end to guarantee the boundedness of the numerical solution for any fixed Δt.

We now propose a second order operator splitting method for Eq. (12). It is a symmetric combination of two half step evolution operators $\mathcal{H}^{\Delta t/2}$, $\mathcal{F}^{\Delta t/2}$ and a full step nonlinear evolution operator $\mathcal{N}_{\beta}^{\Delta t}$ in between. In order to make the nonlinear evolution operator $\mathcal{N}_{\beta}^{\Delta t}$ to be second order accurate, we use a mid-point rule using $\beta_{n+\frac{1}{2}} := \beta(\mathbf{c}^{n+\frac{1}{2}})$.

$$\text{STEP 1. } \mathbf{c}^{n+\frac{1}{2}} = \left(\mathcal{N}_{\beta_n}^{\Delta t/2}\mathcal{H}^{\Delta t/2}\mathcal{F}^{\Delta t/2}\right)\mathbf{c}^n, \tag{18}$$

$$\text{STEP 2. } \mathbf{c}^{n+1} = \left(\mathcal{F}^{\Delta t/2}\mathcal{H}^{\Delta t/2}\mathcal{N}_{\beta_{n+\frac{1}{2}}}^{\Delta t}\mathcal{H}^{\Delta t/2}\mathcal{F}^{\Delta t/2}\right)\mathbf{c}^n, \tag{19}$$

where $\beta_{n+\frac{1}{2}}$ is computed using $\mathbf{c}^{n+\frac{1}{2}}$ given in the first step of the operator splitting method. It is worth remarking that $\left(\mathcal{H}^{\Delta t/2}\mathcal{F}^{\Delta t/2}\right)\mathbf{c}^n$ appeared in STEP 1 can be reused in STEP 2 and the boundedness of $\mathbf{c}^{n+1}$ (or stability of the method) is obtained if $\mathcal{F}^{\Delta t/2}$ is applied at the end.

Example 1 (*Phase Separation of a Quaternary System*)**.** We consider a quaternary system in one-dimensional space, $\Omega = [0, 1]$. An estimate of the convergence rate is obtained by performing a number of simulations for a sample initial problem on a set of increasingly finer time steps. The initial conditions are

$$c_i(x, 0) = 0.25 + 0.05\sin((i+3)\sqrt{8}x) \quad \text{for } i = 1, 2, 3.$$

Note that we only solve c_1, c_2, c_3 since $c_4 = 1 - c_1 - c_2 - c_3$ by the constraint (9). The numerical solutions are computed with $h = 1/128$, $\epsilon = 0.01$, and $\Delta t = T_f/2^k$ for $k = 2, \ldots, 10$. For each time step, we integrate to time $T_f = 0.005$. The error is computed by comparison with a quadruply over-resolved numerical reference solution shown in Fig. 1(a). Fig. 1(b) shows relative l_2 errors of the solutions for different time step sizes by the first and second order methods described in (15) and (18)–(19), respectively. The numerical results show that the proposed methods provides the expected order accuracy in time.

In order to see the effect of interface thickness parameter ϵ on the numerical error, we consider the same problem in Fig. 1 with $\epsilon = 0.002$ ($T_f = 0.0002$), $\epsilon = 0.01$ ($T_f = 0.005$), and $\epsilon = 0.05$ ($T_f = 0.1$). Fig. 2 shows relative l_2 errors of (a) the first and (b) the second order methods for different ϵ values, respectively. The numerical results show that both first and second order accuracy is achieved for $\Delta t \le 5\epsilon^2$ (marked by arrows in the figures) and the solutions are stable even when $\Delta t \gg 5\epsilon^2$.

