Stability and convergence analysis for a new phase field crystal model with a nonlocal Lagrange multiplier☆

Shimin Lin[a], Junying Cao[b], Jun Zhang[c,d], Tao Sun[e]

[a]School of Science, Jiemei university, Xiamen, Fujian 361021, China
[b]School of Data Science and Information Engineering, Guizhou Minzu University, Guiyang, Guizhou 550025, China
[c]Computational Mathematics Research Center, Guizhou University of Finance and Economics, Guiyang, Guizhou 550025, China
[d]School of Mathematics and Statistics, Guizhou University of Finance and Economics, Guiyang, Guizhou 550025, China
[e]School of Statistics and Mathematics, Shanghai Lixin University of Accounting and Finance, Shanghai, 201209, China

Abstract

In this work, an energy stable numerical scheme is proposed to solve the PFC model with a nonlocal Lagrange multiplier. The construction of the numerical scheme is based on invariant energy quadratization (IEQ) technique to transform a nonlinear system into a linear system, while the time variables is discretized by second order scheme. The stability term in the new scheme can balance the influence of nonlinear term. Moreover, we obtain the results of unconditional energy stability, uniqueness and uniform boundedness of numerical solution, and the numerical scheme is convergent with order of $\mathcal{O}(\delta t^2)$. Several numerical tests are conducted to confirm the theoretical results.

Keywords: Phase field crystal model, Invariant Energy Quadratization, Unconditionally energy stable, Error estimate.

1. Introduction

The phase field crystal model (PFC) has attracted considerable attention recently. This model can capture features of solid-liquid system at atomic scales, and has been proven effective, for instance, in modeling the dynamics of crystal growth, foams, colloidal solidification, etc [1, 2] and predicting epitaxial growth, grain growth, etc [4]. In the work of Elder et al [3, 4], the PFC model was first solved by the phase field method, in which a total free energy functional hand been postulated to generate the periodic structure of a crystal lattice. It's worth noting that the well-known Swift-Hohenberg model (SH), which was first proposed by Swift and Hohenberg in 1997 and then widely been studied in modern physics, star from the same total free energy functional. The SH model

☆The research of Junying Cao was supported by NSFC(Grant Nos. 11901135, 11961009) and Foundation of Guizhou Science and Technology Department (Grant No. [2020]1Y015), the work of Shimin Lin is supported by the NSFC(Grant No. 11901237).

*Corresponding author. Tao Sun
Email addresses: smlin@jmu.edu.cn (Shimin Lin), caojunying@gzmu.edu.cn (Junying Cao), jzhang@mail.gufe.edu.cn (Jun Zhang), sunt@lixin.edu.cn (Tao Sun)

is derive by taking variation of the total free energy functional in L^2 space, then lead to a non-conserved, fourth-order governing PDE system. The difference is that the Elder's PFC model is derive by using the variational approach in H^{-1} space, which result in a sixth-order governing PDE system with conserved total mass. The above process is similar to the derivation of the classical Allen-Cahn (AC) and Cahn-Hilliard (CH) systems, but one important difference is that the stable phase of SH and PFC systems are periodic.

It should be recalled that there is a lot of research work on PFC model, such as implicit quadrature method [6, 7], the convex-splitting method [8, 9, 10, 11, 12, 13], Invariant energy quadratization (IEQ) method [14, 15]. The convex-splitting method can produced an energy stable numerical scheme, but some iterative methods are needed to solve the nonlinear system. On the other hand, IEQ method can generate linear and unconditional energy stable numerical schemes [16], but this method does not perform so well when the mobility parameter become large [17, 18, 19]. In order to ensure the conservation of volume, Rubinstein and Sternberg [5] proposed a non-local AC equation. Inspired by their thoughts, Zhang and Yang [15] constructed a second-order stabilized-IEQ scheme by adding some second-order Douglas-Dupont terms, namely, $S_1(\phi^{n+1} - \phi^{*,n+1}), S_2\Delta^2(\phi^{n+1} - \phi^{*,n+1})$. However, they did not discuss the error estimate of numerical scheme. More importantly, by comparing continuous and discrete equation, the added stability terms do not look so natural.

In this paper, we use IEQ technique to construct a new stable numerical scheme for solving the PFC model with a nonlocal Lagrange multiplier. Firstly, the PFC model is reformulated into a new equivalent form via IEQ technique. Secondly, a second-order unconditional numerical scheme is constructed. It should be noted that the stable term in the scheme has the property of balancing the influence of nonlinear term. Next, we also analyze the error estimate of the time discrete scheme. Error estimate shows that our method can achieve second-order accuracy in time direction. More importantly, we obtained the uniform boundedness of numerical solution, and our analysis method does not use any Lipschitz hypothesis for the nonlinear terms. It is only necessary to obtain a sufficiently small time step. At last, subsequent numerical experiments verify the unconditional energy stability of the numerical method. The correctness of the theoretical analysis is also verified.

