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Error Estimate of Full-Discrete Numerical Scheme for the Nonlocal Allen-Cahn Model

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Abstract In this work, we study the error estimates of the fully discrete Fourier pseudo-spectral numerical scheme for solving the nonlocal volume-conserved Allen-Cahn (AC) equation. The time marching method of the numerical scheme is based on the well-known Invariant Energy Quadratization (IEQ) method. We demonstrate that the proposed fully discrete numerical method is uniquely solvable, unconditionally energy stable, and obtain the optimal error estimate of the scheme for both space and time. Additionally, we conduct several numerical tests to verify the theoretical results.

Keywords nonlocal Allen-Cahn model; uniquely solvable; unconditionally energy stable; error estimate; numerical tests

MR(2020) Subject Classification 35K45; 65J15; 65G20; 65M12

1. Introduction

The phase field model finds wide application in interface problems, encompassing phase separation, viscous fingering, fracture dynamics, vesicle dynamics, and more [1–7]. By employing the variational method in either L^2 (AC equation, [8,9]) or in H^{-1} (Cahn-Hilliard (CH) equation, [10–12]) on the postulated total free energy, one can derive a single or a set of partial differential equations that adhere to the principle of energy dissipation. Remarkably, the AC equation does not conserve volume (or mass), prompting various efforts to modify it while upholding volume conservation. The nonlocal Allen-Cahn equation, introduced by Rubinstein and Sternberg [1], achieves this goal by incorporating an additional nonlocal term into the AC equation. This modification enables the straightforward elimination of volume change and accurate conservation. Given its ability to ensure energy dissipation properties alongside volume conservation, this equation has received significant attention, see [6, 13–19].

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In addition to designing efficient numerical algorithms for local types of phase-field models, the development of numerical algorithms for the nonlocal AC equation also emphasizes the efficient discretization of nonlinear terms to achieve higher order, energy stability, and ease of implementation. The introduction of the nonlocal term in the system poses new challenges for algorithm design and corresponding error analysis. To the authors' knowledge, the current numerical algorithms for this nonlocal model mainly include the following approaches. In [20,21], the second-order convex splitting method was developed. However, due to the unique nature of the convex splitting approach, the resulting scheme is nonlinear and nonlocal, which may result in high computational costs in practice. In [22], various numerical methods such as finite difference and Fourier operator splitting methods are applied to the nonlocal model. However, a corresponding stability analysis for the algorithm was not provided. The well-known Invariant Energy Quadratization (IEQ) method is also used to solve this nonlocal model, as seen in [23]. Although the work provides detailed discussions on the algorithm and error estimates, the error estimates primarily focus on the semi-discrete version in time, assuming continuous space.

In this work, we consider to develop the first error analysis work of the fully-discrete type IEQ scheme [24–29], where space is discretized by the Fourier-Spectral method. The unique solvability and unconditional energy stability of the numerical scheme are also derived. By constructing an appropriate auxiliary interpolation function, the error estimate for the full-discrete method is rigorously proved. At last, we also propose some examples to verify the reliability of the numerical method.

The following is how the rest of this article is organized. In Section 2, we describe the PDE system and show its energy law on a continuous scale. In Section 3, we present two second-order numerical schemes, based on the Crank-Nicolson and backward difference formula, and demonstrate that both schemes abide to the unconditional energy stability. In Section 4, we derive the optimal error estimates for both schemes. Section 5 includes several numerical experiments to verify the theoretical estimates established for the proposed algorithms. Section 6 concludes with some closing remarks.

2. Model and Fourier pseudospectral method

In this section, we mainly describe the nonlocal AC equation and introduce the Fourier pseudospectral method.

2.1. Nonlocal AC equation

We define the free energy

$$E(\phi) = \int_\Omega \frac{\varepsilon^2}{2}|\nabla\phi|^2 + F(\phi)\mathrm{d}x. \tag{2.1}$$

By employing the variational method of (2.1) in L^2, we have

$$\partial_t\phi = \varepsilon^2\Delta\phi - f(\phi), \tag{2.2}$$

where $f(\phi)=\phi^3-\phi$. Adding a nonlocal term, we get the following nonlocal AC model

$$\partial_t \phi=\varepsilon^2\Delta\phi-f(\phi)+\frac{1}{|\Omega|}\int_\Omega f(\phi)\mathrm{d}x. \tag{2.3}$$

Taking the inner product of the above equation with 1, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \phi\mathrm{d}x=0. \tag{2.4}$$

Taking the inner product of (2.3) with ϕ_t, we obtain the energy dissipation of the nonlocal AC model.

$$\frac{\mathrm{d}}{\mathrm{d}t}E(\phi)=-\|\phi_t\|^2\le 0. \tag{2.5}$$

2.2. An introduction of Fourier pseudospectral method

In this paper, we will introduce the spatial discrete method. Given $\varphi(x,y)\in L^2(\Omega)$, $\Omega=(0,1)^2$, the Fourier series of φ is denoted by

$$\varphi(x,y)=\sum_{j,k=-\infty}^{\infty}\widehat{\varphi}_{j,k}e^{2\pi i(jx+ky)}, \tag{2.6}$$

where

$$\widehat{\varphi}_{j,k}=\int_\Omega \varphi(x,y)e^{-2\pi i(jx+ky)}\mathrm{d}x\mathrm{d}y. \tag{2.7}$$

We define S_N as a polynomial space. The projection and interpolation of the Fourier functions are given by

$$\mathcal{P}_N\varphi(x,y)=\sum_{j,k=-N/2}^{N/2-1}\widehat{\varphi}_{j,k}e^{2\pi i(jx+ky)},\quad (\mathcal{I}_N\varphi)(x,y)=\sum_{j,k=-N/2}^{N/2-1}(\widehat{\varphi}_N)_{j,k}e^{2\pi i(jx+ky)}, \tag{2.8}$$

where $(\widehat{\varphi}_N)_{j,k}$ are pseudospectral coefficients. We can find the following error estimates.

$$\|\partial^l\varphi(x,y)-\partial^l\mathcal{P}_N\varphi(x,y)\|\le Ch^{m-l}\|\varphi\|_{H^m},\quad \text{for}\quad 0\le l\le m, \tag{2.9}$$

$$\|\partial^l\varphi(x,y)-\partial^l\mathcal{I}_N\varphi(x,y)\|\le Ch^{m-l}\|\varphi\|_{H^m},\quad \text{for}\quad 0\le l\le m, m>\frac{d}{2}. \tag{2.10}$$

Please see Caunto and Quarteroni [30,31] for more details.