4. A phase-field model for dendritic crystal growth

Another example of the AC type equations with nonlinear source terms is a phase-field model for dendritic crystal growth. The purpose of this section is not developing a best possible numerical method but demonstrating the feasibility of the

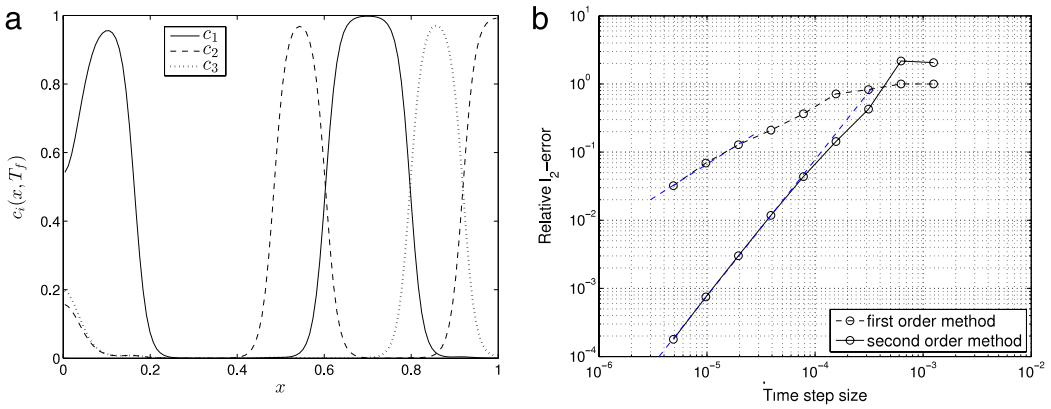
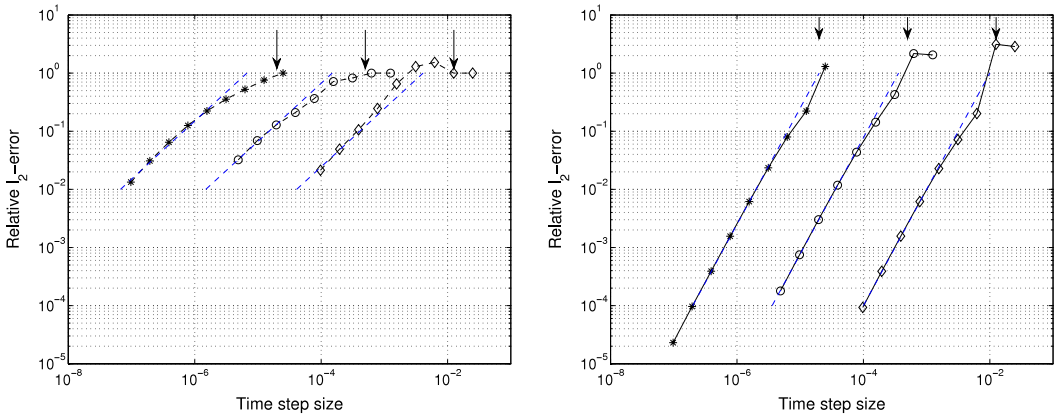


Fig. 1. (a) Reference solution $\mathbf{c}_{\text{ref}}(x, T_f)$ obtained by the second order method at $T_f = 0.005$ with $h = 1/128$, $\epsilon = 0.01$, and $\Delta t = T_f/2^{12}$. (b) Relative l_2 errors of the first and second order methods for different time step sizes. The dashed blue lines indicate the first or the second order convergence slope. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



(a) First order method. (b) Second order method.

Fig. 2. Relative l_2 errors of (a) the first and (b) the second order methods with $\epsilon = 0.002$ ($T_f = 0.0002$, '$*$'), $\epsilon = 0.01$ ($T_f = 0.005$, '$\circ$'), and $\epsilon = 0.05$ ($T_f = 0.1$, '$\diamond$') for different time step sizes, respectively. The dashed blue lines indicate the first or the second order convergence slope. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

simple scheme described in the previous section for this complex system of nonlinear evolution equations of AC type. The two-dimensional phase-field equation for dendritic crystal growth is given by

$$\epsilon^2(\phi)\frac{\partial \phi}{\partial t} = [\phi - \lambda U(1-\phi^2)](1-\phi^2) + \nabla\cdot(\epsilon^2(\phi)\nabla\phi) + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial \epsilon(\phi)}{\partial \phi_x}\right)_x + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial \epsilon(\phi)}{\partial \phi_y}\right)_y, \tag{20}$$

