



# Energy-stable predictor–corrector schemes for the Cahn–Hilliard equation

Jun Zhang<sup>a</sup>, Maosheng Jiang<sup>b</sup>, Yuezheng Gong<sup>c</sup>, Jia Zhao<sup>d,\*</sup>

<sup>a</sup> Guizhou Key Laboratory of Big Data Statistics Analysis, Computational mathematics research center, Guizhou University of Finance and Economics, Guiyang, Guizhou 550025, China

<sup>b</sup> Beijing Computational Science Research Center, Beijing, 100193, China

<sup>c</sup> College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China

<sup>d</sup> Department of Mathematics & Statistics, Utah State University, Logan, UT, 84322, USA

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## ABSTRACT

In this paper, we construct a new class of predictor–corrector time-stepping schemes for the Cahn–Hilliard equation, which are linear, second-order accurate in time, unconditionally energy stable, and uniquely solvable. Then, we present the stability and error estimates of the semi-discrete numerical schemes for solving the Cahn–Hilliard equation with general nonlinear bulk potentials. The semi-discrete scheme is further discretized using the compact central finite difference method. Several numerical examples are shown to verify the theoretical results. In particular, the numerical simulations show that the predictor–corrector schemes reach the second-order convergence rate at relatively larger time-step sizes than the classical linear schemes. The numerical strategies and theoretical tools developed in this article could be readily applied to study other phase-field models or models that can be cast as gradient flow problems.

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## 1. Introduction

During the past few decades, phase-field models, especially the Cahn–Hilliard (C.H.) equation, have been widely studied due to their wide application in image analysis, material science, engineering fluid mechanics, and life science [1–5]. Many numerical methods have been developed to investigate the dynamics of the C.H. equation [6–10]. The C.H. equation is derived from an energy variational approach, i.e., a  $H^{-1}$  gradient flow given the explicit expression of the free energy functional, which could be highly nonlinear and depend on high-order spatial derivatives. To solve the C.H. equation more efficiently, we face two major obstacles. First of all, the nonlinear terms shall be discretized properly. If the nonlinear terms are treated directly explicitly, it will lead to stiff time-step constraints. Many works are focusing on eliminating/weakening such restrictions. See [11–17] and the references therein. Secondly, the energy dissipation properties should be conserved in the discrete level, because the intrinsic property of the C.H. equation is its energy dissipation. Numerical methods that preserve such property are known as energy stable schemes.

One widely used method to design energy stable numerical schemes is the so-called convex splitting approach, which was introduced by [18,19] and popularized by [15,20–22]. In the convex splitting method, the nonlinear terms in the free energy are split into a summation of convex and concave parts, while the convex portion is discretized implicitly, and

\* Corresponding author.

E-mail addresses: [zj654440@163.com](mailto:zj654440@163.com) (J. Zhang), [msjiang@csrc.ac.cn](mailto:msjiang@csrc.ac.cn) (M. Jiang), [gongyuezheng@nuaa.edu.cn](mailto:gongyuezheng@nuaa.edu.cn) (Y. Gong), [jia.zhao@usu.edu](mailto:jia.zhao@usu.edu) (J. Zhao).

the concave part is treated explicitly. The schemes derived from the convex splitting approach are unconditional energy stable and uniquely solvable, but one needs to solve a nonlinear system for each time-marching step.

Another popular approach is the linear stabilization method [11,16,23–27]. The main idea is to discretize the nonlinear term explicitly and then add an artificial stabilization term. It results in linear schemes, which could be solved very efficiently by using the Fast Fourier Transformation (FFT), see [28,29]. While for this method, all prior analytical developments are conditional in the sense that either one makes a Lipschitz assumption on the nonlinearity, or one assumes certain a priori  $L^\infty$  bounds on the numerical solution. In [30,31], these technical restrictions have removed, and an unconditional stability theory of large time-stepping semi-implicit numerical schemes has been established for general phase-field models.

Recently, Guillén-González and Tierra [32] introduced a linear scheme by using a Lagrange multiplier idea [33] to approximate the C.H. equation with double-well bulk free energy, where an equation related to the auxiliary variable  $q(x, t)$  needs to be solved together with the mixed formulation of the C.H. equation for updating the unknown function  $\phi$ . A similar approach was proposed in [34] to solve the nonlinear epitaxial growth model without slope selection, where the discrete equations related to the auxiliary variable  $q(x, t)$  are solved only for updating the modified energies. Its advantages include that it is a linear scheme and unconditionally stable. Unfortunately, this method does not work for other free energies. Yang et al. [27,35–37] made the appropriate improvements based on the Lagrange multiplier method and proposed a new approach, which they named Invariant Energy Quadratization (IEQ) method. This method has been successfully applied to solve thermodynamic and hydrodynamic models. Later, inspired by the IEQ method, Shen et al. propose the scalar auxiliary variable (SAV) approach [38,39]. The critical idea of the IEQ method is that an auxiliary variable is introduced to transform the original PDE system into an equivalent PDE system, where the nonlinear free energy functional for the original system is transformed into a quadratic form for the new system. Afterward, by utilizing the semi-implicit strategies, some energy stable numerical schemes can be obtained generally for gradient flow models and hydrodynamic models.

Unfortunately, due to the stiffness of nonlinear terms in the Cahn–Hilliard equation, even though many of these schemes are shown to be unconditionally energy stable, large time marching step will inevitably introduce truncation errors, contaminating the numerical solutions for long time dynamics simulations, i.e., the semi-implicit method, though stable with large time-step sizes, usually requires small time-step for the sake of accuracy. In order to improve the accuracy of the IEQ method even with large time-step sizes, a new predictor–corrector IEQ approach is proposed to solve the C.H. equation. The essence of the predictor–corrector method is to reduce the extrapolation error of the nonlinear potential and improve numerical accuracy. The predictor–corrector schemes are efficient, as only linear systems need to be solved for each time marching step. Rigorous proofs for energy stability, unique solvability, and error estimates are obtained. Some numerical examples are presented to support our theoretical results, showing that this new approach can reach the order of accuracy with large time-marching step sizes.

The rest of the paper is structured in the following way. In Section 2, we introduce the C.H. equation and reformulate it into an equivalent form using the energy quadratization technique. In Section 3, we propose a class of predictor–corrector numerical schemes to solve the C.H. equation, and we will analyze the unconditional energy stability, unique solvability, and convergence of the newly proposed schemes. In Section 4, several numerical experiments are performed to demonstrate the effectiveness of the predictor–corrector methods. The conclusion of this article is given in Section 5.

## 2. The Cahn–Hilliard equation and its equivalent form after energy quadratization

### 2.1. The Cahn–Hilliard equation

In this work, we study the following free energy

$$E(\phi) = \int_{\Omega} \left( \frac{1}{2} |\nabla \phi|^2 + F(\phi) \right) d\mathbf{x}, \quad (1)$$

where  $\mathbf{x} \in \Omega \subseteq \mathbb{R}^d (d = 2, 3)$ ,  $\phi(\mathbf{x}, t)$  is a scalar function,  $F(\phi)$  is the bulk energy functional (which could be nonlinear).

Using energy variational method for the total energy Eq. (1) in  $H^{-1}(\Omega)$  [40], one can get the following widely-braced C.H. equation

$$\begin{cases} \phi_t = \Delta w, \\ w = \delta E / \delta \phi = -\Delta \phi + f(\phi), \end{cases} \quad (2)$$

subject to the initial and boundary conditions

$$\phi|_{t=0} = \phi_0, \quad (3)$$

$$(i) \phi, w \text{ are periodic ; or } (ii) \partial_{\mathbf{n}} \phi|_{\partial\Omega} = \partial_{\mathbf{n}} w|_{\partial\Omega} = 0. \quad (4)$$

Here  $w = \frac{\delta E}{\delta \phi}$  is the chemical potential, and we use the notation  $f(\phi) = F'(\phi)$ . Taking the  $L^2$  inner product of Eq. (2) with  $-w$ , and  $\phi_t$ , we get the energy dissipation law of the C.H. equation as

$$\frac{dE(\phi)}{dt} = - \int_{\Omega} |\nabla w|^2 d\mathbf{x}. \quad (5)$$

Numerical schemes that preserve the energy dissipation law Eq. (5) in the discrete level are called energy-stable. If such energy-dissipation-law preserving property does not depend on time-step, the numerical scheme is named unconditionally energy-stable.

## 2.2. Energy quadratization

Next, we introduce an equivalent reformulation of Eq. (2) using the IEQ method [41]. Denote the auxiliary variable function

$$q(\phi) = \sqrt{F(\phi) - \frac{\gamma}{2}\phi^2 + B}, \quad (6)$$

with  $\gamma > 0$  the regularized (stabilized) parameter [42], and  $B$  a constant such that  $q(\phi)$  is well-defined. Also, we introduce the notation

$$g(\phi) = 2 \frac{\partial}{\partial \phi} q(\phi) = \frac{f(\phi) - \gamma \phi}{\sqrt{F(\phi) - \frac{\gamma}{2}\phi^2 + B}}. \quad (7)$$

Then, we rewrite Eq. (2) as follows

$$\begin{cases} \phi_t = \Delta w, \\ w = -\Delta \phi + \gamma \phi + g(\phi)q(\phi), \\ q_t = \frac{1}{2}g(\phi)\phi_t, \end{cases} \quad (8)$$

subject to the initial and boundary conditions

$$\phi|_{t=0} = \phi_0, \quad q|_{t=0} = \sqrt{F(\phi_0) - \frac{\gamma}{2}\phi_0^2 + B}, \quad (9)$$

$$(i) \phi, w \text{ are periodic ; or } (ii) \partial_n \phi|_{\partial\Omega} = \partial_n w|_{\partial\Omega} = 0. \quad (10)$$

Note that the transformed equations (8)–(10) are equivalent to the C.H. equations (2)–(4). In addition, the transformed equations (8)–(10) still satisfy the same energy dissipation law as Eqs. (2)–(4). In fact, by taking the  $L^2$  inner product of Eq. (8) with  $w$ ,  $\phi_t$ ,  $2q$ , respectively, we find

$$\frac{d}{dt} E(\phi, q) = - \int_{\Omega} |\nabla w|^2 d\mathbf{x}, \quad (11)$$

where

$$E(\phi, q) = \int_{\Omega} \left( \frac{1}{2} |\nabla \phi|^2 + \frac{\gamma}{2} \phi^2 + q^2 - B \right) d\mathbf{x}. \quad (12)$$

The energy (12) is equivalent to the original energy (1) in time continuous case, by noticing (6).

In the next section, we will develop a class of predictor–corrector schemes for the equivalent system (8)–(10), which in turn solves Eqs. (2)–(4). Then we present several theoretical results.

## 3. Time discretization schemes

We introduce some notations that will be used in the rest of this article. The norms in Sobolev space are defined by  $H^s$  and  $\|\cdot\|_s$  ( $s = 0, \pm 1, \dots$ ), respectively. In particular, the  $L^2(\Omega)$  inner product is denoted by  $(\cdot, \cdot)$  with its norm  $\|\cdot\|$ . We also define the following Sobolev spaces:

$$H_{per}(\Omega) = \{\phi \text{ is periodic}, \phi \in H^1(\Omega) \text{ and } \int_{\Omega} \phi d\mathbf{x} = 0\},$$

and introduce the notations

$$(\bullet)^{n+\frac{1}{2}} = \frac{1}{2}(\bullet)^n + \frac{1}{2}(\bullet)^{n+1}, \quad \overline{(\bullet)}^{n+\frac{1}{2}} = \frac{3}{2}(\bullet)^n - \frac{1}{2}(\bullet)^{n-1}. \quad (13)$$

### 3.1. Second order linear schemes

Let  $N$  be a positive integer,  $t_n = n\delta t$ ,  $n = 0, 1, \dots, N$  be mesh points, and  $\delta t = T/N$  be the uniform time-step, with  $T$  the final time. The reformulated equations (8)–(10) could be solved via the following second-order schemes.

