

On large time-stepping methods for the Cahn–Hilliard equation

Yinnian He ^a, Yunxian Liu ^b, Tao Tang ^{c,*}

^a Faculty of Science, Xi'an Jiaotong University, Xi'an 710049, PR China

^b School of Mathematics and System Sciences, Shandong University, Jinan, Shandong 250100, PR China

^c Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong

Available online 10 August 2006

Abstract

In this work, we will analyze a class of large time-stepping methods for the Cahn–Hilliard equation. The equation is discretized by Fourier spectral method in space and semi-implicit schemes in time. For first-order semi-implicit scheme, the stability and convergence properties are investigated based on an energy approach. Here stability means that the decay of energy is preserved. The numerical experiments are used to demonstrate the effectiveness of the large time-stepping approaches.

© 2006 IMACS. Published by Elsevier B.V. All rights reserved.

MSC: 35Q99; 35R35; 65M12; 65M70

Keywords: Large time-stepping method; Cahn–Hilliard equation; Spectral method; Semi-implicit scheme; Stability; Decay of energy

1. Introduction

We consider the initial-boundary-value problem for the Cahn–Hilliard equation:

$$\partial_t u + \Delta(u - u^3 + \kappa \Delta u) = 0, \quad (x, t) \in \Omega \times \mathbb{R}^+, \quad (1.1)$$

$$u(\cdot, t) \text{ is } L\text{-periodic for all } t \in \mathbb{R}^+, \quad (1.2)$$

$$u(x, 0) = u_0(x), \quad x \in \Omega, \quad (1.3)$$

where the domain $\Omega = (0, L_1) \times (0, L_2)$ is an open set in $\mathbb{R}^2$, κ is a positive constant, $L = (L_1, L_2)$, $u_0: \Omega \rightarrow \mathbb{R}$ is a given initial function. The L -periodic boundary condition (1.2) and the Cahn–Hilliard equation (1.1) lead the conservation of the total mass of the system. The Cahn–Hilliard equation was originally introduced in [3] to describe the complicated phase separation and coarsening phenomena. There has been a significant research interest in simulating the Cahn–Hilliard equation, see, e.g. [9,12,17,18,23] and the references therein. Finite element schemes have been studied with mathematical rigor by Barrett et al. [1] and Elliott et al. [5–8]. Very recently, Feng and Prohl [10] proposed and analyzed a semi-discrete and a fully discrete finite element method for a class of Cahn–Hilliard equation involving a small parameter. Error estimates which are of quasi-optimal order in time and optimal order in space are shown for their proposed methods under minimum regularity assumptions on the initial data and the domain. With

* Corresponding author.

E-mail addresses: heyin@mail.xjtu.edu.cn (Y. He), yxliu@sdu.edu.cn (Y. Liu), ttang@math.hkbu.edu.hk (T. Tang).

finite difference approaches, Sun [19] proposed a linearized finite difference scheme which is uniquely solvable and convergent with order two in a discrete $L^2(\Omega)$ -norm. In [11], a conservative finite difference scheme was proposed to solve the Cahn–Hilliard equation in one space dimension. It is proved that their proposed scheme is stable in the sense that the decay of energy is preserved numerically. In [22], a combined spectral and large-time stepping method was proposed and studied for the nonlinear diffusion equations for thin film epitaxy which are also studied by Li and Liu [16].

Our main interest in this work is to investigate the time-stepping methods for problem (1.1)–(1.3). The classical first order semi-implicit scheme is of the form

$$\frac{u^{n+1} - u^n}{\Delta t} = P_N \Delta f(u^n) - \kappa \Delta^2 u^{n+1}, \quad n \geq 0, \quad (1.4)$$

where P_N is a $L^2(\Omega)$ -projection defined in Section 2, $f(u) = -u + u^3$, Δt is the time-step and $t_n = n\Delta t$, u^n is an approximation to $u(x, t_n)$. In practice, it is known that the semi-implicit treatment in time allows a consistently larger time-step size. Their numerical simulations indicate that the time-step in a semi-implicit method can be two orders of magnitude larger than that in an explicit method. To further improve the stability property of the semi-implicit method (1.4), we propose to add an $\mathcal{O}(\Delta t \partial_t u)$ term to the scheme (1.4):

$$\frac{u^{n+1} - u^n}{\Delta t} = A \Delta(u^{n+1} - u^n) + P_N \Delta f(u^n) - \kappa \Delta^2 u^{n+1}, \quad (1.5)$$

where A is a positive constant. The purpose of adding the extra term is to improve the stability condition so that larger time-steps can be used. In practice, the accuracy in time can be improved by using higher-order semi-implicit schemes. For instance, a second-order backward difference (BDF) for $\partial_t u$ and a second-order Adams–Bashforth (AB) for the explicit treatment of the nonlinear term for (1.1) lead to the following second-order BDF/AB scheme:

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} = P_N \Delta(2f(u^n) - f(u^{n-1})) - \kappa \Delta^2 u^{n+1}. \quad (1.6)$$

Again, to improve stability an $\mathcal{O}(\Delta t^2 \partial_{tt} u)$ term is added in the above scheme, which gives the following second-order time discretization scheme:

$$\frac{3u^{n+1} - 4u^n + u^{n-1}}{2\Delta t} = A \Delta \delta_{tt} u^n + P_N \Delta(2f(u^n) - f(u^{n-1})) - \kappa \Delta^2 u^{n+1}, \quad (1.7)$$

where $\delta_{tt} u^n := u^{n+1} - 2u^n + u^{n-1}$. The purpose of this work is to provide a stability and convergence analysis for (1.5) and (1.7). A detailed numerical comparison for various time discretization schemes will be carried out in this work.

The paper is organized as follows. In Section 2, we provide a theoretical analysis for the semi-implicit method. In particular, for the first-order time-stepping method stability and convergence properties are investigated. Numerical experiments are carried out in Section 3. It will be demonstrated that larger time-steps can be used by adding an extra term consistent with the order of truncation errors. Some concluding remarks are given in the final section.

2. Stability and convergence for semi-implicit method

Let $C_{\text{per}}^\infty(\Omega)$ be the set of all restrictions onto Ω of all real-valued, L -periodic, C^∞ -functions on $\mathbb{R}^2$. For each integer $q \geq 0$, let $H_{\text{per}}^q(\Omega)$ be the closure of $C_{\text{per}}^\infty(\Omega)$ in the usual Sobolev norm $\|\cdot\|_q$, and $H_{\text{per}}^{-q}(\Omega)$ be the dual space of $H_{\text{per}}^q(\Omega)$. Note that $H_{\text{per}}^0(\Omega) = L^2(\Omega)$. We now define the weak solution of (1.1)–(1.3) as follows.

