Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **8**, No. 6, pp. 992-1003

DOI: 10.4208/aamm.2014.m48
December 2016

On a Large Time-Stepping Method for the Swift-Hohenberg Equation

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Received 11 December 2014; Accepted (in revised version) 16 March 2016

Abstract. The main purpose of this work is to contrast and analyze a large time-stepping numerical method for the Swift-Hohenberg (SH) equation. This model requires very large time simulation to reach steady state, so developing a large time step algorithm becomes necessary to improve the computational efficiency. In this paper, a semi-implicit Euler schemes in time is adopted. An extra artificial term is added to the discretized system in order to preserve the energy stability unconditionally. The stability property is proved rigorously based on an energy approach. Numerical experiments are used to demonstrate the effectiveness of the large time-stepping approaches by comparing with the classical scheme.

AMS subject classifications: 65M06, 65Z05

Key words: Large time-stepping method, energy stable, Swift-Hohenberg equation, finite difference method.

1 Introduction

There have been many dynamical models of non-equilibrium system which often results in highly complicated domain structures. There are many well-known models including Cahn-Hilliard equation (for conservative system) [2] and Allen-Cahn model (for non-conservative system) [1] which are used to describe the phase interface, molecular beam epitaxy growth model [11] which is used to describe the height of the thin solid films, the phase field crystal (PFC) equation which is used to describe the defects in crystal. The Swift-Hohenberg (SH) model [10] is a non-conserved form of the PFC equation. Recently, these models are developed to couple with incompressible fluids [3, 14], and the corresponding energy laws are derived.

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The SH model can account for elastic and plastic deformations of the lattice, dislocations, grain boundaries, and many other observable phenomena, see [12]. The models that are minimized by periodic functions were accounted for the periodic structure of a crystal lattice as free energy functionals. This model differs from the CH and AC models in that the stable phase is periodic, see [4]. For SH models, the order parameter is viewed as capturing the inhomogeneities in a fluid associated with Rayleigh-Bénard convection. The theory of the SH problem has been studied for decades. However, both the fourth-order and the nonlinear term make the SH equation stiff and difficult to solve numerically.

The standard Euler integration is known to be unstable for time step Δt above a threshold fixed by lattice spacing Δx [9]. In CH and AC systems, to maintain an interfacial profile, the lattice spacing must be smaller than the interfacial width. As we know for these models such as CH or AC equation, molecular beam epitaxy model and SH model, it takes large time to reach steady state. So developing large time stepping method becomes necessary. The large time stepping idea proposed by Xu and Tang [13] for the molecular beam epitaxy simulation allows rather larger time step than the classical time discretizations, and has been used to solve CH equation by He and Tang [6]. Another method to avoid small time step is to use adaptive time step strategy, which is successfully applied to molecular beam epitaxy model [8] and CH model [15]. The time steps are chosen based on the variation of the energy functional with respect to time variable. In SH system, the time step Δx must be smaller than the periodicity selected by the system. In this paper, we will apply the similar idea in [13] to the simulation of SH model. A large time-stepping method for the SH equation is proposed with an extra term added to the classical Euler approach, which is consistent with the order of the time discretization. The fourth order term is treated implicitly and the concave part is approximated explicitly. The proposed difference scheme is proved to preserve energy stability unconditionally. In this work the energy means the free energy functional corresponding to the SH model in stead of the traditional L^2-norm as discussed in our recent work for epitaxial growth model [7].

This paper is organized as below. In Section 2, the SH model is introduced and the numerical scheme is proposed. In Section 3, we establish the stability analysis about the numerical algorithm. Numerical experiments are presented in Section 4 to show the effectiveness of the proposed scheme. Finally, in Section 5, some concluding remarks are made.