Given periodic functions φ, ψ, we denote the inner product and norm, respectively

$$\|\varphi\|_2^2=\langle\varphi,\varphi\rangle,\quad \langle\varphi,\psi\rangle=\frac{1}{N^2}\sum_{j,k=-N/2}^{N/2-1}\varphi_{j,k}\psi_{j,k}. \tag{2.11}$$

We find that

$$-\langle\varphi,\Delta_N\psi\rangle=\langle\nabla_N\varphi,\nabla_N\psi\rangle \tag{2.12}$$

with

$$\Delta_N\varphi=(D_{Nx}^2+D_{Nx}^2)\varphi,\quad \nabla_N\varphi=(D_{Nx}\varphi,D_{Ny}\varphi)^{\mathrm{T}}, \tag{2.13}$$

where D_N denotes the discrete differentiation matrix.

3. IEQ method for nonlocal AC model

Next, the IEQ method will be studied. Define

$$q = \sqrt{F(\phi) - \gamma\phi^2 + B}, \quad g = \frac{\partial q}{\partial \phi} = \frac{f(\phi) - 2\gamma\phi}{2\sqrt{F(\phi) - \gamma\phi^2 + B}}, \tag{3.1}$$

where $\gamma \geq 0$, A, B are appropriate constants, such that $F(\phi) - \gamma\phi^2 + B \geq A > 0$. Thus, the nonlocal AC model will be rewritten as

$$\partial_t \phi = \varepsilon^2 \Delta\phi - 2qg - 2\gamma\phi + \frac{2}{|\Omega|}\int_\Omega qg + \gamma\phi \mathrm{d}x, \tag{3.2}$$

$$\partial_t q = g\partial_t \phi, \tag{3.3}$$

with $\phi|_{t=0} = \phi^0, q|_{t=0} = \sqrt{F(\phi) - \gamma\phi^2 + B}|_{t=0}$.

Using Crank-Nicolson (CN) scheme for time discretization and pseduspectral for spacial discretization, then we can get the full-discrete scheme as follows

$$\begin{cases} \frac{\phi^{n+1}-\phi^n}{\delta t} - \varepsilon^2 \Delta_N \phi^{n+\frac{1}{2}} + 2g(\phi^\star)q^{n+\frac{1}{2}} + 2\gamma\phi^{n+\frac{1}{2}} - \frac{2}{|\Omega|}\big(\langle g(\phi^\star), q^{n+\frac{1}{2}}\rangle + \gamma\langle\phi^{n+\frac{1}{2}}, 1\rangle\big) = 0, \\ \frac{q^{n+1}-q^n}{\delta t} = g(\phi^\star)\frac{\phi^{n+1}-\phi^n}{\delta t}, \end{cases} \tag{3.4}$$

where $\phi^\star = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}$, $n \geq 1$, with $\phi^\star = \phi^0$ for $n = 0$.

Theorem 3.1 *The full-discrete numerical scheme (3.4) satisfies unconditionally energy stable, that is*

$$E(\phi^{n+1}, q^{n+1}) + \frac{1}{\delta t}\|\phi^{n+1} - \phi^n\|_2^2 = E(\phi^n, q^n) \tag{3.5}$$

with

$$E(\phi^n, q^n) = \frac{\varepsilon^2}{2}\|\nabla_N \phi^n\|_2^2 + \gamma\|\phi^n\|_2^2 + \|q^n\|_2^2.$$

Proof By computing the inner product of the first equation in (3.4) with $(\phi^{n+1} - \phi^n)$ and, we arrive at

$$\begin{aligned} &\frac{1}{\delta t}\|\phi^{n+1} - \phi^n\|_2^2 + \frac{\varepsilon^2}{2}(\|\nabla_N\phi^{n+1}\|_2^2 - \|\nabla_N\phi^n\|_2^2) + \gamma(\|\phi^{n+1}\|_2^2 - \|\phi^n\|_2^2) + \\ &\quad \langle g(\phi^\star)(q^{n+1} + q^n), \phi^{n+1} - \phi^n\rangle - \frac{1}{|\Omega|}\langle g(\phi^\star), q^{n+1} + q^n\rangle\langle\phi^{n+1} - \phi^n, 1\rangle - \\ &\quad \frac{\gamma}{|\Omega|}\langle\phi^{n+1} + \phi^n, 1\rangle\langle\phi^{n+1} - \phi^n, 1\rangle = 0 \end{aligned} \tag{3.6}$$

and

$$\langle\phi^{n+1} - \phi^n, 1\rangle = 0. \tag{3.7}$$

By taking the inner product of the second equation in (3.4) with $\delta t(q^{n+1} + q^n)$, we find

$$\|q^{n+1}\|_2^2 - \|q^n\|_2^2 = \langle g(\phi^\star)(\phi^{n+1} - \phi^n), q^{n+1} + q^n\rangle. \tag{3.8}$$

Thus, we have

$$\frac{1}{\delta t}\|\phi^{n+1}-\phi^n\|_2^2+\frac{\varepsilon^2}{2}(\|\nabla_N\phi^{n+1}\|_2^2-\|\nabla_N\phi^n\|_2^2)+\gamma(\|\phi^{n+1}\|_2^2-\|\phi^n\|_2^2)+\|q^{n+1}\|_2^2-\|q^n\|_2^2=0. \tag{3.9}$$

