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Convergence Analysis for the Invariant Energy Quadratization (IEQ) Schemes for Solving the Cahn–Hilliard and Allen–Cahn Equations with General Nonlinear Potential

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Abstract
In this paper, we carry out stability and error analyses for two first-order, semi-discrete time stepping schemes, which are based on the newly developed invariant energy quadratization approach, for solving the well-known Cahn–Hilliard and Allen–Cahn equations with general nonlinear bulk potentials. Some reasonable sufficient conditions about boundedness and continuity of the nonlinear functional are given in order to obtain optimal error estimates. The well-posedness, unconditional energy stabilities and optimal error estimates of the numerical schemes are proved rigorously. Through the comparisons with some other prevalent schemes for several benchmark numerical examples, we demonstrate the stability and the accuracy of the schemes numerically.

Keywords Cahn–Hilliard · Allen–Cahn · Unconditional energy stability · Invariant energy quadratization · Error estimates

Mathematics Subject Classification 65N12 · 65M12 · 65M70

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1 Introduction

In this paper, we carry out stability analyses and error estimates for two first-order, semi-discrete time-stepping numerical schemes, that are based on the newly developed invariant energy quadratization approach, for solving the Cahn–Hilliard and Allen–Cahn equations with general nonlinear bulk potentials. These two equations are typical representatives of the phase field (diffusive interface) method, which is a popular modeling/numerical tool to resolve the motion of free interfaces between multiple material components, see [3,14,29,31] and the references therein about the extensive theoretical/numerical work, as well as their wide applications in various science and engineering fields.

For algorithm developments of any phase field models, a significant goal is to verify the energy stable property at the discrete level irrespectively of the coarseness of the discretization in time and space. In what follows, those algorithms are called unconditionally energy stable. Scheme with this property is especially preferred since it is not only critical for a numerical scheme to capture the correct long-time dynamics, but also provides sufficient flexibility for dealing with the stiffness issue. Meanwhile, since the dynamics of coarse-graining (macroscopic) process may undergo rapid changes near the interface, the noncompliance of energy dissipation laws may lead to spurious numerical solutions if the mesh and time step size is not carefully controlled.

It is a challenging task to develop unconditionally energy stable schemes to resolve the stiffness issue that is induced by the thin interface for the phase field models. Traditional fully-implicit or explicit discretizations for the nonlinear term can cause severe time step constraints (conditionally energy stable) relying on the interfacial width (cf. [17,34] and the numerical Example 5.1). Many efforts had been done (cf. [13,16,17,21,33–35,47] and the references therein) in the direction of developing unconditionally energy stable schemes without any time step constraints. Among those, the convex splitting approach [16,33,35] and the semi-implicit linear stabilization approach [12,18,26,34] are the two most commonly used numerical techniques. In the convex splitting approach, the convex part of the potential is treated implicitly and the concave part is treated explicitly. The scheme is unconditionally energy stable, however, it usually produces nonlinear type schemes, thus the implementation is complicated and the computational cost might be high. Moreover, it is rather challenging to construct convex–concave combinations for many complicated nonlinear potentials, see [4,5,39,40,42]. The linear stabilization approach treats the nonlinear term explicitly thus it is efficient and very easy to implement. However, in order to remove the time step constraint dependent on the interfacial width, a linear stabilizer term is added and its magnitude usually depends on the interfacial width which in turn results in additional accuracy issues, see [25,26].

Recently, a novel numerical method, called *invariant energy quadratization* (IEQ) approach, has been developed and successfully applied to solve a variety of gradient flow models (cf. [4,5,9,39–42,44,46]). Its essential idea is to transform the bulk potential into a quadratic form (since the nonlinear potential is usually bounded from below) using a set of new variables. For the reformulated model, all nonlinear terms are treated semi-explicitly, which in turn yields a linear and unconditionally energy stable system. This method bypasses those typical challenges such as the justification/adjustment of convexity or implicit/explicit terms, and provides many flexibilities to treat the complicated nonlinear terms since the only request for the nonlinear potential is *bounded from below*.

Although one might think that it could be natural to derive the corresponding error analysis for the IEQ type schemes by analogy with the proof of stability, the reality is quite the opposite.

An exceptional case is the double well potential where many terms can be simplified (cf. Remark 3.1). For general nonlinear potentials, the essential difficulty arises from the way of quadratization to introduce the new variable, that actually leads the new variable to act as a *encapsulation*, making it difficult to estimate the quantitative relation between the new and original variables. To the best of the authors' knowledge, we are not aware of any results about the error analysis of IEQ type schemes with general nonlinear potentials and almost all works had been focused on the remarkable unconditional energy stability. In view of the scarce of error analysis, the main objective of this paper is to derive optimal error estimates for the IEQ schemes for solving the Cahn–Hilliard and Allen–Cahn equations. We give some reasonable sufficient conditions about boundedness and continuity for the nonlinear functionals in order to obtain optimal error estimates. These conditions are naturally satisfied by the commonly used double well potential and regularized logarithmic Flory–Huggins potential. Moreover, the analytical approach developed in this paper is general enough and thus it can work as a standard framework to derive error estimates of IEQ type schemes for various gradient flow models with diverse nonlinear potentials. Through the comparisons with some other prevalent numerical schemes such as the fully-implicit, convex-splitting, stabilized-semi-implicit schemes for some classical benchmark numerical examples, we demonstrate the stability and the accuracy of the proposed IEQ schemes as well.

The rest of paper is organized as follows. In Sect. 2, we give a brief introduction to the Cahn–Hilliard and Allen–Cahn equations. In Sect. 3, for solving the fourth order Cahn–Hilliard equation, we propose the IEQ scheme, prove the unconditional energy stability, and derive the optimal error estimates. In Sect. 4, similar analytical work is performed for solving the second-order Allen–Cahn equation. In Sect. 5, we present some numerical examples to validate the schemes, and compare their performances with some other prevalent schemes. In Sect. 6, some concluding remarks are given.

2 PDE Models and Their Energy Laws

We consider the following Lyapunov energy functional,

$$E(\phi) = \int_{\Omega} \Big(\frac{\epsilon^2}{2} |\nabla \phi|^2 + F(\phi) \Big) d\boldsymbol{x}, \tag{2.1}$$

where $\phi(\boldsymbol{x}, t)$ is the unknown scalar function, $\boldsymbol{x} \in \Omega \subseteq \mathbb{R}^d$ $(d = 2, 3)$, $F(\phi)$ is the nonlinear bulk potential, ϵ is an interface/penalty parameter causing *stiffness* issue into the PDE system when $\epsilon \ll 1$. There are two commonly used nonlinear bulk potentials for $F(\phi)$:

(i) Ginzburg–Landau double-well type potential, cf. [3,29]:

$$F_{db}(x) = \frac{1}{4}(x^2 - 1)^2, \quad x \in (-\infty, \infty); \tag{2.2}$$

(ii) Logarithmic Flory–Huggins potential, cf. [2,3,10,15]:

$$F_{fh}(x) = x \ln x + (1 - x)\ln(1 - x) + \theta(x - x^2), \quad \theta > 0, \quad x \in (0, 1). \tag{2.3}$$

For either of these two nonlinear potentials, we note there always exists a positive constant A such that

$$\begin{cases} F_{db}(x) > -A, & \forall x \in (-\infty, \infty); \\ F_{fh}(x) > -A, & \forall x \in (0, 1), \end{cases} \tag{2.4}$$

where we can simply choose $A = 1$ for both cases.

By applying the variational approach for the total free energy (2.1) in $H^{-1}(\Omega)$, we obtain the Cahn–Hilliard type system that reads as:

$$\phi_t - M\Delta w = 0, \tag{2.5}$$

$$w = -\epsilon^2\Delta\phi + f(\phi), \quad (\boldsymbol{x}, t) \in \Omega \times (0, T], \tag{2.6}$$

where M is the mobility constant, w is the chemical potential, and $f(\phi) = F'(\phi)$. The initial condition is $\phi|_{(t=0)} = \phi_0$. For simplicity, we choose the suitable boundary conditions so that all complexities from the boundary integrals can be removed, i.e.,

$$(i)\ \phi,\ w\ are\ periodic;\ \text{ or } (ii)\ \partial_{\boldsymbol{n}}\phi|_{\partial\Omega} = \partial_{\boldsymbol{n}} w|_{\partial\Omega} = 0. \tag{2.7}$$

By applying the variational approach for the total free energy (2.1) in $L^2(\Omega)$, we obtain the Allen–Cahn type system that reads as:

$$\phi_t + M(-\epsilon^2\Delta\phi + f(\phi)) = 0, \quad (\boldsymbol{x}, t) \in \Omega \times (0, T]. \tag{2.8}$$

Its boundary conditions are

$$(i)\ \phi\ is\ periodic;\ \text{ or } (ii)\ \partial_{\boldsymbol{n}}\phi|_{\partial\Omega} = 0. \tag{2.9}$$

An important feature of the Cahn–Hilliard and Allen–Cahn equations is that they both satisfy energy dissipation law. For the Cahn–Hilliard system (2.5)–(2.6), by taking the L^2 inner product of (2.5) with $-w$, of (2.6) with ϕ_t, performing integration by parts and summing up two equalities, we obtain

$$\frac{d}{dt}E(\phi) = -M\|\nabla w\|^2 \leq 0. \tag{2.10}$$

For the Allen–Cahn system (2.8), by taking the L^2 inner product of with ϕ_t, performing integration by parts, we obtain

$$\frac{d}{dt}E(\phi) = -\frac{1}{M}\|\phi_t\|^2 \leq 0. \tag{2.11}$$

3 Cahn–Hilliard Equation

We first introduce some notations that will be used throughout the paper. We let $L^p(\Omega)$ denote the usual Lebesgue space on Ω with the norm $\|\cdot\|_{L^p}$. The inner product and norm in $L^2(\Omega)$ are denoted by $(\cdot,\cdot)$ and $\|\cdot\|$, respectively. $W^{k,p}(\Omega)$ stands for the standard Sobolev spaces equipped with the standard Sobolev norms $\|\cdot\|_{k,p}$. For $p = 2$, we write $H^k(\Omega)$ for $W^{k,2}(\Omega)$, and the corresponding norm is $\|\cdot\|_k$. We define several Sobolev spaces: $H_{per}(\Omega) = \{\phi\ is\ periodic, \phi \in H^1(\Omega)\}$, $\bar{H}_{per}(\Omega) = \{\phi \in H_{per}(\Omega)\ and\ \int_\Omega \phi d\boldsymbol{x} = 0\}$, and $\bar{H}^1(\Omega) = \{\phi \in H^1(\Omega)\ and\ \int_\Omega \phi d\boldsymbol{x} = 0\}$.

3.1 Unconditional Energy Stable Linear Scheme Using the IEQ Approach

We recall that the main challenge to develop efficient, unconditionally energy stable schemes for solving the system (2.5)–(2.6) lies in how to discretize the nonlinear term $f(\phi)$. Note $F(\phi)$ is bounded from below as (2.4), we choose a positive constant B such that $B > A$, and introduce a new variable $U(\phi)$ through the following *quadratization* formula ([4,5,8,9, 23,27,30,32,37,39–44,46]), that is

$$U(\phi) = \sqrt{F(\phi) + B}. \tag{3.1}$$

Since $F(\phi) + B > -A + B > 0$, we denote $H(\phi) = 2\frac{d}{d\phi}U(\phi) = \frac{f(\phi)}{\sqrt{F(\phi)+B}}$, then the Cahn–Hilliard equation (2.5)–(2.6) can be rewritten as:

$$\phi_t - M\Delta w = 0, \tag{3.2}$$

$$w = -\epsilon^2\Delta\phi + H(\phi)U, \tag{3.3}$$

$$U_t = \frac{1}{2}H(\phi)\phi_t, \tag{3.4}$$

with the initial conditions $\phi|_{t=0} = \phi_0,\ U|_{t=0} = \sqrt{F(\phi_0) + B}$. Note (3.4) is actually an ODE for the new variable U, therefore, the boundary conditions for the new system (3.2)–(3.4) are still (2.7).

The new transformed system (3.2)–(3.4) also follows an energy dissipative law in terms of ϕ and the new variable U. By taking the L^2 inner product of (3.2) with $-w$, of (3.3) with ϕ_t, of (3.4) with $-2U$, performing integration by parts, and summing up all obtained equalities, we can obtain the energy dissipation law of the new system (3.2)–(3.4), that reads as

$$\frac{d}{dt}E(\phi, U) = -M\|\nabla w\|^2, \tag{3.5}$$

where

$$E(\phi, U) = \int_\Omega \left(\frac{\epsilon^2}{2}|\nabla\phi|^2 + U^2\right) d\boldsymbol{x}. \tag{3.6}$$

Note the transformed system (3.2)–(3.4) is exactly equivalent to the original system (2.5)–(2.6) since (3.1) can be easily obtained by integrating (3.4) with respect to the time. Thus the energy law (3.5) for the transformed system is exactly the same as the energy law (2.10) for the original system for the time-continuous case. We will develop energy stable numerical schemes for time stepping of the new transformed system (3.2)–(3.4). Consequently, the proposed schemes should follow the new energy dissipation law (3.5) formally instead of the energy law for the original system (2.10).