The rest of the paper is organized as follows. In Section 2, we will introduce the nonlocal PFC model. In Section 3, the IEQ scheme is studied in detail. Some properties of the newly proposed scheme will be introduced. In Section 4, We will introduce the uniform convergence of numerical method. In Section 5, several numerical experiments are performed to demonstrate the effectiveness of the numerical methods. The conclusion of this article is given in the last section.

2. Phase field crystal model

2.1. Nonlocal phase field crystal model

In this work, we study the nonlocal phase field crystal model that preserves the total volume. In details, for the free energy

$$E(\phi) = \int_\Omega \Big(\frac{\phi}{2}(\Delta + 1)^2 \phi + F(\phi) \Big) d\boldsymbol{x}, \tag{1}$$

where $F(\phi) = \frac{1}{4}\phi^4 - \frac{\eta}{3}\phi^3 - \frac{\epsilon}{2}\phi^2$ be the nonlinear potential function.

The L^2-based PFC model, i.e. SH model, that follows the Allen-Cahn dynamics, namely, by taking the variational derivative of (1) in L^2 space, the obtained equation reads as

$$\frac{1}{M}\partial_t \phi = -(\Delta + 1)^2 \phi - f(\phi), \quad (\boldsymbol{x}, t) \in \Omega \times [0, T], \tag{2}$$

with periodic boundary condition, where $f(\phi) = F'(\phi) = \phi^3 - \eta\phi^2 - \epsilon\phi$. The new PFC model we considered in this paper is the SH model added a nonlocal Lagrange multiplier:

$$\frac{1}{M}\partial_t \phi + (\Delta + 1)^2 \phi + f(\phi) - \frac{1}{|\Omega|}\int_\Omega \phi + f(\phi) d\boldsymbol{x} = 0. \tag{3}$$

By taking the L^2 inner product of (3) with 1, we note that it satisfies the mass conservation property

$$\frac{d}{dt}\int_\Omega \phi d\boldsymbol{x} = 0. \tag{4}$$

By taking the L^2 inner product of (3) with ϕ_t, the following energy dissipation law is obtained

$$\frac{d}{dt}E(\phi) = -\frac{1}{M}\|\phi_t\|^2 \leq 0. \tag{5}$$

3. IEQ technique for nonlocal PFC model

Now we introduce the IEQ scheme. Denote

$$q = \sqrt{F(\phi) - \gamma\phi^2 + A}, \quad g = \frac{\partial q}{\partial \phi} = \frac{f(\phi) - 2\gamma\phi}{2\sqrt{F(\phi) - \gamma\phi^2 + A}}, \tag{6}$$

where $\gamma \geq 0$, The value of A make the inequality $F(\phi) - \gamma\phi^2 + A > 0$ holds. Then, reformulated nonlocal PFC model as

$$\frac{1}{M}\partial_t \phi + (\Delta + 1)^2 \phi + 2qg + 2\gamma\phi - \frac{2}{|\Omega|}\int_\Omega qg + (\gamma + \frac{1}{2})\phi d\boldsymbol{x} = 0, \tag{7}$$

$$\partial_t q = g\partial_t \phi, \tag{8}$$

Let $t_n := n\delta t$, where δt is the time step, set ϕ^n, q^n as approximation of $u(\boldsymbol{x}, t_n), q(\boldsymbol{x}, t_n)$ respectively. we propose the following second order time discrete scheme

$$\frac{1}{M}\frac{\phi^{n+1} - \phi^n}{\delta t} + (\Delta + 1)^2 \phi^{n+\frac{1}{2}} + 2g(\phi^\star)q^{n+\frac{1}{2}} + 2\gamma\phi^{n+\frac{1}{2}} - \frac{2}{|\Omega|}\int_\Omega g(\phi^\star)q^{n+\frac{1}{2}} + (\gamma + \frac{1}{2})\phi^{n+\frac{1}{2}} d\boldsymbol{x} = 0, \tag{9}$$

$$\frac{q^{n+1}-q^n}{\delta t}=g(\phi^\star)\frac{\phi^{n+1}-\phi^n}{\delta t}, \tag{10}$$

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

We have the following energy dissipation properties for the time discrete scheme(9)-(10).

Theorem 3.1. *The time-discrete scheme* (9)-(10) *is unconditionally energy stable. It satisfies the following properties*

$$E(\phi^{n+1},q^{n+1})+\frac{1}{M\delta t}\|\phi^{n+1}-\phi^n\|^2=E(\phi^n,q^n), \tag{11}$$

with discrete energy defined by

$$E(\phi^n,q^n):=\frac{1}{2}\|(\Delta+1)\phi^n\|^2+\gamma\|\phi^n\|^2+\|q^n\|^2. \tag{12}$$