Definition 2.1. A function $u: \Omega \times \mathbb{R}^+ \rightarrow \mathbb{R}$ is called a weak solution of (1.1)–(1.3) if $u \in L^\infty(\mathbb{R}^+; L^2(\Omega)) \cap L^2_{\text{loc}}(\mathbb{R}^+; H_{\text{per}}^2(\Omega))$ and $\partial_t u \in L^2_{\text{loc}}(\mathbb{R}^+; H_{\text{per}}^{-2}(\Omega))$ such that for all $v \in H_{\text{per}}^2(\Omega)$ there holds

$$(\partial_t u, v) + (\nabla(u^3 - u), \nabla v) + \kappa(\Delta u, \Delta v) = 0, \quad t > 0, \text{ a.e.}, \quad (2.1)$$

with the initial condition $u(0) = u_0$, where $(\cdot, \cdot)$ is the standard inner product in $L^2(\Omega)$.

Due to periodic boundary conditions for (1.1)–(1.3), it is natural to use Fourier spectral method. For each integer $N \geq 1$, we introduce the finite dimensional subspace of $H_{\text{per}}^2(\Omega)$:

$$H_N = \text{span} \left\{ 1, \cos \left(2\pi k \cdot \frac{x}{L} \right), \sin \left(2\pi k \cdot \frac{x}{L} \right), 0 < |k| \leq N \right\},$$

where $k = (k_1, k_2)$ and $\frac{x}{L} = (\frac{x_1}{L_1}, \frac{x_2}{L_2})$. Denote also $P_N : L^2(\Omega) \rightarrow H_N$ the $L^2(\Omega)$ -projection onto H_N , which is defined by

$$(P_N u - u, v) = 0, \quad \forall v \in H_N. \quad (2.2)$$

Let $\{\phi_j\}_1^J$ be an orthonormal basis of H_N with respect to the $L^2(\Omega)$ inner product. We define the spectral Galerkin approximation: for each $N \geq 1$, find $u_N(t) \in H_N$ such that

$$(\partial_t u_N, v_N) + (\nabla(u_N^3 - u_N), \nabla v_N) + \kappa(\Delta u_N, \Delta v_N) = 0, \quad \forall v_N \in H_N, \quad (2.3)$$

for all $t > 0$ with $u_N(0) = P_N u_0$. We further define the energy functional of the solution u :

$$E(u) = \frac{\kappa}{2} \|\nabla u\|_0^2 + \frac{1}{4} \|u^2 - 1\|_0^2. \quad (2.4)$$

In [15], some regularity results of the weak solution of (1.1)–(1.3) and convergence properties of the spectral Galerkin approach (2.3) are established. The following results will be useful in our analysis.

Lemma 2.1. [15] *If the initial data in (1.3) satisfies $u_0 \in H_{\text{per}}^4(\Omega)$, then the weak solution $u(t)$ for (1.1)–(1.3) satisfies the following regularity results:*

$$\|u(t)\|_4^2 \leq c_0(\kappa, u_0), \quad \int_0^t \|\partial_t u\|_2^2 ds \leq c_0(\kappa, u_0) + tc(\kappa, u_0), \quad (2.5)$$

for all $t \geq 0$. Similarly, (2.3) admits a unique solution which satisfies

$$\|u_N(t)\|_4^2 \leq c_0(\kappa, u_0), \quad \int_0^t \|\partial_t u_N\|_2^2 ds \leq c_0(\kappa, u_0) + tc(\kappa, u_0), \quad (2.6)$$

where $c(\kappa, u_0)$ and $c_0(\kappa, u_0)$ are two generic positive constants depending on the data (κ, u_0, Ω) .

Lemma 2.2. [15] *Let u be the solution of (1.1)–(1.3) and u_N be the solution of (2.3). If $u_0 \in H_{\text{per}}^4(\Omega)$, then the spectral Galerkin solution $u_N(t)$ satisfies the following error estimate:*

$$\|u(t) - u_N(t)\|_0 \leq N^{-4} c_0(\kappa, u_0) \exp(c(\kappa, u_0)t), \quad \forall t \geq 0. \quad (2.7)$$

Furthermore, if the weak solution u of (1.1)–(1.3) satisfies the following regularity results:

$$\|u(t)\|_q^2 \leq c_0(\kappa, u_0), \quad t \geq 0, \quad q \geq 1, \quad (2.8)$$

then the solution $u_N(t)$ of (2.3) satisfies the following error estimate:

$$\|u(t) - u_N(t)\|_0 \leq N^{-q} c_0(\kappa, u_0) \exp(c(\kappa, u_0)t), \quad \forall t \geq 0. \quad (2.9)$$

2.1. Stability analysis for the first order semi-implicit scheme

In the spectral Galerkin framework, the classical first order semi-implicit scheme is of the form:

$$(d_t u^{n+1}, v) + (\nabla(|u^n|^2 - 1)u^n - \kappa \Delta u^{n+1}, \nabla v) = 0, \quad \forall v \in H_N, \quad (2.10)$$

for all $n \geq 0$ with $u^0 = u_N(0) = P_N u_0$. In (2.10), $d_t u^{n+1} := \frac{1}{\Delta t}(u^{n+1} - u^n)$, where u^n is an approximation of $u_N(x, t_n)$. To increase the size of time-steps, an extra $\mathcal{O}(\Delta t \partial_t u)$ term is added into the left side of (2.10), which gives the following semi-discretized scheme:

$$(d_t u^{n+1}, v) + A(\nabla(u^{n+1} - u^n), \nabla v) + (\nabla(|u^n|^2 - 1)u^n, \nabla v) + \kappa(\Delta u^{n+1}, \Delta v) = 0, \\ \forall v \in H_N(\Omega), \quad (2.11)$$

where A is a positive constant.

Theorem 1. *If A in (2.11) is sufficiently large, then the energy defined by (2.4) is decreasing in time. More precisely, if the positive constant A satisfies*

$$A \geq \max_{x \in \Omega} \left\{ \frac{1}{2} |u^n(x)|^2 + \frac{1}{4} |u^{n+1}(x) + u^n(x)|^2 \right\} - \frac{1}{2}, \quad \forall n \geq 0, \quad (2.12)$$

then for all $m \geq 0$ there holds

$$E(u^m) + \Delta t \sum_{n=1}^{m-1} \|\nabla(A(u^{n+1} - u^n) + (|u^n|^2 - 1)u^n - \kappa \Delta u^{n+1})\|_0^2 \leq E(u_0), \quad (2.13)$$

where $E(u)$ is defined by (2.4) and u_0 is the initial data given by (1.3).