Let $\delta t > 0$ denote the time step size and set $t_n = n\delta t$ for $0 \le n \le N$ with $T = N\delta t$, then a first-order, semi-discrete time discretization IEQ scheme for solving the new transformed system (3.2)–(3.4) reads as,

$$\frac{\phi^{n+1} - \phi^n}{\delta t} - M\Delta w^{n+1} = 0, \tag{3.7}$$

$$w^{n+1} = -\epsilon^2\Delta\phi^{n+1} + H^n U^{n+1}, \tag{3.8}$$

$$U^{n+1} - U^n = \frac{1}{2}H^n(\phi^{n+1} - \phi^n), \tag{3.9}$$

where $H^n = H(\phi^n)$. The boundary conditions are as follows,

$$(i)\ \phi^{n+1},\ w^{n+1}\ \textit{are periodic};\ \text{or}\ (ii)\ \partial_{\boldsymbol{n}}\phi^{n+1}|_{\partial\Omega} = \partial_{\boldsymbol{n}}w^{n+1}|_{\partial\Omega} = 0. \tag{3.10}$$

We show the unconditionally energy stablilty of the scheme (3.7)–(3.9) as follows.

Theorem 3.1 *The scheme (3.7)–(3.9) is unconditionally energy stable in the sense that*

$$E(\phi^{n+1}, U^{n+1}) \le E(\phi^n, U^n) - \delta t M\|\nabla w^{n+1}\|^2, \tag{3.11}$$

where

$$E(\phi^{n+1}, U^{n+1}) = \frac{\epsilon^2}{2}\|\nabla\phi^{n+1}\|^2 + \|U^{n+1}\|^2. \tag{3.12}$$

Proof By taking the L^2 inner product of (3.7) with $-\delta t w^{n+1}$ and performing integration by parts, we derive

$$-(\phi^{n+1} - \phi^n, w^{n+1}) - M\delta t\|\nabla w^{n+1}\|^2 = 0. \tag{3.13}$$

By taking the L^2 inner product of (3.8) with $\phi^{n+1} - \phi^n$, using the identity of

$$2(a, a-b) = a^2 - b^2 + (a-b)^2, \tag{3.14}$$

and performing integration by parts, we get

$$\begin{aligned}(\phi^{n+1} - \phi^n, w^{n+1}) = &\frac{\epsilon^2}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2)\\ &+(H^n U^{n+1}, \phi^{n+1} - \phi^n).\end{aligned}$$

By taking the L^2 inner product of (3.9) with $-2U^{n+1}$ and using (3.14), we get

$$-(\|U^{n+1}\|^2 - \|U^n\|^2 + \|U^{n+1} - U^n\|^2) = -(H^n(\phi^{n+1} - \phi^n), U^{n+1}).$$

By combining the above equations together, we have

$$\begin{aligned}&\frac{\epsilon^2}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2) + \|U^{n+1}\|^2\\ &-\|U^n\|^2 + \|U^{n+1} - U^n\|^2 = -\delta t M\|\nabla w^{n+1}\|^2,\end{aligned}$$

which concludes the energy stability (3.11) by dropping some unnecessary positive terms. □

Remark 3.1 The idea of the IEQ method is to transform the complicated nonlinear potentials into a simple quadratic form in terms of some new variables via a change of variables. When the nonlinear potential is the double well potential, one can choose $B = 0$ and thus this method is exactly the same as the so-called Lagrange multiplier method developed in [20]. We remark that the Lagrange multiplier method in [20] only works for the fourth order polynomial potential ϕ^4 since its derivative ϕ^3 can be decomposed into $\lambda(\phi)\phi$ with $\lambda(\phi) = \phi^2$ which can be viewed as a Lagrange multiplier term. However, for other type potentials, the Lagrange multiplier method is not applicable. For example, one cannot separate a factor of ϕ from the logarithmic term.

Remark 3.2 One can easily construct the second-order version of the IEQ type schemes, for instances, the Adam–Bashforth (BDF2) scheme or the Crank–Nicolson scheme, cf. [9,20, 39]). Due to the page limits, we will not present the error analysis of second-order schemes in this paper since they are quite similar to the first-order scheme.

3.2 Implementations and Well-Posedness

The introduction of the new variable U may lead to an increase of the computational cost if one attempts to solve the coupled system (3.7)–(3.9). In fact, note the nonlinear coefficient H of the new variable U is treated explicitly in (3.8), thus we can rewrite it as follows,

$$U^{n+1} = \frac{1}{2}H^n\phi^{n+1} + U^n - \frac{1}{2}H^n\phi^n. \tag{3.15}$$

Using this equality, (3.8)–(3.9) can be rewritten as

$$\phi^{n+1} - \delta t M \Delta w^{n+1} = \phi^n, \tag{3.16}$$

$$-w^{n+1} + P(\phi^{n+1}) = -H^n U^n + \frac{1}{2} H^n H^n \phi^n, \tag{3.17}$$

where $P(\phi) = -\epsilon^2 \Delta \phi + \frac{1}{2} H^n H^n \phi$. Therefore, in practice one can solve ϕ^{n+1} and w^{n+1} directly from (3.16)–(3.17). Once ϕ^{n+1} is obtained, U^{n+1} is automatically given by (3.15).

The scheme (3.17) includes a variable-coefficient $\frac{1}{2} H^n H^n$ for the term ϕ^{n+1} that leads to time-dependent dense matrices. Explicitly building those time-dependent dense matrices are extremely expensive (note that, if one use finite element methods, the corresponding matrices will be sparse but time-dependent). So in practice, an efficient way is to use a conjugate gradient type solver with preconditioning (PCG), that only needs a subroutine to calculate the matrix–vector product instead of building the mass matrix explicitly. An efficient preconditioner is to replace the variable coefficient term $\frac{1}{2} H^n H^n \phi^{n+1}$ by a term with a constant coefficient being the maximum, i.e., $\frac{1}{2} \|H^n H^n\|_{L^\infty} \phi$.

Furthermore, for any ϕ, ψ satisfy the boundary conditions (3.10), we have

$$(P(\phi), \psi) = \frac{\epsilon^2}{2} (\nabla \phi, \nabla \psi) + \frac{1}{2} (H^n \phi, H^n \psi), \tag{3.18}$$

that means the linear operator $P(\phi)$ is symmetric (self-adjoint). Meanwhile, for ϕ that satisfies the boundary conditions (3.10) and $\int_\Omega \phi d\boldsymbol{x} = 0$, we have

$$(P(\phi), \phi) = \frac{\epsilon^2}{2} \|\nabla \phi\|^2 + \frac{1}{2} \|H^n \phi\|^2 \geq 0, \tag{3.19}$$

where " $=$ " is valid if and only if $\phi \equiv 0$. These facts imply that the linear operator P is symmetric positive definite in $\bar{H}_{per}(\Omega)$ or $\bar{H}^1(\Omega)$.

We now show the well-posedness of the scheme (3.16)–(3.17). In the following arguments, we will only consider the periodic boundary condition for convenience. For the case of homogenous Neumann boundary conditions, as long as the space of $\bar{H}_{per}(\Omega)$ is replaced by $\bar{H}^1(\Omega)$, all theoretical results are still valid.

By taking the L^2 inner product of (3.16) with 1, we derive $\int_\Omega \phi^{n+1} d\boldsymbol{x} = \int_\Omega \phi^n d\boldsymbol{x} = \cdots = \int_\Omega \phi^0 d\boldsymbol{x}$. Let $V_\phi = \frac{1}{|\Omega|} \int_\Omega \phi^0 d\boldsymbol{x}$, $V_w = \frac{1}{|\Omega|} \int_\Omega w^{n+1} d\boldsymbol{x}$, and we define

$$\widehat{\phi}^{n+1} = \phi^{n+1} - V_\phi, \ \widehat{w}^{n+1} = w^{n+1} - V_w, \tag{3.20}$$

then the weak form for (3.16)–(3.17) is the system with unknowns $\phi, w \in (\bar{H}_{per}, \bar{H}_{per})(\Omega)$:

$$(\phi, \mu) + \delta t M (\nabla w, \nabla \mu) = (\widehat{\phi}^n, \mu), \quad \mu \in \bar{H}_{per}(\Omega), \tag{3.21}$$

$$\begin{aligned} &(-w, \psi) + \epsilon^2 (\nabla \phi, \nabla \psi) + \frac{1}{2} (H^n \phi, H^n \psi) \\ &= \left(-H^n U^n + \frac{1}{2} H^n H^n \widehat{\phi}^n, \psi \right), \quad \psi \in \bar{H}_{per}(\Omega). \end{aligned} \tag{3.22}$$

We denote the above linear system as

$$(\boldsymbol{L}(\boldsymbol{X}), \boldsymbol{Y}) = (\boldsymbol{B}, \boldsymbol{Y}), \tag{3.23}$$

where $\boldsymbol{X} = (w, \phi)^T$, $\boldsymbol{Y} = (\mu, \psi)^T$, $\boldsymbol{B} = (\widehat{\phi}^n, -H^n U^n + \frac{1}{2} H^n H^n \widehat{\phi}^n)^T$, and $\boldsymbol{X}, \boldsymbol{Y} \in (\bar{H}_{per}, \bar{H}_{per})(\Omega)$.

The well-posedness of the linear system (3.23) is shown as follows.

Theorem 3.2 *The linear system (3.23) admits a unique solution (w, ϕ) in $(\bar{H}_{per}, \bar{H}_{per})(\Omega)$.*

Proof (i) For any $\boldsymbol{X} = (w, \phi)^T$, $\boldsymbol{Y} = (\mu, \psi)^T$ with $\boldsymbol{X}, \boldsymbol{Y} \in (\bar{H}_{per}, \bar{H}_{per})(\Omega)$, we have

$$(\boldsymbol{L}(\boldsymbol{X}), \boldsymbol{Y}) \le c_1(\|\phi\|_1 + \|w\|_1)(\|\psi\|_1 + \|\mu\|_1), \tag{3.24}$$

where c_1 is a postive constant dependent on δt, M, ϵ and $\|H^n\|_{L^\infty}$. Therefore, the bilinear form $(\boldsymbol{LX}, \boldsymbol{Y})$ is bounded.

(ii) For any $\boldsymbol{X} = (w, \phi)^T \in (\bar{H}_{per}, \bar{H}_{per})(\Omega)$, we derive

$$(\boldsymbol{L}(\boldsymbol{X}), \boldsymbol{X}) = \delta t M\|\nabla w\|^2 + \epsilon^2\|\nabla\phi\|^2 + \frac{1}{2}\|H^n\phi\|^2 \ge c_2(\|w\|_1^2 + \|\phi\|_1^2), \tag{3.25}$$

where c_2 is a constant dependent on δt, M, ϵ. Thus the bilinear form $(\boldsymbol{L}(\boldsymbol{X}), \boldsymbol{Y})$ is coercive. Then from the Lax–Milgram theorem, we conclude that the linear system (3.23) admits a unique solution $(w, \phi) \in (\bar{H}_{per}, \bar{H}_{per})(\Omega)$. Namely, the scheme (3.16)–(3.17) admits a unique solution $(w^{n+1}, \phi^{n+1}) \in (H_{per}, H_{per})(\Omega)$ from (3.20). □

3.3 Error Estimates

We now focus on the error estimates. To simplify the notations, without loss of generality, in the below, we let $M = \epsilon = 1$. We use $x \lesssim y$ to denote there exists a constant C that is independent on δt and n such that $x \le Cy$.

To derive the error estimates of (3.7)–(3.9), we first give the following two Lemmas to establish the quantitative relation between the L^2 and H^1 norms of $H(\phi(t_n)) - H(\phi^n)$ and $\phi(t_n) - \phi^n$ under some reasonable assumptions.

Lemma 3.1 *Suppose* (i) *$F(x)$ is uniformly bounded from below: $F(x) > -A$ for any $x \in (-\infty, \infty)$;* (ii) *$F(x) \in C^2(-\infty, \infty)$; and* (iii) *there exists a positive constant C_0 such that*

$$\max_{n\le M}(\|\phi(t_n)\|_{L^\infty}, \|\phi^n\|_{L^\infty}) \le C_0, \tag{3.26}$$

then we have

$$\|H(\phi(t_n)) - H^n\| \le \widehat{C}_0\|\phi(t_n) - \phi^n\|, \tag{3.27}$$

for $n \le M$, where $\widehat{C}_0$ is a positive constant that is only dependent of C_0, A and B.

Proof First, for any $\theta \in [0, 1]$ (3.26), can ensure $\psi^n = \theta\phi(t_n) + (1-\theta)\phi^n$ is uniformly bounded, i.e., $\psi^n \in [-2C_0, 2C_0]$ for $n \le M$. Thus from assumption (ii), we can always find a positive constant C_1 such that

$$\max_{n\le M}\left(\|F(\psi^n)\|_{L^\infty}, \|f(\psi^n)\|_{L^\infty}, \|f'(\psi^n)\|_{L^\infty}, \|\sqrt{F(\psi^n) + B}\|_{L^\infty}\right) \le C_1. \tag{3.28}$$

Second, for any $x, y \in (-A, \infty)$, by applying the intermediate value Theorem, there exists some value $\xi \in (-A, \infty)$ that is between x and y, such that $\sqrt{x+B} - \sqrt{y+B} = \frac{1}{2\sqrt{\xi+B}}(x-y)$, that implies

$$|\sqrt{x+B} - \sqrt{y+B}| \le \frac{1}{2\sqrt{B-A}}\,|x-y|\,. \tag{3.29}$$

Thus, using (3.28), (3.29), and applying the intermediate value Theorem again, we derive

$$\begin{aligned}\left|\sqrt{F(\phi(t_n))+B}-\sqrt{F(\phi^n)+B}\right| &\leq \frac{1}{2\sqrt{B-A}}\left|F(\phi(t_n))-F(\phi^n)\right| \\ &= \frac{1}{2\sqrt{B-A}}|f(\theta\phi(t_n)+(1-\theta)\phi^n)||\phi(t_n)-\phi^n| \\ &\leq \frac{C_1}{2\sqrt{B-A}}|\phi(t_n)-\phi^n|. \end{aligned} \tag{3.30}$$

Third, for $n \leq M$, from (3.28) and (3.30), we derive

$$\begin{aligned}|H(\phi(t_n))-H^n| &= \left|\frac{f(\phi(t_n))}{\sqrt{F(\phi(t_n))+B}}-\frac{f(\phi^n)}{\sqrt{F(\phi^n)+B}}\right| \\ &= \frac{\left|f(\phi(t_n))\sqrt{F(\phi^n)+B}-f(\phi^n)\sqrt{F(\phi(t_n))+B}\right|}{\sqrt{F(\phi(t_n))+B}\sqrt{F(\phi^n)+B}} \\ &\leq \frac{1}{B-A}\left|f(\phi(t_n))\sqrt{F(\phi^n)+B}-f(\phi^n)\sqrt{F(\phi(t_n))+B}\right| \\ &\leq \frac{1}{B-A}|f(\phi(t_n))|\left|\sqrt{F(\phi(t_n))+B}-\sqrt{F(\phi^n)+B}\right| \\ &\quad + \frac{1}{B-A}\sqrt{F(\phi(t_n))+B}\left|f(\phi^n)-f(\phi(t_n))\right| \\ &\leq \frac{C_1}{B-A}\frac{C_1}{2\sqrt{B-A}}|\phi(t_n)-\phi^n| + \frac{C_1}{B-A}|f'(\psi^n)||\phi(t_n)-\phi^n| \\ &\leq \left(\frac{C_1^2}{2\sqrt{(B-A)^3}}+\frac{C_1^2}{B-A}\right)|\phi(t_n)-\phi^n|, \end{aligned} \tag{3.31}$$

where we have used $\frac{1}{\sqrt{F(x)+B}} \leq \frac{1}{\sqrt{B-A}}$ for any $x \in (-\infty, \infty)$.