Proof. Taking the L^2 inner product of the equation (9) with 1, we find

$$(\phi^{n+1},1)=(\phi^n,1). \tag{13}$$

Taking the L^2 inner product of the equation (9) with $(\phi^{n+1}-\phi^n)$, we have

$$\begin{aligned}&\frac{1}{M\delta t}\|\phi^{n+1}-\phi^n\|^2+\frac{1}{2}\Big(\|(\Delta+1)\phi^{n+1}\|^2-\|(\Delta+1)\phi^n\|^2\Big)+\gamma(\|\phi^{n+1}\|^2-\|\phi^n\|^2)\\&+\Big(g(\phi^\star)(q^{n+1}+q^n),\phi^{n+1}-\phi^n\Big)-\frac{1}{|\Omega|}\Big(g(\phi^\star),q^{n+1}+q^n\Big)\Big(\phi^{n+1}-\phi^n,1\Big)\\&-\frac{\gamma}{|\Omega|}\Big(\phi^{n+1}+\phi^n,1\Big)\Big(\phi^{n+1}-\phi^n,1\Big)=0.\end{aligned} \tag{14}$$

Computing the L^2 inner product of the equation (10) with $\delta t(q^{n+1}+q^n)$, we obtain

$$\|q^{n+1}\|^2-\|q^n\|^2=\Big(g(\phi^\star)(\phi^{n+1}-\phi^n),q^{n+1}+q^n\Big). \tag{15}$$

Substituting (13) and (15) into (14), we have

$$\begin{aligned}&\frac{1}{M\delta t}\|\phi^{n+1}-\phi^n\|^2+\frac{1}{2}\Big(\|(\Delta+1)\phi^{n+1}\|^2-\|(\Delta+1)\phi^n\|^2\Big)\\&+\gamma\Big(\|\phi^{n+1}\|^2-\|\phi^n\|^2\Big)+\|q^{n+1}\|^2-\|q^n\|^2=0,\end{aligned} \tag{16}$$

which yields (11). □

Theorem 3.2. *The time discrete scheme* (9)-(10) *is unique solvable.*

Proof. First, we rewrite the equation (10) as follows

$$q^{n+1}=q^n+g(\phi^\star)(\phi^{n+1}-\phi^n). \tag{17}$$

Then, we reformulate the first equation of (9) as

$$\frac{1}{M\delta t}\phi^{n+1}+\frac{1}{2}(\Delta+1)^2\phi^{n+1}+\gamma\phi^{n+1}+g^2(\phi^\star)\phi^{n+1}-\frac{1}{|\Omega|}\int_\Omega g^2(\phi^\star)\phi^{n+1}+(\gamma+\frac{1}{2})\phi^{n+1}d\boldsymbol{x}=F_1, \tag{18}$$

where

$$F_1=\frac{1}{M\delta t}\phi^n-\frac{1}{2}(\Delta+1)^2\phi^n-\gamma\phi^n-2g(\phi^\star)q^n+g^2(\phi^\star)\phi^n$$

$$+\frac{1}{|\Omega|}\int_\Omega g(\phi^\star)(2q^n - g(\phi^\star)\phi^n) + (\gamma+\frac{1}{2})\phi^n d\boldsymbol{x},$$

is not dependent on ϕ^{n+1}. We introduce $\psi = \phi^{n+1} - c$ and operator

$$\mathcal{L}\psi = \Big[\frac{1}{M\delta t} + \frac{1}{2}(\Delta+1)^2 + \gamma + g^2(\phi^\star) - \frac{1}{|\Omega|}\int_\Omega g^2(\phi^\star)\cdot + (\gamma+\frac{1}{2})\cdot d\boldsymbol{x}\Big]\psi,$$

where $c = (\phi^{n+1}, 1) = \cdots = (\phi^0, 1)$ is a constant, then the equation (18) can be rewritten as

$$\mathcal{L}\psi = F_2. \tag{19}$$

The F_2 is the new right hand side and still independent of ϕ^{n+1}. Then, we can easily shown that there exists a unique solution for ψ. Note that

$$(\mathcal{L}\psi, \psi) = (\frac{1}{M\delta t} + \gamma)\|\psi\|^2 + \frac{1}{2}\|(\Delta+1)\psi\|^2 + \|g(\phi^\star)\psi\|^2. \tag{20}$$

When $\mathcal{L}\psi = 0$, we will derive $\psi = 0$, i.e. there exists a unique solution for (19), which is equivalent to say that there exists a unique solution for (18). □

4. Error estimate

In this section, we will discuss the uniform boundedness results of numerical methods. First, we can rewrite equation (7)-(8) as follows

$$\begin{aligned}\frac{1}{M}\frac{\phi(t^{n+1}) - \phi(t^n)}{\delta t} =& -(\Delta+1)^2\phi(t^{n+\frac{1}{2}}) - 2g(\phi(t^{n+\frac{1}{2}}))q(t^{n+\frac{1}{2}}) - 2\gamma\phi(t^{n+\frac{1}{2}}) \\ &+ \frac{2}{|\Omega|}\int_\Omega g(\phi(t^{n+\frac{1}{2}}))q(t^{n+\frac{1}{2}}) + (\gamma+\frac{1}{2})\phi(t^{n+\frac{1}{2}})d\boldsymbol{x} + R_1^{n+\frac{1}{2}}, \qquad (21)\\ \frac{q(t^{n+1}) - q(t^n)}{\delta t} =& g(\phi(t^{n+\frac{1}{2}})\frac{\phi(t^{n+1}) - \phi(t^n)}{\delta t} + R_2^{n+\frac{1}{2}}. \qquad (22)\end{aligned}$$