This yields (3.5). □

Theorem 3.2 *The numerical scheme (3.4) is unique solvable.*

Proof From (3.4), we find

$$q^{n+1}=q^n+g(\phi^\star)(\phi^{n+1}-\phi^n). \tag{3.10}$$

Thus, we can rewrite the first equation of (3.4) as

$$\frac{1}{\delta t}\phi^{n+1}-\frac{\varepsilon^2}{2}\Delta_N\phi^{n+1}+\gamma\phi^{n+1}+g^2(\phi^\star)\phi^{n+1}-\frac{1}{|\Omega|}\langle g(\phi^\star),g(\phi^\star)\phi^{n+1}\rangle-\frac{\gamma}{|\Omega|}\langle\phi^{n+1},1\rangle=b_1, \tag{3.11}$$

where

$$b_1=\frac{1}{\delta t}\phi^n+\frac{\varepsilon^2}{2}\Delta_N\phi^n-\gamma\phi^n-2g(\phi^\star)q^n+g^2(\phi^\star)\phi^n+\frac{1}{|\Omega|}\langle g(\phi^\star),2q^n-g(\phi^\star)\phi^n\rangle+\frac{\gamma}{|\Omega|}\langle\phi^n,1\rangle.$$

We introduce $\psi=\phi^{n+1}-\alpha$, where

$$\alpha=\langle\phi^{n+1},1\rangle=\cdots=\langle\phi^0,1\rangle.$$

Thus, one can reformulate (3.11) as

$$[\frac{1}{\delta t}-\frac{\varepsilon^2}{2}\Delta_N+\gamma+g^2(\phi^\star)-\frac{1}{|\Omega|}\langle g(\phi^\star),g(\phi^\star)\bullet\rangle-\frac{\gamma}{|\Omega|}\langle\bullet,1\rangle]\psi=b_2, \tag{3.12}$$

where b_2 is defined as some known terms. Thus, the existence for ψ is obvious. Note that

$$\langle\mathcal{L}\psi,\psi\rangle=(\frac{1}{\delta t}+\gamma)\|\psi\|_2^2+\frac{\varepsilon^2}{2}\|\nabla_N\psi\|_2^2+\|g(\phi^\star)\psi\|_2^2. \tag{3.13}$$

When $\mathcal{L}\psi=0$, we will obtain $\psi=0$, then the uniqueness is proved. Thus we get the conclusion of (3.11). □

4. Error estimate

In this part, the fully discrete error estimate of (3.4) will be analyzed. For the sake of simplicity, we now define the following projection function into S_N.

$$\Phi_N(\cdot,t)=\mathcal{P}_N\phi(\cdot,t),\quad Q_N(\cdot,t)=\mathcal{P}_Nq(\cdot,t). \tag{4.1}$$

We have

$$\frac{\partial}{\partial t}\Phi_N=\frac{\partial}{\partial t}\mathcal{P}_N\phi=\mathcal{P}_N\frac{\partial}{\partial t}\phi,\quad \frac{\partial}{\partial t}Q_N=\frac{\partial}{\partial t}\mathcal{P}_Nq=\mathcal{P}_N\frac{\partial}{\partial t}q. \tag{4.2}$$

Then, we can rewrite equations (3.4) as follows

$$\begin{cases}\partial_t\Phi_N=\varepsilon^2\Delta\Phi_N-2g(\Phi_N)Q_N-2\gamma\Phi_N+\frac{2}{|\Omega|}(\langle g(\Phi_N),Q_N\rangle+\gamma\langle\Phi_N,1\rangle)+r_1,\\ \partial_tQ_N=(\Phi_N)\partial_t\Phi_N+r_2,\end{cases} \tag{4.3}$$

where

$$
\begin{aligned}
r_1 =&(\partial_t\Phi_N-\partial_t\phi)-\varepsilon^2(\Delta\Phi_N-\Delta\phi)+2(g(\Phi_N)Q_N-g(\phi)q)+2\gamma(\Phi_N-\phi)+\\
&\frac{2}{|\Omega|}\Big(\int_\Omega gq\mathrm{d}x-\langle g(\Phi_N),Q_N\rangle+\gamma\int_\Omega\phi\mathrm{d}x-\gamma\langle\Phi_N,1\rangle\Big),\\
r_2 =&(\partial_t Q_N-\partial_t q)-(g(\Phi_N)\partial_t\Phi_N-g(\phi)\partial_t\phi).
\end{aligned}
$$

Note that

$$\|\partial_t(\Phi_N-\phi)\|_2\le\|\partial_t(\Phi_N-\phi)\|_{L^2}+\|\partial_t(\mathcal{I}_N\phi-\phi)\|_{L^2}. \tag{4.4}$$

Therefore, we arrive at

$$\|\partial_t(\Phi_N-\phi)\|_2\le Ch^m,\ \|\partial_t(Q_N-q)\|_2\le Ch^m,\ \|\Delta(\Phi_N-\phi)\|_2\le Ch^m. \tag{4.5}$$

The following estimates are obvious

$$
\begin{aligned}
\|Q_N-q\|_{L^2}=&\|\sqrt{F(\Phi_N)-\gamma\Phi_N^2+B}-\sqrt{F(\phi)-\gamma\phi^2+B}\|_{L^2}\\
\le&\|\frac{F(\Phi_N)-F(\phi)+\gamma(\phi^2-\Phi_N^2)}{\sqrt{F(\Phi_N)-\gamma\Phi_N^2+B}\sqrt{F(\phi)-\gamma\phi_N^2+B}}\|_{L^2}\\
\le&C(\|f(\zeta_1)\|_{L^\infty}+\|\phi\|_{L^\infty})\|\phi-\Phi_N\|_{L^2}, && (4.6)\\
\|g(\Phi_N)-g(\phi)\|_{L^2}^2=&\|\frac{f(\Phi_N)-2\gamma\Phi_N}{\sqrt{F(\Phi_N)-\gamma\Phi_N^2+B}}-\frac{f(\phi)-2\gamma\phi}{\sqrt{F(\phi)-\gamma\phi^2+B}}\|_{L^2}\\
\le&C(\|f(\zeta_1)\|_{L^\infty}+\|f'(\zeta_2)\|_{L^\infty}+\|\phi\|_{L^\infty})\|\Phi_N-\phi\|_{L^2}, && (4.7)\\
\|g(\phi)\partial_t q-g(\Phi_N)\partial_t Q_N\|_{L^2}\le&\|\partial_t q\|_{L^\infty}\|g(\phi)-g(\Phi_N)\|_{L^2}+\|g(\Phi_N)\|_{L^\infty}\|\partial_t q-\partial_t Q_N\|_{L^2}. && (4.8)
\end{aligned}
$$