**Scheme 3.1** (Crank–Nicolson (CN) Scheme). Given  $\phi^{n-1}$ ,  $w^{n-1}$ ,  $q^{n-1}$  and  $\phi^n$ ,  $w^n$ ,  $q^n$ , we can obtain  $\phi^{n+1}$ ,  $w^{n+1}$ ,  $q^{n+1}$  via

$$\begin{cases} \frac{\phi^{n+1}-\phi^n}{\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \phi^{n+\frac{1}{2}} + \gamma \phi^{n+\frac{1}{2}} + g(\bar{\phi}^{n+\frac{1}{2}})q^{n+\frac{1}{2}}, \\ \frac{q^{n+1}-q^n}{\delta t} = \frac{1}{2}g(\bar{\phi}^{n+\frac{1}{2}})\frac{\phi^{n+1}-\phi^n}{\delta t}, \end{cases} \quad (14)$$

with  $g(\phi)$  defined in Eq. (7), subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (15)$$

**Scheme 3.2** (Backward Differentiation Formula (BDF) Scheme). Given  $\phi^{n-1}$ ,  $w^{n-1}$ ,  $q^{n-1}$  and  $\phi^n$ ,  $w^n$ ,  $q^n$ , we can obtain  $\phi^{n+1}$ ,  $w^{n+1}$ ,  $q^{n+1}$  via

$$\begin{cases} \frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t} = \Delta w^{n+1}, \\ w^{n+1} = -\Delta \phi^{n+1} + \gamma \phi^{n+1} + g(\bar{\phi}^{n+1})q^{n+1}, \\ \frac{3q^{n+1}-4q^n+q^{n-1}}{2\delta t} = \frac{1}{2}g(\bar{\phi}^{n+1})\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t}, \end{cases} \quad (16)$$

with  $g(\phi)$  defined in Eq. (7), subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (17)$$

**Scheme 3.3** (Leapfrog (LF) Scheme). Given  $\phi^{n-1}$ ,  $w^{n-1}$ ,  $q^{n-1}$  and  $\phi^n$ ,  $w^n$ ,  $q^n$ , we can obtain  $\phi^{n+1}$ ,  $w^{n+1}$ ,  $q^{n+1}$  via

$$\begin{cases} \frac{\phi^{n+1}-\phi^{n-1}}{2\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \frac{\phi^{n+1}+\phi^{n-1}}{2} + \gamma \frac{\phi^{n+1}+\phi^{n-1}}{2} + g(\phi^n)\frac{q^{n+1}+q^{n-1}}{2}, \\ \frac{q^{n+1}-q^{n-1}}{2\delta t} = \frac{1}{2}g(\phi^n)\frac{\phi^{n+1}-\phi^{n-1}}{2\delta t}, \end{cases} \quad (18)$$

with  $g(\phi)$  defined in Eq. (7), subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (19)$$

Schemes 3.1–3.3 have been widely used. Furthermore, they could be easily verified to be unconditionally energy stable and uniquely solvable [41].

### 3.2. Second order predictor–corrector linear schemes

However, Schemes 3.1–3.3 are not accurate with large time-step sizes due to their explicit treatment of nonlinear term  $g$ . In a long time dynamic simulation, the numerical value of  $q$  could eventually deviate away from its original definition in Eq. (6). This could pollute the numerical solutions. Thus, we propose to improve the accuracy of these linear schemes by a predictor–corrector approach.

In the rest of this section, we present the predictor–corrector time discretization schemes first. Afterward, we will show the energy stability, unique solvability, and error estimate. The main idea of the predictor–corrector schemes is as follows.

**Scheme 3.4** (Predictor–corrector CN Scheme). Given  $\phi^{n-1}$ ,  $w^{n-1}$ ,  $q^{n-1}$  and  $\phi^n$ ,  $w^n$ ,  $q^n$ , we can obtain  $\phi^{n+1}$ ,  $w^{n+1}$ ,  $q^{n+1}$  via the following two steps:

- Step 1: Prediction: predict  $\phi_*^{n+1}$  via some efficient and accurate numerical schemes.
- Step 2: Correction: obtain  $(\phi^{n+1}, w^{n+1}, q^{n+1})$  via

$$\begin{cases} \frac{\phi^{n+1}-\phi^n}{\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \phi^{n+\frac{1}{2}} + \gamma \phi^{n+\frac{1}{2}} + g(\frac{\phi_*^{n+1}+\phi^n}{2})q^{n+\frac{1}{2}}, \\ \frac{q^{n+1}-q^n}{\delta t} = \frac{1}{2}g(\frac{\phi_*^{n+1}+\phi^n}{2})\frac{\phi^{n+1}-\phi^n}{\delta t}, \end{cases} \quad (20)$$

subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (21)$$

In a similar manner, we can propose a second-order predictor–corrector scheme based on the backward differentiation formula and leapfrog formula.

**Scheme 3.5** (Predictor–corrector BDF2 Scheme). Given  $\phi^{n-1}, w^{n-1}, q^{n-1}$  and  $\phi^n, w^n, q^n$ , we can obtain  $\phi^{n+1}, w^{n+1}, q^{n+1}$  via the following two steps:

- Step 1: Prediction: predict  $\phi_*^{n+1}$  via some efficient and accurate numerical schemes.
- Step 2: Correction: obtain  $(\phi^{n+1}, w^{n+1}, q^{n+1})$  via

$$\begin{cases} \frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\delta t} = \Delta w^{n+1}, \\ w^{n+1} = -\Delta \phi^{n+1} + \gamma \phi^{n+1} + g(\phi_*^{n+1})q^{n+1}, \\ \frac{3q^{n+1}-4q^n+q^{n-1}}{2\delta t} = \frac{1}{2}g(\phi_*^{n+1})\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{\delta t}, \end{cases} \quad (22)$$

subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (23)$$

**Scheme 3.6** (Predictor–corrector LF Scheme). Given  $\phi^{n-1}, w^{n-1}, q^{n-1}$  and  $\phi^n, w^n, q^n$ , we can obtain  $\phi^{n+1}, w^{n+1}, q^{n+1}$  via the following two steps:

- Step 1: Prediction: predict  $\phi_*^n$  via some efficient and accurate numerical schemes.
- Step 2: Correction: obtain  $(\phi^{n+1}, w^{n+1}, q^{n+1})$  via

$$\begin{cases} \frac{\phi^{n+1}-\phi^{n-1}}{2\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \frac{\phi^{n+1}+\phi^{n-1}}{2} + \gamma \frac{\phi^{n+1}+\phi^{n-1}}{2} + g(\phi_*^n)\frac{q^{n+1}+q^{n-1}}{2}, \\ \frac{q^{n+1}-q^{n-1}}{2\delta t} = \frac{1}{2}g(\phi_*^n)\frac{\phi^{n+1}-\phi^{n-1}}{2\delta t}, \end{cases} \quad (24)$$

subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (25)$$

Note that the prediction and correction steps in the schemes above are fully decoupled. For each prediction time-step, many prediction strategies could be constructed, so long as the predicted value  $\phi_*^{n+1}$  is second-order consistent in time. For instance, here are a couple of choices for the prediction step.

- Case 1: set

$$\phi_*^{n+1} = 2\phi^n - \phi^{n-1}. \quad (26)$$

- Case 2: for  $i = 0, 1, \dots, M-1$ , calculate

$$\begin{cases} \frac{\phi_{i+1}^{n+1}-\phi_i^n}{\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \phi_{i+1}^{n+\frac{1}{2}} + \gamma \phi_{i+1}^{n+\frac{1}{2}} + g(\frac{\phi_i^{n+1}+\phi_i^n}{2})q_{i+1}^{n+\frac{1}{2}}, \\ \frac{q_{i+1}^{n+1}-q_i^n}{\delta t} = \frac{1}{2}g(\frac{\phi_i^{n+1}+\phi_i^n}{2})\frac{\phi_{i+1}^{n+1}-\phi_i^n}{\delta t}, \end{cases} \quad (27)$$

where  $\phi_0^{n+1} = 2\phi^n - \phi^{n-1}$ , subject to the boundary conditions

$$(i) \phi_{i+1}^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi_{i+1}^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (28)$$

Then set  $\phi_*^{n+1} = \phi_M^{n+1}$ .

- Case 3: for  $i = 0, 1, \dots, M-1$ , calculate

$$\begin{cases} \frac{3\phi_{i+1}^{n+1}-4\phi_i^n+\phi^{n-1}}{2\delta t} = \Delta w^{n+1}, \\ w^{n+1} = -\Delta \phi_{i+1}^{n+1} + \gamma \phi_{i+1}^{n+1} + g(\phi_i^{n+1})q_{i+1}^{n+1}, \\ \frac{3q_{i+1}^{n+1}-4q_i^n+q^{n-1}}{2\delta t} = \frac{1}{2}g(\phi_i^{n+1})\frac{3\phi_{i+1}^{n+1}-4\phi_i^n+\phi^{n-1}}{2\delta t}, \end{cases} \quad (29)$$

where  $\phi_0^{n+1} = 2\phi^n - \phi^{n-1}$ , subject to the boundary conditions

$$(i) \phi_{i+1}^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi_{i+1}^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (30)$$

Then set  $\phi_*^{n+1} = \phi_M^{n+1}$ .

- Case 4: for  $i = 0, 1, \dots, M - 1$ , calculate

$$\begin{cases} \frac{\phi_{i+1}^{n+1} - \phi^n}{\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \phi_{i+1}^{n+\frac{1}{2}} + \gamma \phi_{i+1}^{n+\frac{1}{2}} + g\left(\frac{\phi_{i+1}^{n+1} + \phi^n}{2}\right) q_i^{n+\frac{1}{2}}, \\ q_{i+1}^{n+1} = \sqrt{F(\phi_{i+1}^{n+1}) - \frac{\gamma}{2}(\phi_{i+1}^{n+1})^2 + B}, \end{cases} \quad (31)$$

where  $\phi_0^{n+1} = 2\phi^n - \phi^{n-1}$  and  $q_0^{n+\frac{1}{2}} = \bar{q}^{n+\frac{1}{2}}$ , subject to the boundary conditions

$$(i) \phi_{i+1}^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi_{i+1}^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (32)$$

Then set  $\phi_*^{n+1} = \phi_M^{n+1}$ .

**Remark 3.1.** We propose three ways to predict  $\phi_*^{n+1}$ , all of which are commonly used. In fact, given a sufficient precision of  $\phi_*^{n+1}$ , we can also calculate  $\phi^{n+1}$  via correction step. There is no doubt that “Case 2”, “Case 3” and “Case 4” are better than “Case 1” because  $\phi_*^{n+1}$  is close to the exact solution, but “Case 2”, “Case 3” and “Case 4” need more calculation costs. In addition, “Case 2”, “Case 3” and “Case 4” are similar in theoretical analysis, and “Case 2” performs slightly better in numerical simulation. In the last numerical examples, we select “Case 2” as the prediction step to obtain  $\phi_*^{n+1}$ .

**Remark 3.2.** We note that, in gradient flow (especially phase-field) models, an adaptive time-step strategy will be in favor to capture the different time scales during the dynamics, as well as being computationally efficient. However, the broadly used time-adaptive strategies [43,44] could be readily utilized in our proposed schemes to speed up the calculations.

### 3.3. Some theoretical results

As Schemes 3.5 and 3.6 are all similar to Scheme 3.4 we mainly focus on the predictor–corrector CN Scheme 3.4 with the CN predictor, which is summarized as follows.

**Scheme 3.7 (Fixed-point Predictor–corrector CN Scheme).** Given  $\phi^{n-1}, w^{n-1}, q^{n-1}$  and  $\phi^n, w^n, q^n$ , we can obtain  $\phi^{n+1}, w^{n+1}, q^{n+1}$  via the following two steps:

- Step 1: Prediction: while  $\|\phi_{i+1}^{n+1} - \phi_i^{n+1}\| > \varepsilon_0$  and  $i < N$ , for  $i = 0$  to  $N - 1$ , calculate

$$\begin{cases} \frac{\phi_{i+1}^{n+1} - \phi^n}{\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \phi_{i+1}^{n+\frac{1}{2}} + \gamma \phi_{i+1}^{n+\frac{1}{2}} + g\left(\frac{\phi_{i+1}^{n+1} + \phi^n}{2}\right) q_{i+1}^{n+\frac{1}{2}}, \\ \frac{q_{i+1}^{n+1} - q^n}{\delta t} = \frac{1}{2} g\left(\frac{\phi_{i+1}^{n+1} + \phi^n}{2}\right) \frac{\phi_{i+1}^{n+1} - \phi^n}{\delta t}, \end{cases} \quad (33)$$

with  $\phi_0^{n+1} = 2\phi^n - \phi^{n-1}$ , subject to the boundary conditions

$$(i) \phi_{i+1}^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi_{i+1}^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (34)$$

If the loop ends at  $i + 1 = M \leq N$ , set  $\phi_*^{n+1} = \phi_M^{n+1}$ .

- Step 2: Correction: obtain  $(\phi^{n+1}, w^{n+1}, q^{n+1})$  via

$$\begin{cases} \frac{\phi^{n+1} - \phi^n}{\delta t} = \Delta w^{n+\frac{1}{2}}, \\ w^{n+\frac{1}{2}} = -\Delta \phi^{n+\frac{1}{2}} + \gamma \phi^{n+\frac{1}{2}} + g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right) q^{n+\frac{1}{2}}, \\ \frac{q^{n+1} - q^n}{\delta t} = \frac{1}{2} g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right) \frac{\phi^{n+1} - \phi^n}{\delta t}, \end{cases} \quad (35)$$

subject to the boundary conditions

$$(i) \phi^{n+1}, w^{n+1} \text{ are periodic ; or } (ii) \partial_n \phi^{n+1}|_{\partial\Omega} = \partial_n w^{n+1}|_{\partial\Omega} = 0. \quad (36)$$

For Scheme 3.7, we have the following energy stability result.