It is easy to check that $R_i^{n+\frac{1}{2}}(i=1,2)$ satisfies

$$\|R_i^{n+\frac{1}{2}}\| \le C\delta t^2. \tag{23}$$

In order to study uniform boundedness, we write B

$$B = \max_{0\le t\le T}\|\phi(t)\|_{H^2} + 1. \tag{24}$$

Lemma 4.1. *Suppose $\phi \in H^3([0,T]; H^4(\Omega))$. Given $\tau_0 > 0$, when $\delta t < \tau_0$, the following uniform boundedness result yields*

$$\|\phi^k\|_{H^2} \le B, \quad k = 0, 1, \cdots, K = T/\delta t. \tag{25}$$

Proof. We will utilize mathematical induction to prove the above conclusion. First, notice that $\|\phi^0\|_{H^2} \le B$ is clearly true. Suppose $\|\phi^n\|_{H^2} \le B$ for $n \le k$. Then, we need to proof $\|\phi^{k+1}\|_{H^2} \le B$ still holds. Let us define the point-wise error function

$$e_\phi^n = \phi(t^n) - \phi^n, \quad e_q^n = q(t^n) - q^n. \tag{26}$$

We set $M = 1$ for convenience. Subtracting (9)-(10) from (21)-(22) yields

$$\frac{e_\phi^{n+1} - e_\phi^n}{\delta t} = -(\Delta + 1)^2 e_\phi^{n+\frac{1}{2}} - 2\gamma e_\phi^{n+\frac{1}{2}} + \mathcal{N}_1 - \mathcal{N}_2 + R_1^{n+\frac{1}{2}}, \tag{27}$$

$$\frac{e_q^{n+1} - e_q^n}{\delta t} = \mathcal{N}_3 + R_2^{n+\frac{1}{2}}, \tag{28}$$

where

$$\begin{aligned}
\mathcal{N}_1 =& 2\Big(g(\phi^\star)q^{n+\frac{1}{2}} - g(\phi(t^{n+\frac{1}{2}}))q(t^{n+\frac{1}{2}})\Big),\\
\mathcal{N}_2 =& \frac{2}{|\Omega|}\Big(\int_\Omega g(\phi^\star)q^{n+\frac{1}{2}} + (\gamma + \frac{1}{2})\phi^{n+\frac{1}{2}} d\boldsymbol{x} - \int_\Omega g(\phi(t^{n+\frac{1}{2}}))q(t^{n+\frac{1}{2}}) + (\gamma + \frac{1}{2})\phi(t^{n+\frac{1}{2}}) d\boldsymbol{x}\Big),\\
\mathcal{N}_3 =& g(\phi(t^{n+\frac{1}{2}}))\frac{\phi(t^{n+1}) - \phi(t^n)}{\delta t} - g(\phi^\star)\frac{\phi^{n+1} - \phi^n}{\delta t}.
\end{aligned}$$

Taking the inner product of equation (27) with error function $(e_\phi^{n+1} - e_\phi^n)$ gives

$$\begin{aligned}
&\frac{1}{\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \frac{1}{2}\Big(\|(\Delta + 1)e_\phi^{n+1}\|^2 - \|(\Delta + 1)e_\phi^n\|^2\Big) + \gamma\Big(\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2\Big)\\
=&\Big(\mathcal{N}_1, e_\phi^{n+1} - e_\phi^n\Big) - \Big(\mathcal{N}_2, e_\phi^{n+1} - e_\phi^n\Big) + \Big(R_1^{n+\frac{1}{2}}, e_\phi^{n+1} - e_\phi^n\Big).
\end{aligned} \tag{29}$$

Taking the inner product of equation (28) with the error function $\delta t(e_q^{n+1} + e_q^n)$ gives

$$\|e_q^{n+1}\|^2 - \|e_q^n\|^2 = \delta t\Big(\mathcal{N}_3, e_q^{n+1} + e_q^n\Big) + \delta t\Big(R_2^{n+\frac{1}{2}}, e_q^{n+1} + e_q^n\Big). \tag{30}$$

Summing up above equations, we find

$$\begin{aligned}
&\frac{1}{\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \frac{1}{2}\Big(\|(\Delta + 1)e_\phi^{n+1}\|^2 - \|(\Delta + 1)e_\phi^n\|^2\Big)\\
&+ \gamma\Big(\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2\Big) + \|e_q^{n+1}\|^2 - \|e_q^n\|^2\\
=&\Big(\mathcal{N}_1, e_\phi^{n+1} - e_\phi^n\Big) - \Big(\mathcal{N}_2, e_\phi^{n+1} - e_\phi^n\Big) + \Big(R_1^{n+\frac{1}{2}}, e_\phi^{n+1} - e_\phi^n\Big)\\
&+ \delta t\Big(\mathcal{N}_3, e_q^{n+1} + e_q^n\Big) + \delta t\Big(R^{n+\frac{1}{2}}, e_q^{n+1} + e_q^n\Big).
\end{aligned} \tag{31}$$