2 The SH model and the unconditionally stable scheme

Both the SH and PFC models come from minimizing the free energy functional that describes the configurational cost of periodic phase in contact with isotropic phase [5, 10]:

$$E(\phi)=\int_\Omega \left\{\frac{1}{4}\phi^4+\frac{1-\epsilon}{2}\phi-|\nabla\phi|^2+\frac{1}{2}(\Delta\phi)^2\right\}dx, \tag{2.1}$$

where the $\Omega \subset R^D$, $D=2$ or 3, here we consider $D=2$, $\Omega=(0,L)\times(0,L)$, $\phi:\Omega\to R$ is the density field, ϵ is a given small positive constant, ∇ and Δ are the gradient and Laplacian operators, respectively.

The SH model is the non-conserved type dynamics as below

$$\frac{\partial\phi}{\partial t}=-M(\phi)\mu, \tag{2.2}$$

where $M(\phi)$ is a mobility and μ is the chemical potential as

$$\mu=\frac{\delta E}{\delta\phi}=\phi^3+(1-\epsilon)\phi+2\Delta\phi+\Delta^2\phi, \tag{2.3}$$

where $\delta E/\delta\phi$ denotes the variational derivative of E with respect with ϕ.

The PFC model is the conserved dynamics of (2.2):

$$\frac{\partial\phi}{\partial t}=\nabla\cdot(M(\phi)\nabla\mu). \tag{2.4}$$

In [12], a conservative finite difference scheme based on energy splitting was proposed to solve the PFC equation in two space dimension. It is proved that their proposed scheme is stable in the sense that the decay of energy is preserved numerically. Here, we study the numerical scheme of SH equation (2.2) with periodic boundary condition and also suppose that $\Delta\phi$ and $\nabla\phi$ are periodic on Ω. Our main interest is to design an appropriate scheme that allows large time steps.

The classical first order semi-implicit scheme is of the form

$$\frac{\phi^{k+1}-\phi^k}{\Delta t}=-2\Delta_h\phi^k-\Delta_h^2\phi^{k+1}-(1-\epsilon)\phi^{k+1}-(\phi^k)^3,\quad k\geq 0, \tag{2.5}$$

where Δt is the time step and $t_k=k\Delta t$, ϕ^k is an approximation to $\phi(x,t_k)$. Δ_h is the standard central difference approximation to Laplacian operator. 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 (2.5), we propose to add an $\mathcal{O}(\Delta t)$ term to the scheme (2.5):

$$\frac{\phi^{k+1}-\phi^k}{\Delta t}+A(\phi^{k+1}-\phi^k)=-2\Delta_h\phi^k-\Delta_h^2\phi^{k+1}-(1-\epsilon)\phi^{k+1}-(\phi^k)^3, \tag{2.6}$$

where A is a positive constant to be determined later. The purpose for adding the extra terms is to improve the stability condition so that larger time steps can be used. This can be proved theoretically, and will be demonstrated by our numerical results.

3 Stability analysis

We will show the energy stability analysis for the proposed scheme (2.6) and give the choice of the artificial parameter A. We first state the following existing result:

Lemma 3.1. *If $\phi(x,t)$ is a solution of* (2.2)*, then the following energy identity holds:*

$$\frac{d}{dt}E(\phi(t))\leq 0,\quad \forall t\geq 0, \tag{3.1}$$

where $E(\phi)$ is defined in (2.1)*.*

We briefly sketch the proof of Lemma 3.1, which is useful in deriving its discrete case.

Proof. It follows from (2.2) that

$$(\phi_t,\varphi)=(-2\Delta\phi-\Delta^2\phi-\phi^3-(1-\epsilon)\phi,\varphi), \tag{3.2}$$

where $(\cdot,\cdot)$ denotes the standard inner product in the L^2-space.

Taking $\varphi=-\phi_t=2\Delta\phi+\Delta^2\phi+\phi^3+(1-\epsilon)\phi$ in (3.2), we have

$$(\phi_t,-\phi_t)=(\phi_t,2\Delta\phi)+(\phi_t,\Delta^2\phi)+(\phi_t,\phi^3+(1-\epsilon)\phi).$$

We obtain by integration by parts

$$-\frac{d}{dt}\int_\Omega|\nabla\phi|^2dx+\frac{1}{2}\frac{d}{dt}\int_\Omega(\Delta\phi)^2dx+\frac{d}{dt}\int_\Omega\Big(\frac{1}{4}\phi^4+\frac{1-\epsilon}{2}\phi^2\Big)dx=-\|\phi_t\|^2\leq 0.$$