$$\frac{\partial U}{\partial t} = D\Delta U + \frac{1}{2}\frac{\partial \phi}{\partial t}, \tag{21}$$

where ϕ is an order parameter, which varies from negative one in the liquid to positive one in the solid, $\epsilon(\phi)$ is an anisotropy function, λ is a dimensionless parameter that controls the strength of the coupling between the phase and diffusion fields, U is a dimensionless temperature field, and D is the dimensionless thermal diffusivity. For the four-fold symmetry, $\epsilon(\phi)$ is defined as

$$\epsilon(\phi) = (1-3\epsilon_4)\left(1 + \frac{4\epsilon_4}{1-3\epsilon_4}\frac{\phi_x^4 + \phi_y^4}{|\nabla\phi|^4}\right), \tag{22}$$

where ϵ_4 is a parameter for the anisotropy strength in the interface energy. For $F(\phi) = 0.25(\phi^2-1)^2$ and $F'(\phi) = \phi^3 - \phi$, Eq. (20) can be rewritten as follows:

$$\frac{\partial \phi}{\partial t} = -\frac{1}{\epsilon^2(\phi)}F'(\phi) + \Delta\phi + \omega(\phi, U), \tag{23}$$

where the nonlinear source term $\omega(\phi, U)$ is defined as

$$\omega(\phi, U) = \frac{1}{\epsilon^2(\phi)}\left[2\epsilon(\phi)\nabla\epsilon(\phi)\cdot\nabla\phi - 4\lambda U F(\phi) + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_x}\right)_x + \left(|\nabla\phi|^2\epsilon(\phi)\frac{\partial\epsilon(\phi)}{\partial\phi_y}\right)_y\right]. \tag{24}$$

Before we present our method, we redefine the "*free-energy evolution operator*" $\mathcal{F}_\epsilon^{\Delta t}$ depending on $\epsilon(\phi)$ as follows:

$$\mathcal{F}_\epsilon^{\Delta t}(\phi(t^n)) := \phi(t^n + \Delta t),$$

where $\phi(t^n + \Delta t)$ is a solution of the first order nonlinear differential equation,

$$\frac{\partial\phi}{\partial t} = -\frac{F'(\phi)}{\epsilon^2(\phi)}$$

with an initial condition $\phi(t^n)$. Assume that $\epsilon(\phi(t))$ is given as a fixed value $\epsilon_m = \epsilon(\phi(t^m))$, then we have an analytical formula for the evolution operator $\mathcal{F}_{\epsilon_m}^{\Delta t}$ in the physical space,

$$\mathcal{F}_{\epsilon_m}^{\Delta t}(\phi) = \frac{\phi}{\sqrt{\phi^2 + (1-\phi^2)\mathrm{e}^{-\frac{2\Delta t}{\epsilon_m^2}}}} \quad \text{for } \epsilon_m = \epsilon(\phi(t^m)). \tag{25}$$

We also define the "*nonlinear anisotropic evolution operator*" $\mathcal{N}_\omega^{\Delta t}$ as follows:

$$\mathcal{N}_\omega^{\Delta t}(\phi(t^n)) := \phi(t^n + \Delta t),$$

where $\phi(t^n + \Delta t)$ is a solution of the first order nonlinear differential equation

$$\frac{\partial\phi}{\partial t} = \omega(\phi, U)$$

with an initial condition $\phi(t^n)$. Again there is no analytic form of the nonlinear evolution operator so we approximate the evolution operator $\mathcal{N}_\omega^{\Delta t}$ by the Euler method using $\omega_m := \omega(\phi(t^m), U(t^m))$,

$$\mathcal{N}_{\omega_m}^{\Delta t}(\phi) = \phi + \omega(\phi(t^m), U(t^m))\Delta t. \tag{26}$$