Note that

$$\begin{aligned}
\mathcal{N}_1 =& 2q(\phi(t^{n+\frac{1}{2}}))(g(\phi^\star) - g(\phi(t^{n+\frac{1}{2}}))) - g(\phi^\star)\Big((e_q^{n+1} + e_q^n) + q(t^{n+1}) + q(t^n) - q(t^{n+\frac{1}{2}})\Big),\\
\mathcal{N}_2 =& \frac{2}{|\Omega|}\Big(\int_\Omega (g(\phi^\star) - g(\phi(t^{n+\frac{1}{2}})))q(\phi(t^{n+\frac{1}{2}}))d\boldsymbol{x} - \int_\Omega g(\phi^\star)e_q^{n+\frac{1}{2}} d\boldsymbol{x} - \gamma\int_\Omega e_\phi^{n+\frac{1}{2}} d\boldsymbol{x}\Big)\\
&- \frac{1}{|\Omega|}\int_\Omega q(t^{n+1}) + q(t^n) - q(t^{n+\frac{1}{2}})d\boldsymbol{x},\\
\mathcal{N}_3 =& \frac{\phi(t^{n+1}) - \phi(t^n)}{\delta t}(g(\phi(t^{n+\frac{1}{2}})) - g(\phi^\star)) + g(\phi^\star)\frac{e_\phi^{n+1} - e_\phi^n}{\delta t}.
\end{aligned}$$

For the nonlinear terms, we find

$$\begin{aligned}
&\Big|\sqrt{F(\phi(t^{n+\frac{1}{2}})) - \gamma(\phi(t^{n+\frac{1}{2}}))^2 + A} - \sqrt{F(\phi^\star) - \gamma(\phi^\star)^2 + A}\Big|\\
=&\Big|\frac{(F(\phi(t^{n+\frac{1}{2}})) - F(\phi^\star)) - \gamma((\phi(t^{n+\frac{1}{2}}))^2 - (\phi^\star)^2)}{\sqrt{F(\phi(t^{n+\frac{1}{2}})) - \gamma(\phi(t^{n+\frac{1}{2}}))^2 + A} + \sqrt{F(\phi^\star) - \gamma(\phi^\star)^2 + A}}\Big|\\
\leq& C(|e_\phi^n| + |e_\phi^{n-1}| + \delta t^2),
\end{aligned} \tag{32}$$

and

$$
\begin{aligned}
|g(\phi^\star)-g(\phi(t^{n+\frac12}))| =&\Big|\frac{f(\phi^\star)-2\gamma\phi^\star}{2\sqrt{F(\phi^\star)-\gamma(\phi^\star)^2+A}}-\frac{f(\phi(t^{n+\frac12}))-2\gamma\phi(t^{n+\frac12})}{2\sqrt{F(\phi(t^{n+\frac12})-\gamma(\phi(t^{n+\frac12}))^2+A}}\Big|\\
\le&\frac{1}{2A}\Big(|f(\phi^\star)-2\gamma\phi^\star|\Big|\sqrt{F(\phi(t^{n+\frac12}))-\gamma(\phi(t^{n+\frac12}))^2+A}-\sqrt{F(\phi^\star)-\gamma(\phi^\star)^2+A}\Big|\\
&+\sqrt{F(\phi^\star)-\gamma(\phi^\star)^2+A}\Big|(f(\phi^\star)-2\gamma\phi^\star)-(f(\phi(t^{n+\frac12}))-2\gamma\phi(t^{n+\frac12}))\Big|\Big)\\
\le&C(|e_\phi^n|+|e_\phi^{n-1}|+\delta t^2). \qquad (33)
\end{aligned}
$$

The inner product can be handled in a straightforward way

$$
\begin{aligned}
\Big(\mathcal{N}_2,e_\phi^{n+1}-e_\phi^n\Big)\le&3\delta t\|\mathcal{N}_2\|^2+\frac{1}{3\delta t}\|e_\phi^{n+1}-e_\phi^n\|^2\\
\le&C\delta t(\|e_\phi^{n+1}\|^2+\|e_\phi^n\|^2+\|e_\phi^{n-1}\|^2+\|e_q^{n+1}+e_q^n\|^2)+\frac{1}{3\delta t}\|e_\phi^{n+1}-e_\phi^n\|^2, \qquad (34)\\
\Big(R_1^{n+\frac12},e_\phi^{n+1}-e_\phi^n\Big)\le&C\delta t\|R_1^{n+\frac12}\|^2+\frac{1}{3\delta t}\|e_\phi^{n+1}-e_\phi^n\|^2, \qquad (35)\\
\Big(R_2^{n+\frac12},e_q^{n+1}+e_q^n\Big)\le&C\Big(\|R_2^{n+\frac12}\|^2+\|e_q^{n+1}+e_q^n\|^2\Big). \qquad (36)
\end{aligned}
$$