Then

$$
\begin{aligned}
\|g(\phi)q-g(\Phi_N)Q_N\|_2=&\|\mathcal{I}_N(g(\phi)q-g(\Phi_N)Q_N)\|_{L^2}\le Ch^m, && (4.9)\\
\|g(\phi)\partial_t\phi-g(\Phi_N)\partial_t\Phi_N\|_2=&\|\mathcal{I}_N(g(\phi)\partial_t\phi-g(\Phi_N)\partial_t\Phi_N)\|_{L^2}\\
\le&\|g(\phi)\partial_t\phi-g(\Phi_N)\partial_t\Phi_N\|_{L^2}+\|g(\phi)\partial_t\phi-\mathcal{I}_N(g(\phi)\partial_t\phi)\|_{L^2}+\\
&\|g(\Phi_N)\partial_t\Phi_N-\mathcal{I}_N(g(\Phi_N)\partial_t\Phi_N)\|_{L^2}\\
\le&Ch^m. && (4.10)
\end{aligned}
$$

For the last nonlinear term

$$
\begin{aligned}
\int_\Omega gq\mathrm{d}x-\langle g(\Phi_N),Q_N\rangle=&\int_\Omega gq\mathrm{d}x-\langle g,q\rangle+\langle g,q\rangle-\langle g(\Phi_N),Q_N\rangle\\
=&\int_\Omega gq\mathrm{d}x-\langle g,q\rangle+\langle g,q-Q_N\rangle+\langle g-g(\Phi_N),Q_N\rangle. && (4.11)
\end{aligned}
$$

The above inner product error can be deduced from the interpolation approximation result. Combining with (4.5)–(4.11) gives

$$\|r_i\|_2\le Ch^m,\quad i=1,2. \tag{4.12}$$

Based on Eq. (4.3), we have the following consistency result. For simplicity of presentation, let (Φ_N,Q_N) be the approximation solution of (4.3). We also define $(\Phi,Q)=\mathcal{I}_N(\Phi_N,Q_N)$ as the discrete interpolation.

Theorem 4.1 *Assume (ϕ, q) be the exact periodic solution for problem (3.2) and (3.3). If (ϕ, q) is smooth enough, then there hold*

$$\begin{cases} \frac{\Phi^{n+1}-\Phi^n}{\delta t} = \varepsilon^2 \Delta_N \Phi^{n+\frac{1}{2}} - 2g(\Phi^\star) Q^{n+\frac{1}{2}} - 2\gamma \Phi^{n+\frac{1}{2}} + \\ \qquad \frac{2}{|\Omega|}(\langle g(\Phi^\star), Q^{n+\frac{1}{2}}\rangle + \gamma\langle \Phi^{n+\frac{1}{2}}, 1\rangle) + R_1^{n+\frac{1}{2}}, \\ \frac{Q^{n+1}-Q^n}{\delta t} = g(\Phi^\star)\frac{\Phi^{n+1}-\Phi^n}{\delta t} + R_2^{n+\frac{1}{2}}, \end{cases} \tag{4.13}$$

where

$$\Phi^n = \Phi(t_n), \quad Q^n = Q(t_n),$$

and $R_i^{n+\frac{1}{2}}$ $(i = 1, 2)$ satisfies

$$\|R_i\|_{l^2(0,T;l^2)} := \Big(\delta t \sum_{k=0}^{K} \|R_i^{k+\frac{1}{2}}\|_2^2\Big)^{\frac{1}{2}} \le C(\delta t^2 + h^m). \tag{4.14}$$

Proof Applying Taylor expansion and (4.12), we can prove the desired result. □

Lemma 4.2 *Given (i) $F(\phi) - \gamma\phi^2 \in C^3$; (ii) There is a constant $\widehat{C}$ that makes*

$$\max_{n\le k} g\{\|\Phi^n\|_{L^\infty}, \|\phi^n\|_{L^\infty}\} \le \widehat{C}.$$

The following inequalities hold

$$\|g(\Phi^n) - g(\phi^n)\|_2 \le C(\|(\Phi^n - \phi^n)\|_2, \tag{4.15}$$

$$\|\nabla_N g(\Phi^n) - \nabla_N g(\phi^n)\|_2 \le C(\|\nabla_N(\Phi^n - \phi^n)\|_2 + \|\Phi^n - \phi^n\|_2). \tag{4.16}$$

Proof Using the similar arguments in (4.7), we can conclude the above proof. □

Lemma 4.3 *Let $\{u^n\}_{n=0}^{k+1}$ be the function of the grid point. We obtain*

$$\|u^{k+1}\| \le \sum_{n=0}^{k} \|u^{n+1} + u^n\| + \|u^0\|.$$

In order to study uniform boundedness, we define μ as

$$\mu = \max_{0\le t\le T} \|\Phi(t)\|_{L^\infty} + 1.$$

Lemma 4.4 *Assume $F(\phi) - \gamma\phi^2 \in C^3$ and the exact solution is smooth enough. Given τ_0 and h_0, when $\tau_0 < \delta t, h_0 < h$, the following uniform boundedness result yields*

$$\|\phi^k\|_{L^\infty} \le \mu, \quad k = 0, 1, \ldots, K = T/\delta t. \tag{4.17}$$

Proof We can easily find that $\|\phi^0\|_{L^\infty} \le \nu$ is clearly true. Suppose

$$\|\phi^n\|_{L^\infty} \le \nu \text{ for } n \le k.$$

Next, we will prove $\|\phi^{k+1}\|_{L^\infty} \le \nu$. Denote

$$\widetilde{e}_\phi^n = \Phi^n - \phi^n, \ \widetilde{e}_q^n = Q^n - q^n. \tag{4.18}$$