Finally, let $\widehat{C}_0 = \frac{C_1^2}{2\sqrt{(B-A)^3}} + \frac{C_1^2}{B-A}$, we derive

$$\begin{aligned}\|H(\phi(t_n))-H^n\| &= \left(\int_\Omega |H(\phi(t_n))-H(\phi^n)|^2 d\boldsymbol{x}\right)^{\frac{1}{2}} \leq \widehat{C}_0\left(\int_\Omega |\phi(t_n)-\phi^n|^2 d\boldsymbol{x}\right)^{\frac{1}{2}} \\ &= \widehat{C}_0\|\phi(t_n)-\phi^n\|.\end{aligned}$$

□

Remark 3.3 Lemma 3.1 establishes a quantitative relation between the L^2 norm of $H(\phi(t_n)) - H(\phi^n)$ and $\phi(t_n) - \phi^n$ under some reasonable assumptions, where the Lipschitz property (3.29) of the quadratization function $\sqrt{x+B}$ $(x > -A)$ plays a critical role. We note assumptions (i) and (ii) are automatically valid for the fourth order polynomial type double-well potential. Indeed, for the double well potential, one can choose $B = 0$ and $H^n = \phi^n$, thus Lemma 3.1 is trivial and the error analysis is straightforward for this case, see [20]. However, for the logarithmic Flory–Huggins potential, $B \neq 0$ and assumption (ii) is not true since the domain is the open interval (0, 1) instead of $(-\infty, \infty)$. This issue can be overcome by extending the logarithmic functional near the domain boundary with a continuous, convex, piecewise function, see [10,15,39]. Such a regularized method is also a common practice to remove the difficulty about that any small fluctuation near the domain boundary (0, 1) can cause the overflow, numerically. In this way, the domain is regularized to $(-\infty, \infty)$ and thus the assumptions (ii) will become valid.

Similarly, we further establish the relation between their H^1 norms, as follows.

Lemma 3.2 *Suppose* (i) *$F(x)$ is uniformly bounded from below: $F(x) > -A$ for any $x \in (-\infty, \infty)$;* (ii) *$F(x) \in C^3(-\infty, \infty)$; and* (iii) *there exists a positive constant D_0 such that*

$$\max_{n\le M}(\|\phi(t_n)\|_{L^\infty}, \|\phi^n\|_{L^\infty}, \|\nabla\phi(t_n)\|_{L^3}) \le D_0, \tag{3.32}$$

then we have

$$\|\nabla H(\phi(t_n)) - \nabla H^n\| \le \widehat{D}_0(\|\phi(t_n) - \phi^n\| + \|\nabla\phi(t_n) - \nabla\phi^n\|), \tag{3.33}$$

for $n \le M$, where $\widehat{D}_0$ is a positive constant dependent on Ω, D_0, A and B.

Proof First, from assumption (ii) and (iii), for any $\psi^n = \theta\phi(t_n) + (1-\theta)\phi^n$ where $\theta \in [0, 1]$, we can always find a positive constant D_1 that is dependent on D_0, such that

$$\max_{n\le M}\Big(\|F(\psi^n)\|_{L^\infty}, \|f(\psi^n)\|_{L^\infty}, \|f'(\psi^n)\|_{L^\infty}, \|f''(\psi^n)\|_{L^\infty}, \|F(\psi^n) + B\|_{L^\infty}\Big) \le D_1. \tag{3.34}$$

Second, for convenience, we denote $G(u) = f'(u)(F(u) + B) - \frac{1}{2}f^2(u)$. From (3.34), assumption (i), (ii) and (iii), we derive

$$\begin{aligned}
|\nabla H(\phi(t_n)) - \nabla H(\phi^n)| &= |H'(\phi(t_n))\nabla\phi(t_n) - H'(\phi^n)\nabla\phi^n| \\
&\le |\nabla\phi(t_n)||H'(\phi(t_n)) - H'(\phi^n)| + |H'(\phi^n)||\nabla\phi(t_n) - \nabla\phi^n| \\
&\le |\nabla\phi(t_n)||H'(\phi(t_n)) - H'(\phi^n)| + \left|\frac{G(\phi^n)}{(F(\phi^n) + B)^{\frac{3}{2}}}\right| |\nabla\phi(t_n) - \nabla\phi^n| \\
&\le |\nabla\phi(t_n)||H'(\phi(t_n)) - H'(\phi^n)| + \frac{\frac{3}{2}D_1^2}{(B - A)^{\frac{3}{2}}}|\nabla\phi(t_n) - \nabla\phi^n|,
\end{aligned} \tag{3.35}$$

where we have used $|G(\phi^n)| \le \frac{3}{2}D_1^2$ from (3.34) and $\frac{1}{(F(\phi^n)+B)^{\frac{3}{2}}} \le \frac{1}{(B-A)^{\frac{3}{2}}}$ from assumption (i).

Third, we estimate

$$\begin{aligned}
|H'(\phi(t_n)) - H'(\phi^n)| &= \left|\frac{G(\phi(t_n))}{(F(\phi(t_n)) + B)^{\frac{3}{2}}} - \frac{G(\phi^n)}{(F(\phi^n) + B)^{\frac{3}{2}}}\right| \\
&= \frac{\left|(F(\phi^n) + B)^{\frac{3}{2}}G(\phi(t_n)) - (F(\phi(t_n)) + B)^{\frac{3}{2}}G(\phi^n)\right|}{(F(\phi(t_n)) + B)^{\frac{3}{2}}(F(\phi^n) + B)^{\frac{3}{2}}} \\
&\le \frac{1}{(B - A)^3}\left|(F(\phi^n) + B)^{\frac{3}{2}}G(\phi(t_n)) - (F(\phi(t_n)) + B)^{\frac{3}{2}}G(\phi^n)\right| \\
&\le \frac{1}{(B - A)^3}\left|(F(\phi^n) + B)^{\frac{3}{2}} - (F(\phi(t_n)) + B)^{\frac{3}{2}}\right||G(\phi(t_n))| \\
&\quad + \frac{1}{(B - A)^3}(F(\phi(t_n)) + B)^{\frac{3}{2}}\left|f'(\phi(t_n))(F(\phi(t_n)) + B) - f'(\phi^n)(F(\phi^n) + B)\right| \\
&\quad + \frac{1}{(B - A)^3}(F(\phi(t_n)) + B)^{\frac{3}{2}}\frac{1}{2}\left|f^2(\phi^n) - f^2(\phi(t_n))\right| \\
&\le \frac{\frac{3}{2}D_1^2}{(B - A)^3}\left|(F(\phi^n) + B)^{\frac{3}{2}} - (F(\phi(t_n)) + B)^{\frac{3}{2}}\right| \qquad (:\ \text{term } I_1)
\end{aligned}$$

$$+\frac{D_1^{\frac{3}{2}}}{(B-A)^3}\left|f'(\phi(t_n))(F(\phi(t_n))+B)-f'(\phi^n)(F(\phi^n)+B)\right| \quad (\because \text{ term } I_2)$$
$$+\frac{1}{2}\frac{D_1^{\frac{3}{2}}}{(B-A)^3}\left|f^2(\phi^n)-f^2(\phi(t_n))\right| \quad (\because \text{ term } I_3). \tag{3.36}$$

For term I_1, by applying the intermediate value theorem twice and using (3.34), we derive

$$\begin{aligned} I_1 &\le \frac{\frac{3}{2}D_1^2}{(B-A)^3}\frac{3}{2}\sqrt{(\xi_1+B)}\Big|F(\phi^n)-F(\phi(t_n))\Big| \\ &\le \frac{\frac{3}{2}D_1^2}{(B-A)^3}\frac{3}{2}\sqrt{(\xi_1+B)}|f(\xi_2)|\Big|\phi^n-\phi(t_n)\Big| \\ &\le \frac{\frac{9}{4}D_1^3\sqrt{(2D_1+B)}}{(B-A)^3}\Big|\phi^n-\phi(t_n)\Big|, \end{aligned} \tag{3.37}$$

where $\xi_1=\theta_1F(\phi(t_n))+(1-\theta_1)F(\phi^n)$, $\xi_2=\theta_2\phi(t_n)+(1-\theta_2)\phi^n$ for some $\theta_1,\theta_2\in[0,1]$, $\sqrt{\xi_1+B}\le\sqrt{2D_1+B}$ and $f(\xi_2)\le D_1$.

For term I_2, using the intermediate value Theorem for F and f' and (3.34), we derive

$$\begin{aligned} I_2 &\le \frac{D_1^{\frac{3}{2}}}{(B-A)^3}\Big(\left|f'(\phi(t_n))(F(\phi(t_n))-F(\phi^n))\right|+\left|(f'(\phi(t_n))-f'(\phi^n))(F(\phi^n)+B)\right|\Big) \\ &\le \frac{D_1^{\frac{5}{2}}}{(B-A)^3}\Big(\left|(F(\phi(t_n))-F(\phi^n))\right|+\left|f'(\phi(t_n))-f'(\phi^n)\right|\Big)\le\frac{D_1^{\frac{7}{2}}}{(B-A)^3}|\phi^n-\phi(t_n)|. \end{aligned} \tag{3.38}$$

For term I_3, using the intermediate value theorem for f and (3.34), we derive

$$\begin{aligned} I_3 &\le \frac{1}{2}\frac{D_1^{\frac{3}{2}}}{(B-A)^3}|f(\phi(t_n))+f(\phi^n)||f(\phi(t_n))-f(\phi^n)| \\ &\le \frac{D_1^{\frac{5}{2}}}{(B-A)^3}|f(\phi(t_n))-f(\phi^n)|\le\frac{D_1^{\frac{7}{2}}}{(B-A)^3}|\phi^n-\phi(t_n)|. \end{aligned} \tag{3.39}$$

Thus, by combining (3.37)–(3.39), and denote $\widehat{D}_1=\frac{\frac{9}{4}D_1^3\sqrt{(2D_1+B)}}{(B-A)^3}+\frac{2D_1^{\frac{7}{2}}}{(B-A)^3}$, we have

$$|H'(\phi(t_n)-H'(\phi^n)|\le\widehat{D}_1|\phi^n-\phi(t_n)|. \tag{3.40}$$

Therefore, from (3.35), we derive

$$\begin{aligned} \|\nabla H(\phi(t_n))-\nabla H(\phi^n)\|^2 &= \int_\Omega|\nabla H(\phi(t_n))-\nabla H(\phi^n)|^2dx \\ &\le 2\int_\Omega|\nabla\phi(t_n)|^2\widehat{D}_1^2|\phi(t_n)-\phi^n|^2+\frac{\frac{9}{4}D_1^4}{(B-A)^3}|\nabla\phi(t_n)-\nabla\phi^n|^2dx \\ &= 2\widehat{D}_1^2\int_\Omega|\nabla\phi(t_n)|^2|\phi(t_n)-\phi^n|^2dx+\frac{\frac{9}{2}D_1^4}{(B-A)^3}\|\nabla\phi(t_n)-\nabla\phi^n\|^2 \\ &\le 2\widehat{D}_1^2\|\nabla\phi(t_n)\|_{L^3}^2\|\phi(t_n)-\phi^n\|_{L^6}^2+\frac{\frac{9}{2}D_1^4}{(B-A)^3}\|\nabla\phi(t_n)-\nabla\phi^n\|^2 \end{aligned}$$

$$
\begin{aligned}
&\le 2\widehat{D}_1^2 D_0^2 C_\Omega^2 \|\phi(t_n)-\phi^n\|_1^2 + \frac{\frac{9}{2}D_1^4}{(B-A)^3}\|\phi(t_n)-\phi^n\|_1^2\\
&= \widehat{D}_0^2 \|\phi(t_n)-\phi^n\|_1^2, \qquad (3.41)
\end{aligned}
$$

where $\widehat{D}_0^2 = 2\widehat{D}_1^2 D_0^2 C_\Omega^2 + \frac{\frac{9}{2}D_1^4}{(B-A)^3}$, that concludes (3.33). □

We now establish the error estimates for scheme (3.7)–(3.9). To this end, we formulate the Cahn–Hilliard system (3.2)–(3.4) as a truncation form:

$$
\frac{\phi(t_{n+1})-\phi(t_n)}{\delta t} = \Delta w(t_{n+1}) + R_\phi^{n+1}, \qquad (3.42)
$$

$$
w(t_{n+1}) = -\Delta\phi(t_{n+1}) + H(\phi(t_n))U(t_{n+1}) + R_w^{n+1}, \qquad (3.43)
$$

$$
U(t_{n+1}) - U(t_n) = \frac{1}{2}H(\phi(t_n))(\phi(t_{n+1})-\phi(t_n)) + \delta t R_u^{n+1}, \qquad (3.44)
$$

where

$$
\begin{cases}
R_\phi^{n+1} = \dfrac{\phi(t_{n+1})-\phi(t_n)}{\delta t} - \phi_t(t_{n+1}),\\
R_w^{n+1} = H(\phi(t_{n+1}))U(t_{n+1}) - H(\phi(t_n))U(t_{n+1}),\\
R_u^{n+1} = \dfrac{U(t_{n+1})-U(t_n)}{\delta t} - U_t(t_{n+1}) + \dfrac{1}{2}H(\phi(t_{n+1}))\phi_t(t_{n+1}) - \dfrac{1}{2}H(\phi(t_n))\dfrac{\phi(t_{n+1})-\phi(t_n)}{\delta t}.
\end{cases} \qquad (3.45)
$$

We assume the exact solution ϕ, w, U of the system (3.2)–(3.4) possesses the following regularity conditions,

$$
\begin{cases}
\phi \in L^\infty(0,T;H^2(\Omega)), \quad U \in L^\infty(0,T;W^{1,\infty}(\Omega)), \quad w \in L^\infty(0,T;H^1(\Omega)),\\
\phi_t \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^\infty), \quad \phi_{tt}, U_{tt} \in L^2(0,T;L^2(\Omega)).
\end{cases} \qquad (3.46)
$$

One can easily establish the following estimates for the truncation errors, provided that the exact solutions of the system (3.2)–(3.4) satisfy (3.46).