**Theorem 3.3 (Unconditionally Energy Stability).** The time discrete Scheme 3.7 is unconditionally energy stable. And it follows the energy dissipation law as

$$E(\phi^{n+1}, q^{n+1}) + \delta t \|\nabla(-\Delta \phi^{n+\frac{1}{2}} + \gamma \phi^{n+\frac{1}{2}} + g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right) q^{n+\frac{1}{2}})\|^2 = E(\phi^n, q^n), \quad (37)$$

where  $E(\phi^{n+1}, q^{n+1}) = \frac{1}{2} \|\nabla \phi^{n+1}\|^2 + \frac{\gamma}{2} \|\phi^{n+1}\|^2 + \|q^{n+1}\|^2 - B|\Omega|$ . In particular,

$$E(\phi^{n+1}, q^{n+1}) \leq E(\phi^n, q^n).$$

**Proof.** Computing the  $L^2$  inner product of the first equation in Eq. (33) with  $2\delta t w^{n+\frac{1}{2}}$  and using integrating by parts, we get

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

Taking the  $L^2$  inner product of the second equation in Eq. (33) with  $2(\phi^{n+1} - \phi^n)$  to arrive at

$$2(w^{n+\frac{1}{2}}, \phi^{n+1} - \phi^n) = \|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \gamma(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) + 2\left(g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)q^{n+\frac{1}{2}}, \phi^{n+1} - \phi^n\right).$$

Computing the  $L^2$  inner product of the third equation in Eq. (33) with  $2(q^{n+1} + q^n)\delta t$ , we obtain

$$2\|q^{n+1}\|^2 - 2\|q^n\|^2 = \left(g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)(\phi^{n+1} - \phi^n), q^{n+1} + q^n\right).$$

Summing the equations above up, we derive

$$\|\nabla \phi^{n+1}\|^2 - \|\nabla \phi^n\|^2 + \gamma(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) + 2\|q^{n+1}\|^2 - 2\|q^n\|^2 = -2\delta t \|\nabla w^{n+\frac{1}{2}}\|^2,$$

i.e.

$$E(\phi^{n+1}, q^{n+1}) + \delta t \|\nabla(-\Delta \phi^{n+\frac{1}{2}} + \gamma \phi^{n+\frac{1}{2}} + g(\frac{\phi_*^{n+1} + \phi^n}{2})q^{n+\frac{1}{2}})\|^2 = E(\phi^n, q^n).$$

That is Eq. (37).  $\square$

In a similar proving strategy, we can obtain the following corollary.

**Corollary 3.1.** For the prediction step Eq. (33), it holds

$$E(\phi_{i+1}^{n+1}, q_{i+1}^{n+1}) \leq E(\phi^n, q^n), \quad \forall i = 0, 1, \dots, M-1, \quad (38)$$

where  $E(\phi_{i+1}^{n+1}, q_{i+1}^{n+1}) = \frac{1}{2}\|\nabla \phi_{i+1}^{n+1}\|^2 + \frac{\gamma}{2}\|\phi_{i+1}^{n+1}\|^2 + \|q_{i+1}^{n+1}\|^2 - B|\Omega|$ .

The detailed proof is omitted for simplicity. In addition to the unconditional energy stability, the unique solvability could also be shown as follows.

**Theorem 3.4 (Unique Solvability).** The predictor–corrector Scheme 3.7 is uniquely solvable.

**Proof.** First, from the third equation of Eq. (35), we find

$$q^{n+1} = q^n + \frac{1}{2}g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right)(\phi^{n+1} - \phi^n). \quad (39)$$

Then, we can rewrite Eq. (35) as follows

$$\begin{cases} \phi^{n+1} - \frac{1}{2}\delta t \Delta w^{n+1} = Q_1, \\ P(\phi^{n+1}) - w^{n+1} = Q_2, \end{cases} \quad (40)$$

where

$$\begin{cases} Q_1 = \phi^n + \frac{1}{2}\delta t \Delta w^n, \\ Q_2 = \Delta \phi^n - \gamma \phi^n + g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right)\left(\frac{1}{2}g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right)\phi^n - 2q^n\right) + w^n, \\ P(\phi) = -\Delta \phi + \gamma \phi + \frac{1}{2}g^2\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right)\phi. \end{cases} \quad (41)$$

Thus, we can solve  $(\phi^{n+1}, w^{n+1})$  directly from Eq. (40). Once we get  $\phi^{n+1}$ , the  $q^{n+1}$  is automatically obtained in Eq. (39). Moreover, when  $\phi$  satisfies the boundary condition Eq. (10), we have

$$(P(\phi), \phi) = (\nabla \phi, \nabla \phi) + \gamma(\phi, \phi) + \frac{1}{2}\left(g^2\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right)\phi, \phi\right) = (\phi, P(\phi)). \quad (42)$$

Then, the linear operator  $P(\phi)$  is self-adjoint. Furthermore, if  $\int_{\Omega} \phi d\mathbf{x} = 0$ , we have

$$(P(\phi), \phi) = \|\nabla \phi\|^2 + \gamma\|\phi\|^2 + \frac{1}{2}\|g\left(\frac{\phi_*^{n+1} + \phi^n}{2}\right)\phi\|^2 \geq C_{\Omega}\|\phi\|_1^2. \quad (43)$$

Thus the operator  $P(\phi)$  is positive define. Computing the  $L^2$  inner product of the first equation in Eq. (35) with 1, we obtain

$$\int_{\Omega} \phi^{n+1} d\mathbf{x} = \int_{\Omega} \phi^n d\mathbf{x} = \dots = \int_{\Omega} \phi^0 d\mathbf{x}.$$

Set  $v_{\phi} = \frac{1}{|\Omega|} \int_{\Omega} \phi^0 d\mathbf{x}$ ,  $v_w = \frac{1}{|\Omega|} \int_{\Omega} w^{n+1} d\mathbf{x}$ , and denote

$$\widehat{\phi}^{n+1} = \phi^{n+1} - v_{\phi}, \quad \widehat{w}^{n+1} = w^{n+1} - v_w.$$

From Eq. (40), we find  $(\widehat{\phi}, \widehat{w}) \in (H_{per}, H_{per})$  is the solution of the following equations

$$\begin{cases} (\phi, \mu) + \frac{1}{2} \delta t (\nabla w, \mu) = (Q_3, \mu), & \mu \in H_{per}(\Omega), \\ (P(\phi), \psi) - (w, \psi) = (Q_4, \psi), & \psi \in H_{per}(\Omega). \end{cases} \quad (44)$$

We denote the above system (44) as

$$(\mathcal{L}X, Y) = (\mathcal{F}, Y), \quad (45)$$

where  $X = (w, \phi)$ ,  $Y = (\mu, \psi)$ ,  $\mathcal{F} = (Q_3, Q_4)$  with  $X, Y \in (H_{per}, H_{per})$ , we can obtain that

$$(\mathcal{L}X, Y) \leq C(\|\phi\|_1 + \|w\|_1)(\|\psi\|_1 + \|\mu\|_1). \quad (46)$$

Thus, the bilinear form  $(\mathcal{L}X, Y)$  is bounded. In addition, we have

$$(\mathcal{L}X, X) = \frac{\delta t}{2} \|\nabla w\|^2 + (P(\phi), \phi) \geq C(\|w\|_1^2 + \|\phi\|_1^2), \quad (47)$$

using the Poincaré inequality. Then the bilinear form  $(\mathcal{L}X, Y)$  is positive definite, it is easy to show that exists a unique solution  $(w, \phi) \in (H_{per}, H_{per})$  for Eq. (45) by using Lax–Milgram theorem. Thus, linear Scheme 3.7 admits a unique solution.  $\square$

### 3.4. Error estimate for the time-discrete scheme

In this part, we present the error estimate of the time-discrete predictor–corrector Scheme 3.7. Scheme 3.4 with other predictors could be analyzed in a similar manner. In particular, if we choose the extrapolation predictor equation (26), Scheme 3.4 reduces to the Crank–Nicolson IEQ Scheme 3.1. In other words, our proof strategies also work for linear IEQ Schemes 3.1–3.3.

To this end we will prove  $\|\phi^{n+1}\|_{L^\infty}$  is uniformly bounded. First, let us denote the error functions

$$e_{i,\phi}^n = \phi(t_n) - \phi_i^n, \quad e_{i,\phi}^n = \phi(t_n) - \phi^n, \quad e_{i,q}^n = q(t_n) - q_i^n, \quad e_q^n = q(t_n) - q^n.$$

and the truncation error functions

$$\begin{aligned} r_1^n &:= \frac{\phi(t_{n+1}) - \phi(t_n)}{\delta t} - \phi_t(t_{n+\frac{1}{2}}), & r_2^n &:= \frac{\phi(t_{n+1}) + \phi(t_n)}{2} - \phi(t_{n+\frac{1}{2}}), \\ r_3^n &:= \frac{q(t_{n+1}) - q(t_n)}{\delta t} - q_t(t_{n+\frac{1}{2}}), & r_4^n &:= \frac{q(t_{n+1}) + q(t_n)}{2} - q(t_{n+\frac{1}{2}}), \\ r_5^n &:= \frac{w(t_{n+1}) + w(t_n)}{2} - w(t_{n+\frac{1}{2}}). \end{aligned}$$

By using Taylor series expansion, we find

$$\|r_1^n\| \leq C\delta t^2, \quad \|r_2^n\| \leq C\delta t^2, \quad \|r_3^n\| \leq C\delta t^2, \quad \|r_4^n\| \leq C\delta t^2, \quad \|r_5^n\| \leq C\delta t^2. \quad (48)$$

The next three lemmas [36] will help us to handle the bound of nonlinear terms.

**Lemma 3.5.** Given that (a)  $F(x) \in C^2(-\infty, +\infty)$ ; (b) there exists a constant  $A$ , such that  $F(x) - \frac{\gamma}{2}x^2 > -A$ ,  $\forall x \in (-\infty, +\infty)$ ; (c) there exists a positive constant  $C_1$  such that

$$\max_{n \leq k} \left\{ \|\phi(t_n)\|_{L^\infty}, \|\phi^n\|_{L^\infty}, \|\phi_i^{n+1}\|_{L^\infty} \right\} \leq C_1, \quad (49)$$

it holds

$$\max_{n \leq k} \left\{ \|F_1(\chi^n)\|_{L^\infty}, \|f_1(\chi^n)\|_{L^\infty}, \|f_1'(\chi^n)\|_{L^\infty}, \|\sqrt{F_1(\chi^n) + B}\|_{L^\infty} \right\} \leq C_2, \quad (50)$$

where  $\chi^n = \varepsilon_1 \phi(t_n) + \varepsilon_2 \phi^n + \varepsilon_3 \phi_i^{n+1}$ ,  $\varepsilon_1, \varepsilon_2, \varepsilon_3 \in [0, 1]$ ,  $F_1(x) = F(x) - \frac{\gamma}{2}x^2$ ,  $f_1 = F_1'$ . Moreover, we have

$$\|g(\phi(t_n)) - g(\phi^n)\| \leq C_3 \|\phi(t_n) - \phi^n\|, \quad (51)$$

where  $C_3$  are constants which are dependent on  $C_1, C_2, A, B$ .



**Proof.** The inequality (50) is obtained by combining assumptions (a) and (c). By using the Lagrange mean value theorem, we find

$$\begin{aligned} |g(\phi(t_n)) - g(\phi^n)| &= \left| \frac{f_1(\phi(t_n))}{\sqrt{F_1(\phi(t_n)) + B}} - \frac{f_1(\phi^n)}{\sqrt{F_1(\phi^n) + B}} \right| \\ &= \left| \frac{f_1(\phi(t_n))\sqrt{F_1(\phi^n) + B} - f_1(\phi^n)\sqrt{F_1(\phi(t_n)) + B}}{\sqrt{F_1(\phi(t_n)) + B}\sqrt{F_1(\phi^n) + B}} \right| \\ &\leq \left| \frac{f_1(\phi(t_n))(\sqrt{F_1(\phi^n) + B} - \sqrt{F_1(\phi(t_n)) + B})}{\sqrt{F_1(\phi(t_n)) + B}\sqrt{F_1(\phi^n) + B}} \right| \\ &\quad + \left| \frac{\sqrt{F_1(\phi(t_n)) + B}(f_1(\phi(t_n)) - f_1(\phi^n))}{\sqrt{F_1(\phi(t_n)) + B}\sqrt{F_1(\phi^n) + B}} \right| \\ &\leq C|\phi(t_n) - \phi^n|. \end{aligned}$$

This concludes the proof.  $\square$

**Lemma 3.6.** Given that (a)  $F(x) \in C^3(-\infty, +\infty)$ ; (b) there is a constant  $A$ , such that  $F(x) - \frac{\gamma}{2}x^2 > -A, \forall x \in (-\infty, +\infty)$ ; (c) there exists a positive constant  $C_4$  such that

$$\max_{n \leq k} \left\{ \|\phi(t_n)\|_{L^\infty}, \|\phi^n\|_{L^\infty}, \|\phi_i^{n+1}\|_{L^\infty} \right\} \leq C_4.$$

The following inequalities hold

$$\begin{aligned} \max_{n \leq k} \left\{ \|F_1(\chi^n)\|_{L^\infty}, \|f_1(\chi^n)\|_{L^\infty}, \|f_1'(\chi^n)\|_{L^\infty}, \|f_1''(\chi^n)\|_{L^\infty}, \|\sqrt{F_1(\chi^n) + B}\|_{L^\infty} \right\} &\leq C_5, \\ \|\nabla g(\phi(t_n)) - \nabla g(\phi^n)\| &\leq C_6\|\phi(t_n) - \phi^n\|_1. \end{aligned}$$

The proof is similar to Lemma 3.5. We thus omit it here for simplicity.