Subtracting (3.4) from (4.13) yields

$$\begin{cases} \frac{\widetilde{e}_\phi^{n+1}-\widetilde{e}_\phi^n}{\delta t} = \varepsilon^2\Delta_N \widetilde{e}_\phi^{n+\frac{1}{2}} - 2\gamma \widetilde{e}_\phi^{n+\frac{1}{2}} + \mathcal{NLN}_1 - \mathcal{NLN}_2 + R_1^{n+\frac{1}{2}}, \\ \frac{\widetilde{e}_q^{n+1}-\widetilde{e}_q^n}{\delta t} = \mathcal{NLN}_3 + R_2^{n+\frac{1}{2}}, \end{cases} \tag{4.19}$$

where

$$\begin{aligned} \mathcal{NLN}_1 =& 2(g(\phi^\star)q^{n+\frac{1}{2}} - g(\Phi^\star)Q^{n+\frac{1}{2}}), \\ \mathcal{NLN}_2 =& \frac{2}{|\Omega|}(\langle g(\phi^\star), q^{n+\frac{1}{2}}\rangle - \langle g(\Phi^\star), Q^{n+\frac{1}{2}}\rangle + \gamma\langle \phi^{n+\frac{1}{2}} - \Phi^{n+\frac{1}{2}}, 1\rangle), \\ \mathcal{NLN}_3 =& g(\Phi^{n+\frac{1}{2}})\frac{\Phi^{n+1}-\Phi^n}{\delta t} - g(\phi^\star)\frac{\phi^{n+1}-\phi^n}{\delta t}. \end{aligned}$$

According to the hypothesis, we find

$$\|\Phi_N\|_{L^\infty(0,T;W^{2,\infty})} \le C, \quad \text{i.e.,} \quad \|\Phi^n\|_{L^\infty} \le C, \quad \|\nabla\Phi^n\|_{L^\infty} \le C. \tag{4.20}$$

To simplify the notations, we let $\varepsilon = 1$. Computing the inner product of (4.19) with $(\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n)$ and $\delta t(\widetilde{e}_q^{n+1} + \widetilde{e}_q^n)$ gives

$$\begin{aligned} &\frac{1}{\delta t}\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2 + \frac{1}{2}(\|\nabla_N \widetilde{e}_\phi^{n+1}\|_2^2 - \|\nabla_N \widetilde{e}_\phi^n\|_2^2) + \gamma(\|\widetilde{e}_\phi^{n+1}\|_2^2 - \|\widetilde{e}_\phi^n\|_2^2) \\ &= \langle \mathcal{NLN}_1, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle - \langle \mathcal{NLN}_2, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle + \langle R_1^{n+\frac{1}{2}}, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle. \end{aligned} \tag{4.21}$$

And

$$\|\widetilde{e}_q^{n+1}\|_2^2 - \|\widetilde{e}_q^n\|_2^2 = \delta t\langle \mathcal{NLN}_3, \widetilde{e}_q^{n+1} + \widetilde{e}_q^n\rangle + \delta t\langle R_2^{n+\frac{1}{2}}, \widetilde{e}_q^{n+1} + \widetilde{e}_q^n\rangle. \tag{4.22}$$

Thus, we have

$$\begin{aligned} &\frac{1}{\delta t}\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2 + \frac{1}{2}(\|\nabla_N \widetilde{e}_\phi^{n+1}\|_2^2 - \|\nabla_N \widetilde{e}_\phi^n\|_2^2) + \gamma(\|\widetilde{e}_\phi^{n+1}\|_2^2 - \|\widetilde{e}_\phi^n\|_2^2) + \|\widetilde{e}_q^{n+1}\|_2^2 - \|\widetilde{e}_q^n\|_2^2 \\ &= \langle \mathcal{NLN}_1, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle - \langle \mathcal{NLN}_2, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle + \langle R_1^{n+\frac{1}{2}}, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle + \\ &\quad \delta t\langle \mathcal{NLN}_3, \widetilde{e}_q^{n+1} + \widetilde{e}_q^n\rangle + \delta t\langle R_2^{n+\frac{1}{2}}, \widetilde{e}_q^{n+1} + \widetilde{e}_q^n\rangle. \end{aligned} \tag{4.23}$$

Note that

$$\begin{aligned} \mathcal{NLN}_1 =& (Q^{n+1} + Q^n)(g(\phi^\star) - g(\Phi^{n+\frac{1}{2}})) - g(\phi^\star)(\widetilde{e}_q^{n+1} + \widetilde{e}_q^n), \\ \mathcal{NLN}_2 =& \frac{2}{|\Omega|}(\langle g(\phi^\star) - g(\Phi^\star), Q^{n+\frac{1}{2}}\rangle - \langle g(\phi^\star), \widetilde{e}_q^{n+\frac{1}{2}}\rangle - \gamma\langle \widetilde{e}_\phi^{n+\frac{1}{2}}, 1\rangle), \\ \mathcal{NLN}_3 =& \frac{\Phi^{n+1}-\Phi^n}{\delta t}(g(\Phi^{n+\frac{1}{2}}) - g(\phi^\star)) + g(\phi^\star)\frac{\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n}{\delta t}. \end{aligned}$$

We have the following error estimates

$$\begin{aligned} \langle \mathcal{NLN}_2, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle &\le 6\delta t\|\mathcal{NLN}_2\|_2^2 + \frac{1}{6\delta t}\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2 \\ &\le C\delta t(\|\widetilde{e}_\phi^{n+1}\|_2^2 + \|\widetilde{e}_\phi^n\|_2^2 + \|\widetilde{e}_\phi^{n-1}\|_2^2 + \|\widetilde{e}_q^{n+1} + \widetilde{e}_q^n\|_2^2) + \frac{1}{6\delta t}\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2, \end{aligned} \tag{4.24}$$

$$\langle R_1^{n+\frac{1}{2}}, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle \le C\delta t\|R_1^{n+\frac{1}{2}}\|_2^2 + \frac{1}{6\delta t}\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2, \tag{4.25}$$

$$\langle R_2^{n+\frac{1}{2}}, \widetilde{e}_q^{n+1} + \widetilde{e}_q^n\rangle \le C(\|R_2^{n+\frac{1}{2}}\|_2^2 + \|\widetilde{e}_q^{n+1} + \widetilde{e}_q^n\|_2^2). \tag{4.26}$$