Proof. Taking $v = (A(u^{n+1} - u^n) + (|u^n|^2 - 1)u^n - \kappa \Delta u^{n+1})\Delta t$ in (2.11) and using the equalities

$$2a(a - b) = a^2 - b^2 + (a - b)^2, \quad 2ab = a^2 + b^2 - (a - b)^2, \quad (2.14)$$

we have

$$0 = \|\nabla(A(u^{n+1} - u^n) + (|u^n|^2 - 1)u^n - \kappa \Delta u^{n+1})\|_0^2 \Delta t + A\|u^{n+1} - u^n\|_0^2 \\ + \frac{\kappa}{2} (\|\nabla u^{n+1}\|_0^2 - \|\nabla u^n\|_0^2 + \|\nabla(u^{n+1} - u^n)\|_0^2) + I_n, \quad (2.15)$$

where

$$I_n = ((|u^n|^2 - 1)u^n, u^{n+1} - u^n) \\ = \frac{1}{2} (|u^n|^2 - 1, |u^{n+1}|^2 - |u^n|^2 - |u^{n+1} - u^n|^2) \\ = \frac{1}{2} (1 - |u^n|^2, |u^{n+1} - u^n|^2) - \frac{1}{2} \|u^{n+1}\|_0^2 + \frac{1}{2} \|u^n\|_0^2 - \frac{1}{4} \| |u^{n+1}|^2 - |u^n|^2 \|_0^2 + \frac{1}{4} \|u^{n+1}\|_{L^4}^4 - \frac{1}{4} \|u^n\|_{L^4}^4 \\ = \frac{1}{2} (1 - |u^n|^2 - \frac{1}{2} |u^{n+1} + u^n|^2, |u^{n+1} - u^n|^2) + \frac{1}{4} \| |u^{n+1}|^2 - 1 \|_0^2 - \frac{1}{4} \| |u^n|^2 - 1 \|_0^2. \quad (2.16)$$

Combining (2.15) and (2.16) yields

$$0 \geq \|\nabla(A(u^{n+1} - u^n) + (|u^n|^2 - 1)u^n - \kappa \Delta u^{n+1})\|_0^2 \Delta t + E(u^{n+1}) - E(u^n) \\ + \left(A + \frac{1}{2} - \frac{1}{2} |u^n|^2 - \frac{1}{4} |u^{n+1} + u^n|^2, |u^{n+1} - u^n|^2 \right),$$

which gives the desired result (2.13) provided that the assumption (2.12) is satisfied. $\square$

We point out that the condition for A , i.e. (2.12), is not a satisfactory one in the sense that the right-hand side of (2.12) depends also on A . In other words, it is an implicit relationship for A . An ideal condition will be that the right-hand side of (2.12) depends only on the values of u^n , but not on u^{n+1} . If this is the case, we can obtain an explicit way to compute the value of A (which depends only in time) at each time level. In any case, the condition (2.12) only serves as some intuited way in computations. If the solution of (2.11) is convergent (as Δt is sufficiently small and N is sufficiently large) then the condition (2.12) can be roughly regarded as

$$A \geq \frac{3}{2} \max_{t \geq 0} |u(x, t)|^2 - \frac{1}{2}, \quad \text{a.e. in } \Omega.$$

However, for some larger values of A , the computations of (2.11) may lead to divergent solutions.

2.2. Error estimate of the first order scheme

In this subsection, we will consider the error estimate for the first order time-stepping scheme (2.11). To do this, the following lemmas are useful.

Lemma 2.3. [16,20] *There hold*

$$\|v\|_{L^4}^4 \leq c_0 \|v\|_0^2 \|v\|_1^2, \quad \forall v \in H_{\text{per}}^1(\Omega), \quad (2.17)$$

$$\|v\|_{L^\infty}^4 \leq c_1 \|v\|_0^2 (\|v\|_0^2 + \|\Delta v\|_0^2), \quad \forall v \in H_{\text{per}}^2(\Omega), \quad (2.18)$$

where c_0 and c_1 are positive constants depending on Ω .

Lemma 2.4. [13,14] *Let y_n, d_n, h_n and Δt be non-negative numbers such that*

$$y_{n+1} - y_n \leq d_n y_n \Delta t + h_n \Delta t, \quad \forall n \geq 0. \quad (2.19)$$

Then for all $m \geq 1$,

$$y_m \leq \exp\left(\Delta t \sum_{n=0}^{m-1} d_n\right) \left(y_0 + \Delta t \sum_{n=0}^{m-1} h_n\right). \quad (2.20)$$

Theorem 2. *Let $u(t)$ be the solution of (1.1)–(1.3) and u^n be the solution of (2.11). If Δt and A are chosen such that*

$$\Delta t \leq \frac{2\kappa}{\kappa + 8/7}, \quad (2.21)$$

$$A \geq 3 \max_{x \in \Omega} \left\{ |u^n(x)|^2 + |u_N(x, t_n) - u^n(x)|^2 \right\} - 1, \quad \forall n \geq 0, \quad (2.22)$$

and if $u_0 \in H_{\text{per}}^4(\Omega)$ and u satisfies the regularity result (2.8), then we have the following error estimate:

$$\|u(t_m) - u^m\|_0 \leq c_0(\kappa, u_0) e^{c(\kappa, u_0)t_m} (\Delta t + N^{-q}), \quad q \geq 4. \quad (2.23)$$

Proof. Let $e^m = u_N(t_m) - u^m$, where u_N is the spectral Galerkin solution of (2.3). Integrating (2.3) from t_n to t_{n+1} gives

$$\begin{aligned} & \frac{1}{\Delta t} (u_N(t_{n+1}) - u_N(t_n), v) + A(\nabla(u_N(t_{n+1}) - u_N(t_n)), \nabla v) \\ & + (\Delta(u_N(t_n) - u_N^3(t_n)), v) + \kappa(\Delta u_N(t_{n+1}), \Delta v) = (E^{n+1}, v), \quad \forall v \in H_N(\Omega), \end{aligned} \quad (2.24)$$

for all $n \geq 0$, where

$$\begin{aligned} (E^{n+1}, v) = & -A \left(\int_{t_n}^{t_{n+1}} \Delta(\partial_t u_N) dt, v \right) + \frac{1}{\Delta t} \left(\int_{t_n}^{t_{n+1}} (t - t_{n+1}) \Delta(\partial_t u_N - 3u_N^2 \partial_t u_N) dt, v \right) \\ & + \frac{\kappa}{\Delta t} \left(\int_{t_n}^{t_{n+1}} (t - t_n) \Delta \partial_t u_N dt, \Delta v \right). \end{aligned}$$

Subtracting (2.24) from (2.11) yields

$$\begin{aligned} & \frac{1}{\Delta t} (e^{n+1} - e^n, v) + A(\nabla(e^{n+1} - e^n), \nabla v) + \kappa(\Delta e^{n+1}, \Delta v) \\ & + (3|u^n|^2 - 1, \nabla e^n \cdot \nabla v) + 3(2u_N(t_n)e^n - |e^n|^2, \nabla u_N(t_n) \cdot \nabla v) = (E^{n+1}, v), \end{aligned} \quad (2.25)$$

for all $v \in H_N(\Omega)$ and $n \geq 0$. Taking $v = e^{n+1}$ in (2.25) and using (2.14) yields

$$\begin{aligned}
& \frac{1}{2\Delta t} (\|e^{n+1}\|_0^2 - \|e^n\|_0^2 + \|e^{n+1} - e^n\|_0^2) + \kappa \|\Delta e^{n+1}\|_0^2 + \frac{A}{2} (\|\nabla e^{n+1}\|_0^2 - \|\nabla e^n\|_0^2 + \|\nabla(e^{n+1} - e^n)\|_0^2) \\
& + \frac{1}{2} (3|u^n|^2 - 1, |\nabla e^{n+1}|^2 + |\nabla e^n|^2 - |\nabla(e^{n+1} - e^n)|^2) \\
& + 3(|e^n|^2 + 2u^n e^n, \nabla u_N(t_n) \cdot \nabla e^{n+1}) = (E^{n+1}, e^{n+1}).
\end{aligned} \quad (2.26)$$