Lemma 3.3 *Under the regularity conditions* (3.46)*, the truncation errors satisfy*

$$
\delta t \sum_{n=0}^{[\frac{T}{\delta t}]} (\|R_\phi^{n+1}\|^2 + \|R_w^{n+1}\|_1^2 + \|R_u^{n+1}\|^2) \lesssim \delta t^2. \qquad (3.47)
$$

Proof Since the proof is rather straight forward, we leave this to the interested readers. □

To derive the error estimates, we denote the error functions as

$$
\begin{cases}
e_\phi^n = \phi(t_n) - \phi^n, \quad e_w^n = w(t_n) - w^n,\\
e_u^n = U(t_n) - U^n, \quad e_H^n = H(\phi(t_n)) - H(\phi^n).
\end{cases} \qquad (3.48)
$$

By subtracting (3.7)–(3.9) from (3.42)–(3.44), we derive the error equations:

$$
\frac{e_\phi^{n+1} - e_\phi^n}{\delta t} = \Delta e_w^{n+1} + R_\phi^{n+1}, \qquad (3.49)
$$

$$
e_w^{n+1} = -\Delta e_\phi^{n+1} + e_H^n U(t_{n+1}) + H^n e_u^{n+1} + R_w^{n+1}, \qquad (3.50)
$$

$$
e_u^{n+1} - e_u^n = \frac{1}{2}(e_H^n(\phi(t_{n+1})-\phi(t_n)) + H^n(e_\phi^{n+1} - e_\phi^n)) + \delta t R_u^{n+1}. \qquad (3.51)
$$

We first prove the L^∞ stability of ϕ^n, which plays the key point in the error estimates. From (3.46), we define a positive constant κ such that

$$\kappa = \max_{0\le t\le T} \|\phi(t)\|_{L^\infty} + 1. \tag{3.52}$$

The preliminary result is given in the following lemma.

Lemma 3.4 *Suppose* (i) $F(x)$ *is uniformly bounded from below:* $F(x) > -A$ *for any* $x \in (-\infty, \infty)$*;* (ii) $F(x) \in C^3(-\infty, \infty)$*; and* (iii) *the exact solutions of* (3.2)–(3.4) *satisfy the regularity conditions* (3.46)*, then there exists a positive constant* s_0 *that is given in the proof, such that when* $\delta t \le s_0$*, the solution* ϕ^n *of* (3.7)–(3.9) *is uniformly bounded as*

$$\|\phi^n\|_{L^\infty} \le \kappa, n = 0, 1, \ldots, N = \frac{T}{\delta t}. \tag{3.53}$$

Proof We use the mathematical induction to prove this Lemma.

For $n = 0$, $\|\phi^0\|_{L^\infty} \le \kappa$ is true naturally. Assuming that $\|\phi^n\|_{L^\infty} \le \kappa$ is valid for all $n \le M$, we show $\|\phi^{M+1}\|_{L^\infty} \le \kappa$ is also valid through the following two steps.

(i) By taking the L^2 inner product of (3.49) with $\delta t e_w^{n+1}$, we obtain

$$(e_\phi^{n+1} - e_\phi^n, e_w^{n+1}) + \delta t\|\nabla e_w^{n+1}\|^2 = \delta t(R_\phi^{n+1}, e_w^{n+1}). \tag{3.54}$$

By taking the L^2 inner product of (3.50) with $-(e_\phi^{n+1} - e_\phi^n)$, we obtain

$$\begin{aligned}&-(e_w^{n+1}, e_\phi^{n+1} - e_\phi^n) + \frac{1}{2}(\|\nabla e_\phi^{n+1}\|^2 - \|\nabla e_\phi^n\|^2 + \|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|^2)\\ &= -(e_H^n U(t_{n+1}) + H^n e_u^{n+1}, e_\phi^{n+1} - e_\phi^n) - (R_w^{n+1}, e_\phi^{n+1} - e_\phi^n).\end{aligned} \tag{3.55}$$

By taking the L^2 inner product of (3.51) with $2e_u^{n+1}$, we get

$$\begin{aligned}&\|e_u^{n+1}\|^2 - \|e_u^n\|^2 + \|e_u^{n+1} - e_u^n\|^2\\ &= (e_H^n(\phi(t_{n+1}) - \phi(t_n)) + H^n(e_\phi^{n+1} - e_\phi^n), e_u^{n+1}) + 2\delta t(R_u^{n+1}, e_u^{n+1}).\end{aligned} \tag{3.56}$$

By taking the L^2 inner product of (3.49) with $\delta t e_\phi^{n+1}$, we get

$$\frac{1}{2}(\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2 + \|e_\phi^{n+1} - e_\phi^n\|^2) = \delta t(\Delta e_w^{n+1}, e_\phi^{n+1}) + \delta t(R_\phi^{n+1}, e_\phi^{n+1}). \tag{3.57}$$

By taking the L^2 inner product of (3.50) with $\delta t e_w^{n+1}$, we derive

$$\delta t\|e_w^{n+1}\|^2 = -\delta t(\Delta e_\phi^{n+1}, e_w^{n+1}) + \delta t(e_H^n U(t_{n+1}) + H^n e_u^{n+1}, e_w^{n+1}) + \delta t(R_w^{n+1}, e_w^{n+1}). \tag{3.58}$$

Combining (3.54)–(3.58) together, we obtain

$$\begin{aligned}&\frac{1}{2}(\|e_\phi^{n+1}\|^2 + \|\nabla e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2 - \|\nabla e_\phi^n\|^2)\\ &\quad + (\|e_u^{n+1}\|^2 - \|e_u^n\|^2) + \delta t(\|e_w^{n+1}\|^2 + \|\nabla e_w^{n+1}\|^2)\\ &\quad + \frac{1}{2}(\|e_\phi^{n+1} - e_\phi^n\|^2 + \|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|^2) + \|e_u^{n+1} - e_u^n\|^2\\ &= -(e_H^n U(t_{n+1}), e_\phi^{n+1} - e_\phi^n) + \big(e_H^n(\phi(t_{n+1}) - \phi(t_n)), e_u^{n+1}\big)\\ &\quad + \delta t(e_H^n U(t_{n+1}) + H^n e_u^{n+1}, e_w^{n+1})\end{aligned}$$

$$
- (R_w^{n+1}, e_\phi^{n+1} - e_\phi^n) + \delta t (R_\phi^{n+1}, e_w^{n+1}) + 2\delta t (R_u^{n+1}, e_u^{n+1}) \\
+ \delta t (R_\phi^{n+1}, e_\phi^{n+1}) + \delta t (R_w^{n+1}, e_w^{n+1}). \tag{3.59}
$$

By using Lemmas 3.1, 3.2 and (3.46), for $n \leq M$, we estimate terms on the right hand side as follows.

$$
\begin{aligned}
|(e_H^n U(t_{n+1}), e_\phi^{n+1} - e_\phi^n)| &= \delta t |(e_H^n U(t_{n+1}), \frac{e_\phi^{n+1} - e_\phi^n}{\delta t})| \\
&= \delta t |(e_H^n U(t_{n+1}), \Delta e_w^{n+1} + R_\phi^{n+1})| \\
&= \delta t |(\nabla (e_H^n U(t_{n+1})), \nabla e_w^{n+1}) + (e_H^n U(t_{n+1}), R_\phi^{n+1})| \\
&= \delta t |(U(t_{n+1}) \nabla e_H^n + e_H^n \nabla U(t_{n+1}), \nabla e_w^{n+1}) \\
&\quad + (e_H^n U(t_{n+1}), R_\phi^{n+1})| \\
&\leq \delta t \|U(t_{n+1})\|_{L^\infty} \|\nabla e_H^n\| \|\nabla e_w^{n+1}\| \\
&\quad + \delta t \|e_H^n\| \|\nabla U(t_{n+1})\|_{L^\infty} \|\nabla e_w^{n+1}\| \\
&\quad + \delta t \|e_H^n\| \|U(t_{n+1})\|_{L^\infty} \|R_\phi^{n+1}\| \\
&\lesssim \delta t \|\nabla e_H^n\| \|\nabla e_w^{n+1}\| + \delta t \|e_H^n\| \|\nabla e_w^{n+1}\| + \delta t \|e_H^n\| \|R_\phi^{n+1}\| \\
&\lesssim \frac{1}{4} \delta t \|\nabla e_w^{n+1}\|^2 + \delta t \|\nabla e_H^n\|^2 + \delta t \|e_H^n\|^2 + \delta t \|R_\phi^{n+1}\|^2 \\
&\lesssim \frac{1}{4} \delta t \|\nabla e_w^{n+1}\|^2 + \delta t \|\nabla e_\phi^n\|^2 + \delta t \|e_\phi^n\|^2 + \delta t \|R_\phi^{n+1}\|^2;
\end{aligned} \tag{3.60}
$$

$$
\begin{aligned}
\left|\left(e_H^n(\phi(t_{n+1}) - \phi(t_n)), e_u^{n+1}\right)\right| &\leq \|e_H^n\|_{L^4} \|\phi(t_{n+1}) - \phi(t_n)\|_{L^4} \|e_u^{n+1}\| \\
&\lesssim \delta t \|e_H^n\|_{L^4} \|e_u^{n+1}\| \\
&\lesssim \delta t \|e_H^n\|_{L^4}^2 + \delta t \|e_u^{n+1}\|^2 \\
&\lesssim \delta t (\|e_H^n\|^2 + \|\nabla e_H^n\|^2) + \delta t \|e_u^{n+1}\|^2 \\
&\lesssim \delta t (\|e_\phi^n\|^2 + \|\nabla e_\phi^n\|^2) + \delta t \|e_u^{n+1}\|^2;
\end{aligned} \tag{3.61}
$$

$$
\begin{aligned}
\delta t |(e_H^n U(t_{n+1}) + H^n e_u^{n+1}, e_w^{n+1})| &\leq \delta t (\|e_H^n\| \|U(t_{n+1})\|_{L^\infty} + \|H^n\|_{L^\infty} \|e_u^{n+1}\|) \|e_w^{n+1}\| \\
&\lesssim \delta t (\|e_H^n\| + \|e_u^{n+1}\|) \|e_w^{n+1}\| \\
&\lesssim \frac{1}{6} \delta t \|e_w^{n+1}\|^2 + \delta t \|e_H^n\|^2 + \delta t \|e_u^{n+1}\|^2 \\
&\lesssim \frac{1}{6} \delta t \|e_w^{n+1}\|^2 + \delta t \|e_\phi^n\|^2 + \delta t \|e_u^{n+1}\|^2,
\end{aligned} \tag{3.62}
$$

where, $\|H^n\|_{L^\infty}$ is bounded since $\|\phi^n\|_{L^\infty}$ is bounded, f is continuous, and $F(x) > -A$;

$$
\begin{aligned}
|(R_w^{n+1}, e_\phi^{n+1} - e_\phi^n)| &= \delta t \left| \left(R_w^{n+1}, \frac{e_\phi^{n+1} - e_\phi^n}{\delta t} \right) \right| \\
&= \delta t |(R_w^{n+1}, \Delta e_w^{n+1} + R_\phi^{n+1})| \\
&= \delta t |(\nabla R_w^{n+1}, \nabla e_w^{n+1}) + (R_w^{n+1}, R_\phi^{n+1})|
\end{aligned}
$$

$$
\begin{aligned}
&\le \delta t\|\nabla R_w^{n+1}\|\|\nabla e_w^{n+1}\| + \delta t\|R_w^{n+1}\|\|R_\phi^{n+1}\| \\
&\lesssim \frac{1}{4}\delta t\|\nabla e_w^{n+1}\|^2 + \delta t\|\nabla R_w^{n+1}\|^2 + \delta t\|R_w^{n+1}\|^2 + \delta t\|R_\phi^{n+1}\|^2;
\end{aligned} \tag{3.63}
$$

$$
|\delta t(R_\phi^{n+1}, e_w^{n+1})| \le \delta t\|R_\phi^{n+1}\|\|e_w^{n+1}\| \lesssim \frac{1}{6}\delta t\|e_w^{n+1}\|^2 + \delta t\|R_\phi^{n+1}\|^2; \tag{3.64}
$$

$$
2\delta t|(R_u^{n+1}, e_u^{n+1})| \lesssim \delta t\|R_u^{n+1}\|^2 + \delta t\|e_u^{n+1}\|^2; \tag{3.65}
$$

$$
|\delta t(R_\phi^{n+1}, e_\phi^{n+1})| \lesssim \delta t\|R_\phi^{n+1}\|^2 + \delta t\|e_\phi^{n+1}\|^2; \tag{3.66}
$$

$$
|\delta t(R_w^{n+1}, e_w^{n+1})\| \le \delta t\|R_w^{n+1}\|\|e_w^{n+1}\| \lesssim \frac{1}{6}\delta t\|e_w^{n+1}\|^2 + \delta t\|R_w^{n+1}\|^2. \tag{3.67}
$$