And

$$\begin{aligned}
&\langle \mathcal{NLN}_1, \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle + \delta t\langle \mathcal{NLN}_3, \widetilde{e}_q^{n+1} + \widetilde{e}_q^n\rangle\\
&= \langle (Q^{n+1}+Q^n)(g(\phi^\star) - g(\Phi^{n+\frac12})) - g(\phi^\star)(e_q^{n+1}+e_q^n), \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle +\\
&\quad \langle (\Phi^{n+1}-\Phi^n)(g(\Phi^{n+\frac12}) - g(\phi^\star)) + g(\phi^\star)(e_\phi^{n+1}-e_\phi^n), \widetilde{e}_q^{n+1}+\widetilde{e}_q^n\rangle\\
&= \langle (Q^{n+1}+Q^n)(g(\phi^\star) - g(\Phi^{n+\frac12})), \widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\rangle + \langle (\Phi^{n+1}-\Phi^n)(g(\Phi^{n+\frac12}) - g(\phi^\star)), \widetilde{e}_q^{n+1}+\widetilde{e}_q^n\rangle\\
&\le \|Q^{n+1}+Q^n\|_4\|g(\phi^\star)-g(\Phi^{n+\frac12})\|_4\|\widetilde{e}_\phi^{n+1}-\widetilde{e}_\phi^n\|_2 +\\
&\quad \|\Phi^{n+1}-\Phi^n\|_4\|g(\Phi^{n+\frac12})-g(\phi^\star)\|_4\|\widetilde{e}_q^{n+1}+\widetilde{e}_q^n\|_2\\
&\le C\delta t(\|\widetilde{e}_\phi^n\|_2^2 + \|\widetilde{e}_\phi^{n-1}\|_2^2 + \|\nabla_N\widetilde{e}_\phi^n\|_2^2 + \|\nabla_N\widetilde{e}_\phi^{n-1}\|_2^2 + \delta t^4 + \|\widetilde{e}_q^{n+1}+\widetilde{e}_q^n\|_2^2) +\\
&\quad \frac{1}{6\delta t}\|\widetilde{e}_\phi^{n+1}-\widetilde{e}_\phi^n\|_2^2. \qquad (4.27)
\end{aligned}$$

Combining with (4.23)–(4.27), we have

$$\begin{aligned}
&\frac12(\|\nabla_N\widetilde{e}_\phi^{n+1}\|_2^2 - \|\nabla_N\widetilde{e}_\phi^n\|_2^2) + \gamma(\|\widetilde{e}_\phi^{n+1}\|_2^2 - \|\widetilde{e}_\phi^n\|_2^2) + \|\widetilde{e}_q^{n+1}\|_2^2 - \|\widetilde{e}_q^n\|_2^2 + \frac{1}{2\delta t}\|\widetilde{e}_\phi^{n+1}-\widetilde{e}_\phi^n\|_2^2\\
&\quad \le C\delta t(\delta t^4 + h^{2m}) + C\delta t\big(\|\widetilde{e}_\phi^{n+1}\|_2^2 + \|\widetilde{e}_\phi^n\|_2^2 + \|\widetilde{e}_\phi^{n-1}\|_2^2 + \|\nabla_N\widetilde{e}_\phi^n\|_2^2 + \|\nabla_N\widetilde{e}_\phi^{n-1}\|_2^2 +\\
&\qquad \|\widetilde{e}_q^{n+1}\|_2^2 + \|\widetilde{e}_q^n\|_2^2\big). \qquad (4.28)
\end{aligned}$$

Summing (4.28) for $n = 1, \ldots, k$, we deduce that

$$\widetilde{E}^{k+1} + \frac{1}{2\delta t}\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2 \le C(\widetilde{E}^1 + (\delta t^2 + h^m)^2) + C\delta t\sum_{n=1}^k \widetilde{E}^{n+1}, \qquad (4.29)$$

where

$$\widetilde{E}^{k+1} = \frac12\|\nabla_N\widetilde{e}_\phi^{k+1}\|_2^2 + \gamma\|\widetilde{e}_\phi^{k+1}\|_2^2 + \|\widetilde{e}_q^{k+1}\|_2^2.$$

We find

$$\widetilde{E}^1 \le C(\delta t^2 + h^m)^2. \qquad (4.30)$$

By using Grownwall inequality, we get

$$\widetilde{E}^{k+1} + \frac{1}{2\delta t}\sum_{n=1}^k\|\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n\|_2^2 \le C(\delta t^2 + h^m)^2. \qquad (4.31)$$

As can be seen from first equation of (4.19)

$$\begin{aligned}
\|\Delta_N(\widetilde{e}_\phi^{n+1} + \widetilde{e}_\phi^n)\|_2^2 \le & Cg(\|\mathcal{NLN}_1\|_2^2 + \|\mathcal{NLN}_2\|_2^2 + \|\widetilde{e}_\phi^{n+1} + \widetilde{e}_\phi^n\|_2^2 +\\
& \|\frac{\widetilde{e}_\phi^{n+1} - \widetilde{e}_\phi^n}{\delta t}\|_2^2 + \|R_1^{n+\frac12}\|_2^2). \qquad (4.32)
\end{aligned}$$

From Lemma 4.3, (4.31) and (4.32), we arrive at

$$\|\Delta_N\widetilde{e}_\phi^{k+1}\|_2 \le \sum_{n=0}^k\|\Delta_N(\widetilde{e}_\phi^{n+1} + \widetilde{e}_\phi^n)\|_2 \le C(\delta t + \delta t^{-1}h^m). \qquad (4.33)$$

Thus

$$\|\phi^{k+1}\|_{L^\infty} \le \|\widetilde{e}_\phi^{k+1}\|_{L^\infty} + \|\Phi^{k+1}\|_{L^\infty} \le C\|e_\phi^{k+1}\|_{H^1}^{\frac12}\|e_\phi^{k+1}\|_{H^2}^{\frac12} + \|\Phi^{k+1}\|_{L^\infty}$$

$$\leq \widetilde{C}(\delta t^3 + \delta t h^m + \delta t^{-1} h^{2m})^{\frac{1}{2}} + \|\Phi^{k+1}\|_{L^\infty}. \tag{4.34}$$

When

$$\widetilde{C}(\delta t^3 + \delta t h^m + \delta t^{-1} h^{2m})^{\frac{1}{2}} \leq 1,$$

we find

$$\|\phi^{k+1}\|_{L^\infty} \leq 1 + \|\Phi^{k+1}\|_{L^\infty} \leq \mu. \tag{4.35}$$

This completes the proof. □

Theorem 4.5 *Under the assumption of Lemma 4.4, the following estimation results hold.*

$$\|\phi(t_{k+1}) - \phi^{k+1}\|_{H^1} + \|q(\phi(t_{k+1})) - q(\phi^{k+1})\|_2 \leq C(\delta t^2 + h^m). \tag{4.36}$$

Proof By using the technique of Lemma 4.4, we can obtain the following estimation

$$\widetilde{E}^{k+1} \leq C(\delta t^2 + h^m)^2. \tag{4.37}$$

Using trigonometric inequalities and the conclusion of (2.9) and (2.10), we can get the above results. □

5. Numerical experiments

In this part, some numerical experiments will be proposed to verify our analysis results. In the following tests, all the numerical experiments are fixed in a bounded domain $\Omega = (0, 2\pi)^2$, and we also choose periodic boundary conditions.