Using the Young inequality, the Schwartz inequality and Lemma 2.3, we estimate the second last term in (2.26):

$$3(2u^n e^n, \nabla u_N(t_n) \cdot \nabla e^{n+1}) \geq -\frac{3}{2} \|u^n \nabla e^{n+1}\|_0^2 - 6(|e^n|^2, 6|\nabla u_N(t_n)|^2), \quad (2.27)$$

and

$$\begin{aligned}
& 3(|e^n|^2, \nabla u_N(t_n) \cdot \nabla e^{n+1}) \\
& = \frac{3}{2} (|e^n|^2, -|\nabla(e^{n+1} - e^n)|^2 + |\nabla e^n|^2 + |\nabla e^{n+1}|^2) + 3(|e^n|^2, \nabla u^n \cdot \nabla e^{n+1}) \\
& \geq \frac{3}{2} (|e^n|^2, -|\nabla(e^{n+1} - e^n)|^2 + |\nabla e^n|^2) - \frac{3}{2} (|e^n|^2, |\nabla u^n|^2) \\
& \geq \frac{3}{2} (|e^n|^2, -|\nabla(e^{n+1} - e^n)|^2) - \frac{3}{2} \|e^n\|_{L^\infty}^2 \|\nabla u^n\|_0^2 \\
& \geq \frac{3}{2} (|e^n|^2, -|\nabla(e^{n+1} - e^n)|^2) - \frac{3}{2} c_1^{\frac{1}{2}} \|e^n\|_0 (\|e^n\|_0 + \|\Delta e^n\|_0) \|\nabla u^n\|_0^2 \\
& \geq \frac{3}{2} (|e^n|^2, -|\nabla(e^{n+1} - e^n)|^2) - \frac{\kappa}{16} \|\Delta e^n\|_0^2 - \frac{3}{2} c_1 \|\nabla u^n\|_0^2 (c_1^{-1/2} + 6\kappa^{-1} \|\nabla u^n\|_0^2) \|e^n\|_0^2.
\end{aligned} \quad (2.28)$$

Similarly, the last term in (2.26) can be estimated:

$$\begin{aligned}
(E^{n+1}, e^{n+1}) & \leq \int_{t_n}^{t_{n+1}} ((A+1) \|\Delta \partial_t u_N\|_0 + 3 \|\Delta(u_N^2 \partial_t u_N)\|_0) dt \|e^{n+1}\|_0 + \kappa \int_{t_n}^{t_{n+1}} \|\Delta \partial_t u_N\|_0 dt \|\Delta e^{n+1}\|_0 \\
& \leq \frac{1}{8} \|e^{n+1}\|_0^2 + \frac{\kappa}{16} \|\Delta e^{n+1}\|_0^2 + 4(\kappa + (A+1)^2) \Delta t \int_{t_n}^{t_{n+1}} \|\Delta \partial_t u_N\|_0^2 dt \\
& \quad + 36 \Delta t \int_{t_n}^{t_{n+1}} \|\Delta(u_N^2 \partial_t u_N)\|_0^2 dt.
\end{aligned} \quad (2.29)$$

We can also estimate the last term above:

$$\begin{aligned}
& \int_{t_n}^{t_{n+1}} \|\Delta(u_N^2 \partial_t u_N)\|_0^2 dt \\
& \leq 2 \int_{t_n}^{t_{n+1}} \|2\partial_t u_N |\nabla u_N|^2 + 2u_N \partial_t u_N \Delta u_N\|_0^2 dt + 4 \int_{t_n}^{t_{n+1}} \|4u_N \nabla u_N \cdot \nabla \partial_t u_N + u_N^2 \Delta \partial_t u_N\|_0^2 dt \\
& \leq 16 \int_{t_n}^{t_{n+1}} (\|\partial_t u_N\|_{L^\infty}^2 \|\nabla u_N\|_{L^4}^4 + \|u_N\|_{L^\infty}^2 \|\partial_t u_N\|_{L^\infty}^2 \|\Delta u_N\|_0^2) dt \\
& \quad + 8 \int_{t_n}^{t_{n+1}} (16\|u_N\|_{L^\infty}^2 \|\nabla u_N\|_{L^4}^2 \|\nabla \partial_t u_N\|_{L^4}^2 + \|u_N\|_{L^\infty}^4 \|\Delta \partial_t u_N\|_0^2) dt \\
& \leq 40(c_1 + 5c_0 c_1^{1/2}) \int_{t_n}^{t_{n+1}} \|u_N\|_2^4 (\|\partial_t u_N\|_0^2 + \|\Delta \partial_t u_N\|_0^2) dt.
\end{aligned}$$

Using the Young inequality and the Schwartz inequality gives

$$\frac{1}{2}(\|\nabla e^{n+1}\|_0^2 + \|\nabla e^n\|_0^2) \leq \frac{7\kappa}{16}(\|\Delta e^{n+1}\|_0^2 + \|\Delta e^n\|_0^2) + \frac{1}{7\kappa}(2\|e^{n+1} - e^n\|_0^2 + 3\|e^n\|_0^2),$$

and

$$\frac{1}{8}\|e^{n+1}\|_0^2 \leq \frac{1}{4}\|e^{n+1} - e^n\|_0^2 + \frac{1}{4}\|e^n\|_0^2.$$

Applying the above inequalities to (2.26) and using Lemma 2.1 yields

$$\begin{aligned} & \|e^{n+1}\|_0^2 - \|e^n\|_0^2 + A(\|\nabla e^{n+1}\|_0^2 - \|\nabla e^n\|_0^2)\Delta t + \kappa(\|\Delta e^{n+1}\|_0^2 - \|\Delta e^n\|_0^2)\Delta t \\ & + \left(1 - \left(\frac{1}{2} + \frac{4}{7\kappa}\right)\Delta t\right)\|e^{n+1} - e^n\|_0^2 + \left(A + 1 - 3\max_{x \in \Omega}\{|u^n(x)|^2 + |e^n(x)|^2\}, |\nabla(e^{n+1} - e^n)|^2\right)\Delta t \\ & \leq d_n\|e^n\|_0^2\Delta t + 8(\kappa + (1 + A)^2 + c_0(\kappa, u_0))\Delta t^2 \int_{t_n}^{t_{n+1}} (\|\partial_t u_N\|_0^2 + \|\Delta \partial_t u_N\|_0^2) dt, \end{aligned} \quad (2.30)$$

where

$$d_n = \kappa^{-1} + \frac{1}{2} + 3c_1^{1/2}\|\nabla u^n\|_0^2(c_1^{-1/2} + 6\kappa^{-1}\|\nabla u^n\|_0^2). \quad (2.31)$$

Using (2.21)–(2.22) and setting

$$\begin{aligned} y_n &= \|e^n\|_0^2 + A\|\nabla e^n\|_0^2 + \kappa\|\Delta e^n\|_0^2, \\ h_n &= 8(\kappa + (1 + A)^2 + c_0(\kappa, u_0))\Delta t \int_{t_n}^{t_{n+1}} (\|\partial_t u_N\|_0^2 + \|\Delta \partial_t u_N\|_0^2) dt, \end{aligned}$$

we deduce from (2.30) that $y_{n+1} - y_n \leq d_n y_n + h_n$ for $n \geq 0$. Using Lemma 2.4, together with Lemma 2.1 and Theorem 1, yield

$$\|e^m\|_0^2 + A\|\nabla e^m\|_0^2 + \kappa\|\Delta e^m\|_0^2 \leq c_0(\kappa, u_0)e^{c(\kappa, u_0)t_m}\Delta t^2. \quad (2.32)$$

This result, together with Lemma 2.2, leads to the desired estimate (2.23). $\square$

The condition (2.21) indicates that Δt is linearly proportional to κ . It will be seen in the next section that if κ is very small then the time-step Δt has to be also very small in order to preserve solution accuracy.