Note the definition of energy functional $E(\phi)$, this completes the proof. □

Theorem 3.1. *For any $A>0$ and $\Delta t>0$, the finite difference scheme* (2.6) *is solvable.*

Proof. The numerical scheme (2.6) leads to a linear algebra system, and the coefficient matrix is of the form

$$\Big(\frac{1}{\Delta t}+A\Big)I+\Delta_h^2,$$

which always has positive eigenvalues. So the system is solvable. □

Theorem 3.2. *If the constant A in* (2.6) *is sufficiently large, then the following energy inequality holds:*

$$E_h(\phi^{k+1})\leq E_h(\phi^k), \tag{3.3}$$

where E_h is the discrete form of the energy functional defined in (2.1)*. More precisely, the positive constant A satisfies*

$$A\geq\max_{x\in\Omega}\Big\{\frac{1}{2}((\phi^k)^2+1-\epsilon)+\frac{1}{4}(\phi^{k+1}+\phi^k)^2\Big\}, \tag{3.4}$$

where ϕ^k and ϕ^{k+1} are the numerical solutions of (2.6)*.*

Proof. For any L-periodic $H^2(\Omega)$ function φ, it follows from (2.6) that

$$\frac{1}{\Delta t}(\phi^{k+1}-\phi^k,\varphi)_h+A((\phi^{k+1}-\phi^k),\varphi)_h+I(\varphi)=0, \tag{3.5}$$

where $(\cdot,\cdot)_h$ denotes the standard discrete inner product in the L^2-space, and

$$I(\varphi)=(\Delta_h^2\phi^{k+1}+2\Delta_h\phi^k+(\phi^k)^3+(1-\epsilon)\phi^{k+1},\varphi)_h. \tag{3.6}$$

Letting $\varphi=\phi^{k+1}-\phi^k$, observe that

$$\frac{1}{\Delta t}\|\phi^{k+1}-\phi^k\|_h^2+A(\phi^{k+1}-\phi^k,\phi^{k+1}-\phi^k)_h+I=0, \tag{3.7}$$

where $\|\cdot\|_h$ denotes the discrete L^2-norm and

$$I=(\Delta^2\phi^{k+1}+2\Delta_h\phi^k+(\phi_h^k)^3+(1-\epsilon)\phi^{k+1},\phi^{k+1}-\phi^k)_h.$$

Below we always use the equalities

$$b(a-b)=\frac{1}{2}(a^2-b^2-(a-b)^2) \quad \text{and} \quad a(a-b)=\frac{1}{2}(a^2-b^2+(a-b)^2).$$

We divide I into three parts as $I=I_1+I_2+I_3$, where

$$\begin{aligned} I_1&=(\Delta_h^2\phi^{k+1},\phi^{k+1}-\phi^k)_h=(\Delta_h\phi^{k+1},\Delta_h(\phi^{k+1}-\phi^k))_h\\ &=\frac{1}{2}\|\Delta_h\phi^{k+1}\|_h^2-\frac{1}{2}\|\Delta_h\phi^k\|_h^2+\frac{1}{2}\|\Delta_h(\phi^{k+1}-\phi^k)\|_h^2, \end{aligned} \tag{3.8a}$$

$$\begin{aligned} I_2&=2(\Delta_h\phi^k,\phi^{k+1}-\phi^k)_h=-2(\nabla_h\phi^k,\nabla_h(\phi^{k+1}-\phi^k))_h\\ &=-\|\nabla_h\phi^{k+1}\|_h^2+\|\nabla_h\phi^k\|_h^2+\|\nabla_h(\phi^{k+1}-\phi^k)\|_h^2, \end{aligned} \tag{3.8b}$$