5.1. Convergence test for time and space

First, let us test the convergence with respect to δt. We set $B = 4$, $\gamma = 1$, $\varepsilon = 0.1$, then we can reformulate q and g as

$$q = \sqrt{\frac{1}{4}(\phi^2 - 3)^2 + 2}, \quad g = \frac{\phi^3 - 3\phi}{\sqrt{\frac{1}{4}(\phi^2 - 3)^2 + 2}}. \tag{5.1}$$

We set

$$\phi^0 = \sin^2 x \sin^2 y, \quad q|_{t=0} = \sqrt{F(\phi^0) - \phi^0 + 4}. \tag{5.2}$$

Then fix $T = 1$, we choose $N_x = 128$, $N_y = 128$, so that the spatial errors can be ignored. Because the exact solution is unknown, we use the numerical solution of (3.4) in the case $dt = 10^{-5}$ as the reference solution. The L^2, H^1 errors and the corresponding convergence orders of ϕ and q are showed in Table 1. From this table, we can find the second-order accuracy of time direction for ϕ and q. The errors in spatial direction and convergence orders for ϕ and q are presented in Table 2. It can be seen from the table that the convergence order in the spatial direction does not increase linearly, but it may increase exponentially.

δt	L^2-error for ϕ	Order	H^1-error for ϕ	Order	L^2-error for q	Order
$\frac{1}{10}$	6.1328E-04		7.7563E-04		3.4379E-03	
$\frac{1}{20}$	1.5562E-04	1.9784	2.0493E-04	1.9202	1.2628E-03	1.4449
$\frac{1}{100}$	6.3314E-06	1.9894	8.6801E-06	1.9644	6.7348E-05	1.8212
$\frac{1}{200}$	1.5868E-06	1.9963	2.1878E-06	1.9882	1.7440E-05	1.9491
$\frac{1}{1000}$	6.3606E-08	1.9987	8.8104E-08	1.9958	7.1761E-07	1.9824
$\frac{1}{2000}$	1.5904E-08	1.9997	2.2040E-08	1.9990	1.7998E-07	1.9952
$\frac{1}{10000}$	6.3406E-10	2.0020	8.7657E-10	2.0035	7.1507E-09	2.0042

Table 1 The L^2 and H^1 errors and convergence orders for ϕ and q with various time steps

h	L^2-error for ϕ	Order	H^1-error for ϕ	Order	L^2-error for q	Order
$\frac{1}{4}$	2.5248E-01		7.0066E-01		6.4374E-02	
$\frac{1}{8}$	7.1668E-02	1.8167	3.3464E-01	1.0660	2.2671E-02	1.5055
$\frac{1}{16}$	9.9324E-03	2.8511	8.3228E-02	2.0074	4.4243E-03	2.3573
$\frac{1}{24}$	1.5900E-03	4.5183	1.9533E-02	3.5748	9.6891E-04	3.7455
$\frac{1}{32}$	2.7500E-04	6.0995	4.4659E-03	5.1294	2.1416E-04	5.2468
$\frac{1}{48}$	9.2603E-06	8.3633	2.2403E-04	7.3802	1.0264E-05	7.4926
$\frac{1}{96}$	5.1312E-10	14.1394	2.4701E-08	13.1468	9.8363E-10	13.3492

Table 2 The L^2 and H^1 errors and convergence orders for ϕ and q with various spatial steps

5.2. Dynamic evolution of solutions

In the next experiments, we will scheme (3.4) to study the dynamic evolution of the solutions.

Example 5.1 Set $\gamma = 1$, $B = 5$, $\varepsilon = 0.1$, $\delta t = 0.001$, $N = 256$, and we choose the initial condition as

$$\phi^0 = 0.05 \sin x \sin y, \quad q|_{t=0} = \sqrt{F(\phi^0) - \phi^0 + 5}. \tag{5.3}$$

Example 5.2 In order to test the properties for the nonlocal Allen-Cahn model, we choose the same initial value as in [32]. We set $\gamma = 1, B = 5, \varepsilon = 0.01, \delta t = 0.001, N = 256$, and we choose the initial as

$$\begin{aligned}\phi^0 =& \frac{1}{2}\big(1 - \tanh\frac{\sqrt{(x-0.65)^2+(y-0.5)^2}-0.1}{\varepsilon}\tanh\frac{\sqrt{(x-0.35)^2+(y-0.5)^2}-0.1}{\varepsilon}\times \\ &\tanh\frac{\sqrt{(x-0.5)^2+(y-0.65)^2}-0.1}{\varepsilon}\tanh\frac{\sqrt{(x-0.5)^2+(y-0.35)^2}-0.1}{\varepsilon}\big).\end{aligned} \tag{5.4}$$