For the last nonlinear term, we find

$$
\begin{aligned}
&\Big(\mathcal{N}_1,e_\phi^{n+1}-e_\phi^n\Big)+\delta t\Big(\mathcal{N}_3,e_q^{n+1}+e_q^n\Big)\\
=&\Big(2q(\phi(t^{n+\frac12}))(g(\phi^\star)-g(\phi(t^{n+\frac12})))-g(\phi^\star)(q(t^{n+1})+q(t^n)-q(t^{n+\frac12})),e_\phi^{n+1}-e_\phi^n\Big)\\
&+\Big((\phi(t^{n+1})-\phi(t^n))(g(\phi(t^{n+\frac12}))-g(\phi^\star)),e_q^{n+1}+e_q^n\Big)\\
\le&C\delta t\Big(\|e_\phi^n\|^2+\|e_\phi^{n-1}\|^2+\delta t^4+\|e_q^{n+1}+e_q^n\|^2\Big)+\frac{1}{3\delta t}\|e_\phi^{n+1}-e_\phi^n\|^2. \qquad (37)
\end{aligned}
$$

Combing with (32)-(37), we have

$$
\begin{aligned}
&\frac12\Big(\|(\Delta+1)e_\phi^{n+1}\|^2-\|(\Delta+1)e_\phi^n\|^2\Big)+\gamma\Big(\|e_\phi^{n+1}\|^2-\|e_\phi^n\|^2\Big)+\|e_q^{n+1}\|^2-\|e_q^n\|^2\\
\le&C\delta t^5+C\delta t\Big(\|e_\phi^{n+1}\|^2+\|e_\phi^n\|^2+\|e_\phi^{n-1}\|^2+\|e_q^{n+1}\|^2+\|e_q^n\|^2\Big). \qquad (38)
\end{aligned}
$$

Summing (38) for $n=1,\cdots,k$, we deduce that

$$
E^{k+1}\le E^1+C\delta t^4+C\delta t\sum_{n=1}^{k}E^{n+1}, \qquad (39)
$$

where

$$
E^{k+1}=\frac12\|(\Delta+1)e_\phi^{k+1}\|^2+\gamma\|e_\phi^{k+1}\|^2+\|e_q^{k+1}\|^2.
$$

It is easy to check that

$$
E^1\le C_1\delta t^4. \qquad (40)
$$

Applying discrete Gronwall inequality to derive that

$$
E^{k+1}\le C_2\delta t^4. \qquad (41)
$$

Thus

$$\|e_{\phi}^{k+1}\|_{H^2} \leq C_3 \delta t^2. \tag{42}$$

If we set $\tau_0 = \sqrt{\frac{1}{C_3}}$, then for all $\delta t \leq \sqrt{\frac{1}{C_3}}$, it holds

$$\|e_{\phi}^{k+1}\|_{H^2} \leq 1. \tag{43}$$

This ends the proof. □

Theorem 4.2. *Suppose the assumption of Lemma* (4.1)*, the following error estimate holds.*

$$\|\phi(t_{k+1}) - \phi^{k+1}\|_{H^2} + \|q(\phi(t_{k+1})) - q(\phi^{k+1})\| \leq C\delta t^2. \tag{44}$$

5. Numerical examples

In this section, we present some numerical tests for the validation of the developed model, as well as the efficiency and accuracy of the proposed IEQ scheme.

5.1. Temporal convergence rate

Firstly, we test the temporal convergence rate. Set the computational domain as $\Omega = [0, 2\pi]^2$, and the order parameters as $M = 1, \gamma = 1, \eta = 0, \varepsilon = -1, A = 5$, a forcing function is added to the right hand side of system (7),(8) such that the exact solution is given by

$$\phi(x, y, t) = \cos(t)\sin(2x)\sin(4y).$$

We use 129^2 Fourier modes so the spatial discretization error is negligible compared with the time discretization error. Table 5.1 show the H^2-error for ϕ, L^2-error for auxiliary variable q between the numerical solution and the exact solution at $t = 1$ with different time step sizes, we observe that the numerical solution ϕ and q both are second-order convergent, which is consistent with our theoretical estimate.

δt	H^2-error for ϕ	order	L^2-error for q	order
0.1	0.00270143071312333	-	7.60230673887e-05	
0.05	0.00174737253973162	0.629	2.04847554780988e-05	1.892
0.01	7.15201988020057e-05	1.986	8.11109066356989e-07	2.006
0.005	1.7879511693599e-05	2.000	2.02514354280915e-07	2.002
0.001	7.15166099298328e-07	2.000	8.09242682881422e-09	2.001
0.0005	1.787911221463e-07	2.000	2.02285458496778e-09	2.000
0.0001	7.151654506629e-09	2.000	8.09058107565712e-11	2.000

Table 1: numerical error for ϕ and q at time $t = 1$

5.2. Benchmark simulations

In this subsection, we implement several long-time benchmark simulations to investigate whether the nonlocal PFC model solved by IEQ method can recover the same dynamical behaviors that had been simulated by the classical Elder's PFC model.