**Lemma 3.7.** Denote  $\{u^n\}_{n=0}^{N-1}$  to be sequences of function on  $\Omega$ . It holds

$$|u^{n+1}| \leq \sum_{m=0}^n |u^{m+1} + u^m| + |u^0|.$$

**Proof.** To prove it, we utilize the mathematical induction. For  $n = 0$ , it is easy to see that  $|u^1| \leq |u^1 + u^0| + |u^0|$ . If  $n = k - 1$ , suppose that  $|u^k| \leq \sum_{m=0}^{k-1} |u^{m+1} + u^m| + |u^0|$ . When  $n = k$ , we can obtain

$$\begin{aligned} |u^{k+1}| - |u^0| &= |u^{k+1}| - |u^k| + |u^k| - |u^0| \\ &\leq \sum_{m=0}^{k-1} |u^{m+1} + u^m| + |u^{k+1}| - |u^k| \leq \sum_{m=0}^k |u^{m+1} + u^m|. \end{aligned}$$

This completes the proof.  $\square$

We also need to make the following regularity assumptions.

$$\begin{aligned} \phi &\in L^\infty(0, T; H^2(\Omega)) \cap L^\infty(0, T; W^{1,\infty}(\Omega)), \quad \phi_t \in L^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; L^\infty(\Omega)), \\ q &\in L^\infty(0, T; W^{1,\infty}(\Omega)), \quad q_{tt}, \phi_{tt} \in L^2(0, T; L^2(\Omega)), \quad w \in L^\infty(0, T; H^2(\Omega)). \end{aligned} \quad (52)$$

Here, we define  $\nu$  as

$$\nu = \max_{0 \leq t \leq T} \|\phi(t)\|_{L^\infty} + 1. \quad (53)$$

We will show that  $\|\phi^n\|$  and  $\|\phi_{i+1}^{n+1}\|_{L^\infty}$  are uniformly bounded in the following lemma.

**Lemma 3.8** (Uniform  $L_\infty$  Bound). Given that  $F(x) - \frac{\gamma}{2}x^2 > -A$  for all  $x \in (-\infty, +\infty)$ ,  $F(x) \in C^3(-\infty, +\infty)$  and the system (8)–(10) has a unique solution, which satisfies the assumptions (52), there is a positive constant  $\tau$ , when  $\delta t < \tau$ , the solution of Eqs. (33)–(35) is bounded as follows

$$\|\phi^{n+1}\|_{L^\infty} \leq \nu, \|\phi_{i+1}^{n+1}\|_{L^\infty} \leq \nu \quad n = 0, 1, \dots, K = T/\delta t, 0 \leq i \leq M - 1. \quad (54)$$

**Proof.** We present the proof using mathematical induction. When  $n = 0$ , it is easy to verify  $\|\phi^0\|_{L^\infty} \leq \nu$ . For  $i = 0$ , subtracting Eq. (33) from Eq. (8) gives

$$\left(\frac{e_{1,\phi}^1 - e_\phi^0}{\delta t}, \varphi\right) = -(\nabla e_w^{\frac{1}{2}}, \nabla \varphi) + (r_1^0 - \Delta r_5^0, \varphi), \quad (55)$$

$$(e_w^{\frac{1}{2}}, \theta) = (r_5^0 + \Delta r_2^n - \gamma r_2^0, \theta) + \gamma \left(\frac{e_{1,\phi}^1 + e_\phi^0}{2}, \theta\right) + \left(\nabla \frac{e_{1,\phi}^1 + e_\phi^0}{2}, \nabla \theta\right) + (g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g(\phi^0)q_1^{\frac{1}{2}}, \theta), \quad (56)$$

$$\left(\frac{e_{1,q}^1 - e_q^0}{\delta t}, \psi\right) = (r_3^0, \psi) + \frac{1}{2}(g(\phi(t_{\frac{1}{2}}))\phi_t(t_{\frac{1}{2}}) - g(\phi^0)\frac{\phi_1^1 - \phi^0}{\delta t}, \psi). \quad (57)$$

By taking  $\varphi = \delta t e_{1,\phi}^1, 2\delta t e_w^{\frac{1}{2}}$  in Eq. (55), we derive

$$\begin{aligned} \|e_{1,\phi}^1\|^2 &= -\delta t(\nabla e_w^{\frac{1}{2}}, \nabla e_{1,\phi}^1) + \delta t(r_1^0 - \Delta r_5^0, e_{1,\phi}^1), \\ 2(e_{1,\phi}^1, e_w^{\frac{1}{2}}) &= -2\delta t\|\nabla e_w^{\frac{1}{2}}\|^2 + 2\delta t(r_1^0 - \Delta r_5^0, e_w^{\frac{1}{2}}). \end{aligned}$$

By taking  $\theta = 2e_{1,\phi}^1, 2\delta t e_w^{\frac{1}{2}}$  in Eq. (56), we find

$$\begin{aligned} 2(e_w^{\frac{1}{2}}, e_{1,\phi}^1) &= 2(r_5^0 + \Delta r_2^n - \gamma r_2^0, e_{1,\phi}^1) + \gamma \|e_{1,\phi}^1\|^2 + \|\nabla e_{1,\phi}^1\|^2 + 2(g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g(\phi^0)q_1^{\frac{1}{2}}, e_{1,\phi}^1), \\ 2\delta t\|e_w^{\frac{1}{2}}\|^2 &= 2\delta t(r_5^0 + \Delta r_2^n - \gamma r_2^0, e_w^{\frac{1}{2}}) + \gamma \delta t(e_{1,\phi}^1, e_w^{\frac{1}{2}}) + \delta t(\nabla e_{1,\phi}^1, \nabla e_w^{\frac{1}{2}}) \\ &\quad + 2\delta t(g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g(\phi^0)q_1^{\frac{1}{2}}, e_w^{\frac{1}{2}}). \end{aligned}$$

By taking  $\psi = 2\delta t e_{1,q}^1$  in Eq. (57), that is

$$2\|e_{1,q}^1\|^2 = 2\delta t(r_3^0, e_{1,q}^1) + \delta t(g(\phi(t_{\frac{1}{2}}))\phi_t(t_{\frac{1}{2}}) - g(\phi^0)\frac{\phi_1^1 - \phi^0}{\delta t}, e_{1,q}^1).$$

Summing above equations up, we get

$$\begin{aligned} &\|e_{1,\phi}^1\|^2 + \gamma \|e_{1,\phi}^1\|^2 + 2\|e_{1,q}^1\|^2 + 2\delta t\|e_w^{\frac{1}{2}}\|^2 \\ &= \delta t(r_1^0 - \Delta r_5^0, e_{1,\phi}^1) + 2\delta t(r_1^0 - \Delta r_5^0, e_w^{\frac{1}{2}}) - 2(r_5^0 + \Delta r_2^n - \gamma r_2^0, e_{1,\phi}^1) \\ &\quad + 2\delta t(r_5^0 + \Delta r_2^n - \gamma r_2^0, e_w^{\frac{1}{2}}) + 2\delta t(r_3^0, e_{1,q}^1) \\ &\quad - 2(g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g(\phi^0)q_1^{\frac{1}{2}}, e_{1,\phi}^1) + 2\delta t(g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g(\phi^0)q_1^{\frac{1}{2}}, e_w^{\frac{1}{2}}) \\ &\quad + \delta t(g(\phi(t_{\frac{1}{2}}))\phi_t(t_{\frac{1}{2}}) - g(\phi^0)\frac{\phi_1^1 - \phi^0}{\delta t}, e_{1,q}^1). \end{aligned}$$

By using Cauchy-Schwarz and Young's inequality, we obtain

$$\begin{aligned} \delta t(r_1^0 - \Delta r_5^0, e_{1,\phi}^1) &\leq C\delta t^6 + \gamma \|e_{1,\phi}^1\|^2, \\ 2\delta t(r_1^0 - \Delta r_5^0, e_w^{\frac{1}{2}}) &\leq C\delta t^5 + \frac{\delta t}{3}\|e_w^{\frac{1}{2}}\|^2, \\ 2\delta t(r_5^0 + \Delta r_2^n - \gamma r_2^0, e_w^{\frac{1}{2}}) &\leq C\delta t^5 + \frac{\delta t}{3}\|e_w^{\frac{1}{2}}\|^2, \\ 2\delta t(r_3^0, e_{1,q}^1) &\leq C\delta t^5 + \delta t\|e_{1,q}^1\|^2, \\ -2(r_5^0 + \Delta r_2^n - \gamma r_2^0, e_{1,\phi}^1) &= -2\delta t(r_5^0 + \Delta r_2^n - \gamma r_2^0, r_1^0 - \Delta r_5^0 + \Delta e_w^{\frac{1}{2}}) \leq C\delta t^5 + \frac{\delta t}{2}\|\nabla e_w^{\frac{1}{2}}\|^2. \end{aligned}$$

For the nonlinear term, we find that

$$\begin{aligned} &-2(g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g_0^{\frac{1}{2}}q_1^{\frac{1}{2}}, e_{1,\phi}^1) + \delta t(g(\phi(t_{\frac{1}{2}}))\phi_t(t_{\frac{1}{2}}) - g(\phi^0)\frac{\phi_1^1 - \phi^0}{\delta t}, e_{1,q}^1) \\ &= -2\delta t(q(\phi(t_{\frac{1}{2}}))(g(\phi(t_{\frac{1}{2}})) - g(\phi^0)) + g(\phi^0)(-r_4^0 + \frac{e_{1,q}^1}{2}), \frac{e_{1,\phi}^1 - e_\phi^0}{\delta t}) \\ &\quad + \delta t(\phi_t(t_{\frac{1}{2}})(g(\phi(t_{\frac{1}{2}})) - g(\phi^0)) + g(\phi^0)(-r_1^0 + \frac{e_{1,\phi}^1 - e_\phi^0}{\delta t}), e_{1,q}^1) \\ &= -2\delta t(q(\phi(t_{\frac{1}{2}}))(g(\phi(t_{\frac{1}{2}})) - g(\phi^0)) - g(\phi^0)r_4^0, r_1^0 - \Delta r_5^0 + \Delta e_w^{\frac{1}{2}}) \end{aligned}$$

$$\begin{aligned}
& + \delta t(\phi(t_{\frac{1}{2}}))(g(\phi(t_{\frac{1}{2}})) - g(\phi^0)) - g(\phi^0)r_1^0, e_{1,q}^1) \\
& \leq C\delta t(\delta t^2 + \|e_{1,q}^1\|^2) + \frac{\delta t}{2}\|\nabla e_w^{\frac{1}{2}}\|^2,
\end{aligned}$$

and

$$2\delta t(g(\phi(t_{\frac{1}{2}}))q(\phi(t_{\frac{1}{2}})) - g(\phi^0)q_1^{\frac{1}{2}}, e_w^{\frac{1}{2}}) \leq C\delta t(\delta t^2 + \|e_{1,q}^1\|^2) + \frac{\delta t}{3}\|e_w^{\frac{1}{2}}\|^2.$$

Combining the above equations together, we get

$$\|e_{1,\phi}^1\|^2 + 2\|e_{1,q}^1\| + \delta t\|e_w^{\frac{1}{2}}\|^2 \leq C\delta t^3 + C_7\delta t\|e_{1,q}^1\|^2.$$

When  $C_7\delta t \leq 1$ , we immediately obtain  $\|e_{1,\phi}^1\|^2 + \|e_{1,q}^1\| + \delta t\|e_w^{\frac{1}{2}}\|^2 \leq C\delta t^3$ .