Combining the above estimates with (3.59), we obtain

$$
\begin{aligned}
&\|e_\phi^{n+1}\|^2 + \|\nabla e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2 - \|\nabla e_\phi^n\|^2 + 2(\|e_u^{n+1}\|^2 - \|e_u^n\|^2) \\
&\quad + \delta t(\|e_w^{n+1}\|^2 + \|\nabla e_w^{n+1}\|^2) \\
&\lesssim \delta t(\|e_\phi^n\|^2 + \|\nabla e_\phi^n\|^2 + \|e_u^{n+1}\|^2 + \|e_\phi^{n+1}\|^2) \\
&\quad + \delta t(\|R_w^{n+1}\|^2 + \|\nabla R_w^{n+1}\|^2 + \|R_\phi^{n+1}\|^2 + \|R_u^{n+1}\|^2).
\end{aligned} \tag{3.68}
$$

Summing up the above inequality from $n = 0$ to m ($m \le M$) and using Lemma 3.3, we have

$$
\begin{aligned}
&\|e_\phi^{m+1}\|^2 + \|\nabla e_\phi^{m+1}\|^2 + 2\|e_u^{m+1}\|^2 + \delta t\sum_{n=0}^{m}(\|e_w^{n+1}\|^2 + \|\nabla e_w^{n+1}\|^2) \\
&\lesssim \delta t\sum_{n=0}^{m}(\|e_\phi^n\|^2 + \|\nabla e_\phi^n\|^2 + \|e_u^{n+1}\|^2 + \|e_\phi^{n+1}\|^2) \\
&\quad + \delta t\sum_{n=0}^{m}(\|R_w^{n+1}\|_1^2 + \|R_\phi^{n+1}\|^2 + \|R_u^{n+1}\|^2) \\
&\lesssim \delta t\sum_{n=0}^{m}(\|e_\phi^{n+1}\|^2 + \|\nabla e_\phi^{n+1}\|^2 + \|e_u^{n+1}\|^2) + \delta t^2.
\end{aligned}
$$

Then, by using the Gronwall's inequality, there exist two positive constants s_1, s_2 such that when $\delta t \le s_1$, the following inequality holds for any $m \le M$,

$$
\|e_\phi^{m+1}\|^2 + \|\nabla e_\phi^{m+1}\|^2 + \|e_u^{m+1}\|^2 + \delta t\sum_{n=0}^{m}(\|e_w^{n+1}\|^2 + \|\nabla e_w^{n+1}\|^2) \le s_2\delta t^2. \tag{3.69}
$$

(ii) By using the H^2 regularity of elliptic problem of (3.8), and (3.69), there exists a positive constant s_3 such that we have

$$
\begin{aligned}
\|\phi^{M+1}\|_2 &\lesssim \|w^{M+1}\| + \|H^M U^{M+1}\| \\
&\lesssim \|e_w^{M+1}\| + \|w(t_{M+1})\| + \|H^M\|_{L^\infty}(\|U(t_{M+1})\| + \|e_u^{M+1}\|) \\
&\le s_3.
\end{aligned} \tag{3.70}
$$

Thus, from (3.70) and (3.46), we can find a positive constant s_4 to get

$$
\|e_\phi^{M+1}\|_2 \le \|\phi^{M+1}\|_2 + \|\phi(t_{M+1})\|_2 \le s_4. \tag{3.71}
$$

Furthermore, from (3.69) and (3.71), we derive

$$\begin{aligned}\|\phi^{M+1}\|_{L^\infty} &= \|e_\phi^{M+1}\|_{L^\infty} + \|\phi(t_{M+1})\|_{L^\infty} \\ &\le C_\Omega \|e_\phi^{M+1}\|_1^{\frac{1}{2}} \|e_\phi^{M+1}\|_2^{\frac{1}{2}} + \|\phi(t_{M+1})\|_{L^\infty} \\ &\le C_\Omega \sqrt[4]{s_2}\sqrt{\delta t}\sqrt{s_4} + \|\phi(t_{M+1})\|_{L^\infty}. \end{aligned} \tag{3.72}$$

where we have used the Sobolev inequality $\|\phi\|_{L^\infty} \le C_\Omega \|\phi\|_1^{\frac{1}{2}} \|\phi\|_2^{\frac{1}{2}}$ where C_Ω is a constant that only depends on Ω.

Thus, if $C_\Omega \sqrt[4]{s_2}\sqrt{\delta t}\sqrt{s_4} \le 1$, i.e., $\delta t \le \frac{1}{C_\Omega^2 \sqrt{s_2} s_4}$, we have

$$\|\phi^{M+1}\|_{L^\infty} \le 1 + \|\phi(t_{M+1})\|_{L^\infty} = \kappa. \tag{3.73}$$

Then we obtain the conclusion (3.53) by induction provided that $\delta t \le s_0 = min(s_1, \frac{1}{C_\Omega^2 \sqrt{s_2} s_4})$. □

Theorem 3.3 *Suppose the conditions of* Lemma 3.4 *hold, then for* $0 \le m \le \frac{T}{\delta t} - 1$, *there holds*

$$\|e_\phi^{m+1}\|^2 + \|\nabla e_\phi^{m+1}\|^2 + \|e_u^{m+1}\|^2 + \delta t \sum_{n=0}^{m} (\|e_w^{n+1}\|^2 + \|\nabla e_w^{n+1}\|^2) \lesssim \delta t^2. \tag{3.74}$$

Proof Since $\|\phi^n\|_{L^\infty} \le \kappa$ for any $0 \le n \le \frac{T}{\delta t}$ when $\delta t \le s_0$, by following the first step in the proof of Lemma 3.4, we obtain the conclusion (3.74). □

Corollary 3.1 *Suppose the conditions of* Lemma 3.4 *hold, then for* $0 \le m \le \frac{T}{\delta t} - 1$, *there holds*

$$\Big| \|\nabla\phi^{m+1}\| - \|\nabla\phi(t_{m+1})\| \Big| \lesssim \delta t, \quad \left| \|U^{m+1}\| - \sqrt{\int_\Omega (F(\phi(t_{m+1})) + B) d\boldsymbol{x}} \ \right| \lesssim \delta t. \tag{3.75}$$

Proof The conclusion is easily obtained from Theorem 3.3, the triangle inequality, and note $U(t) = \sqrt{F(\phi(t)) + B}$ by integrating (3.4). □

Remark 3.4 From Corollary 3.1, the discrete energy (3.12) is actually the first-order approximation to the original energy (2.1) at $t = t_{m+1}$, which will be verified by Table 1 in the Sect. 5.3.

4 Allen–Cahn Equation

4.1 Unconditional Energy Stable Linear Scheme Using the IEQ Approach

For the Allen–Cahn equation, by using the same quadratization formula, we obtain a transformed PDE system as:

$$\phi_t + M(-\epsilon^2 \Delta\phi + H(\phi)U) = 0, \tag{4.1}$$

$$U_t = \frac{1}{2} H(\phi)\phi_t, \tag{4.2}$$

where the new variable U is defined as (3.1). The initial conditions $\phi|_{t=0} = \phi_0,\ U|_{t=0} = \sqrt{F(\phi_0) + B}$ and boundary conditions are (2.9). By taking the L^2 inner product of (4.1) with ϕ_t, and of (4.2) with $-2U$, performing integration by parts, and summing up two equalities, we can obtain the energy dissipation law of the new system (4.1)–(4.2), that reads as

$$\frac{d}{dt}E(\phi, U) = -\frac{1}{M}\|\phi_t\|^2. \tag{4.3}$$

The first-order, semi-discrete in time, IEQ scheme for solving the Allen–Cahn system (4.1)–(4.2) reads as follows,

$$\frac{\phi^{n+1} - \phi^n}{\delta t} + M(-\epsilon^2 \Delta\phi^{n+1} + H^n U^{n+1}) = 0, \tag{4.4}$$

$$U^{n+1} - U^n = \frac{1}{2}H^n(\phi^{n+1} - \phi^n), \tag{4.5}$$

where $H^n = H(\phi^n)$. The boundary conditions are:

$$(i)\ \phi^{n+1} \textit{ is periodic}; \text{ or } (ii)\ \partial_{\boldsymbol{n}}\phi^{n+1}|_{\partial\Omega} = 0. \tag{4.6}$$

The unconditional energy stability of the scheme (4.4)–(4.5) is shown as follows.

Theorem 4.1 *The scheme* (4.4)–(4.5) *is unconditionally energy stable in the sense that*

$$E(\phi^{n+1}, U^{n+1}) \le E(\phi^n, U^n) - \frac{1}{M\delta t}\|\phi^{n+1} - \phi^n\|^2. \tag{4.7}$$

Proof By taking the L^2 inner product of (4.4) with $\frac{1}{M}(\phi^{n+1} - \phi^n)$ and using (3.14), we get

$$\begin{aligned}&\frac{1}{M\delta t}\|\phi^{n+1} - \phi^n\|^2 + \frac{\epsilon^2}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2)\\ &\quad + (H^n U^{n+1}, \phi^{n+1} - \phi^n) = 0.\end{aligned} \tag{4.8}$$

By taking the L^2 inner product of (4.5) with $2U^{n+1}$ and using (3.14), we get

$$\|U^{n+1}\|^2 - \|U^n\|^2 + \|U^{n+1} - U^n\|^2 = (H^n(\phi^{n+1} - \phi^n), U^{n+1}).$$

By combining the above equations together, we have

$$\begin{aligned}&\frac{\epsilon^2}{2}(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2)\\ &\quad + \|U^{n+1}\|^2 - \|U^n\|^2 + \|U^{n+1} - U^n\|^2 = -\frac{1}{M\delta t}\|\phi^{n+1} - \phi^n\|^2,\end{aligned} \tag{4.9}$$

which concludes the energy stability (4.7) by dropping some unnecessary positive terms. □

4.2 Implementations and Well-Posedness

Similar to the Cahn–Hilliard equation, we can rewrite (4.5) as follows,

$$U^{n+1} = \frac{1}{2}H^n\phi^{n+1} + U^n - \frac{1}{2}H^n\phi^n, \tag{4.10}$$

then (4.4) can be rewritten as

$$\frac{1}{M\delta t}\phi^{n+1} - \epsilon^2\Delta\phi^{n+1} + \frac{1}{2}H^n H^n\phi^{n+1} = \frac{1}{M\delta t}\phi^n - H^n U^n + \frac{1}{2}H^n H^n\phi^n. \tag{4.11}$$

Therefore, in practice one can solve ϕ^{n+1} directly from (4.11) and then update U^{n+1} by (4.10).

The weak form for (4.11) can be written as the following system with unknowns $\phi \in H_{per}(\Omega)$,

$$\frac{1}{M\delta t}(\phi,\psi)+\epsilon^2(\nabla\phi,\nabla\psi)+\frac{1}{2}(H^n\phi,H^n\psi)=(b,\psi),\quad \psi\in H_{per}(\Omega). \tag{4.12}$$

where $b=\frac{1}{M\delta t}\phi^n-H^nU^n+\frac{1}{2}H^nH^n\phi^n$. We denote the above linear system as

$$(L(\phi),\psi)=(b,\psi),\quad \phi,\psi\in H_{per}(\Omega). \tag{4.13}$$

The well-posedness of the linear system (4.13) is shown as follows.

Theorem 4.2 *The linear system (4.13) admits a unique solution $\phi \in H_{per}(\Omega)$. Furthermore, the bilinear form $(L(\phi),\psi)$ is symmetric positive definite.*

Proof (i) For any $\phi,\psi\in H_{per}(\Omega)$, we have

$$(L(\phi),\psi)\le\widehat{c}_1\|\phi\|_1\|\psi\|_1, \tag{4.14}$$

where $\widehat{c}_1$ is a positive constant dependent on $\delta t, M, \epsilon$ and $\|H^n\|_{L^\infty}$. Therefore, the bilinear form $(L(\phi),\psi)$ is bounded.

(ii) For any $\phi\in H_{per}(\Omega)$, we derive

$$(L(\phi),\phi)=\frac{1}{\delta t M}\|\phi\|^2+\epsilon^2\|\nabla\phi\|^2+\frac{1}{2}\|H^n\phi\|^2\ge\widehat{c}_2\|\phi\|_1^2, \tag{4.15}$$

where $\widehat{c}_2$ is a constant dependent on $\delta t, M, \epsilon$. Thus the bilinear form $(L(\phi),\psi)$ is coercive. Then from the Lax–Milgram theorem, we conclude that the linear system (4.13) admits a unique solution $\phi\in H_{per}(\Omega)$.