and

$$\begin{aligned} I_3&=((\phi^k)^3+(1-\epsilon)\phi^{k+1},\phi^{k+1}-\phi^k)_h\\ &=((\phi^k)^2,\phi^k(\phi^{k+1}-\phi^k))_h+(1-\epsilon)(\phi^{k+1},\phi^{k+1}-\phi^k))_h\\ &=\frac{1}{2}((\phi^k)^2,(\phi^{k+1})^2-(\phi^k)^2-(\phi^{k+1}-\phi^k)^2)_h\\ &\quad+\frac{1}{2}(1-\epsilon)((\phi^{k+1})^2-(\phi^k)^2+(\phi^{k+1}-\phi^k)^2,1)_h\\ &=\frac{1}{4}((\phi^{k+1})^4-(\phi^k)^4-((\phi^{k+1})^2-(\phi^k)^2)^2,1)_h-\frac{1}{2}((\phi^k)^2,(\phi^{k+1}-\phi^k)^2)_h\\ &\quad+\frac{1}{2}(1-\epsilon)((\phi^{k+1})^2-(\phi^k)^2+(\phi^{k+1}-\phi^k)^2,1)_h\\ &=K+\frac{1}{4}\|(\phi^{k+1})^2+1-\epsilon\|_h^2-\frac{1}{4}\|(\phi^k)^2+1-\epsilon\|_h^2, \end{aligned} \tag{3.9}$$

where

$$K=\Big(-\frac{1}{2}((\phi^k)^2-(1-\epsilon))-\frac{1}{4}(\phi^{k+1}+\phi^k)^2,(\phi^{k+1}-\phi^k)^2\Big)_h.$$

With the above estimation for I_1, I_2 and I_3, we re-estimate (3.7) to get

$$\begin{aligned}&\frac{1}{\Delta t}\|\phi^{k+1}-\phi^k\|_h^2+E_h(\phi^{k+1})-E_h(\phi^k)+\frac{1}{2}\|\Delta_h(\phi^{k+1}-\phi^k)\|_h^2+\|\nabla_h(\phi^{k+1}-\phi^k)\|_h^2\\&\quad+\Big(A-\frac{1}{2}((\phi^k)^2-1+\epsilon)-\frac{1}{4}(\phi^{k+1}+\phi^k)^2,(\phi^{k+1}-\phi^k)^2\Big)_h=0.\end{aligned}\tag{3.10}$$

Note that the last term in (3.10) can be made nonnegative provided that

$$A\geq\max_{x\in\Omega}\Big\{\frac{1}{2}((\phi^k)^2-1+\epsilon)+\frac{1}{4}(\phi^{k+1}+\phi^k)^2\Big\}.\tag{3.11}$$

This completes the proof. □

We point out that the condition for A, i.e., (3.4), is not a satisfactory one in the sense that the expression of A depends also on the unknown solution. In other words, A is given in an implicit form. An ideal condition is expected that the right-hand side of (3.4) depends only on the values of ϕ^k instead of ϕ^{k+1}. If this is the case, we can obtain an explicit way to compute the value of A (which depends only on time) at each time level. In any case, the condition (3.4) only serves as some intuited way in computations. Moreover, if the numerical solution is convergent in $L^\infty((0,T),W_1^\infty(\Omega))$ as $\Delta t\to 0$, then the constant A can be chosen to satisfy

$$A\geq\frac{3}{2}|\phi^k|^2-\frac{1}{2}(1-\epsilon)\quad\text{a.e. in }\Omega\times(0,T].\tag{3.12}$$

Remark 3.1. The numerical scheme (2.6) with the parameter A satisfying (3.4) is unconditionally stable in the sense that energy decays with respect to time.

4 Numerical experiments

In the previous sections, we discussed the time discretization for the SH model and its stability analysis. For discretization in space, we apply the central finite difference scheme. The main objective of this section is to verify the stability of the proposed numerical scheme dependent on the choice of the artificial parameter A. We carry out two numerical experiments, one is with smooth initial data and the other is with random initial data.

Example 4.1. The initial condition is

$$\phi_0(x,y)=0.025(\sin x+\cos y),$$

with $\Omega=[0,2\pi]\times[0,2\pi]$. Periodic boundary conditions are adopted. This example is used to test the advantage of A in improving numerical stability.