And we define the "*thermal evolution operator*" $\mathcal{M}^{\Delta t}$ as follows:

$$\mathcal{M}^{\Delta t}(U(t^n)) := U(t^n + \Delta t),$$

where $U(t^n + \Delta t)$ is a solution of the first order differential equation

$$\frac{\partial U}{\partial t} = \frac{1}{2}\frac{\partial\phi}{\partial t}$$

with an initial condition $U(t^n)$ and the order parameter $\phi(t)$. Then, we have a formula for the evolution operator $\mathcal{M}^{\Delta t}$

$$\mathcal{M}^{\Delta t}(U) = U + \frac{\phi(t^n + \Delta t) - \phi(t^n)}{2}, \tag{27}$$

whose numerical accuracy is governed by the accuracy of $\phi(t)$.

A first order operator splitting method for the solution $\phi^n \approx \phi(t^n)$ and $U^n \approx U(t^n)$ from Eqs. (21) and (23) can be described as follows:

$$\phi^{n+1} = \left(\mathcal{F}_{\epsilon_n}^{\Delta t}\mathcal{H}^{\Delta t}\mathcal{N}_{\omega_n}^{\Delta t}\right)\phi^n \quad \text{and} \quad U^{n+1} = \left(\mathcal{H}^{D\Delta t}\mathcal{M}^{\Delta t}\right)U^n. \tag{28}$$

We propose a second order stable operator splitting method for Eqs. (21) and (23):

$$\text{STEP 1. } \phi^{n+\frac{1}{2}} = \left(\mathcal{N}_{\omega_n}^{\Delta t/2}\mathcal{H}^{\Delta t/2}\mathcal{F}_{\epsilon_n}^{\Delta t/2}\right)\phi^n, \tag{29}$$

$$U^{n+\frac{1}{2}} = \left(\mathcal{M}^{\Delta t/2}\mathcal{H}^{D\Delta t/2}\right)U^n, \tag{30}$$

$$\text{STEP 2. } \phi^{n+1} = \left(\mathcal{F}_{\epsilon_*}^{\Delta t/2}\mathcal{H}^{\Delta t/2}\mathcal{N}_{\omega_{n+\frac{1}{2}}}^{\Delta t}\mathcal{H}^{\Delta t/2}\mathcal{F}_{\epsilon_n}^{\Delta t/2}\right)\phi^n, \tag{31}$$

$$U^{n+1} = \left(\mathcal{H}^{D\Delta t/2}\mathcal{M}^{\Delta t}\mathcal{H}^{D\Delta t/2}\right)U^n, \tag{32}$$

where $\omega_{n+\frac{1}{2}} = \omega(\phi^{n+\frac{1}{2}}, U^{n+\frac{1}{2}})$ can be computed from the results in STEP 1 and $\epsilon_* = \epsilon(\phi^*)$ is given by a predictor step for the computation of ϕ^*,

$$\phi^* = \left(\mathcal{F}_{\epsilon_{n+\frac{1}{2}}}^{\Delta t/2}\mathcal{H}^{\Delta t/2}\mathcal{N}_{\omega_{n+\frac{1}{2}}}^{\Delta t}\mathcal{H}^{\Delta t/2}\mathcal{F}_{\epsilon_n}^{\Delta t/2}\right)\phi^n.$$