Let  $n = 0, i = 0$  in Eq. (33), we find

$$\begin{aligned}
\|\Delta\phi_1^{\frac{1}{2}}\|^2 & \leq 3\left(\|w^{\frac{1}{2}}\|^2 + C\|g(\phi^0)\|_{L^\infty}^2|q_1^{\frac{1}{2}}|^2 + \gamma\|\phi_1^{\frac{1}{2}}\|^2\right) \\
& \leq C\left(\|w(t_1)\|^2 + \|w(t_0)\|^2 + \|e_w^1\|^2 + \|e_{1,q}^1\|^2 + \|q(t_1)\|^2 + \|q(t_0)\|^2 + \|\phi(t_1)\|^2 + \|\phi(t_0)\|^2 + \|e_{1,\phi}^1\|^2\right) \\
& \leq C.
\end{aligned}$$

Therefore, we derive  $\|\Delta e_{1,\phi}^1\|^2 \leq 2\|\Delta\phi_1^1\|^2 + 2\|\Delta\phi(t_1)\|^2 \leq C$ . Then

$$\|\phi_1^1\|_{L^\infty} \leq \|e_{1,\phi}^1\|_{L^\infty} + \|\phi(t_1)\|_{L^\infty} \leq C\|e_{1,\phi}^1\|_1^{\frac{1}{2}}\|e_{1,\phi}^1\|_2^{\frac{1}{2}} + \|\phi(t_1)\|_{L^\infty} \leq C_8\delta t^{\frac{3}{4}} + \|\phi(t_1)\|_{L^\infty}.$$

When  $C_8\delta t^{\frac{3}{4}} \leq 1$ , we have

$$\|\phi_1^1\|_{L^\infty} \leq 1 + \|\phi(t_1)\|_{L^\infty} \leq \nu. \quad (58)$$

Suppose  $i = j \geq 1$ ,  $\|\phi_j^1\|_{L^\infty} \leq \nu$  holds, next we will show  $\|\phi_{j+1}^1\|_{L^\infty} \leq \nu$  is still valid. Subtracting Eq. (33) from Eq. (8) at  $t_{\frac{1}{2}}$  by applying Cauchy-Schwarz, Young's inequality and Lemmas 3.5–3.6, we obtain

$$\|e_{j+1,\phi}^1\|^2 + 2\|e_{j+1,q}^1\|^2 + \delta t\|e_w^{\frac{1}{2}}\|^2 \leq C\delta t^5 + C_9\delta t\|e_{j,\phi}^1\|^2 + C_{10}\delta t\|e_{j+1,q}^1\|^2. \quad (59)$$

If  $C_{10}\delta t \leq 1$ , we arrive at

$$\|e_{j+1,\phi}^1\|^2 + \|e_{j+1,q}^1\|^2 + \delta t\|e_w^{\frac{1}{2}}\|^2 \leq C\delta t^5 + C_9\delta t\|e_{j,\phi}^1\|^2. \quad (60)$$

By using a simple recursion formula, we derive

$$\|e_{j+1,\phi}^1\|^2 + \|e_{j+1,q}^1\|^2 + \delta t\|e_w^{\frac{1}{2}}\|^2 \leq d^j\|e_{1,\phi}^1\|^2 + C\delta t^5\left(\frac{1-d^j}{1-d}\right), \quad (61)$$

where  $d = C_9\delta t$ , if  $d < 1/2$ , we have

$$\|e_{j+1,\phi}^1\|^2 + \|e_{j+1,q}^1\|^2 + \delta t\|e_w^{\frac{1}{2}}\|^2 \leq C\delta t^3. \quad (62)$$

From Eq. (33), we find

$$\begin{aligned}
\|\Delta\phi_{j+1}^{\frac{1}{2}}\|^2 & \leq 3\left(\|w^{\frac{1}{2}}\|^2 + C_\Omega\|g(\phi_j^{\frac{1}{2}})\|_{L^\infty}^2|q_{j+1}^{\frac{1}{2}}|^2 + \gamma\|\phi_{j+1}^{\frac{1}{2}}\|^2\right) \\
& \leq C\left(\|w(t_1)\|^2 + \|w(t_0)\|^2 + \|e_w^1\|^2 + \|e_{j+1,q}^1\|^2 + \|q(t_1)\|^2 + \|q(t_0)\|^2\right. \\
& \quad \left.+ \|\phi(t_1)\|^2 + \|\phi(t_0)\|^2 + \|e_{j+1,\phi}^1\|^2\right) \\
& \leq C.
\end{aligned}$$

Therefore  $\|\Delta e_{j+1,\phi}^1\|^2 \leq 2\|\Delta\phi_{j+1}^1\|^2 + 2\|\Delta\phi(t_1)\|^2 \leq C$ . Then, we derive that

$$\|\phi_{j+1}^1\|_{L^\infty} \leq \|e_{j+1,\phi}^1\|_{L^\infty} + \|\phi(t_1)\|_{L^\infty} \leq C\|e_{j+1,\phi}^1\|_1^{\frac{1}{2}}\|e_{j+1,\phi}^1\|_2^{\frac{1}{2}} + \|\phi(t_1)\|_{L^\infty} \leq C_{11}\delta t^{\frac{3}{4}} + \|\phi(t_1)\|_{L^\infty}.$$

When  $C_{11}\delta t^{\frac{3}{4}} \leq 1$ , we derive

$$\|\phi_{j+1}^1\|_{L^\infty} \leq \nu. \quad (63)$$

Suppose  $\|\phi^k\|_{L^\infty} \leq \nu$ , and  $\|\phi_{i+1}^{k+1}\|_{L^\infty} \leq \nu, \forall 0 \leq i \leq M-1$ . Next, we will prove that  $\|\phi^{k+1}\|_{L^\infty} \leq \nu, \|\phi_{i+1}^{k+2}\|_{L^\infty} \leq \nu$  is still valid. First, for  $i = 0$ , subtracting Eq. (33) from Eq. (8) at  $t_{n+\frac{1}{2}}$ , and taking the inner product with  $\varphi, \theta, \psi$ , respectively,

$$\left(\frac{e_{1,\phi}^{n+1} - e_\phi^n}{\delta t}, \varphi\right) = -(\nabla e_w^{n+\frac{1}{2}}, \nabla \varphi) + (r_1^n - \Delta r_5^n, \varphi), \quad (64)$$

$$\begin{aligned} (e_w^{n+\frac{1}{2}}, \theta) &= (r_5^n + \Delta r_2^n - \gamma r_2^n, \theta) + \gamma \left(\frac{e_{1,\phi}^{n+1} + e_\phi^n}{2}, \theta\right) + \left(\nabla \frac{e_{1,\phi}^{n+1} + e_\phi^n}{2}, \nabla \theta\right) \\ &\quad + \left(g(\phi(t_{n+\frac{1}{2}}))q(\phi(t_{n+\frac{1}{2}})) - g\left(\frac{\phi_0^{n+1} + \phi^n}{2}\right)q_1^{n+\frac{1}{2}}, \theta\right), \end{aligned} \quad (65)$$

$$\left(\frac{e_{1,q}^{n+1} - e_q^n}{\delta t}, \psi\right) = (r_3^n, \psi) + \frac{1}{2} \left(g(\phi(t_{n+\frac{1}{2}}))\phi_t(t_{n+\frac{1}{2}}) - g\left(\frac{\phi_0^{n+1} + \phi^n}{2}\right)\frac{\phi_1^{n+1} - \phi^n}{\delta t}, \psi\right). \quad (66)$$

Taking  $\varphi = \delta t(e_{1,\phi}^{n+1} + e_\phi^n), 2\delta t e_w^{n+\frac{1}{2}}$  in Eq. (64),  $\theta = 2(e_{1,\phi}^{n+1} - e_\phi^n), 2\delta t e_w^{n+\frac{1}{2}}$  in Eq. (65),  $\psi = 2\delta t(e_{1,q}^{n+1} + e_q^n)$  in Eq. (66). Following the previous proof, we arrive at

$$\begin{aligned} &\|e_{1,\phi}^{n+1}\|_1^2 - \|e_\phi^n\|_1^2 + \gamma(\|e_{1,\phi}^{n+1}\|^2 - \|e_\phi^n\|^2) + 2\delta t\|e_w^{n+\frac{1}{2}}\|_1^2 + 2(\|e_{1,q}^{n+1}\|^2 - \|e_q^n\|^2) \\ &= \delta t(r_1^n - \Delta r_5^n, e_{1,\phi}^{n+1} + e_\phi^n) + 2\delta t(r_1^n - \Delta r_5^n, e_w^{n+\frac{1}{2}}) + 2\delta t(r_3^n, e_{1,q}^{n+1} + e_q^n) \\ &\quad - 2(r_5^n + \Delta r_2^n - \gamma r_2^n, e_{1,\phi}^{n+1} - e_\phi^n) + 2\delta t(r_5^n + \Delta r_2^n - \gamma r_2^n, e_w^{n+\frac{1}{2}}) \\ &\quad - 2\left(g(\phi(t_{n+\frac{1}{2}}))q(\phi(t_{n+\frac{1}{2}})) - g\left(\frac{\phi_0^{n+1} + \phi^n}{2}\right)q_1^{n+\frac{1}{2}}, e_{1,\phi}^{n+1} - e_\phi^n\right) \\ &\quad + 2\left(g(\phi(t_{n+\frac{1}{2}}))q(\phi(t_{n+\frac{1}{2}})) - g\left(\frac{\phi_0^{n+1} + \phi^n}{2}\right)q_1^{n+\frac{1}{2}}, e_w^{n+\frac{1}{2}}\right) \\ &\quad + \delta t\left(g(\phi(t_{n+\frac{1}{2}}))\phi_t(t_{n+\frac{1}{2}}) - g\left(\frac{\phi_0^{n+1} + \phi^n}{2}\right)\frac{\phi_1^{n+1} - \phi^n}{\delta t}, e_{1,q}^{n+1} + e_q^n\right). \end{aligned} \quad (67)$$

Applying again the Cauchy-Schwarz, Young's inequality and Lemmas 3.5–3.6, we obtain that

$$\begin{aligned} &\|e_{1,\phi}^{n+1}\|_1^2 - \|e_\phi^n\|_1^2 - \gamma\|e_\phi^n\|^2 + 2\|e_{1,q}^{n+1}\|^2 - 2\|e_q^n\|^2 + \delta t\|e_w^{n+\frac{1}{2}}\|_1^2 \\ &\leq C_{12}\delta t\|e_{1,q}^{n+1}\|^2 + C\delta t(\delta t^4 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2). \end{aligned}$$

Given  $C_{12}\delta t \leq 1$ , we can get

$$\|e_{1,\phi}^{n+1}\|_1^2 \leq \|e_\phi^n\|_1^2 + \gamma\|e_\phi^n\|^2 + 2\|e_q^n\|^2 + C\delta t(\delta t^4 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2). \quad (68)$$

Subtracting Eq. (33) from Eq. (8) at  $t_{n+\frac{1}{2}}$ , we can derive

$$\begin{aligned} &\|e_{i+1,\phi}^{n+1}\|_1^2 - \|e_\phi^n\|_1^2 - \gamma\|e_\phi^n\|^2 + 2\|e_{i+1,q}^{n+1}\|^2 - 2\|e_q^n\|^2 + \delta t\|e_w^{n+\frac{1}{2}}\|_1^2 \\ &\leq C_{13}\delta t\|e_{i+1,q}^{n+1}\|^2 + C\delta t(\delta t^4 + \|e_{i,\phi}^{n+1}\|_1^2 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2). \end{aligned}$$

When  $C_{13}\delta t \leq 1$ , we arrive at

$$\|e_{i+1,\phi}^{n+1}\|_1^2 \leq C_{14}\delta t\|e_{i,\phi}^{n+1}\|_1^2 + C(\delta t^5 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2).$$

It is easy to see that

$$\|e_{i+1,\phi}^{n+1}\|_1^2 \leq h^i\|e_{1,\phi}^{n+1}\|_1^2 + C(\delta t^5 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2)\frac{1-h^i}{1-h}.$$

where  $h = C_{14}\delta t$ , when  $h < 1/2$ , then we get

$$\|e_{i+1,\phi}^{n+1}\|_1^2 \leq \|e_{1,\phi}^{n+1}\|_1^2 + C(\delta t^5 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2), i-1 \leq M. \quad (69)$$

Similarly, subtracting Eq. (35) from Eq. (8), and combining with (68)–(69), we arrive at

$$\begin{aligned} &\|e_\phi^{n+1}\|_1^2 - \|e_\phi^n\|_1^2 + \gamma(\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2) + 2(\|e_q^{n+1}\|^2 - \|e_q^n\|^2) + \delta t\|e_w^{n+\frac{1}{2}}\|_1^2 \\ &\leq C\delta t^5 + C\delta t(\|e_{*,\phi}^{n+1}\|_1^2 + \|e_\phi^n\|_1^2 + \|e_q^{n+1}\|^2) \\ &\leq C\delta t^5 + C\delta t(\|e_q^{n+1}\|_1^2 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2). \end{aligned}$$

Summing up the equation above for  $n = 0, \dots, k$ , we find

$$\|e_\phi^{k+1}\|_1^2 + \|e_q^{k+1}\|^2 + \delta t \sum_{n=1}^k \|e_w^{n+\frac{1}{2}}\|_1^2 \leq C \sum_{n=0}^k (\|e_\phi^n\|_1^2 + \|e_q^n\|^2).$$

Applying Gronwall's lemma, we derive

$$\|e_\phi^{k+1}\|_1^2 + \|e_q^{k+1}\|^2 + \delta t \sum_{n=1}^k \|e_w^{n+\frac{1}{2}}\|_1^2 \leq C\delta t^4.$$

Combining with Eqs. (35) and (8), and we find that

$$\begin{aligned} \|\Delta e_\phi^{n+\frac{1}{2}}\|^2 &\leq C \left( \|\Delta r_2^n\|^2 + \|r_2^n\|^2 + \|r_5^n\|^2 + \|e_\phi^{n+\frac{1}{2}}\|^2 + \|e_w^{n+\frac{1}{2}}\|^2 \right. \\ &\quad \left. + \|g(\phi(t_{n+\frac{1}{2}}))q(t_{n+\frac{1}{2}}) - g(\frac{\phi_*^{n+1} + \phi^n}{2})q^{n+\frac{1}{2}}\|^2 \right) \\ &\leq C\delta t^4. \end{aligned}$$