Table 1: Example 4.1: stability comparison with different parameter A in (2.6), $\Delta t_{\max}$ denotes the maximum time step allowed in the numerical computation.

	$A=0$	$A=1$	$A=2$
$\epsilon=0.1$	$\Delta t_{\max}\approx 0.8$	$\Delta t_{\max}\approx 0.8$	$\Delta t_{\max}\approx 0.8$
$\epsilon=0.01$	$\Delta t_{\max}\approx 0.3$	$\Delta t_{\max}\approx 0.8$	$\Delta t_{\max}\approx 0.8$
$\epsilon=0.001$	$\Delta t_{\max}\approx 0.05$	$\Delta t_{\max}\approx 0.8$	$\Delta t_{\max}\approx 0.8$

It is observed from the Table 1, the introduce of the parameter A may improve the stability of the scheme. For large ϵ, the stability does not strongly depend on A, however,

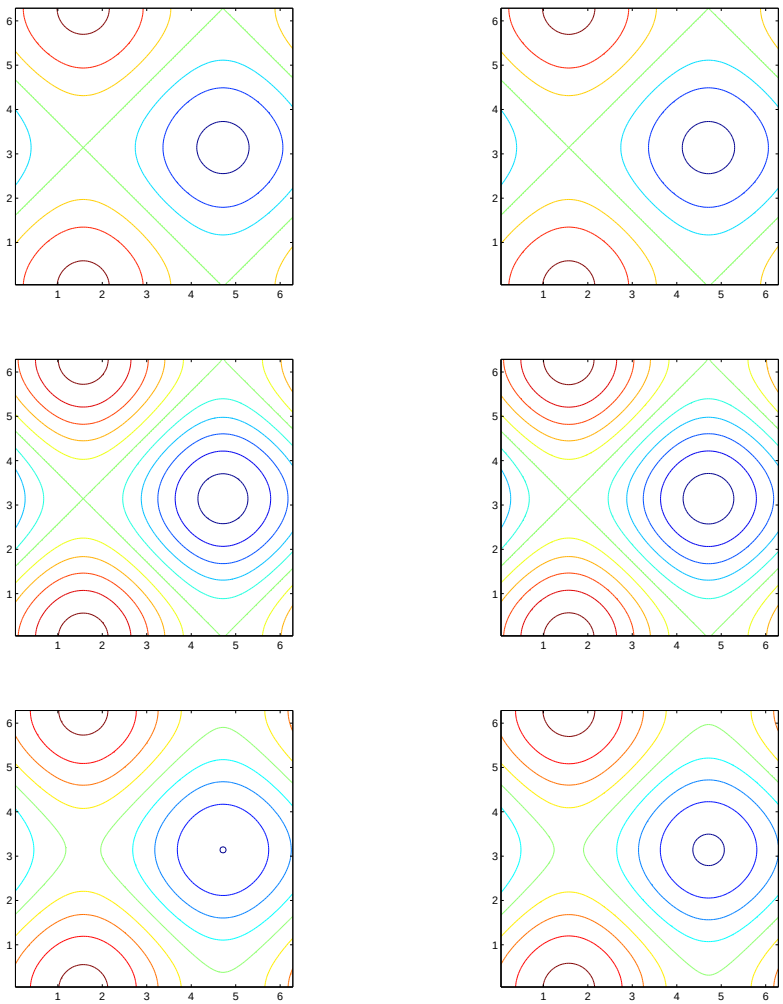

Figure 1: Example 4.1: Solution contours with $\epsilon=0.01$ at $t=0.1$,1 and 5.0. Left: $A=0$, $\Delta t=0.3$ (from top to bottom); right: $A=1$, $\Delta t=0.8$, $N=128$.