5.2.1. Crystal growth in a supercooled liquid

The First example presents the growth of a poly-crystal in a supercooled liquid. The computational domain is set as $\Omega = [0, 800]^2$, the order parameters take the values $M = 1, \gamma = 0, \eta = 0, \varepsilon = 0.25, A = 4$. To define the initial configuration, we first set $\phi(x, y, 0) = \bar{\phi}$, where $\bar{\phi}$ is a constant. Secondly, we modify this constant configuration by setting some perfect crystallites in small square patches of the domain as illustrated in the first subfigure of Fig5.2.1 or Fig5.2.1. We use the following expression to define the crystallites

$$\phi(x_l, y_l) = \bar{\phi} + C\left(\cos(\frac{p}{\sqrt{3}}y_l)\cos(px_l) - 0.5\cos(\frac{2p}{\sqrt{3}}y_l)\right), \tag{45}$$

where x_l and y_l define a local system of cartesian coordinates that is oriented with the crystallite lattice. The parameters $\bar{\phi}, C$ and p take the values $\bar{\phi} = 0.285, C = 0.446$, and $q = 0.66$. To generate crystallites with different orientations, we formulate the local coordinates (x_l, y_l) by using an affine transformation of the global coordinates (x, y), that produces a rotation given by and angle θ, i.e.,

$$\begin{aligned} x_l(x, y) =& x\sin\theta + y\cos\theta, \\ y_l(x, y) =& -x\cos\theta + y\sin\theta. \end{aligned}$$

All the above initial configurations are consistent with those in [4, 15, 20]. We perform the simulations by using the second order IEQ scheme with time step $\delta t = 0.1$, and 1025^2 Fourier modes to discretize spaces.

Figure 1: The dynamical behaviors of the crystal growth with one initial crystallite arbitrarily deposited in a supercooled liquid for PFC model.

Fig 5.2.1 shows snapshots of the numerical solution at several computational times where the initial condition is set to be a single crystallite that is placed at the center of the domain with $\theta = 0$. Fig 5.2.1 presents close view for several snapshots. We observe that the crystals form hexagonal lattice structure in the end. We further simulate evolution of three crystallites with different orientations. Setting the initial conditions to be three arbitrarily deposited crystallites with $\theta = -\frac{\pi}{4}, 0, \frac{\pi}{4}$ respectively. Several snapshots and close views of the phase variable ϕ are shown in Fig 5.2.1, Fig 5.2.1. We observe the growth of the crystalline phase and the motion of well-defined crystal-liquid interfaces. The dislocation lines are formed due to the different alignment of the initial crystallites. This results present similar features to those obtained in references mentioned above. Fig 5.2.1, Fig 5.2.1 present time evolution of discrete energy defined in (12) and total mass $\int_\Omega \phi d\boldsymbol{x}$.

These results verify the conclusion of Theorem 3.1 and equation (13), i.e. the numerical solution obtained by the IEQ method satisfies the energy dissipation law and guarantees the conservation of total mass.

Figure 2: The dynamical behaviors of the crystal growth with three initial crystallites arbitrarily deposited in a supercooled liquid for PFC model.

5.2.2. Phase transition behaviors

In Fig 3, and Fig 4, we simulate the phase transition behaviors of nonlocal PFC model. Initial condition reads as

$$\phi(x, y, 0) = \bar{\phi}(1 + \text{rand}(x, y)),$$

where $\bar{\phi}$ is the mean density of solid and liquid, $\text{rand}(x, y)$ is the random numbers in the rang of $[-1, 1]$. We set computational domain $[0, 256]^2$, the parameters take the values $\bar{\phi} = 0.07, M = 1, r = 0, A = 4$. The only difference between the two examples is that the parameter η and ϵ is set to $\eta = 0, \epsilon = 0.3$ in Fig 5.2.2 and $\eta = 1, \epsilon = 0.1$ in Fig 5.2.2. We perform the simulations by using the second-order scheme IEQ with time step $\delta = 0.1$ and 513^2 Fourier modes to discretize spaces.

Figure 3: The dynamical behaviors of the phase separation behaviors for PFC model with $\eta = 0, \epsilon = 0.3$.

Figure 4: The dynamical behaviors of the phase separation behaviors for PFC model with $\eta = 1, \epsilon = 0.1$.

In Fig 3, Fig 4, we present the snapshots of phase transition behaviors of the density field ϕ at different computational times. We observe the formation of rolls in Fig 5.2.2 and hexagons in Fig 5.2.2 respectively. These results are similar to those of SH model [15, 21]. The time evolution of discrete energy and total mass $\int_\Omega \phi d\boldsymbol{x}$ are show in Fig 5.2.2, Fig 5.2.2, we come to the same conclusion that IEQ method is effective in solving the nonlocal phase field crystal model.