From Lemma 3.7, we find

$$\|\Delta e_\phi^{k+1}\| \leq C\delta t. \quad (70)$$

On the other hand, it holds that

$$\begin{aligned} \|\phi^{k+1}\|_{L^\infty} &\leq \|e_\phi^{k+1}\|_{L^\infty} + \|\phi(t_{k+1})\|_{L^\infty} \\ &\leq C\|e_\phi^{k+1}\|_1^{\frac{1}{2}}\|e_\phi^{k+1}\|_2^{\frac{1}{2}} + \|\phi(t_{k+1})\|_{L^\infty} \\ &\leq C_{15}\delta t^{\frac{3}{2}} + \|\phi(t_{k+1})\|_{L^\infty}. \end{aligned}$$

Given  $C_{15}\delta t^{\frac{3}{2}} \leq 1$ , we derive

$$\|\phi^{k+1}\|_{L^\infty} \leq 1 + \|\phi(t_{k+1})\|_{L^\infty} \leq \nu.$$

Next we will prove  $\|\phi_{i+1}^{k+2}\|_{L^\infty} \leq \nu$ ,  $0 \leq i \leq M-1$ . Subtracting Eq. (33) from Eq. (8) at  $t_{k+\frac{3}{2}}$ ,  $i = 0$ . Similarly, we can derive

$$\|e_{1,\phi}^{k+2}\|_1^2 + \|e_{1,q}^{k+2}\|^2 + \delta t \|e_w^{k+\frac{3}{2}}\|_1^2 \leq C\delta t^4. \quad (71)$$

Subtracting Eq. (33) from Eq. (8) at  $t_{k+\frac{3}{2}}$ ,  $i = 0$ , we obtain

$$\begin{aligned} \|\Delta e_{1,\phi}^{k+\frac{3}{2}}\|^2 &\leq C \left( \|\Delta r_2^{k+1}\|^2 + \|r_2^{k+1}\|^2 + \|r_5^{k+1}\|^2 + \|e_{1,\phi}^{k+\frac{3}{2}}\|^2 + \|e_w^{k+\frac{3}{2}}\|^2 \right. \\ &\quad \left. + \|g(\phi(t_{k+\frac{3}{2}}))q(t_{k+\frac{3}{2}}) - g(\frac{\phi_0^{k+2} + \phi^{k+1}}{2})q_1^{k+\frac{3}{2}}\|^2 \right) \leq C\delta t^{\frac{9}{4}}. \end{aligned}$$

Combining with (70), we derive  $\|\Delta e_{1,\phi}^{k+2}\| \leq C\delta t$ . Thus

$$\begin{aligned} \|\phi_1^{k+2}\|_{L^\infty} &\leq \|e_{1,\phi}^{k+2}\|_{L^\infty} + \|\phi(t_{k+2})\|_{L^\infty} \\ &\leq C\|e_{1,\phi}^{k+2}\|_1^{\frac{1}{2}}\|e_{1,\phi}^{k+2}\|_2^{\frac{1}{2}} + \|\phi(t_{k+2})\|_{L^\infty} \leq C_{16}\delta t^{\frac{3}{2}} + \|\phi(t_{k+2})\|_{L^\infty}. \end{aligned}$$

Given  $C_{16}\delta t^{\frac{3}{2}} \leq 1$ , we derive

$$\|\phi_1^{k+2}\|_{L^\infty} \leq 1 + \|\phi(t_{k+2})\|_{L^\infty} \leq \nu. \quad (72)$$

Supposing  $\|\phi_i^{k+2}\|_{L^\infty} \leq \nu$ , we will prove  $\|\phi_{i+1}^{k+2}\|_{L^\infty} \leq \nu$  still holds. Similarly, we have

$$\begin{aligned} &\|e_{i+1,\phi}^{k+2}\|_1^2 - \|e_\phi^{k+1}\|_1^2 - \gamma \|e_\phi^{k+1}\|^2 + 2\|e_{i+1,q}^{k+2}\|^2 - 2\|e_q^{k+1}\|^2 + \delta t \|e_w^{k+\frac{3}{2}}\|_1^2 \\ &\leq C_{17}\delta t \|e_{i+1,q}^{k+2}\|^2 + C\delta t(\delta t^4 + \|e_{i,\phi}^{k+2}\|_1^2 + \|e_\phi^{k+1}\|_1^2 + \|e_q^{k+1}\|^2). \end{aligned}$$

Given  $C_{17}\delta t \leq 1$ , we can obtain

$$\|e_{i+1,\phi}^{k+2}\|_1^2 + \|e_{i+1,q}^{k+2}\|^2 + \delta t \|e_w^{k+\frac{3}{2}}\|_1^2 \leq C_{18}\delta t \|e_{i,\phi}^{k+2}\|^2 + C\delta t^4.$$

That is

$$\|e_{i+1,\phi}^{k+2}\|_1^2 + \|e_{i+1,q}^{k+2}\|^2 + \delta t \|e_w^{k+\frac{3}{2}}\|_1^2 \leq l^i \|e_{1,\phi}^{k+2}\|_1^2 + C\delta t^4 \frac{1-l^i}{1-l},$$

where  $l = C_{18}\delta t$ . When  $l < 1/2$ , we get

$$\|e_{i+1,\phi}^{k+2}\|_1^2 + \|e_{i+1,q}^{k+2}\|^2 + \delta t \|e_w^{k+\frac{3}{2}}\|_1^2 \leq C\delta t^4.$$

Thus, we find

$$\begin{aligned} \|\Delta e_{i+1,\phi}^{k+2} + \Delta e_{\phi}^{k+1}\|^2 &\leq C \left( \|\Delta r_2^{k+1}\|^2 + \|r_2^{k+1}\|^2 + \|r_5^{k+1}\|^2 + \|e_{i+1,\phi}^{k+\frac{3}{2}}\|^2 + \|e_w^{k+\frac{3}{2}}\|^2 \right. \\ &\quad \left. + 2\|g(\phi(t_{k+\frac{3}{2}}))q(t_{k+\frac{3}{2}}) - g(\frac{\phi_i^{k+2} + \phi^{k+1}}{2})q_{i+1}^{k+\frac{3}{2}}\|^2 \right) \leq C\delta t^{\frac{9}{4}}. \end{aligned}$$

Then, we derive  $\|\Delta e_{i+1,\phi}^{k+2}\| \leq C\delta t$ . Furthermore

$$\begin{aligned} \|\phi_{i+1,\phi}^{k+2}\|_{L^\infty} &\leq \|e_{i+1,\phi}^{k+2}\|_{L^\infty} + \|\phi(t_{k+2})\|_{L^\infty} \\ &\leq C_\Omega \|e_{i+1,\phi}^{k+2}\|_1^{\frac{1}{2}} \|e_{i+1,\phi}^{k+2}\|_2^{\frac{1}{2}} + \|\phi(t_{k+2})\|_{L^\infty} \leq C_{19}\delta t^{\frac{3}{2}} + \|\phi(t_{k+2})\|_{L^\infty}. \end{aligned}$$

Given  $C_{19}\delta t^{\frac{3}{2}} \leq 1$ , we derive  $\|\phi_{i+1,\phi}^{k+2}\|_{L^\infty} \leq 1 + \|\phi(t_{k+2})\|_{L^\infty} \leq \nu$ . This concludes the proof.  $\square$

**Remark 3.9.** Our algorithm can also be extended to other schemes with various predictors. For a given predictor algorithm, we only need the infinite norm of predictor  $\phi_*^{n+1}$  is uniformly bounded, which is usually true. Then we can prove that the numerical solution  $\phi^{n+1}$  from the corrected step also satisfies the infinite norm uniformly bounded.

**Theorem 3.10** (Error Estimate). *Scheme 3.7 is second-order convergent in time. In particular, under the assumption of Lemma 3.8, we have*

$$\|\phi(t_{k+1}) - \phi^{k+1}\|_1 + \|q(\phi(t_{k+1})) - q(\phi^{k+1})\| + \delta t \sum_{n=0}^k \|w(t_{n+\frac{1}{2}}) - w^{n+\frac{1}{2}}\|_1 \leq C\delta t^2. \quad (73)$$

**Proof.** Subtracting Eq. (33) from Eq. (8) at  $t_{n+\frac{1}{2}}$ , and taking the  $L^2$  inner product with  $\varphi$ ,  $\theta$ ,  $\psi$ , respectively,

$$\left( \frac{e_{i+1,\phi}^{n+1} - e_{\phi}^n}{\delta t}, \varphi \right) = -(\nabla e_w^{n+\frac{1}{2}}, \nabla \varphi) + (r_1^n - \Delta r_5^n, \varphi), \quad (74)$$

$$\begin{aligned} (e_w^{n+\frac{1}{2}}, \theta) &= (r_5^n + \Delta r_2^n - \gamma r_2^n, \theta) + \gamma \left( \frac{e_{i+1,\phi}^{n+1} + e_{\phi}^n}{2}, \theta \right) + \left( \nabla \frac{e_{i+1,\phi}^{n+1} + e_{\phi}^n}{2}, \nabla \theta \right) \\ &\quad + \left( g(\phi(t_{n+\frac{1}{2}}))q(\phi(t_{n+\frac{1}{2}})) - g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)q_{i+1}^{n+\frac{1}{2}}, \theta \right), \end{aligned} \quad (75)$$

$$\left( \frac{e_{i+1,q}^{n+1} - e_q^n}{\delta t}, \psi \right) = (r_3^n, \psi) + \frac{1}{2} \left( g(\phi(t_{n+\frac{1}{2}}))\phi_t(t_{n+\frac{1}{2}}) - g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)\frac{\phi_{i+1}^{n+1} - \phi^n}{\delta t}, \psi \right). \quad (76)$$

Taking  $\varphi = \delta t(e_{i+1,\phi}^{n+1} + e_{\phi}^n)$ ,  $2\delta t e_w^{n+\frac{1}{2}}$  in Eq. (74),  $\theta = 2(e_{i+1,\phi}^{n+1} - e_{\phi}^n)$ ,  $2\delta t e_w^{n+\frac{1}{2}}$  in Eq. (75),  $\psi = 2\delta t(e_{i+1,q}^{n+1} + e_q^n)$  in Eq. (76). Following the previous proof, we arrive at

$$\begin{aligned} &\|e_{i+1,\phi}^{n+1}\|_1^2 - \|e_{\phi}^n\|_1^2 + \gamma(\|e_{i+1,\phi}^{n+1}\|^2 - \|e_{\phi}^n\|^2) + 2\delta t\|e_w^{n+\frac{1}{2}}\|_1^2 + 2(\|e_{i+1,q}^{n+1}\|^2 - \|e_q^n\|^2) \\ &= \delta t(r_1^n - \Delta r_5^n, e_{i+1,\phi}^{n+1} + e_{\phi}^n) + 2\delta t(r_1^n - \Delta r_5^n, e_w^{n+\frac{1}{2}}) + 2\delta t(r_3^n, e_{i+1,q}^{n+1} + e_q^n) \\ &\quad - 2(r_5^n + \Delta r_2^n - \gamma r_2^n, e_{i+1,\phi}^{n+1} - e_{\phi}^n) + 2\delta t(r_5^n + \Delta r_2^n - \gamma r_2^n, e_w^{n+\frac{1}{2}}) \\ &\quad - 2\left(g(\phi(t_{n+\frac{1}{2}}))q(\phi(t_{n+\frac{1}{2}})) - g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)q_{i+1}^{n+\frac{1}{2}}, e_{i+1,\phi}^{n+1} - e_{\phi}^n\right) \\ &\quad + 2(g(\phi(t_{n+\frac{1}{2}}))q(\phi(t_{n+\frac{1}{2}})) - g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)q_{i+1}^{n+\frac{1}{2}}, e_w^{n+\frac{1}{2}}) \\ &\quad + \delta t(g(\phi(t_{n+\frac{1}{2}}))\phi_t(t_{n+\frac{1}{2}}) - g\left(\frac{\phi_i^{n+1} + \phi^n}{2}\right)\frac{\phi_{i+1}^{n+1} - \phi^n}{\delta t}, e_{i+1,q}^{n+1} + e_q^n). \end{aligned} \quad (77)$$

Using Cauchy–Schwarz, Young’s inequality, and Lemma 3.8, we get that

$$\begin{aligned} &\|e_{i+1,\phi}^{n+1}\|_1^2 - \|e_{\phi}^n\|_1^2 - \gamma\|e_{\phi}^n\|^2 + 2\|e_{i+1,q}^{n+1}\|^2 - 2\|e_q^n\|^2 + \delta t\|e_w^{n+\frac{1}{2}}\|_1^2 \\ &\leq C_{20}\delta t\|e_{i+1,q}^{n+1}\|^2 + C\delta t(\delta t^4 + \|e_{i,\phi}^{n+1}\|_1^2 + \|e_{\phi}^n\|_1^2 + \|e_q^n\|^2). \end{aligned}$$