Furthermore, for any $\phi,\psi\in H_{per}(\Omega)$ we have $(L(\phi),\psi)=(\phi,L\psi)$ that means the bilinear form is symmetric. Meanwhile, for $\phi\in H_{per}(\Omega)$, we have $(L(\phi),\phi)\ge 0$ and the “ $=''$ is valid if and only if $\phi\equiv 0$, that means the bilinear form is positive definite. □

4.3 Error Estimates

For simplicity, we still assume $\epsilon = M = 1$, and then formulate the Allen–Cahn system (4.1)–(4.2) as a truncation form:

$$\frac{\phi(t_{n+1})-\phi(t_n)}{\delta t}-\Delta\phi(t_{n+1})+H(\phi(t_n))U(t_{n+1})=R_\phi^{n+1}, \tag{4.16}$$

$$U(t_{n+1})-U(t_n)=\frac{1}{2}H(\phi(t_n))(\phi(t_{n+1})-\phi(t_n))+\delta t R_u^{n+1}, \tag{4.17}$$

where

$$\begin{cases} R_\phi^{n+1}=\dfrac{\phi(t_{n+1})-\phi(t_n)}{\delta t}-\phi_t(t_{n+1})-H(\phi(t_{n+1}))U(t_{n+1})+H(\phi(t_n))U(t_{n+1}),\\ R_u^{n+1}=\dfrac{U(t_{n+1})-U(t_n)}{\delta t}-U_t(t_{n+1})+\dfrac{1}{2}H(\phi(t_{n+1}))\phi_t(t_{n+1})-\dfrac{1}{2}H(\phi(t_n))\dfrac{\phi(t_{n+1})-\phi(t_n)}{\delta t}. \end{cases} \tag{4.18}$$

We assume the exact solution ϕ, U of the system (4.1)–(4.2) possesses the following regularity conditions,

$$\begin{cases} \phi \in L^\infty(0,T;H^2(\Omega)), \quad U \in L^\infty(0,T;L^\infty(\Omega)), \\ \phi_t \in L^\infty(0,T;L^\infty(\Omega)), \quad U_{tt}, \phi_{tt} \in L^2(0,T;L^2(\Omega)). \end{cases} \tag{4.19}$$

One can easily establish the following estimates for the truncation errors, provided that the exact solutions of (4.1)–(4.2) satisfy the regularity conditions (4.19).

Lemma 4.1 *If the exact solutions of* (4.1)–(4.2) *satisfy the regularity conditions* (4.19)*, then the truncation errors satisfy*

$$\delta t \sum_{n=0}^{[\frac{T}{\delta t}]} (\|R_\phi^{n+1}\|^2 + \|R_u^{n+1}\|^2) \lesssim \delta t^2. \tag{4.20}$$

Proof Since the proof is rather standard, due to the page limit, we leave it to the interested readers. □

To derive the error estimates, we denote the error functions as

$$e_\phi^n = \phi(t_n) - \phi^n, \quad e_H^n = H(\phi(t_n)) - H(\phi^n), \quad e_u^n = U(t_n) - U^n. \tag{4.21}$$

By subtracting (4.4)–(4.5) from (4.16)–(4.17), we derive the error equations:

$$\frac{e_\phi^{n+1} - e_\phi^n}{\delta t} - \Delta e_\phi^{n+1} + e_H^n U(t_{n+1}) + H^n e_u^{n+1} = R_\phi^{n+1}, \tag{4.22}$$

$$e_u^{n+1} - e_u^n = \frac{1}{2}(e_H^n(\phi(t_{n+1}) - \phi(t_n)) + H^n(e_\phi^{n+1} - e_\phi^n)) + \delta t R_u^{n+1}. \tag{4.23}$$

Let $\kappa = \max_{0 \le t \le T} \|\phi(t)\|_{L^\infty} + 1$, we first prove the L^∞ stability of solution ϕ^n.

Lemma 4.2 *Suppose* (i) *$F(x)$ is uniformly bounded from below: $F(x) > -A$ for any $x \in (-\infty, \infty)$;* (ii) *$F(x) \in C^3(-\infty, \infty)$; and* (iii) *the exact solutions of* (4.1)–(4.2) *satisfy the regularity conditions* (4.19)*, then there exists a positive constant $\widehat{s_0}$ that is given in the proof, such that when $\delta t \le \widehat{s_0}$, the solution ϕ^n of* (4.4)–(4.5) *is uniformly bounded as*

$$\|\phi^n\|_{L^\infty} \le \kappa, n = 0, 1, \ldots, N = \frac{T}{\delta t}. \tag{4.24}$$

Proof For $n = 0$, $\|\phi^0\|_{L^\infty} \le \kappa$ is true naturally. Assuming that $\|\phi^n\|_{L^\infty} \le \kappa$ is valid for all $n \le M$, we show $\|\phi^{M+1}\|_{L^\infty} \le \kappa$ is also valid through the following two steps.

(i) By taking the L^2 inner product of (4.22) with $e_\phi^{n+1} - e_\phi^n$, we get

$$\begin{aligned} &\frac{1}{\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \frac{1}{2}(\|\nabla e_\phi^{n+1}\|^2 - \|\nabla e_\phi^n\|^2 + \|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|^2) \\ &+ (e_H^n U(t_{n+1}), e_\phi^{n+1} - e_\phi^n) + (H^n e_u^{n+1}, e_\phi^{n+1} - e_\phi^n) = (R_\phi^{n+1}, e_\phi^{n+1} - e_\phi^n). \end{aligned} \tag{4.25}$$

By taking the L^2 inner product of (4.23) with $2e_u^{n+1}$, we get

$$\begin{aligned} &\|e_u^{n+1}\|^2 - \|e_u^n\|^2 + \|e_u^{n+1} - e_u^n\|^2 - (e_H^n(\phi(t_{n+1}) \\ &-\phi(t_n)), e_u^{n+1}) - (H^n(e_\phi^{n+1} - e_\phi^n), e_u^{n+1}) = 2\delta t(R_u^{n+1}, e_u^{n+1}). \end{aligned} \tag{4.26}$$

By taking the L^2 inner product of (4.22) with $2\delta t e_\phi^{n+1}$, we get

$$\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2 + \|e_\phi^{n+1} - e_\phi^n\|^2 + 2\delta t\|\nabla e_\phi^{n+1}\|^2 \\ +2\delta t(e_H^n U(t_{n+1}), e_\phi^{n+1}) + 2\delta t(H^n e_u^{n+1}, e_\phi^{n+1}) = 2\delta t(R_\phi^{n+1}, e_\phi^{n+1}). \tag{4.27}$$

By combining the above three equalities, we derive

$$\begin{aligned}
&\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2 + \frac{1}{2}(\|\nabla e_\phi^{n+1}\|^2 - \|\nabla e_\phi^n\|^2) + \|e_u^{n+1}\|^2 - \|e_u^n\|^2 + 2\delta t\|\nabla e_\phi^{n+1}\|^2 \\
&\quad + \frac{1}{\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \|e_\phi^{n+1} - e_\phi^n\|^2 + \|e_u^{n+1} - e_u^n\|^2 + \frac{1}{2}\|\nabla e_\phi^{n+1} - \nabla e_\phi^n\|^2 \\
&= -(e_H^n U(t_{n+1}), e_\phi^{n+1} - e_\phi^n) + (e_H^n(\phi(t_{n+1}) - \phi(t_n)), e_u^{n+1}) \\
&\quad - 2\delta t(e_H^n U(t_{n+1}), e_\phi^{n+1}) - 2\delta t(H^n e_u^{n+1}, e_\phi^{n+1}) \\
&\quad + 2\delta t(R_\phi^{n+1}, e_\phi^{n+1}) + 2\delta t(R_u^{n+1}, e_u^{n+1}) + (R_\phi^{n+1}, e_\phi^{n+1} - e_\phi^n).
\end{aligned} \tag{4.28}$$

By applying Lemmas 3.1, 3.2, and regularity conditions (4.19), for $n \le M$, we estimate terms on the right hand side:

$$\begin{aligned}
|(e_H^n U(t_{n+1}), e_\phi^{n+1} - e_\phi^n)| &\le \|e_H^n\|\|U(t_{n+1})\|_{L^\infty}\|e_\phi^{n+1} - e_\phi^n\| \\
&\lesssim \|e_H^n\|\|e_\phi^{n+1} - e_\phi^n\| \\
&\lesssim \frac{1}{2\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \delta t\|e_H^n\|^2 \\
&\lesssim \frac{1}{2\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \delta t\|e_\phi^n\|^2;
\end{aligned} \tag{4.29}$$

$$\begin{aligned}
\left|\left(e_H^n(\phi(t_{n+1}) - \phi(t_n)), e_u^{n+1}\right)\right| &\le \|e_H^n\|_{L^4}\|\phi(t_{n+1}) - \phi(t_n)\|_{L^4}\|e_u^{n+1}\| \\
&\lesssim \delta t\|e_H^n\|_{L^4}\|e_u^{n+1}\| \\
&\lesssim \delta t\|e_H^n\|_{L^4}^2 + \delta t\|e_u^{n+1}\|^2 \\
&\lesssim \delta t(\|e_H^n\|^2 + \|\nabla e_H^n\|^2) + \delta t\|e_u^{n+1}\|^2 \\
&\lesssim \delta t(\|e_\phi^n\|^2 + \|\nabla e_\phi^n\|^2) + \delta t\|e_u^{n+1}\|^2;
\end{aligned} \tag{4.30}$$

$$\begin{aligned}
2\delta t|(e_H^n U(t_{n+1}), e_\phi^{n+1})| &\le 2\delta t\|e_H^n\|\|U(t_{n+1})\|_{L^\infty}\|e_\phi^{n+1}\| \\
&\lesssim \delta t\|e_H^n\|\|e_\phi^{n+1}\| \\
&\lesssim \delta t\|e_H^n\|^2 + \delta t\|e_\phi^{n+1}\|^2 \\
&\lesssim \delta t\|e_\phi^n\|^2 + \delta t\|e_\phi^{n+1}\|^2;
\end{aligned} \tag{4.31}$$

$$\begin{aligned}
2\delta t|(H^n e_u^{n+1}, e_\phi^{n+1})| &\le 2\delta t\|H^n\|_{L^\infty}\|e_u^{n+1}\|\|e_\phi^{n+1}\| \\
&\lesssim \delta t\|e_u^{n+1}\|\|e_\phi^{n+1}\| \\
&\lesssim \delta t\|e_u^{n+1}\|^2 + \delta t\|e_\phi^{n+1}\|^2;
\end{aligned} \tag{4.32}$$

$$\begin{aligned}
2\delta t|(R_\phi^{n+1}, e_\phi^{n+1}) + (R_u^{n+1}, e_u^{n+1})| &\le 2\delta t(\|R_\phi^{n+1}\|\|e_\phi^{n+1}\| + \|R_u^{n+1}\|\|e_u^{n+1}\|) \\
&\le \delta t(\|R_\phi^{n+1}\|^2 + \|R_u^{n+1}\|^2) + \delta t\|e_\phi^{n+1}\|^2 + \delta t\|e_u^{n+1}\|^2;
\end{aligned} \tag{4.33}$$

and

$$|(R_\phi^{n+1}, e_\phi^{n+1} - e_\phi^n)| \le \|R_\phi^{n+1}\| \|e_\phi^{n+1} - e_\phi^n\| \lesssim \frac{1}{2\delta t}\|e_\phi^{n+1} - e_\phi^n\|^2 + \delta t \|R_\phi^{n+1}\|^2. \quad (4.34)$$

By combining the above estimates with (4.28), we derive

$$\begin{aligned}&\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2 + \frac{1}{2}(\|\nabla e_\phi^{n+1}\|^2 - \|\nabla e_\phi^n\|^2) + \|e_u^{n+1}\|^2 - \|e_u^n\|^2 + 2\delta t \|\nabla e_\phi^{n+1}\|^2 \\ &\lesssim \delta t(\|e_\phi^n\|^2 + \|\nabla e_\phi^n\|^2 + \|e_\phi^{n+1}\|^2 + \|e_u^{n+1}\|^2) + \delta t(\|R_\phi^{n+1}\|^2 + \|R_u^{n+1}\|^2).\end{aligned}$$

Summing up the above inequality from $n = 0$ to m ($m \le M$) and dropping some unnecessary positive terms, we get

$$\|e_\phi^{m+1}\|^2 + \frac{1}{2}\|\nabla e_\phi^{m+1}\|^2 + \|e_u^{m+1}\|^2 \lesssim \delta t \sum_{n=0}^{m}(\|e_\phi^{n+1}\|^2 + \|\nabla e_\phi^{n+1}\|^2 + \|e_u^{n+1}\|^2) + \delta t^2.$$

By Gronwall's inequality, there exist two positive constants $\widehat{s}_1, \widehat{s}_2$ such that when $\delta t \le \widehat{s}_1$,

$$\|e_\phi^{m+1}\|^2 + \|\nabla e_\phi^{m+1}\|^2 + \|e_u^{m+1}\|^2 \le \widehat{s}_2 \delta t^2. \quad (4.35)$$

(ii) By using the H^2 regularity of elliptic problem (4.4) and the estimate (4.35), there exists a positive constant $\widehat{s}_3$, such that the following inequality holds,

$$\begin{aligned}\|\phi^{M+1}\|_2 &\lesssim \left\|\frac{\phi^{M+1} - \phi^M}{\delta t}\right\| + \|H(\phi^M)U^{M+1}\| \\ &\lesssim \left\|\frac{e_\phi^{M+1} - e_\phi^M}{\delta t}\right\| + \left\|\frac{\phi(t_{M+1}) - \phi(t_M)}{\delta t}\right\| + \|H(\phi^M)\|_{L^\infty}\|\|U^{M+1}\| \le \widehat{s}_3,\end{aligned} \quad (4.36)$$

that implies, there exists a constant $\widehat{s}_4$ such that,

$$\|e_\phi^{M+1}\|_2 \le \|\phi(t_{M+1})\|_2 + \|\phi^{M+1}\|_2 \le \widehat{s}_4. \quad (4.37)$$