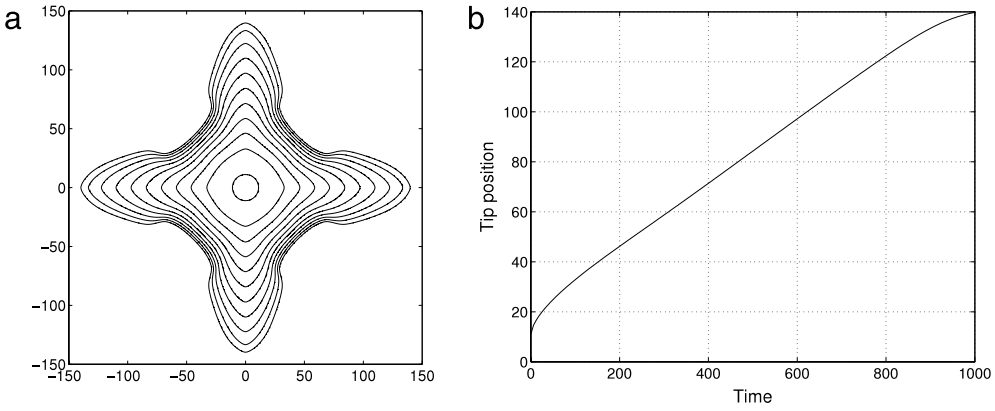


Fig. 3. (a) Sequence of interfaces of the reference solution $\phi_{\text{ref}}(x, y, t)$ at $t = 0, 100, \ldots, 1000$ (from inside to outside) obtained by the second order method with $R_0 = 40d_0$, $d_0 = 0.2770$, $\Delta = -0.55$, $\epsilon_4 = 0.05$, $\lambda = 3.1913$, $D = 2$, $h = 300/900$, and $\Delta t = 100/2^{12}$. (b) Tip position $P_{\text{ref}}(t)$ of the reference solution as a function of time.

The method for ϕ^n is nothing but a symmetric combination of two half step evolution operators $\mathcal{H}^{\Delta t/2}$, $\mathcal{F}_\epsilon^{\Delta t/2}$ and a full step anisotropic evolution operator $\mathcal{N}_\omega^{\Delta t}$ in between. The computation for U^n is again a symmetric combination of half step evolution operator $\mathcal{H}^{\Delta t/2}$ and a full step thermal evolution operator $\mathcal{M}^{\Delta t}$ in between. Similar properties on the stability and the order of accuracy are expected as in Example 1.

Example 2 (*Dendritic Crystal Growth with Four-Fold Symmetry*)**.** In order to measure the accuracy of the proposed method for solving Eqs. (21) and (23), we take the initial conditions as

$$\phi(x, y, 0) = \tanh\left(\frac{R_0 - \sqrt{x^2 + y^2}}{\sqrt{2}}\right) \quad \text{and} \quad U(x, y, 0) = \begin{cases} 0 & \text{if } \phi > 0 \\ \Delta & \text{else} \end{cases}$$

on the domain $\Omega = [-150, 150]^2$. The level set $\phi = 0$ represents a circle of radius R_0. We choose $R_0 = 40d_0$ (the capillary length d_0 is defined as $d_0 = a_1/\lambda$ [42–44] with $a_1 = 5\sqrt{2}/8$ [17,42,45] and $\lambda = 3.1913$ [42]), $\Delta = -0.55$, $\epsilon_4 = 0.05$, $D = 2$, $h = 300/900$, and $\Delta t = 100/2^k$ for $k = 4, \ldots, 10$. For each time step, we integrate to time $T_f = 1000$. The error is computed by comparison with a quadruply over-resolved numerical reference solution (Fig. 3(a)). The tip position is an important parameter in the phase-field simulation and can be inferred from the numerical solution by using a third-order polynomial to interpolate ϕ, using neighbor and next-neighbor grid point values. The tip position $P_{\text{ref}}(t)$ of the reference solution as a function of time is shown in Fig. 3(b).

Figs. 4 (a, c) and (b, d) show relative l_2 errors of $\phi(x, y, T)$ and $U(x, y, T)$ at $T = 100, \ldots, 400$ for different time step sizes obtained by the first and second order methods, respectively. The simulation numerically demonstrates that the method provides the expected order of accuracy for both the order parameter ϕ and the temperature field U even for relatively large time steps and the solution remains to be bounded for arbitrarily large time step sizes.