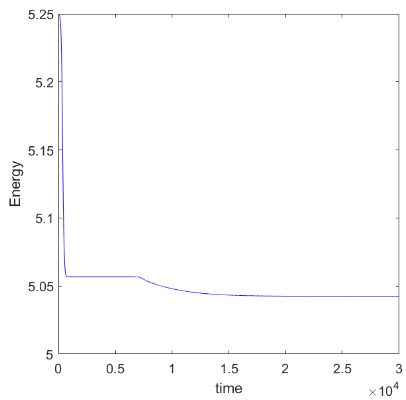

Figure 1 The energy evolution with Example 5.1

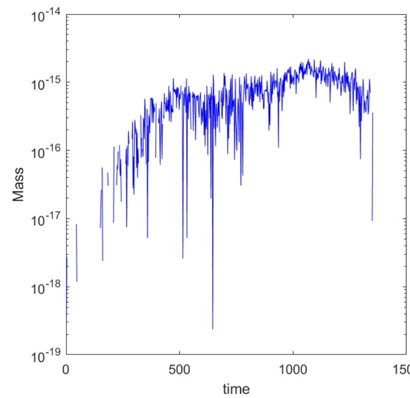

Figure 2 The mass of numerical solution

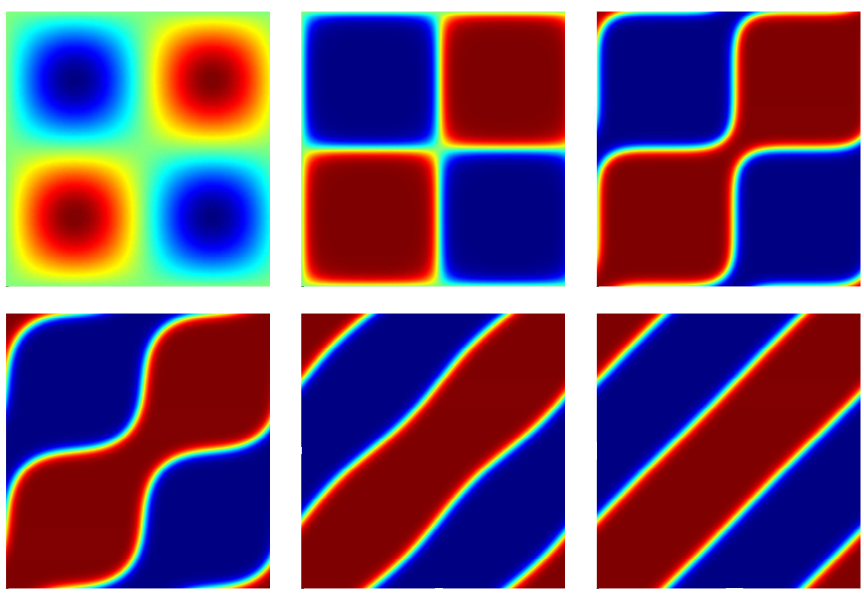

Figure 3 Coarsening dynamics of ϕ by using scheme (3.4) with $t = 0, 6, 80, 100, 200, 300$, respectively

The evolution of energy are plotted in Figure 1 for Example 5.1, and Figure 5 for Example 5.2, we can clearly see that it decreases with time. This also shows that the scheme (3.4) is unconditional energy stable. To verify that ϕ can keep the total mass. We plot the graph to show the error of the total mass. The results are summarized in Figures 2 and 6. We conclude that the full-discrete almost preserves mass conservation for ϕ. In Figures 3 and 4, we propose the snapshots of phase separation of the field ϕ. It can be seen from the figure that our numerical scheme can maintain long-term stability.

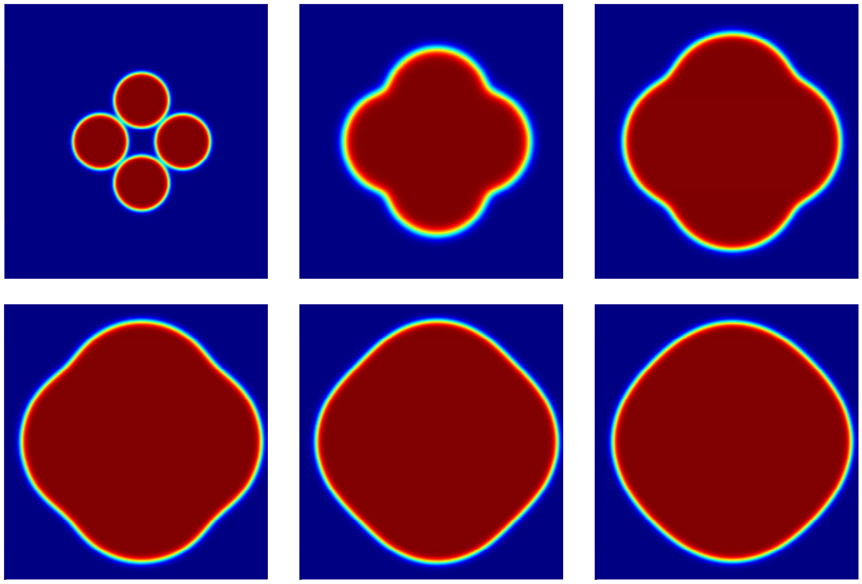

Figure 4 Coarsening dynamics of ϕ by using scheme (3.4) with $t = 0, 6, 10, 20, 50, 100$, respectively

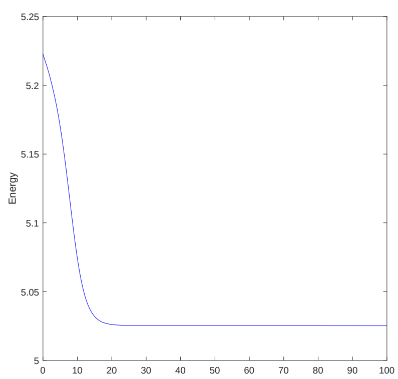

Figure 5 The energy evolution with Example 5.2

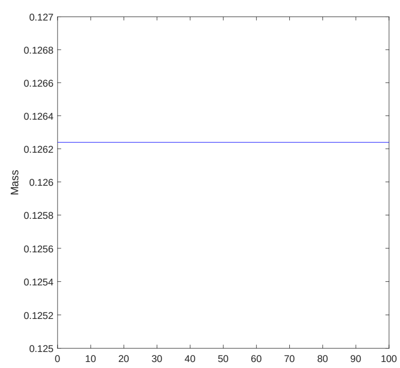

Figure 6 The mass of numerical solution

6. Conclusion

In this work, we develop a full-discrete, second-order accurate in time, and unconditionally energy stable numerical method to solve nonlocal AC equation. We use the Fourier pseudo-spectral method to discretize the spatial direction and the IEQ for the nonlinear and nonlocal terms. The uniqueness, unconditional energy stability and error estimate of the numerical method are obtained. Several numerical examples are proposed to confirm the stability and convergence for the full-discrete method, numerically.

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