Therefore, by (4.37) and (4.35), we obtain

$$\begin{aligned}\|\phi^{M+1}\|_{L^\infty} &\le \|e_\phi^{M+1}\|_{L^\infty} + \|\phi(t_{M+1})\|_{L^\infty} \\ &\le C_\Omega \|e_\phi^{M+1}\|_1^{\frac{1}{2}} \|e_\phi^{M+1}\|_2^{\frac{1}{2}} + \|\phi(t_{M+1})\|_{L^\infty} \\ &\le C_\Omega \sqrt[4]{\widehat{s}_2}\sqrt{\delta t}\sqrt{\widehat{s}_4} + \|\phi(t_{M+1})\|_{L^\infty} \le \kappa,\end{aligned} \quad (4.38)$$

as long as $\delta t \le \frac{1}{C_\Omega^2 \sqrt{\widehat{s}_2 \widehat{s}_4}}$. Thus the proof is finished by setting $\widehat{s}_0 = min(\widehat{s}_1, \frac{1}{C_\Omega^2 \sqrt{\widehat{s}_2 \widehat{s}_4}})$. □

Theorem 4.3 *Suppose the conditions of* Lemma 4.2 *hold, then for* $0 \le m \le \frac{T}{\delta t} - 1$, *there holds*

$$\|e_\phi^{m+1}\|^2 + \|\nabla e_\phi^{m+1}\|^2 + \|e_u^{m+1}\|^2 \lesssim \delta t^2. \quad (4.39)$$

Proof When $\delta t \le \widehat{s}_0$, we have $\|\phi^n\|_{L^\infty} \le \kappa$ for any $0 \le n \le \frac{T}{\delta t}$. Thus, by following the first step in the proof of Lemma 4.2, we obtain the conclusion (4.39). □

Remark 4.1 For the Allen–Cahn equation, although we consider only time discrete schemes in this study, the error analyses can be carried over to any consistent finite-dimensional Galerkin approximations since the proofs are all based on a variational formulation with all test functions in the same space as the space of the trial functions. However, for the fully

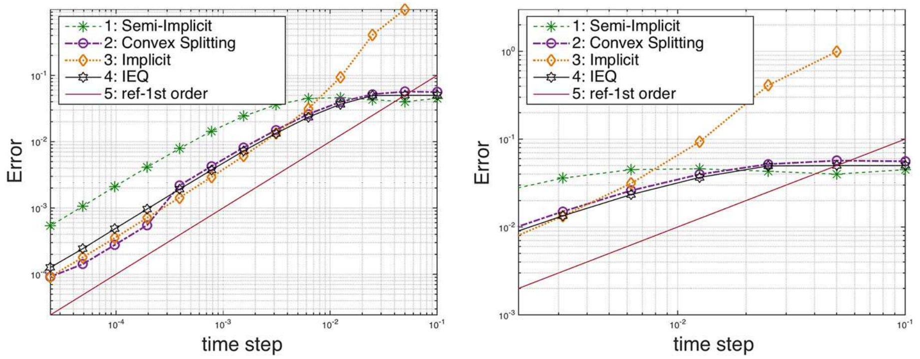


Fig. 1 The L^2 numerical errors at $t = 0.1$ for the approximate phase variable ϕ of the presumed exact solution (5.2), that are computed using four different first-order schemes: stabilized-semi-implicit, convex-splitting, fully-implicit, and IEQ schemes. The left subfigure is the accuracy curve for $\delta t \in [1e-6, 1e-1]$), and the right subfigure is a close-up view for larger time steps, i.e., $\delta t \in [1e-3, 1e-1]$)

discrete IEQ scheme of the Cahn–Hilliard equations, we are not clear on how to derive the corresponding error analysis using the Galerkin type approximations, where the challenge is to estimate (3.60) since it is not easy to find a proper discrete space for $e_H^n U(t_{n+1})$.

5 Numerical Tests

We now present several two dimensional numerical examples to validate the proposed schemes and demonstrate their accuracy, energy stability and efficiency. Here, we choose the periodic boundary conditions and set the computational domain as $\Omega = [0, 2\pi]^2$. We use the Fourier-spectral method to discretize the space, where 129×129 Fourier modes are used for 2D simulations.

If not explicitly specified, the default values of order parameters are set as follows,

$$M = \epsilon = 6e - 2. \tag{5.1}$$

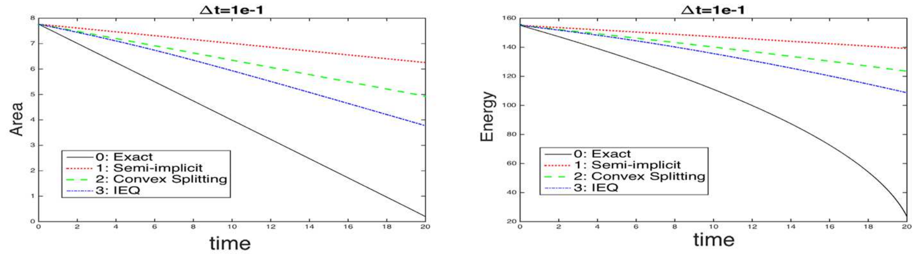
5.1 Accuracy Test

We first perform numerical simulations to test the convergence rates of the IEQ scheme for solving the Allen–Cahn equation (2.8) with the double well potential. We assume the following function

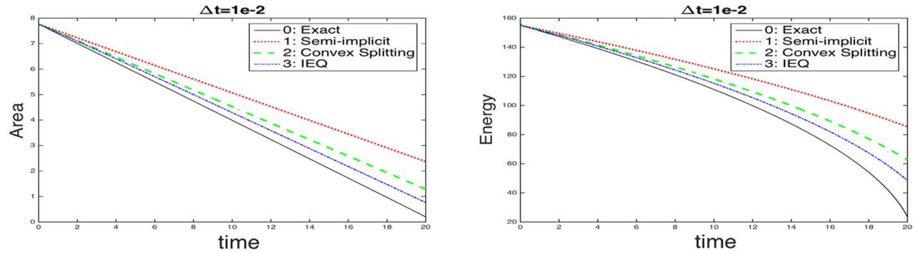
$$\phi(x, y, t) = \sin(x)\cos(y)\cos(t) \tag{5.2}$$

to be the exact solution, and impose some suitable force fields such that the given solution can satisfy the system (2.8). We compare four schemes here, including three unconditionally energy stable schemes: the IEQ scheme (4.4)–(4.5), the convex splitting scheme (see Eqn. (7) in [16]), and the stabilized-semi-implicit scheme (see Eqn. (2.6) with stabilizer $S = 2$ in [34]), and one conditionally energy stable fully-implicit scheme (see Eqn. (7) in [17]).

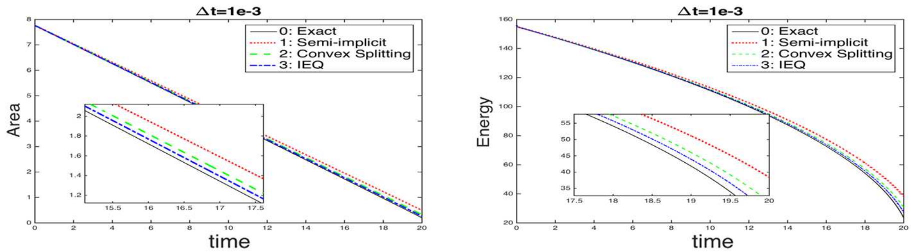
In Fig. 1, we plot the L^2 errors of the phase variable ϕ between the numerically simulated solution and the exact solution at $t = 0.1$ with different time step sizes. Some remarkable features are listed as follows.



(a) $\delta t = 1\text{e}{-}1$.



(b) $\delta t = 1\text{e}{-}2$.



(c) $\delta t = 1\text{e}{-}3$.

Fig. 2 Time evolution of the area and total free energy functional using the three schemes: stabilized semi-implicit, convex-splitting, and IEQ, for three different time steps **a** $\delta t = 1\text{e} - 1$, **b** $\delta t = 1\text{e} - 2$, and **c** $\delta t = 1\text{e} - 3$. For each subfigure, the left one is the area, and the right one is the total free energy. The small inset figure is a close-up view for corresponding time intervals

- When $\delta t \leq 1\text{e} - 2$, all four schemes achieve almost perfect first-order accuracy in time. But obviously, the magnitude of errors computed by the stabilized-semi-implicit scheme is much bigger than that of the other three schemes.
- When $\delta t > 1\text{e} - 2$, the IEQ, convex-splitting, and stabilized-semi-implicit schemes only present 0th order of accuracy.
- For the fully-implicit scheme, although apparently it always keeps the first-order accuracy for all time steps, its performance is actually worse than others since, (i) when $\delta t = 0.1$, it blows up quickly thus the point of $\delta t = 0.1$ does not show up in Fig. 1; and (ii) when $\delta t \geq 0.01$, the magnitude of errors computed by it is much bigger than that of the other three schemes.
- For the stabilized-semi-implicit scheme, since the stabilizing term $\frac{S}{\epsilon^2}(\phi^{n+1} - \phi^n)$ introduces an extra consistency error of $\frac{S\delta t}{\epsilon^2}\phi_t(\xi_n)$, this scheme does not enter the convergence zone for relative big time step size.

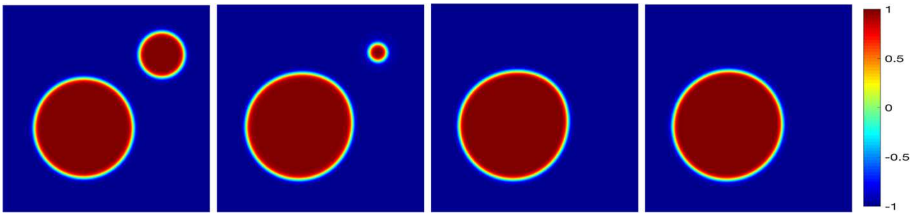


Fig. 3 Snapshots of the phase field variable ϕ are taken at $t = 0.2$, 1.02, 1.14, and 2, by using the initial condition (5.3) and the time step $\delta t = 1\mathrm{e}-3$

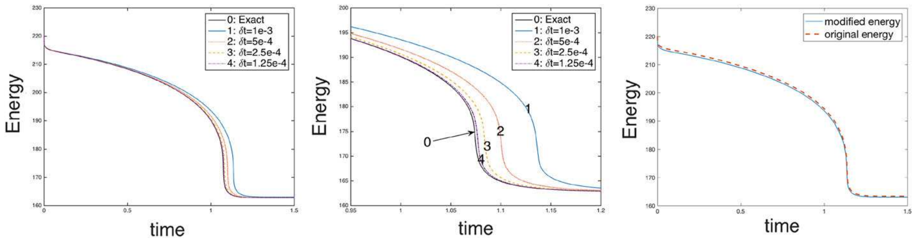


Fig. 4 Time evolution of the total free energy functional using four time steps, $\delta t = 1\mathrm{e}-3$, $5\mathrm{e}-4$, $2.5\mathrm{e}-4$ and $1.25\mathrm{e}-4$. The left subfigure is the energy profile for $t \in [0, 1.5]$, the middle subfigure is a close-up view for $t \in [0.95, 1.2]$, and the right subfigure is the comparison of the modified energy and the original energy with the time step $\delta t = 1\mathrm{e}-3$

Therefore, in this example, when concerning the stability or accuracy, the three unconditionally energy stable schemes (IEQ, convex-splitting, and stabilized-semi-implicit) perform better than the fully-implicit scheme. Furthermore, the performance of the stabilized-semi-implicit scheme is slightly worse than that of the IEQ and convex-splitting schemes.

5.2 Coarsening Effects for the Allen–Cahn Equation

In this example, we compare the accuracy of three unconditionally energy stable schemes, the IEQ, convex-splitting, and stabilized-semi-implicit schemes, for a benchmark problem of coarsening effects for the Allen–Cahn equation. We set the initial condition as

$$\phi(x, y, t = 0) = -\tanh\Big(\frac{(x-\pi)^2 + (y-\pi)^2 - \frac{\pi}{2}^2}{4\epsilon}\Big). \tag{5.3}$$

The initial profile of ϕ is a circular interface which is unstable, it will shrink and eventually disappear. Since the exact solutions are not known, we choose the solution computed by the fully-implicit scheme with a very tiny time step size $\delta t = 1\mathrm{e}-5$ as the benchmark solution.

In Fig. 2, we plot the time evolution curves of the area and the total free energy obtained by the IEQ, stabilized-semi-implicit, and convex-splitting schemes, with three time step sizes $\delta t = 1\mathrm{e}-1$, $1\mathrm{e}-2$, and $1\mathrm{e}-3$. For each time step, we can observe that the magnitude of errors is: IEQ scheme $<$ convex-splitting scheme $<$ stabilized-semi-implicit scheme.