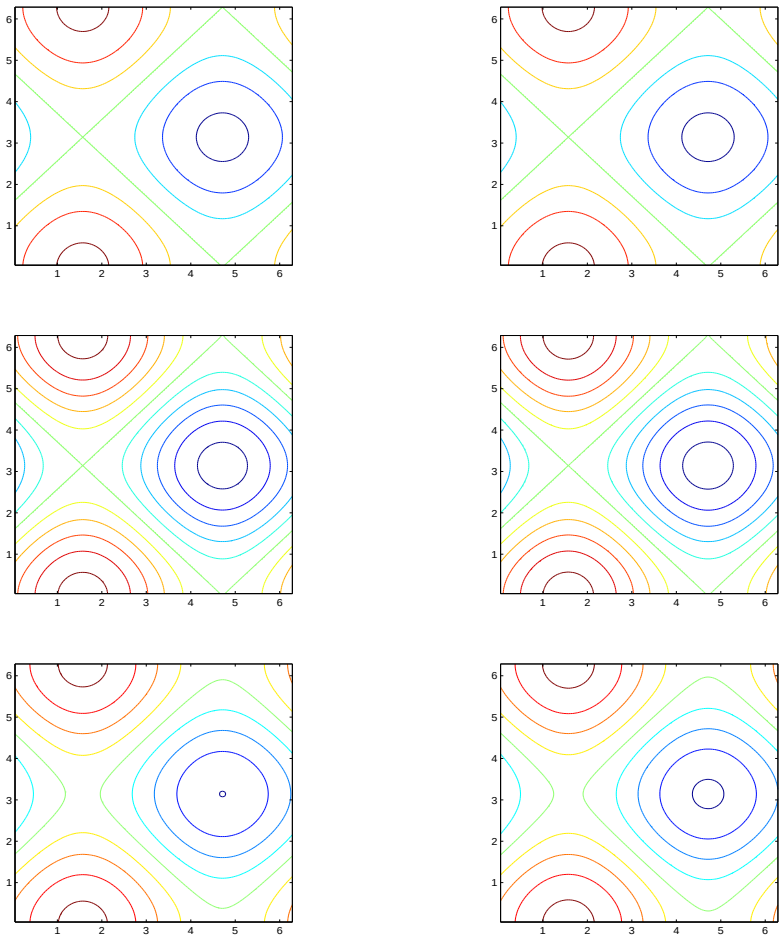

Figure 2: Example 4.1: Same as Fig. 1, except with $N=512$.

for small ϵ, the A does improve the stability greatly and as a result the range of applicable time steps is enlarged. In Figs. 1, we show the contour lines of the solution with $\epsilon=0.01$ at different times. It is obvious that the numerical solution obtained with larger time step (corresponding to $A=1$) is agree with the one obtained with small time step (corresponding to $A=0$). To further confirm the correctness of the solution in Figs. 1, we refine the mesh to do the same computation and present the results in Figs. 2.

Example 4.2. Consider the problem (2.2) in 2D with ϕ_0 being random data. The simulations are carried out in the domain $\Omega=[0,2\pi]^2$, with a double 2π-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.

Let $\Delta t_{\max}$ denote the largest possible time step which allows stable numerical com-