5. Conclusions

We proposed a simple and stable second order numerical scheme for the AC type equations with nonlinear source terms. The methods are based on the operator splitting scheme for the subequations with the free-energy, the heat, and the nonlinear evolution terms. Unlike the methods for the classical AC equation, it is critical to combine these three subequations in proper order in order to ensure the second order accuracy and stability. The second order of accuracy can be achieved by symmetrically combining two half step evolution operators $\mathcal{H}^{\Delta t/2}$, $\mathcal{F}^{\Delta t/2}$ and a full step nonlinear evolution operator in between. It is important to utilize the existence of semi-analytic formula for the subequations with the free-energy evolution term and the heat evolution term and a simple mid-point rule provides the second order approximation of the nonlinear evolution operator. It is also important to evaluate $\mathcal{F}^{\Delta t}$ at the end to guarantee the boundedness of the solution. The simulations such as the phase separation and the dendritic crystal growth numerically demonstrate the feasibility of the simple scheme as a stable and second order method for the AC type evolution equations with nonlinear source terms.

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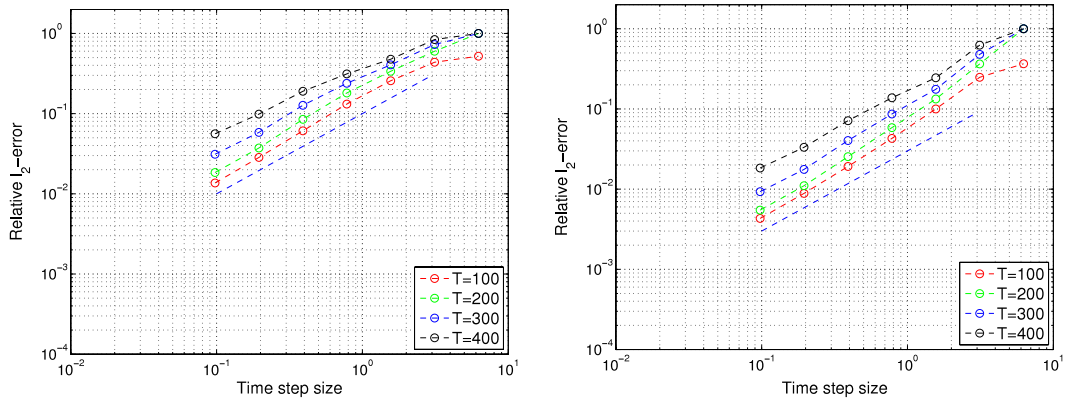
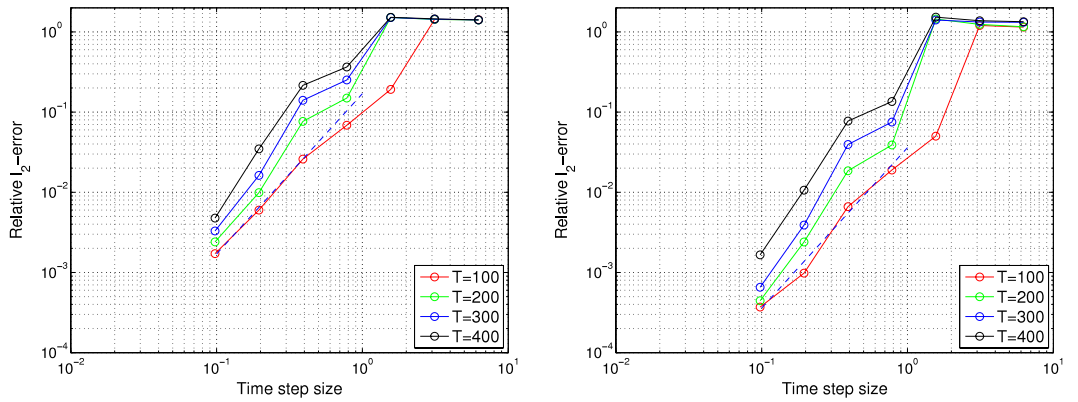


(a) $\phi(x, y, T)$, First order.

(b) $U(x, y, T)$, First order.



(c) $\phi(x, y, T)$, Second order.

(d) $U(x, y, T)$, Second order.

Fig. 4. Relative l_2 errors of $\phi(x, y, T)$ and $U(x, y, T)$ at $T = 100, \ldots, 400$ for different time step sizes obtained by the first and the second order methods, respectively. The dashed blue lines indicate the first or the second order convergence slope. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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