When  $C_{20}\delta t \leq 1$ , we obtain that

$$\|e_{i+1,\phi}^{n+1}\|_1^2 \leq C_{21}\delta t\|e_{i,\phi}^{n+1}\|_1^2 + C(\delta t^5 + \|e_{\phi}^n\|_1^2 + \|e_{\phi}^{n-1}\|_1^2 + \|e_q^n\|^2).$$

That is

$$\|e_{i+1,\phi}^{n+1}\|_1^2 \leq z^i \|e_{1,\phi}^{n+1}\|_1^2 + C(\delta t^5 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2) \left( \frac{1-z^i}{1-z} \right),$$

with  $z = C_{21}\delta t$ , when  $z < 1/2$ , we have

$$\|e_{i+1,\phi}^{n+1}\|_1^2 \leq \|e_{1,\phi}^{n+1}\|_1^2 + C(\delta t^5 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2).$$

Similarly, subtracting Eq. (35) from Eq. (8), and noticing (68), we arrive at

$$\begin{aligned} & \|e_\phi^{n+1}\|_1^2 - \|e_\phi^n\|_1^2 + \gamma(\|e_\phi^{n+1}\|^2 - \|e_\phi^n\|^2) + 2(\|e_q^{n+1}\|^2 - \|e_q^n\|^2) + \delta t \|e_w^{n+\frac{1}{2}}\|_1^2 \\ & \leq C\delta t^5 + C\delta t(\|e_{1,\phi}^{n+1}\|_1^2 + \|e_\phi^n\|_1^2 + \|e_q^{n+1}\|^2) \\ & \leq C\delta t^5 + C\delta t(\|e_q^{n+1}\|^2 + \|e_\phi^n\|_1^2 + \|e_\phi^{n-1}\|_1^2 + \|e_q^n\|^2). \end{aligned}$$

Summing up above equation for  $n = 0, \dots, k$ , we find

$$\|e_\phi^{k+1}\|_1^2 + \|e_q^{k+1}\|^2 + \delta t \sum_{n=1}^k \|e_w^{n+\frac{1}{2}}\|_1^2 \leq C \sum_{n=0}^k (\|e_\phi^n\|_1^2 + \|e_q^{n+1}\|^2).$$

Applying Gronwall's lemma, we have

$$\|e_\phi^{k+1}\|_1^2 + \|e_q^{k+1}\|^2 + \delta t \sum_{n=1}^k \|e_w^{n+\frac{1}{2}}\|_1^2 \leq C\delta t^4.$$

Then, we get the desired result.  $\square$

#### 4. Numerical examples

In this section, we present some numerical experiments to verify our theoretical results. In all the numerical examples below, we set the numerical stopping criterion as  $N = 10$  and  $\varepsilon_0 = 10^{-12}$ .

##### 4.1. Spatial discretization

For the spatial discretization, we choose the standard second-order compact central finite difference method. Mainly consider a rectangular domain  $\Omega = [0, L_x] \times [0, L_y]$ . We discretize it with uniform meshes. Interested readers can refer to [45–47] for details.

##### 4.2. Temporal and spatial convergence test

Consider the C.H. equation

$$\begin{cases} \partial_t \phi = \lambda \Delta w, \\ w = -\varepsilon^2 \Delta \phi + \phi^3 - \phi, \end{cases}$$

subject to the boundary conditions

$$(i) \phi, w \text{ are periodic ; or } (ii) \partial_n \phi|_{\partial\Omega} = \partial_n w|_{\partial\Omega} = 0. \quad (78)$$

This is derived by choosing the free energy  $E = \int_\Omega \frac{\varepsilon^2}{2} |\nabla \phi|^2 + \frac{1}{4}(\phi^2 - 1)^2 d\mathbf{x}$  and taking the  $H^{-1}$  gradient flow with mobility  $\lambda$ . We can reformulate it with IEQ method by introducing the auxiliary variable  $q$  and the function  $g(\phi)$  are derived as

$$q = \frac{1}{2}(\phi^2 - 1 - \gamma), \quad g(\phi) = 2\phi. \quad (79)$$

Consider the square domain  $[0, 1] \times [0, 1]$  with  $512 \times 512$  uniform meshes. The initial profile for  $\phi$  is chosen as

$$\phi(\mathbf{x}, t = 0) = 0.45 \cos(4\pi x) \cos(4\pi y). \quad (80)$$

The model parameters are chosen as  $\varepsilon = 10^{-2}$ ,  $\lambda = 10^{-2}$  and  $\gamma = 1$ .

**Scheme 3.1** is tested first. First of all, we present the time convergence test. For simplicity, we only show the results for the case with periodic boundary conditions. The convergence rates are summarized in the left part of Table 1, where we observe second-order convergence when the time-step is small enough, which is consistent with our theoretical results. Then we test the predictor–corrector C.N. **Scheme 3.7** with the same initial values and parameters as above. The result is summarized in the right part of Table 1, where we observe robust second-order convergence in time, even with large

**Table 1**

The  $L^2$  numerical errors of  $\phi$  at  $t = 0.5$  are computed by linear CN Scheme 3.1 and the predictor–corrector CN Scheme 3.4 using various temporal resolutions.

$\delta t$	Linear CN Scheme 3.1		Predictor–corrector CN Scheme 3.7	
	$L^2$ – Error	Order	$L^2$ – Error	Order
0.2	6.5620		0.4236	
0.1	2.5722	1.351	0.1070	1.984
0.05	0.7780	1.725	0.0267	2.003
0.025	0.2085	1.900	0.0067	2.001
0.0125	0.0534	1.963	0.0017	2.001
0.00625	0.0135	1.989	0.0004	2.004
0.003125	0.0033	2.010	0.0001	2.016

**Table 2**

Spatial mesh refinement test for  $\phi$  at  $t = 0.5$ . The results are calculated using predictor–corrector CN Scheme 3.7.

$N$	Error		Order	
	$L^\infty$	$L^2$	$L^\infty$	$L^2$
64	–	–	–	–
192	6.5018	2.6455	–	–
320	0.2818	0.1375	1.9553	2.4341
448	0.0746	0.0372	2.0096	2.0501
576	0.0303	0.0153	2.0048	2.0218
704	0.0153	0.0077	2.0029	2.0124

time-step sizes. By comparing the results in Table 1, we observe that the predictor–corrector schemes reach the optimal second-order convergence rate faster than the linear IEQ schemes.

Next, we conduct the mesh refinement test using predictor–corrector C.N. Scheme 3.7. We use the same model, parameters, and other settings as above. To avoid the temporal errors affecting the spatial convergence results, we use a small time-step  $\delta t = 10^{-4}$ , along with various  $N^2$  spatial meshes, where we choose  $N = 64, 192, 320, 448, 576$  and  $704$ . The errors are calculated as the difference between numerical solutions by adjacent meshes at the coarse  $64^2$  mesh points. The results are summarized in Table 2. It is shown that the numerical schemes have second-order accuracy in space in both  $L^2$  norms and  $L^\infty$  norm.

#### 4.3. Coarsening dynamics

In this section, we further test predictor–corrector Scheme 3.7 on the coarsening dynamics. We use the same model as above, and choose the domain as  $[0, 2\pi] \times [0, 2\pi]$  with  $512 \times 512$  uniform meshes. The initial profile

$$\phi(x, t = 0) = 10^{-3} \text{rand}(-1, 1) \quad (81)$$

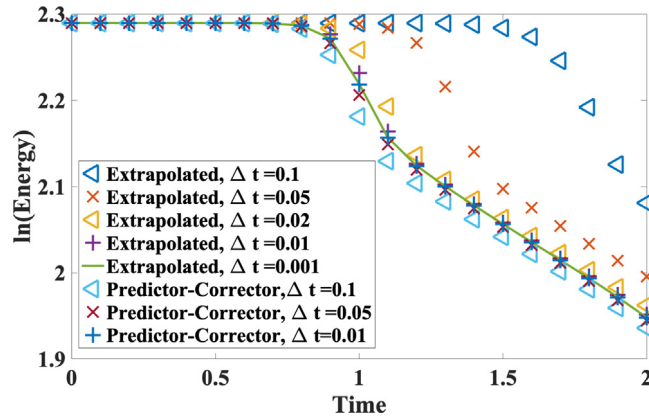
is used, and the model parameters are  $\gamma = 1$ ,  $\lambda = 0.1$  and  $\varepsilon = 0.05$ .

In the first case, we pick the periodic boundary condition. We test both IEQ CN Scheme 3.1 and the fixed-point predictor–corrector CN Scheme 3.7 with different time-step sizes. The results are summarized in Fig. 1. When the time-step is large (saying  $\delta t = 0.1$ ), even though Scheme 3.1 preserves the energy dissipating property, its numerical predicted energy is already largely deviated from the correct energy, as shown in Fig. 1. When the time-step size is small enough (saying  $\delta t = 0.01$ ), IEQ CN Scheme 3.1 predicts accurate results. On the contrary, for fixed-point predictor–corrector C.N. Scheme 3.7, its numerical prediction is already accurate enough even with large time-step  $\delta t = 0.1$ , i.e., the predictor–corrector scheme provides better numerical accuracy at large time-step size.

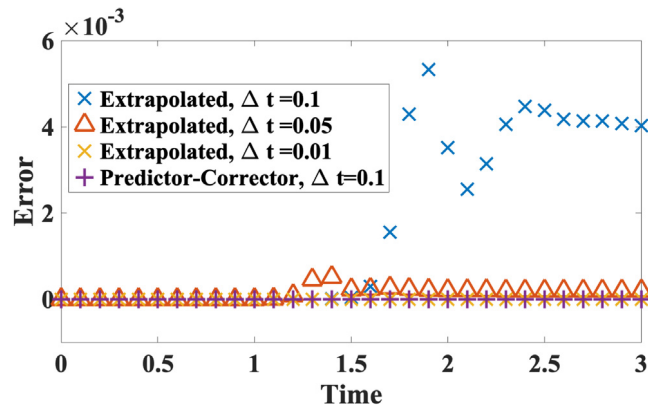
To better compare these two schemes, the  $L^2$  norm on the difference between numerical solution  $q$  and Eq. (79) (the original definition of  $q$ ) are summarized in Fig. 2. Notice, due to the numerical discretization for the equation of  $q$ , numerical truncation errors are introduced inevitably. We observe, when the time-step is large, Scheme 3.1 introduces large errors, deviating  $q$  from its original definition (79). On the other hand, for the predictor–corrector Scheme 3.7, it predicts dramatically accurate results, that is the errors between  $q$  and (79) are negligible.

From the comparisons above, we observe predictor–corrector Scheme 3.7 predicts accurate numerical results. In addition, using Scheme 3.7, with  $512^2$  meshes and time-step size  $\delta t = 10^{-2}$ , we simulate the long-time coarsening dynamics, where the results are summarized in Fig. 3. We observe the two phases evolve and separate with time passing by. Eventually, it reaches a steady state, where a trip pattern is formed by noticing the periodic boundary condition. The numerical solver captures the phase separation properly, i.e., it demonstrates the effectiveness of the newly proposed predictor–corrector schemes.





**Fig. 1.** Comparisons of the calculated energies using different numerical schemes with various time-step sizes. In this figure, the numerical energies using linear CN Scheme 3.1 and predictor–corrector CN Scheme 3.7 with different time-step sizes are summarized together.



**Fig. 2.** Numerical error between  $q$  and its original definition in (79). This figure shows that large time-step size would introduce numerical error for  $q$ , so that it deviates from its original definition in Eq. (79). But the predictor–corrector scheme provides more accurate results.

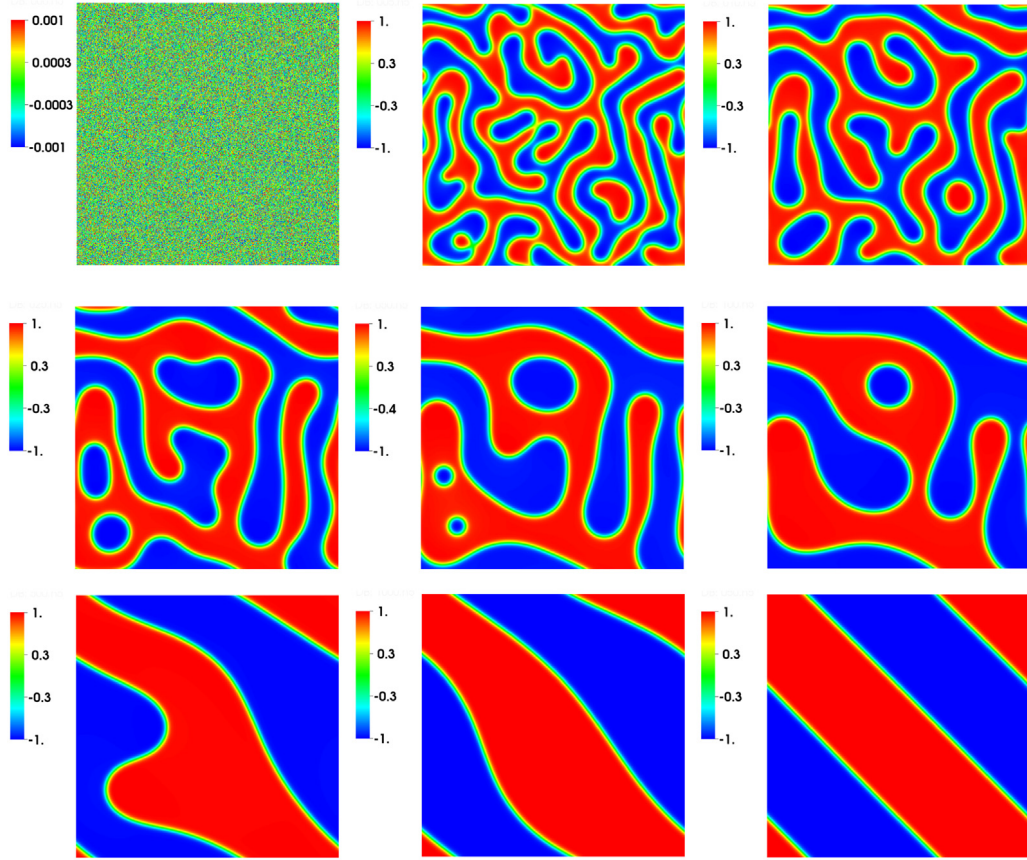
In addition, we study the coarsening dynamics with the same model parameters as above, but with Neumann boundary condition. We use predictor–corrector Scheme 3.7, along with  $512^2$  meshes and time-step  $\delta t = 10^{-2}$ . The simulation results are summarized in Fig. 4. We notice that when we use the physical boundary condition, it resolve different dynamics (due to the interaction with boundaries). Mainly, we observe dramatically different coarsening dynamics with different boundary conditions, and the dynamics evolve slower than the case with periodic boundary condition, as it does not reach the equilibrium state at  $t = 10\,000$ , but the case with periodic boundary condition already reaches the equilibrium state at  $t = 5000$  as shown in Fig. 3.