Table 1 The relative errors $e_{|E}(t^n)$ between the discrete energy $E(\phi^n, U^n)$ and the free energy of the exact solution $E(\phi(t^n))$ at $t^n = 0.8, 1, 1.2$, in which, the discrete free energy $E(\phi^n, U^n)$ is computed using five different time steps $\delta t = 1e-3, 5e-4, 2.5e-4, 1.25e-4$ and $6.25e-5$

δt	$e_{\|E}(t=0.8)$	Order	$e_{\|E}(t=1)$	Order	$e_{\|E}(t=1.2)$	Order
$1e-3$	$9.20e-3$		$2.20e-2$		$6.50e-3$	
$5e-4$	$4.50e-3$	1.03	$1.07e-2$	1.04	$3.10e-3$	1.07
$2.5e-4$	$2.10e-3$	1.09	$4.40e-3$	1.23	$1.50e-3$	1.04
$1.25e-4$	$9.36e-4$	1.17	$1.50e-3$	1.55	$6.34e-4$	1.24
$6.25e-5$	$3.19e-4$	1.55	$6.38e-4$	1.23	$2.59e-4$	1.29

5.3 Coarsening Effects for the Cahn–Hilliard Equation

In this example, we perform the numerical simulation using the IEQ scheme (3.7)–(3.9) for a benchmark problem of coarsening effects for the Cahn–Hilliard equation, see [5,6]. We set the initial condition as

$$\phi(x, y, t=0) = \sum_{i=1}^{2} -\tanh\left(\frac{\sqrt{(x-x_i)^2 + (y-y_i)^2 - r_i}}{1.2\epsilon}\right) + 1, \tag{5.4}$$

where $(x_1, y_1, r_1) = (\pi - 0.7, \pi - 0.6, 1.5)$ and $(x_2, y_2, r_2) = (\pi + 1.65, \pi + 1.6, 0.7)$.

In Fig. 3, we show the evolutions of the phase field variable ϕ at various time by using the time step $\delta t = 1e-3$. We observe the coarsening effect that the small circle is absorbed into the big circle, and the total absorption happens at around $t = 1.2$. In Fig. 4, we compare the time evolution of the discrete energy $E(\phi^n, U^n)$ [defined in (3.12)] up to the equilibrium for four different time steps with the exact (benchmark) solution, that is computed by the fully-implicit scheme with a tiny time step size $\delta t = 1e-6$. We observe that all four energy curves show decays monotonically, which numerically confirms that the IEQ algorithm is unconditionally energy stable. When δt gets smaller, the four energy curves present behaviors of asymptotic approximations to that of the exact solution. We also compare the modified energy (3.6) and (2.1) with the time step $\delta t = 1e-3$ and the both energies agree very well. Theoretically, the approximation of $E(\phi^n, U^n) \to E(\phi(t^n))$ is of first-order accuracy from the Corollary 3.1. We verify it by presenting the relative error $e_{|E}(t = t^n)$ that is defined as

$$e_{|E}(t = t^n) := \frac{|E(\phi^n, U^n) - E(\phi(t^n))|}{E(\phi(t^n))}. \tag{5.5}$$

We choose three time points of $t^n = 0.8, 1, 1.2$, and the discrete energy $E(\phi^n, U^n)$ is computed by using five different time steps $\delta t = 1e-3, 5e-4, 2.5e-4, 1.25e-4$ and $6.25e-5$. The computed results are shown in Table 1, where we observe that the order asymptotically match the first-order accuracy in time.

6 Concluding Remarks

We carry out the stability and error analysis of two first-order, semi-discrete time stepping schemes for solving the Cahn–Hilliard and Allen–Cahn equations, respectively. Some general, sufficient conditions about the boundedness/continuity of the nonlinear functional are given in order to obtain the optimal error estimates. These conditions are naturally satisfied by the commonly use polynomial type double well potential. For the logarithmic Flory–Huggins potentials of the regularized version, these conditions are appropriate as well. By utilizing the Lipschitz property of the quadratic formula together with the mathematical inductions, we rigorously derive the optimal error estimates for the first-order IEQ schemes. The analytical approach developed in this paper is general enough and thus it can work as a standard framework to derive error estimates of IEQ type schemes for various gradient flow models with diverse nonlinear potentials. For the fully discrete scheme of the Allen–Cahn equation, the error analyses can be carried over without any further difficulties when using finite-dimensional Galerkin approximations ([1,7,11,19,22,24,28,36,38,45,48]). But for Cahn–Hilliard equation, there maybe exist some substantial challenges to derive the convergence analysis for the fully discrete version with Galerkin approximations, which will be considered in the future work.

References

1. An, N., Huang, C., Yu, X.: Error analysis of direct discontinuous Galerkin method for two-dimensional fractional diffusion-wave equation. Appl. Math. Comput. **349**, 148–157 (2019)
2. Cahn, J.W., Allen, S.M.: A microscopic theory for domain wall motion and its experimental varification in Fe–Al alloy domain growth kinetics. J. Phys. Colloq. **C7**, C7–51 (1977)
3. Cahn, J.W., Hilliard, J.E.: Free energy of a nonuniform system. I. Interfacial free energy. J. Chem. Phys. **28**, 258–267 (1958)
4. Chen, C., Yang, X.: Efficient numerical scheme for a dendritic solidification phase field model with melt convection. J. Comput. Phys. **388**, 41–62 (2019)
5. Chen, C., Yang, X.: Fast, provably unconditionally energy stable, and second-order accurate algorithms for the anisotropic Cahn–Hilliard Model. Comput. Methods Appl. Mech. Eng. **351**, 35–59 (2019)
6. Chen, F., Shen, J.: Efficient energy stable schemes with spectral discretization in space for anisotropic Cahn–Hilliard systems. Commun. Comput. Phys. **05**, 1189–1208 (2013)
7. Chen, H., Zhou, Z., Wang, H.: An optimal-order error estimate for an H^1-Galerkin mixed method for a pressure equation in compressible porous medium flow. Int. J. Numer. Anal. Model. **9**, 132–148 (2012)
8. Chen, L., Zhao, J., Yang, X.: Regularized linear schemes for the molecular beam epitaxy model with slope selection. Appl. Numer. Math. **128**, 139–156 (2018)
9. Chen, R., Yang, X., Zhang, H.: Second order, linear and unconditionally energy stable schemes for a hydrodynamic model of smectic-A liquid crystals. SIAM J. Sci. Comput. **39**, A2808–A2833 (2017)
10. Copetti, M.I.M., Elliott, C.M.: Numerical analysis of the Cahn–Hilliard equation with a logarithmic free energy. Numer. Math. **63**(4), 39–65 (1992)
11. Du, G., Zuo, L.: Local and parallel finite element method for the mixed Navier–Stokes/Darcy model with Beavers–Joseph interface conditions. Acta Math. Sci. **37**, 1331–1347 (2017)
12. Du, Q., Ju, L., Li, X., Qiao, Z.: Stabilized linear semi-implicit schemes for the nonlocal Cahn–Hilliard equation. J. Comput. Phys. **363**, 39–54 (2018)
13. Du, Q., Ju, L., Li, X., Qiao, Z.: Maximum principle preserving exponential time differencing schemes for the nonlocal Allen–Cahn equation. SIAM J. Numer. Anal. **57**(2), 875–898 (2019)
14. Du, Q., Liu, C., Wang, X.: A phase field approach in the numerical study of the elastic bending energy for vesicle membranes. J. Comput. Phys. **198**, 450–468 (2004)
15. Elliott, C.M., Garcke, H.: On the Cahn–Hilliard equation with degenerate mobility. SIAM J. Math. Anal. **27**, 404–423 (1996)
16. Eyre, D.J.: Unconditionally gradient stable time marching the Cahn–Hilliard equation. In: Computational and Mathematical Models of Microstructural Evolution of Materials Research Society Symposium Proceedings, vol. 529 pp. 39–46, San Francisco (1998)
17. Feng, X., Prol, A.: Numerical analysis of the Allen–Cahn equation and approximation for mean curvature flows. Numer. Math. **94**, 33–65 (2003)
18. Gao, Y., He, X., Mei, L., Yang, X.: Decoupled, linear, and energy stable finite element method for Cahn–Hilliard–Navier–Stokes–Darcy phase field model. SIAM J. Sci. Comput. **40**, B110–B137 (2018)
19. Gong, W., Hinze, M., Zhou, Z.: Finite element method and a priori error estimates for Dirichlet boundary control problems governed by parabolic PDEs. J. Sci. Comput. **66**, 941–967 (2016)

20. Guillén-González, F., Tierra, G.: On linear schemes for a Cahn–Hilliard diffuse interface model. J. Comput. Phys. **234**, 140–171 (2013)
21. He, Y., Liu, Y., Tang, T.: On large time-stepping methods for the Cahn–Hilliard equation. J. Appl. Numer. Math. **57**, 616–628 (2007)
22. Huang, C., Martin, S., An, N.: Optimal L^∞ (L^2) error analysis of a direct discontinuous Galerkin method for a time-fractional reaction–diffusion problem. BIT Numer. Math. **58**, 661–690 (2018)
23. Huang, Q., Yang, X., He, X.: Numerical approximations for a smectic-A liquid crystal flow model: first-order, linear, decoupled and energy stable schemes. Discret. Contin. Dyn. Syst. B **23**, 2177–2192 (2018)
24. Jia, L., Chen, H., Wang, H.: Mixed-type Galerkin variational principle and numerical simulation for a generalized nonlocal elastic model. J. Sci. Comput. **71**, 660–681 (2017)
25. Li, D., Qiao, Z.: On second order semi-implicit Fourier spectral methods for 2d Cahn–Hilliard equations. J. Sci. Comput. **70**(1), 301–341 (2017)
26. Li, D., Qiao, Z., Tang, T.: Characterizing the stabilization size for semi-implicit Fourier-spectral method to phase field equations. SIAM J. Numer. Anal. **54**(3), 1653–1681 (2016)
27. Li, H., Ju, L., Zhang, C., Peng, Q.: Unconditionally energy stable linear schemes for the diffuse interface model with Peng–Robinson equation of state. J. Sci. Comput. **75**, 993–1015 (2018)
28. Li, Y., Chen, H., Wang, H.: A mixed-type Galerkin variational formulation and fast algorithms for variable-coefficient fractional diffusion equations. Math. Methods Appl. Sci. **40**, 5018–5034 (2017)
29. Liu, C., Shen, J.: A phase field model for the mixture of two incompressible fluids and its approximation by a Fourier-spectral method. Phys. D **179**(3–4), 211–228 (2003)
30. Liu, Z., Li, X.: Efficient modified techniques of invariant energy quadratization approach for gradient flows. Appl. Math. Lett. **98**, 206–214 (2019)
31. Lowengrub, J.S., Ratz, A., Voigt, A.: Phase field modeling of the dynamics of multicomponent vesicles spinodal decomposition coarsening budding and fission. Phys. Rev. E **79**(3), 031926 (2009)
32. Peng, Q., Li, H., Xu, Z.: Energy stable linear schemes for mass-conserved gradient flows with Peng–Robinson equation of state. East Asian J. Appl. Math. **9**, 212–232 (2019)
33. Shen, J., Wang, C., Wang, S., Wang, X.: Second-order convex splitting schemes for gradient flows with Ehrlich–Schwoebel type energy: application to thin film epitaxy. SIAM J. Numer. Anal **50**, 105–125 (2012)
34. Shen, J., Yang, X.: Numerical approximations of Allen–Cahn and Cahn–Hilliard equations. Discret. Contin. Dyn. Syst. A **28**, 1669–1691 (2010)
35. Wang, C., Wise, S.M.: An energy stable and convergent finite-difference scheme for the modified phase field crystal equation. SIAM J. Numer. Anal. **49**, 945–969 (2011)
36. Wang, F., Chen, H., Wang, H.: Finite element simulation and efficient algorithm for fractional Cahn–Hilliard equation. J. Comput. Appl. Math. **356**, 248–266 (2019)
37. Xu, C., Chen, C., Yang, X., He, X.: Numerical approximations for the hydrodynamics coupled binary surfactant phase field model: second-order, linear, unconditionally energy stable schemes. Commun. Math. Sci. **17**, 835–858 (2019)
38. Yang, Q., Zhang, X.: Discontinuous Galerkin immersed finite element methods for parabolic interface problems. J. Comput. Appl. Math. **299**, 127–139 (2016)
39. Yang, X.: Linear, first and second order and unconditionally energy stable numerical schemes for the phase field model of homopolymer blends. J. Comput. Phys. **327**, 294–316 (2016)
40. Yang, X.: Efficient linear, stabilized, second order time marching schemes for an anisotropic phase field dendritic crystal growth model. Comput. Methods Appl. Mech. Eng. **347**, 316–339 (2019)
41. Yang, X., Ju, L.: Efficient linear schemes with unconditionally energy stability for the phase field elastic bending energy model. Comput. Methods Appl. Mech. Eng. **315**, 691–712 (2017)
42. Yang, X., Yu, H.: Efficient second order unconditionally stable schemes for a phase field moving contact line model using an invariant energy quadratization approach. SIAM J. Sci. Comput. **40**, B889–B914 (2018)
43. Yang, X., Zhao, J., He, X.: Linear, second order and unconditionally energy stable schemes for the viscous Cahn–Hilliard equation with hyperbolic relaxation using the invariant energy quadratization method. J. Comput. Appl. Math. **343**, 80–97 (2018)
44. Yang, X., Zhao, J., Wang, Q., Shen, J.: Numerical approximations for a three components Cahn–Hilliard phase-field model based on the invariant energy quadratization method. Math. Model. Methods Appl. Sci. **27**, 1993–2030 (2017)
45. Yuan, Y., Sun, T., Li, C., Liu, Y., Yang, Q.: Mixed volume element combined with characteristic mixed finite volume element method for oil–water two phase displacement problem. J. Comput. Appl. Math. **340**, 404–419 (2018)

46. Zhang, J., Chen, C., Yang, X.: A novel decoupled and stable scheme for an anisotropic phase-field dendritic crystal growth model. Appl. Math. Lett. **95**, 122–129 (2019)
47. Zhao, J., Wang, Q., Yang, X.: Numerical approximations to a new phase field model for immiscible mixtures of nematic liquid crystals and viscous fluids. Comput. Methods Appl. Mech. Eng. **310**, 77–97 (2016)
48. Zhou, Z., Chen, F., Chen, H.: Local discontinuous Galerkin approximation of non-Fickian diffusion model in viscoelastic polymers. Appl. Anal. **94**, 819–839 (2015)

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