3. Numerical experiments

A complete numerical algorithm also requires a discretization strategy in space. Since Fourier spectral method is one of the most suitable spatial approximation methods for periodic problems [2,4,21], it will be employed to handle the spatial discretization. To demonstrate the main ideas of the numerical schemes, we begin by considering the problem (1.1)–(1.3) in one space dimension. We use the following Fourier transformations:

$$\hat{u}(k, t) = \frac{1}{N} \sum_{j=0}^{N-1} u(x_j, t) e^{-ikx_j}, \quad -N/2 \leq k \leq N/2 - 1 \quad (3.1)$$

$$u^N(x_j, t) = \sum_{k=-N/2}^{N/2-1} \hat{u}(k, t) e^{ikx_j}, \quad 0 \leq j \leq N - 1. \quad (3.2)$$

Denote $f(u) = -u + u^3$. Taking Fourier transforms to (1.1) gives, for $0 \leq j \leq N - 1$,

$$\sum_{k=-N/2}^{N/2-1} \frac{d}{dt} \hat{u}(k, t) e^{ikx_j} = - \sum_{k=-N/2}^{N/2-1} \hat{f}(k, t) k^2 e^{ikx_j} - \kappa \sum_{k=-N/2}^{N/2-1} \hat{u}(k, t) k^4 e^{ikx_j}, \quad (3.3)$$

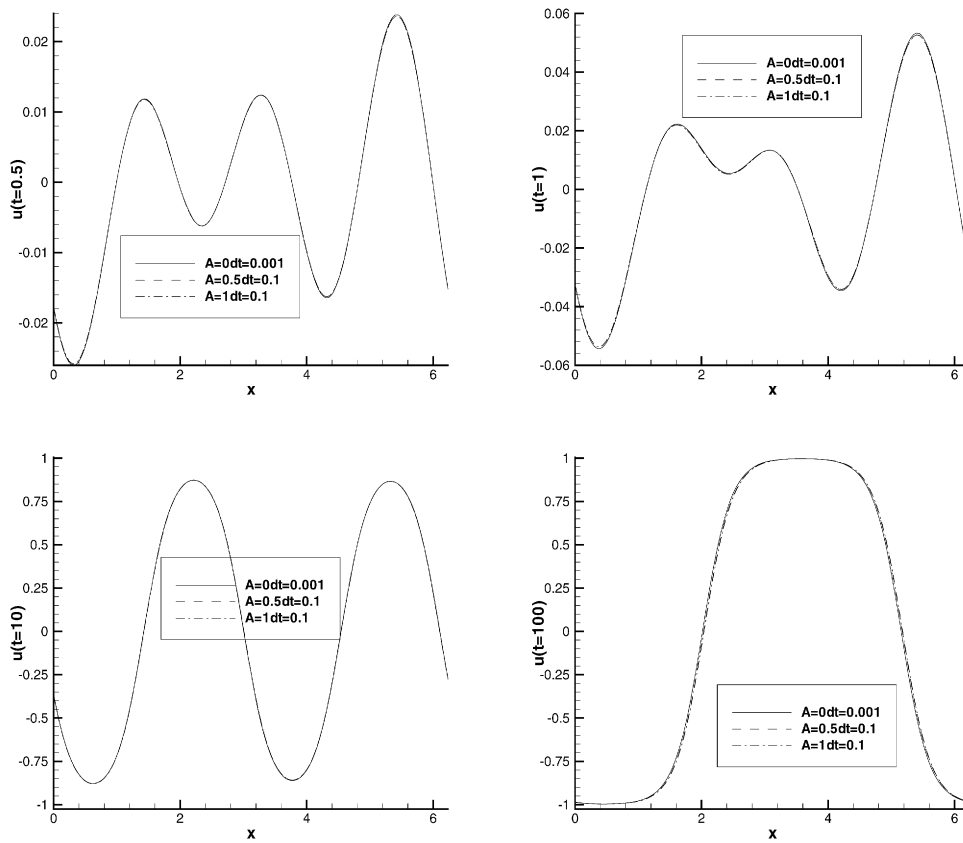


Fig. 1. Numerical results obtained by using the second-order time-stepping method with $N = 128$. $\kappa = 0.1$.

Table 1
 $\Delta t_{\max}$ with different κ and A

κ	A	Δt_c for scheme (3.6)	Δt_c for scheme (3.7)
$\kappa = 0.1$	$A = 0$	$\Delta t_c \approx 0.2$	$\Delta t_c \approx 0.06$
	$A = 0.5$	$\Delta t_c > 1$	$\Delta t_c \approx 0.15$
	$A = 1$	$\Delta t_c > 1$	$\Delta t_c \approx 0.8$
$\kappa = 0.01$	$A = 0$	$\Delta t_c \approx 0.02$	$\Delta t_c \approx 0.004$
	$A = 0.5$	$\Delta t_c \approx 0.2$	$\Delta t_c \approx 0.013$
	$A = 1$	$\Delta t_c \approx 0.2$	$\Delta t_c \approx 0.07$
$\kappa = 0.001$	$A = 0$	$\Delta t_c \approx 0.003$	$\Delta t_c \approx 0.0004$
	$A = 0.5$	$\Delta t_c \approx 0.013$	$\Delta t_c \approx 0.0013$
	$A = 1$	$\Delta t_c \approx 0.03$	$\Delta t_c \approx 0.005$

where

$$\hat{f}(k, t) = \frac{1}{N} \sum_{j=0}^{N-1} f(u(x_j, t)) e^{-ikx_j}, \quad -N/2 \leq k \leq N/2 - 1.$$

Consequently, we have an ODE system in the Fourier space

$$\frac{d}{dt} \hat{u}(k, t) = -k^2 \hat{f}(k, t) - \kappa k^4 \hat{u}(k, t), \quad -N/2 \leq k \leq N/2 - 1. \quad (3.4)$$

The ODE system (3.4) can be approximated by using the classical first-order semi-implicit method:

$$\hat{u}^{n+1}(k) = \hat{u}^n(k) - k^2 \Delta t \hat{f}^n(k) - \kappa k^4 \Delta t \hat{u}^{n+1}(k), \quad -N/2 \leq k \leq N/2 - 1. \quad (3.5)$$