#### 4.4. Coarsening dynamics of the Cahn–Hilliard equation with the Flory–Huggins bulk potential

Notice that, in the proposed numerical schemes and error estimates, the explicit expression of the bulk potential is not specified. Thus, the proposed numerical methodology applies to a wide class of problems. To demonstrate it, we use the proposed numerical scheme to solve the Cahn–Hilliard equation with the Flory–Huggins bulk potential in this section.

This Flory–Huggins bulk potential is derived from studying the polymer solutions, which takes account of the differences of molecular sizes in the solvent and solute. The expression of the Flory–Huggins bulk free energy functional is derived as

$$F(\phi) = \frac{1}{N_1} \phi \ln \phi + \frac{1}{N_2} (1 - \phi) \ln(1 - \phi) + \chi \phi(1 - \phi), \quad (82)$$



**Fig. 3.** Coarsening dynamics using the C.H. equation with the periodic boundary condition. The profile of  $\phi$  at time slots  $t = 0, 5, 10, 50, 100, 500, 1000, 5000$  are shown.

where  $N_1$  and  $N_2$  are the molecular sizes for the two phases, and  $\chi$  is a mixing parameter. Consider the C.H. equation

$$\begin{cases} \partial_t \phi = \lambda \Delta w, \\ w = -\varepsilon^2 \Delta \phi + \left( \frac{1}{N_1} \phi \ln \phi + \frac{1}{N_2} (1 - \phi) \ln(1 - \phi) + \chi \phi(1 - \phi) \right), \end{cases}$$

with periodic boundary condition.

Following the energy quadratization idea in previous sections, we introduce the auxiliary variable  $q$  and function  $g$  as follows

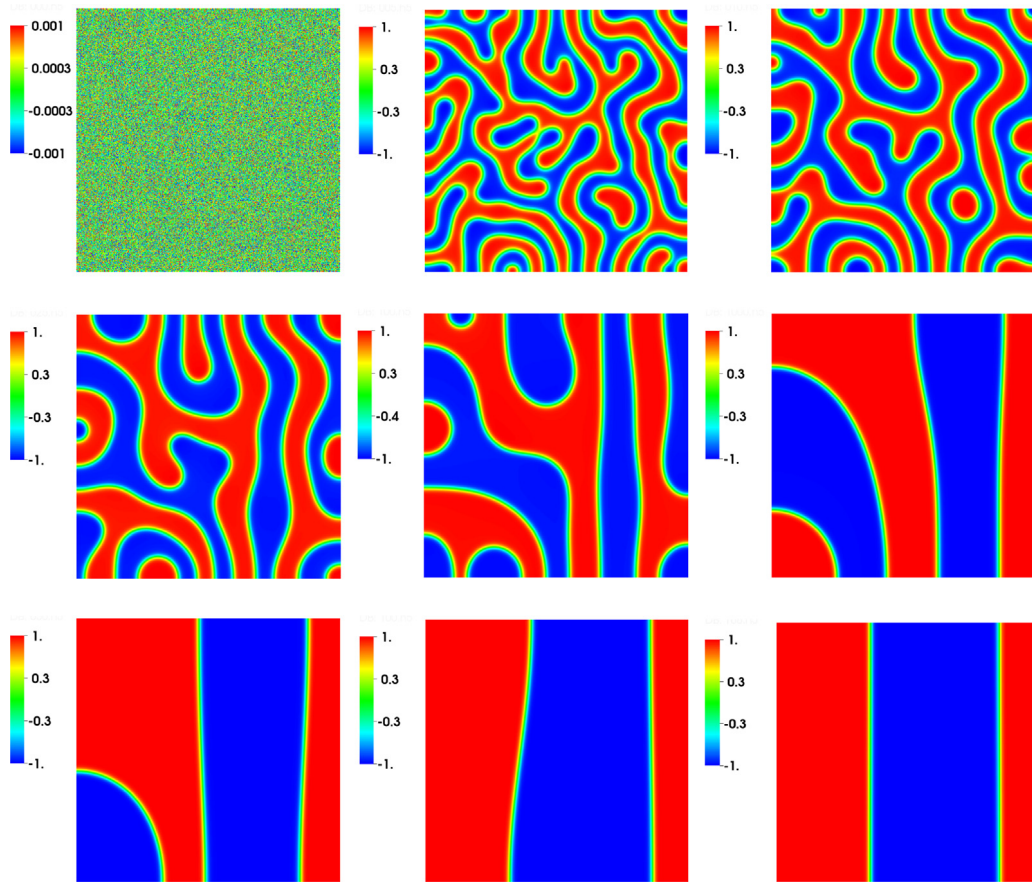
$$q = \sqrt{F - \frac{1}{2} \gamma \phi^2 + B}, \quad g(\phi) = 2 \frac{\partial q}{\partial \phi} = \frac{\frac{\partial F}{\partial \phi} - \gamma \phi}{\sqrt{F - \frac{1}{2} \gamma \phi^2 + B}}. \quad (83)$$

We remark that, during numerical calculation, there might exist singularity due to the logarithm function in  $g$ . We can regularize  $g$  as

$$g(\phi) = \frac{\partial q}{\partial \phi} = \frac{\frac{\partial \hat{F}}{\partial \phi} - \gamma \phi}{\sqrt{\hat{F} - \frac{1}{2} \gamma \phi^2 + B}}, \quad (84)$$

where the regularized  $\hat{F}$  is defined by

$$\hat{F}(\phi) = \begin{cases} \frac{1}{N_1} \phi \ln \phi + \frac{1}{N_2} \left[ \frac{(1-\phi)^2}{2\sigma} + (1-\phi) \ln \sigma - \frac{\sigma}{2} \right] + \chi \phi(1-\phi), & \text{if } \phi \geq 1-\sigma, \\ \frac{1}{N_1} \phi \ln \phi + \frac{1}{N_2} (1-\phi) \ln(1-\phi) + \chi \phi(1-\phi), & \text{if } \sigma \leq \phi \leq 1-\sigma, \\ \frac{1}{N_1} \left[ \frac{\phi^2}{2\sigma} + \phi \ln \sigma - \frac{\sigma}{2} \right] + \frac{1}{N_2} (1-\phi) \ln(1-\phi) + \chi \phi(1-\phi), & \text{if } \phi \leq \sigma. \end{cases} \quad (85)$$



**Fig. 4.** Coarsening dynamics using the C.H. equation with Neumann boundary condition. The profile of  $\phi$  at time slots  $t = 0, 5, 10, 25, 100, 1000, 5000, 10\,000, 26\,800$  are shown.

Consider the initial profile  $\phi(\mathbf{x}, t = 0) = 0.3 + 0.001\text{rand}(-1, 1)$  and domain  $[0, 20] \times [0, 20]$ . We use the model parameters  $\chi = 2.5$ ,  $N_1 = N_2 = 1$ ,  $\lambda = 1$ ,  $\varepsilon = 0.05$ ,  $\gamma = 1$ ,  $\sigma = 10^{-3}$  and  $B = 10$ .

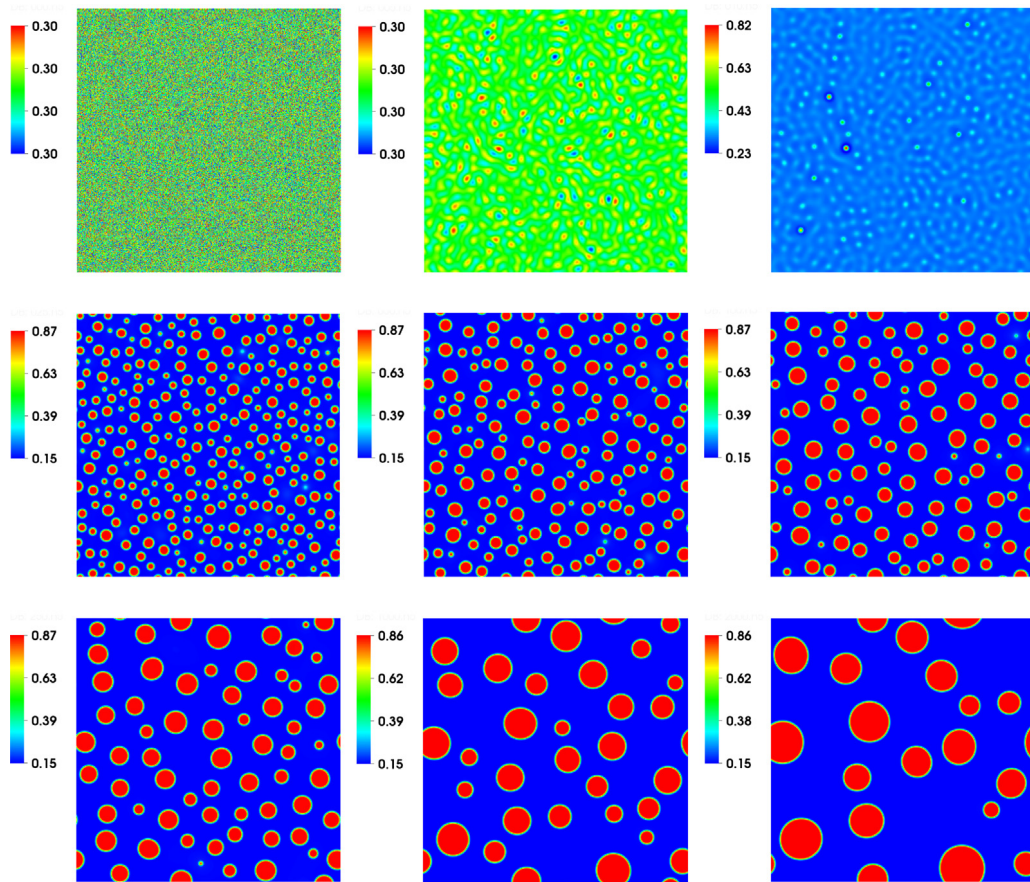
In this case, we consider the periodic boundary condition. We use predictor–corrector Scheme 3.7, along with  $512^2$  meshes and time-step  $\delta t = 10^{-3}$ . The coarsening dynamics with the Flory–Huggins bulk potential are summarized in Fig. 5. We observe phase transitions with a huge quantity of small droplets emerging, which is dramatically different from the coarsening dynamics predicted by the Cahn–Hilliard equation with the double-well potential.

## 5. Conclusion

The C.H. equation, one of the most important equations in phase-field models, has been widely used to study a variety of applications in the fields of biology, engineering, material science, soft matter physics, and many others. One of the existing critical numerical issues is to develop unconditionally energy stable numerical approximation, such that large time-step is durable. In this article, we construct a class of predictor–corrector schemes, improving the accuracy of the schemes derived from the energy quadratization approach. Rigorous results on convergence and error estimates are obtained, showing the second-order convergence of our proposed predictor–corrector schemes. In particular, as the linear IEQ schemes are special cases of our general predictor–corrector schemes, our theoretical results also apply directly to linear IEQ schemes. Besides, due to the generality of the theoretical and numerical strategy, the results in this paper could be readily used to propose unconditionally energy stable numerical approximations for other phase-field models or gradient flow models, and conduct rigorous convergence and error estimate as well. These topics will be pursued in our later research.

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**Fig. 5.** Coarsening dynamics using the C.H. equation with the Flory–Huggins free energy. This profile of  $\phi$  at time  $t = 0, 0.5, 1, 2.5, 5, 10, 25, 100, 200$  are shown.

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