6. Conclusion

In this article, we have constructed a second order, unconditional energy stable numerical method for nonlocal PFC model. Stability, uniqueness and convergence in time direction are proved. Theoretical proof and numerical experiments show that the constructed numerical scheme can achieve the second-order accuracy of time. A large number of numerical experiments show that our algorithm can better simulate the dynamic behavior of the nonlocal PFC model.

[1] N. Guttenberg, N. Goldenfeld, and J. A Dantzig. Emergence of foams from the breakdown of the phase field crystal model. *Physical Review E*, 81(6):065301, 2010.

[2] S. V. Teeffelen, R. Backofen, A. Voigt, and H. Löwen. Derivation of the phase-field-crystal model for colloidal solidification. *Physical Review E*, 79(5):051404, 2009.

[3] K. R. Elder, M. Katakowski, M. Haataja, and M. Grant. Modeling Elasticity in Crystal Growth. *Physical Review Letters*, 88(24):245701, 2002.

[4] K. R. Elder, and M. Grant. Modeling elastic and plastic deformations in nonequilibrium processing using phase field crystals. *Physical Review E*, 70(5):051605, 2004.

[5] J. Rubinstein, and P. Sternberg. Nonlocal reaction-diffusion equations and nucleation. *Ima Journal of Applied Mathematics*, 84(3):249-264, 1992.

[6] M. Elsey, and B. Wirth. A simple and efficient scheme for phase field crystal simulation. *Esaim Mathematical Modelling and Numerical Analysis*, 47(5):1413-1432, 2013.

[7] X. Yang, and D. Han. Linearly first- and second-order, unconditionally energy stable schemes for the phase field crystal model. *Journal of Computational Physics*, 330:1116-1134, 2017.

[8] C. Wang, and S. M. Wise. An energy stable and convergent finite-difference scheme for the modified phase field crystal equation. *SIAM Journal on Numerical Analysis*, 49:945-969, 2011.

[9] J. Shen, C. Wang, X. Wang, and S. M. Wise. Second-order convex splitting schemes for gradient flows with Ehrlich-Schwoebel type energy: application to thin film epitaxy. *SIAM Journal on Numerical Analysis*, 50:105-125, 2012.

[10] J. Zhao, X. Yang, J. Li, and Q. Wang. Energy stable numerical schemes for a hydrodynamic model of nematic liquid crystals. *SIAM Journal on Scientific Computing*, 38: A3264-A3290, 2016.

[11] Z. Hu, S. M. Wise, C. Wang,and J. S. Lowengrub. Stable and efficient finite-difference nonlinear-multigrid schemes for the phase field crystal equation. *Journal of Computational Physics*, 228: 5323-5339, 2009.

[12] P. Vignal, L. Dalcin, D. L. Brown, N. Collier, and V. M. Calo. An energy-stable convex splitting for the phase-field crystal equation. *Computers and Structures*, 158: 355-368, 2015.

[13] J. Shin, G. L. Hyun, and J. Lee. First and second order numerical methods based on a new convex splitting for phase-field crystal equation. *Journal of Computational Physics*, 327: 519-542, 2016.

[14] X. Yang, and D. Han. Linearly first-and second-order, unconditionally energy stable schemes for the phase field crystal model. *Journal of Computational Physics*, 330: 1116-1134, 2017.

[15] J. Zhang, and X. Yang. Numerical approximations for a new L2-gradient flow based Phase field crystal model with precise nonlocal mass conservation. *Computer Physics Communications*, 243: 51-67, 2019.

[16] J. Zhang, J. Zhao and Y. Gong Error analysis of full-discrete invariant energy quadratization schemes for the Cahn-Hilliard type equation. *Journal of Computational and Applied Mathematics*, 372:112719, 2020.

[17] J. Zhang, M. Jiang, Y. Gong, and J. Zhao. Energy-stable predictor-corrector schemes for the Cahn-Hilliard equation. *Journal of Computational and Applied Mathematics*, 376:112832, 2020.

[18] J. Zhang, and X. Yang. A fully decoupled, linear and unconditionally energy stable numerical scheme for a melt-convective phase-field dendritic solidification model. *Computer Methods in Applied Mechanics and Engineering*, 363:112779, 2020.

[19] J. Zhang, and X. Yang. Efficient, second oder accurate, and unconditionally energy stable numerical scheme for a new hydrodynamics coupled binary phase-field surfactant system. *Computer Physics Communications*, https://doi.org/10.1016/j.cpc.2019.107122, 2020.

[20] H. Gomez, and X. Nogueira. An unconditionally energy-stable method for the phase field crystal equation. *Computer Methods in Applied Mechanics and Engineering*, 249: 52-61, 2012

[21] H. Gomez, and X. Nogueira. A new space-time discretization for the Swift-Hohenberg equation that strictly respects the Lyapunov functional. *Communications in Nonlinear Science and Numerical Simulation*, 17(12): 4930-4946, 2012