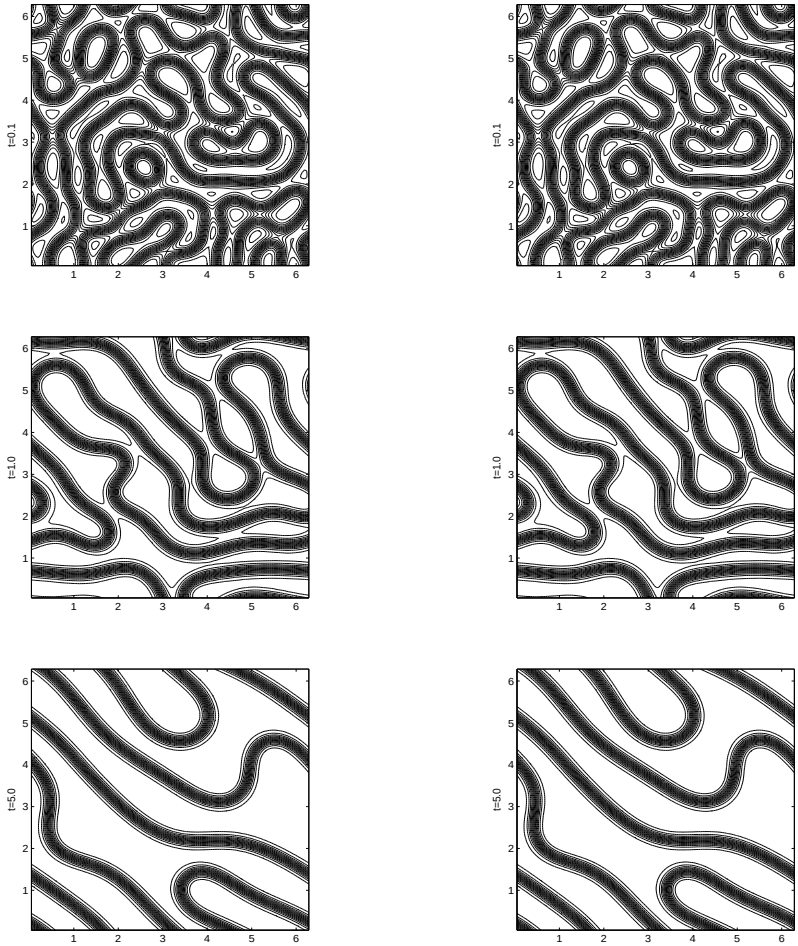

Figure 3: Example 4.2: Solution contours with $\epsilon=0.01$ at $t=0.1$,1 and 5. Left: $A=0$, $\Delta t=0.01$; right: $A=1$, $\Delta t=0.1$, $N=128$.

putation. To demonstrate convergence property of the proposed numerical schemes, we present some numerical simulations for the SH equation (2.2) with different parameter settings. In Figs. 3, we present the solution contour lines for $\epsilon=0.01$ at different time levels. If we set $A=0$, the largest time step allow is $\Delta t_{\max}=0.0001$, while $\Delta t_{\max}=0.001$ if we set the parameter A as $A=1$. It is seen from Figs. 3, there is no significant difference caused by parameters $(A,\Delta t)=(0,0.0001)$ and $(A,\Delta t)=(1,0.001)$. We also test the case $\epsilon=0.001$ in (2.6). The solution contours are shown in Figs. 4, and it is seen that the parameter A can improve the stability clearly.

In Figs. 5, we set the mesh as 512×512 with random data at each grid point, the same observation as Figs. 4 is found.