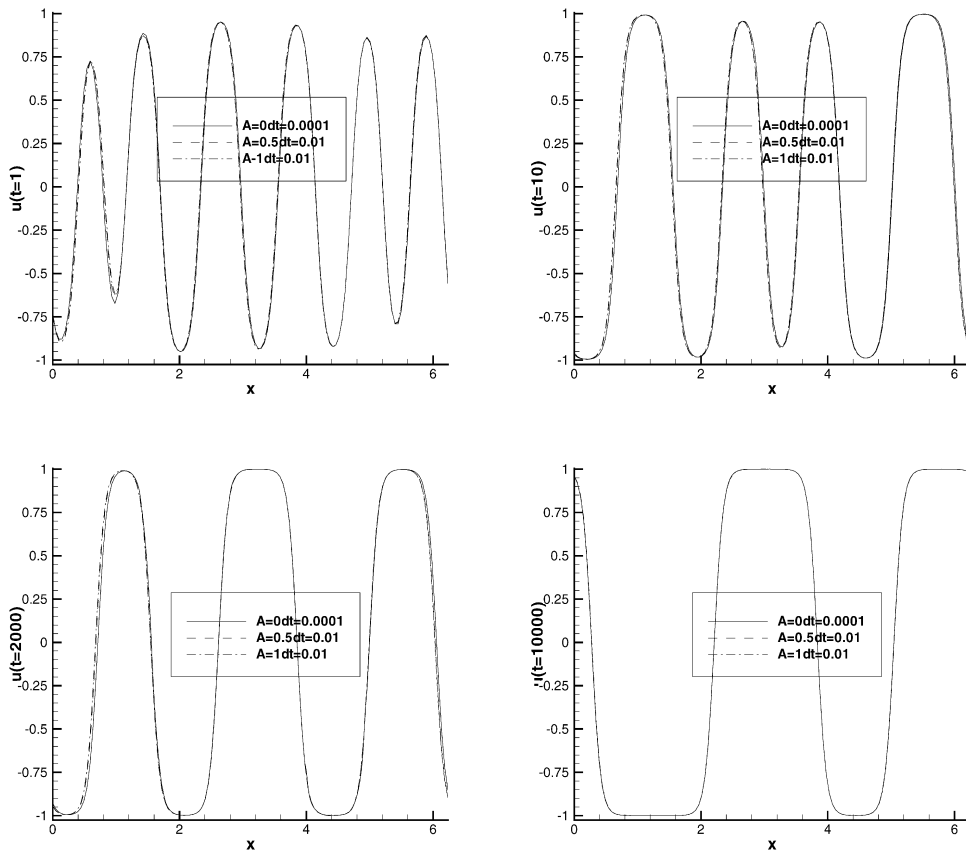


Fig. 2. Numerical results obtained by using the second-order time-stepping method with $N = 128$, $\kappa = 0.01$.

Table 2

Numerical errors obtained by using the second-order time-stepping scheme (3.7) with $\kappa = 0.001$ and $N = 256$

	Δt	L^2 -error	L^∞ -error
$A = 0$	$\Delta t = 0.00005$	3.98E-5	1.32E-4
	$\Delta t = 0.0001$	1.62E-4	5.40E-4
	$\Delta t = 0.0005$	unstable	unstable
$A = 0.25$	$\Delta t = 0.00005$	5.55E-5	1.85E-4
	$\Delta t = 0.0001$	2.21E-4	7.36E-4
	$\Delta t = 0.0005$	2.70E-3	8.98E-3
$A = 0.5$	$\Delta t = 0.00005$	7.11E-5	2.37E-4
	$\Delta t = 0.0001$	2.78E-4	9.27E-4
	$\Delta t = 0.0005$	3.01E-3	1.00E-2
$A = 1$	$\Delta t = 0.00005$	1.02E-4	3.40E-4
	$\Delta t = 0.0001$	3.89E-4	1.30E-3
	$\Delta t = 0.0005$	3.46E-3	1.15E-2

If we add an $\mathcal{O}(u_t \Delta t)$ term as discussed in the last two sections, we need to solve a modified system

$$\hat{u}^{n+1}(k) = \hat{u}^n(k) - Ak^2 \Delta t (\hat{u}^{n+1}(k) - \hat{u}^n(k)) - k^2 \Delta t \hat{f}^n(k) - \kappa k^4 \Delta t \hat{u}^{n+1}(k), \quad (3.6)$$

for $-N/2 \leq k \leq N/2 - 1$. The corresponding second-order BDF/AB scheme is of the form:

$$\begin{aligned} & \frac{3\hat{u}^{n+1}(k) - 4\hat{u}^n(k) + \hat{u}^{n-1}(k)}{2\Delta t} \\ &= -Ak^2 (\hat{u}^{n+1}(k) - 2\hat{u}^n(k) + \hat{u}^{n-1}(k)) - k^2 [2\hat{f}^n(k) - \hat{f}^{n-1}(k)] - \kappa k^4 \hat{u}^{n+1}(k), \end{aligned} \quad (3.7)$$