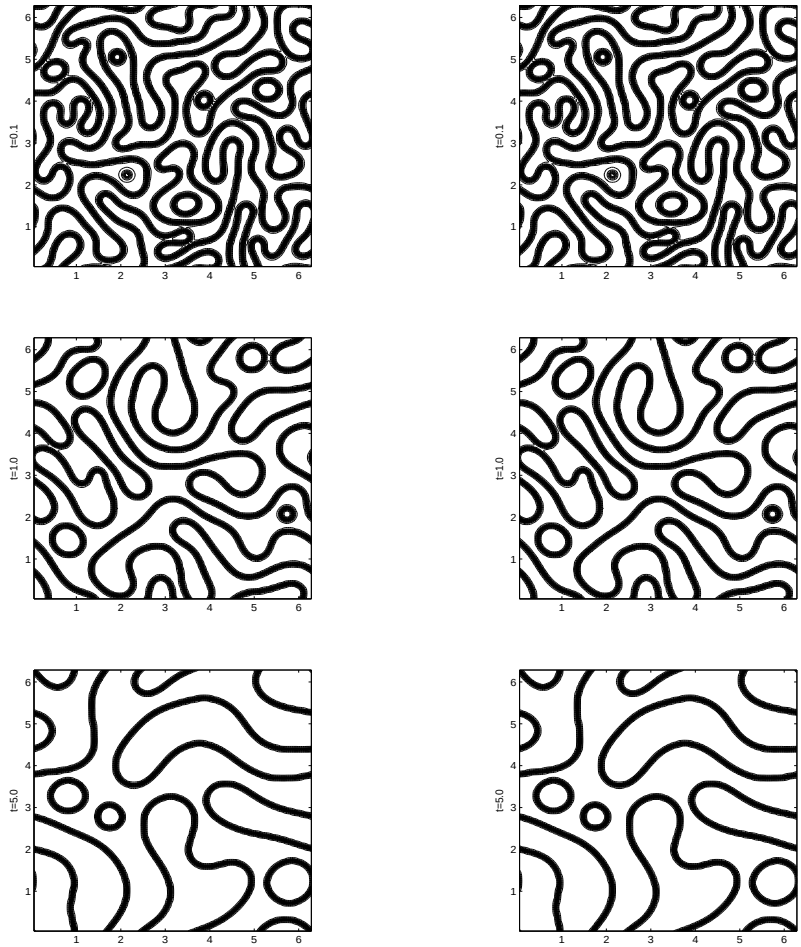

Figure 4: Example 4.2: Same as Fig. 3, except with $\epsilon = 0.001$.

5 Conclusions

In this work, we performed a preliminary study of large time stepping techniques for the SH equation. It is known that the time steps 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 stability analysis has been performed, which provides simple conditions on choice of the parameter which depends on the numerical solutions. High order time discretization is expected to further improve the stability, which will be reported later. The method proposed here can be easily generalized to a class of PDEs derived from the variational derivative of some energy functions, because

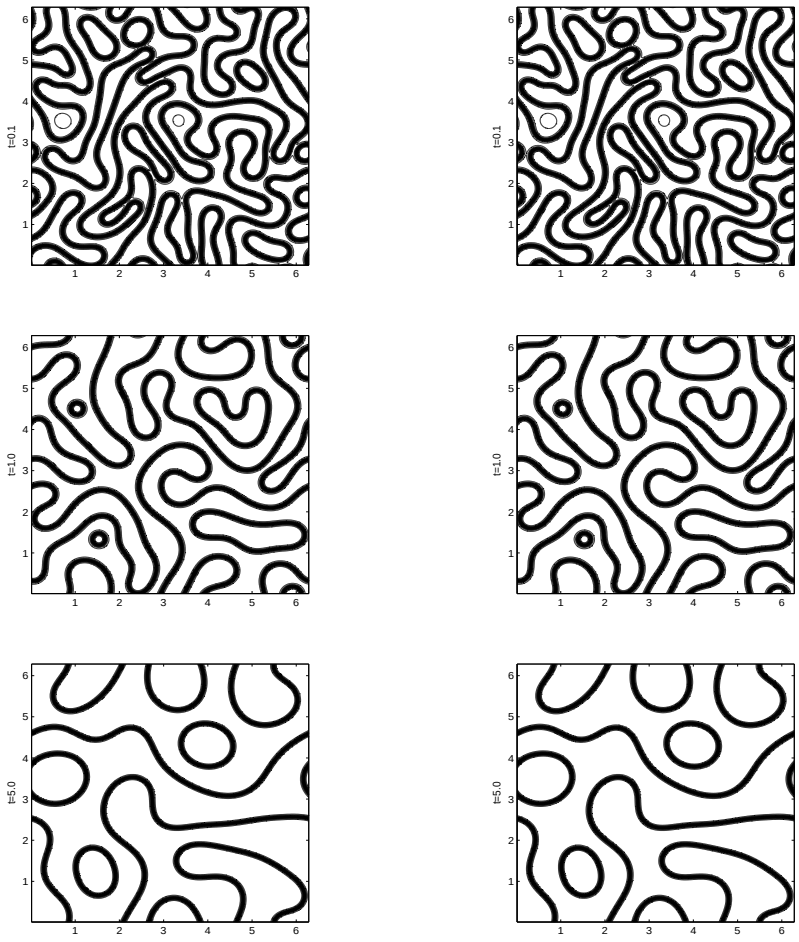

Figure 5: Example 4.2: Same as Fig. 4, except $N=512$.

the energy laws are always expected to preserve in discrete sense.

Acknowledgements

The research of Z. R. Zhang was partially supported by the Fundamental Research Funds for the Central Universities and National NSF of China under grant Nos. 11271048, 1130021 and 11571054.

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