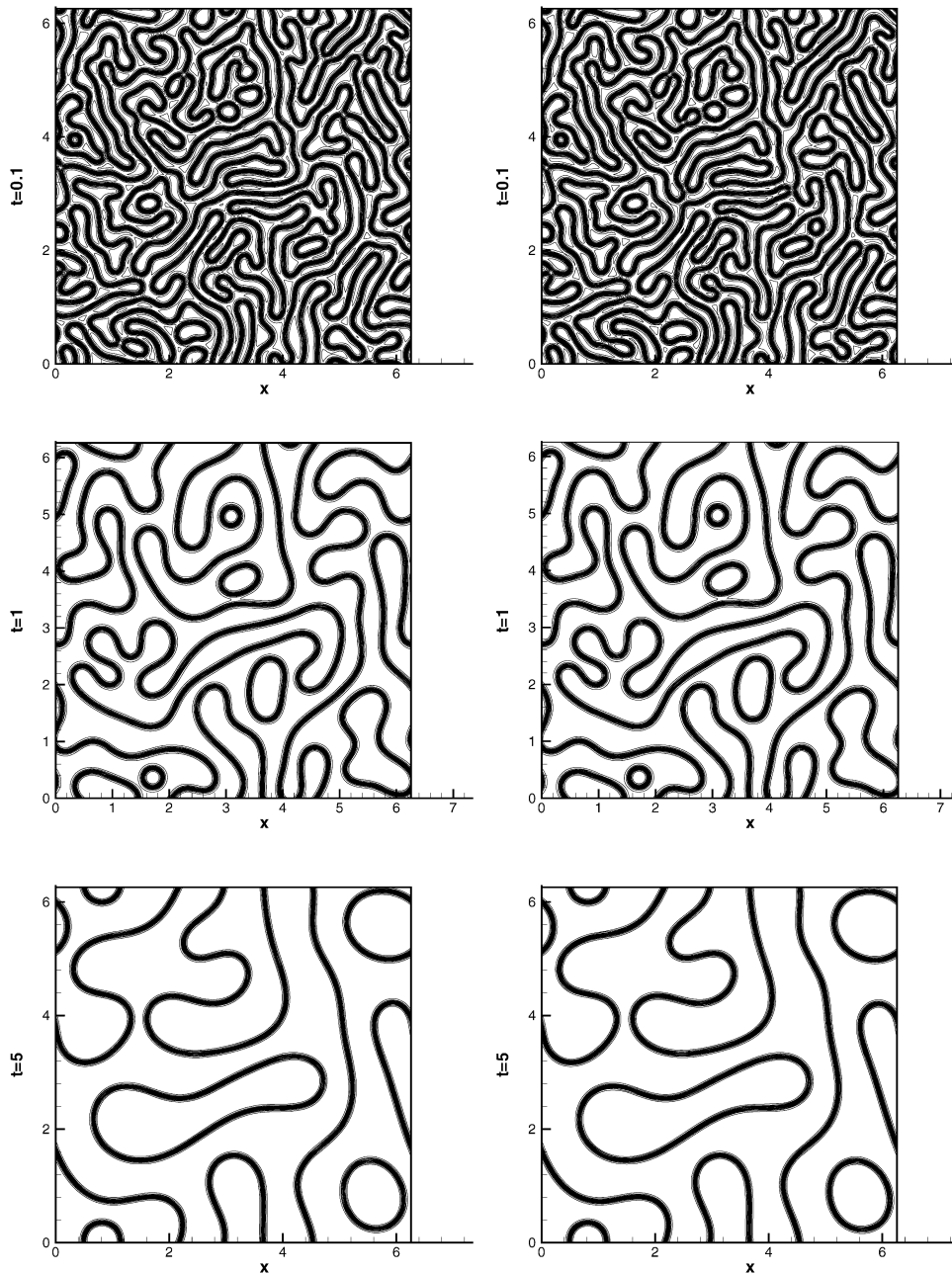
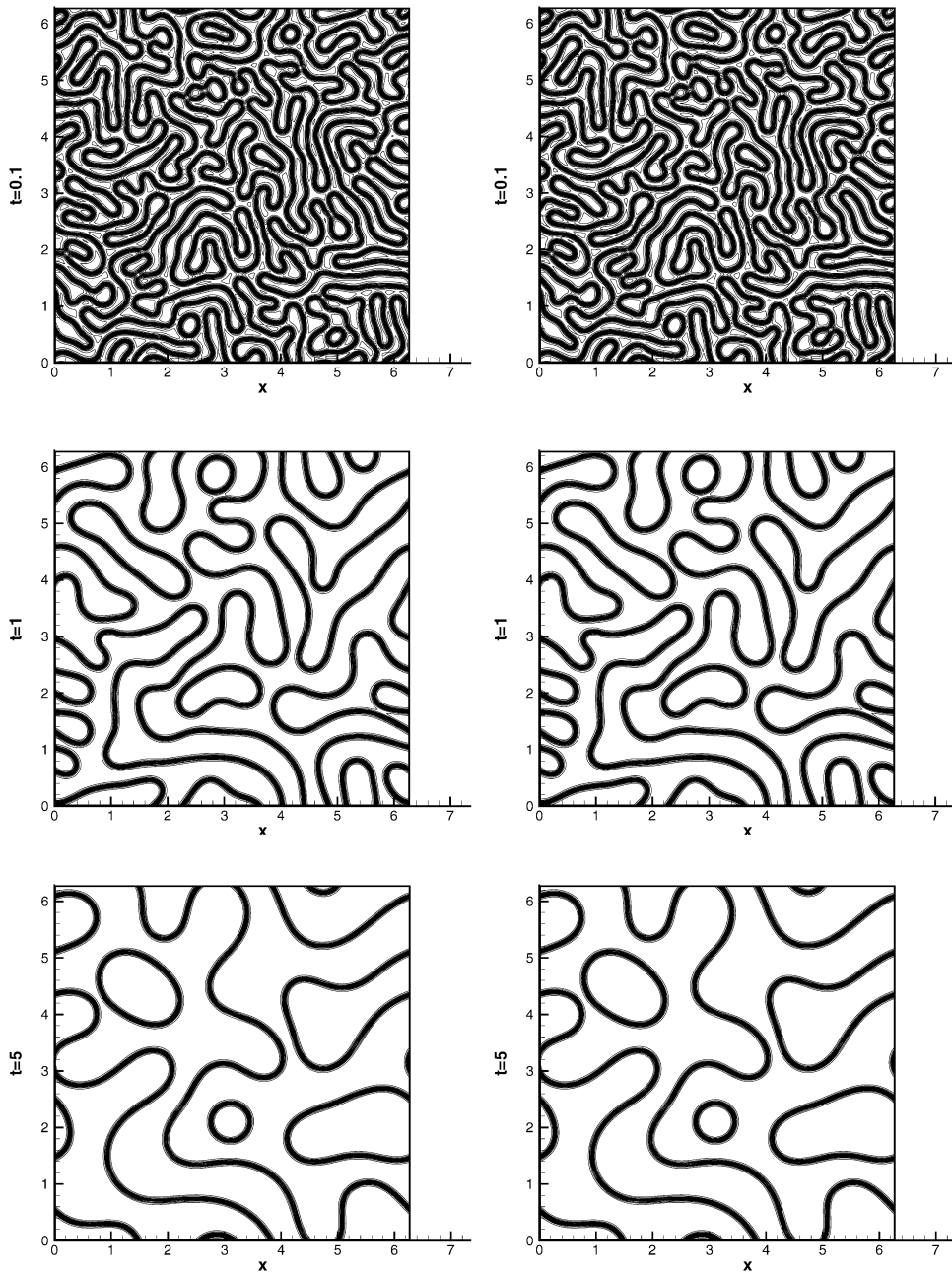


Fig. 3. Solution of $\kappa = 0.001$ at $t = 0.1, 1$ and 5 . Left: $A = 0$, $\Delta t = 0.0001$; right: $A = 0.5$, $\Delta t = 0.0005$. $N = 256$.

for $-N/2 \leq k \leq N/2 - 1$. The schemes (3.6) and (3.7) can be easily extended to two space dimensions, and we will omit the details here. Standard FFTs have been used to speed up the computations.

We first investigate the stability issue. Consider the problem (1.1)–(1.3) in 1D with u_0 being a random data. Define Δt_c to be the largest possible time which allows stable numerical computation. In other words, if the time-step is larger than Δt_c then the numerical solution will blow up. In Table 1, we list the values of Δt_c with different κ and different choices of A , from which it is observed that time-steps can be increased a few times larger by adding a non-zero A term in both first and second order semi-implicit schemes.

To demonstrate convergence property of the proposed numerical schemes, we present some numerical simulations for the Cahn–Hilliard equation (1.1) with the second-order scheme (3.7). The simulations are carried out in the do-

Fig. 4. Same as Fig. 3, except with $N = 512$.

main $\Omega = [0, 2\pi]^2$, with a double periodic boundary condition. The initial condition is a random state by assigning a random number varying from -0.05 to 0.05 to each grid point. The spatial discretization is based on a Fourier pseudospectral approximation with N denoting the number of the Fourier mode.

Figs. 1 and 2 show the solutions for $\kappa = 0.1$ and $\kappa = 0.01$ with different values of A and Δt : Fig. 1 with $(A, \Delta t) = (0, 0.01), (0.5, 0.1), (1, 0.1)$ and Fig. 2 with $(A, \Delta t) = (0, 0.0001), (0.5, 0.01), (1, 0.01)$. It is observed that there is a good agreement between the numerical results obtained by using standard semi-implicit time-stepping method (i.e., $A = 0$) with small Δt and the modified method (3.7) with larger Δt . Qualitatively, the results in Figs. 1 and 2 are in good agreement with those presented in [11], where $\Delta t = 1/1200$ is used.

We now turn to time accuracy comparison. Since the exact solution of (1.1) is unknown, we use numerical results of the second-order scheme (3.7) with $\Delta t = 10^{-7}$ and $N = 256$ as the “exact” solution. In our computations, we set $\kappa = 0.001$ and the final time $T = 1$. Table 2 shows the L^2 -errors and L^∞ -errors obtained by using the second-order scheme (3.7). It is seen that the numerical errors are almost the same for computations with and without using the A terms, and larger time-steps can be used by adding an A term.

For 2D problems, we plot the contour lines of the solution at different times with $A = 0$, $\Delta t = 10^{-4}$ and $A = 0.5$, $\Delta t = 5 \times 10^{-4}$, respectively. Figs. 3 and 4 show the solution comparisons with 256 Fourier modes (i.e., $N = 256$) and 512 modes, respectively. The agreement in each case is excellent. It is noted that the corresponding solutions in Figs. 3 and 4 are different, since the random data using different sampling size N gives different initial condition.

4. Conclusions

In this work, we performed a preliminary study of larger time stepping techniques for the Cahn–Hilliard equation. It is known that the time-step in a semi-implicit method can be orders of magnitude larger than that in an explicit method. In this work, it is demonstrated that the classical semi-implicit method can be further improved by simply adding a linear term consistent with the truncation errors in time. This treatment can be used to increase the time-step size a few times larger. Some preliminary error and stability analysis has been performed, which provides some simple conditions on the magnitude of the extra term.

The future works along this direction are to carry out more rigorous analysis for the large time-stepping techniques, including more realistic condition for A . The conditions (2.12) and (2.22) depend on the numerical solutions and are therefore unsatisfactory. Theoretical analysis for higher order schemes of type (3.7) also seems challenging.

Acknowledgements

The research of Y. He was supported in part by National Science Foundation of China Grant #10371095. The research of Y. Liu was supported in part by National Science Foundation of China Grant #10501031. This project was supported by CERG Grants of Hong Kong Research Grant Council, FRG grants of Hong Kong Baptist University, and NSAF Grant #10476032 of National Science Foundation of China.

References

- [1] J.W. Barrett, J.F. Blowey, H. Garcke, On fully practical finite element approximations of degenerate Cahn–Hilliard systems, *M2AN Math. Model. Numer. Anal.* 35 (2001) 713–748.
- [2] J.P. Boyd, Chebyshev and Fourier Spectral Methods, second ed., Dover, Mineola, NY, 2001.
- [3] J.W. Cahn, J.E. Hilliard, Free energy of a non-uniform system I: Interfacial free energy, *J. Chem. Phys.* 28 (1958) 258–267.
- [4] B. Costa, W.-S. Don, D. Gottlieb, R. Sendersky, Two-dimensional multi-domain hybrid spectral-WENO methods for conservation laws, *Commun. Comput. Phys.* 1 (2006) 550–577.
- [5] C.M. Elliot, D.A. French, Numerical studies of the Cahn–Hilliard equation for phase separation, *IMA J. Appl. Math.* 38 (1987) 97–128.
- [6] C.M. Elliot, D.A. French, A nonconforming finite element method for the two-dimensional Cahn–Hilliard equation, *SIAM J. Numer. Anal.* 26 (1989) 884–903.
- [7] C.M. Elliot, D.A. French, D.A. Milner, A second order splitting method for the Cahn–Hilliard equation, *Numer. Math.* 54 (1989) 575–590.
- [8] C.M. Elliot, S. Larsson, Error estimates with smooth and nonsmooth data for a finite element method for the Cahn–Hilliard equation, *Math. Comp.* 58 (1992) 603–630.
- [9] L.Q. Chen, J. Shen, Applications of semi-implicit Fourier-spectral method to phase field equations, *Comput. Phys. Comm.* 108 (1998) 147–158.
- [10] X.B. Feng, A. Prohl, Error analysis of a mixed finite element method for the Cahn–Hilliard equation, *Numer. Math.* 99 (2004) 47–84.
- [11] D. Furihata, A stable and conservative finite difference scheme for the Cahn–Hilliard equation, *Numer. Math.* 87 (2001) 675–699.
- [12] M.E. Gurtin, On the two-phase Stefan problem with interfacial energy and entropy, *Acta Rat. Mech. Anal.* 96 (1988) 199–243.
- [13] Y.N. He, K.T. Li, Asymptotic behavior and time discretization analysis for the nonstationary Navier–Stokes problem, *Numer. Math.* 98 (4) (2004) 647–673.
- [14] Y.N. He, K.T. Li, Convergence and stability of finite element nonlinear Galerkin method for the Navier–Stokes equations, *Numer. Math.* 79 (1998) 77–106.
- [15] Y.N. He, Y.X. Liu, Stability and convergence of the spectral Galerkin method for the Cahn–Hilliard equation, in preparation.
- [16] B. Li, J.G. Liu, Thin film epitaxy with or without slope selection, *Eur. J. Appl. Math.* 14 (2003) 713–743.
- [17] E.V.L. Mello, O.T.S. Filho, Numerical study of the Cahn–Hilliard equation in one, two and three dimensions, *Phys. A* 347 (2005) 429–443.
- [18] R.L. Pego, Front migration in the nonlinear Cahn–Hilliard equation, *Proc. Roy. Soc. London A* 422 (1989) 261–278.

- [19] Z.Z. Sun, A second-order accurate linearized difference scheme for the two-dimensional Cahn–Hilliard equation, *Math. Comp.* 64 (1995) 1463–1471.
- [20] R. Temam, *Navier–Stokes Equations, Theory and Numerical Analysis*, third ed., North-Holland, Amsterdam, 1983.
- [21] D. Xiu, J. Shen, An efficient spectral method for acoustic scattering from rough surfaces, *Commun. Comput. Phys.* 1 (2007) 54–72.
- [22] C. Xu, T. Tang, Stability analysis of large time-stepping methods for epitaxial growth models, *SIAM J. Numer. Anal.* (2006), in press.
- [23] J. Zhu, L.-Q. Chen, J. Shen, V. Tikare, Coarsening kinetics from a variable-mobility Cahn–Hilliard equation: Application of a semi-implicit Fourier spectral method, *Phys. Rev. E* 60 (4) (1999) 3564–3572.