

# Efficient linear and unconditionally energy stable schemes for the modified phase field crystal equation

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**Abstract** In this paper, we construct efficient schemes based on the scalar auxiliary variable block-centered finite difference method for the modified phase field crystal equation, which is a sixth-order nonlinear damped wave equation. The schemes are linear, conserve mass and unconditionally dissipate a pseudo energy. We prove rigorously second-order error estimates in both time and space for the phase field variable in discrete norms. We also present some numerical experiments to verify our theoretical results and demonstrate the robustness and accuracy.

**Keywords** modified phase field crystal, scalar auxiliary variable, energy stability, error estimate, numerical experiments

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## 1 Introduction

The phase field crystal (PFC) model was developed in [3, 4] to model the crystallization process in the purification of solid compounds. It has been used to model the evolution of the atomic-scale crystal growth on diffusive time scales. In the PFC model, the phase field variable is introduced to describe the phase transition from the liquid phase to the crystal phase. The model is versatile and able to simulate various phenomena, such as grain growth, epitaxial growth, reconstructive phase transitions, material hardness and crack propagations. Numerical methods and simulations for the PFC model have been studied extensively, including the finite element method [5], the finite difference method [12, 18, 20], the local discontinuous Galerkin method [6] and the Fourier-spectral method [10, 19].

The modified phase field crystal (MPFC) equation was introduced in [15] to model phase-field crystals with elastic interactions. The MPFC equation can be viewed as a perturbed gradient flow with respect to a free energy, and is a sixth-order nonlinear damped wave equation. However, as pointed out in [16], the original free energy of the MPFC equation may increase in time on some time intervals. Thus, a pseudo energy is introduced in [16] and shown to be dissipative. There exist a number of works on the numerical

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approximations of the MPFC model. First- and second-order accurate nonlinear convex splitting schemes have been proposed in [2, 16], and are proved to be unconditionally energy stable and convergent. A nonlinear multigrid method is used to solve the nonlinear system at each time step [1]. Guo and Xu [7] developed first- and second-order nonlinear convex splitting schemes and a first-order linear energy stable scheme, coupled with local discontinuous Galerkin (LDG) methods in space. Very recently, Li et al. [8] proposed unconditionally energy stable schemes based on the “invariant energy quadratization” (IEQ) approach for the MPFC model but without the convergence proof. The convergence analysis is challenging due to the nonlinear hyperbolic nature of the MPFC equation. To the best of our knowledge, there is no second-order convergence analysis on any linear scheme for the MPFC equation.

The main goals of this paper are to construct linear and unconditionally energy stable schemes based on the recently proposed scalar auxiliary variable (SAV) approach [13, 14], and to carry out a rigorous error analysis. More specifically, we construct two SAV block-centered finite difference schemes for the MPFC equation based on the Euler backward and Crank-Nicolson schemes, respectively, and show that they are unconditionally energy stable with a suitably defined pseudo energy. In addition, we establish second-order convergence in both time and space in a discrete  $L^\infty(0, T; H^3(\Omega))$  norm.

The rest of the paper is organized as follows. In Section 2, we describe the MPFC model and reformulate it using the SAV approach. In Section 3, we construct fully discrete schemes for the reformulated MPFC equation by the block-centered finite difference method, and show that the scheme conserves mass and is unconditionally energy stable. In Section 4, we derive the error estimate for the MPFC model. In Section 5, some numerical experiments are presented to verify the accuracy of the proposed numerical schemes. In Section 6, we give a summary.

## 2 The MPFC model and its semi-discretization in time

We describe in this section the MPFC model and its reformulation using the SAV approach, construct a second-order SAV semi-discretization scheme and show that it preserves mass and dissipates a pseudo energy.

### 2.1 The MPFC model and its SAV reformulation

Consider the free energy (see [1, 2, 7])

$$E(\phi) = \int_{\Omega} \left\{ \frac{1}{2}(\Delta\phi)^2 - |\nabla\phi|^2 + \frac{\alpha}{2}\phi^2 + F(\phi) \right\} d\mathbf{x}, \quad (2.1)$$

where  $\Omega \subset \mathbb{R}^d$  ( $d = 1, 2, 3$ ). The phase field variable  $\phi$  is introduced to represent the concentration field of a coarse-grained temporal average of the density of atoms. It holds that  $F(\phi) = \frac{1}{4}\phi^4$ . Here,  $\alpha = 1 - \epsilon$  with  $\epsilon \ll 1$ . Then the MPFC model is designed to describe the elastic interactions

$$\begin{cases} \frac{\partial^2 \phi}{\partial t^2} + \beta \frac{\partial \phi}{\partial t} = M \Delta \mu, & \mathbf{x} \in \Omega, \quad t > 0, \\ \mu = \Delta^2 \phi + 2\Delta\phi + \alpha\phi + F'(\phi), & \mathbf{x} \in \Omega, \quad t > 0, \\ \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \end{cases} \quad (2.2)$$

where  $\beta > 0$ . The PFC and MPFC equations have close relationship. However, we should keep in mind that the original energy (2.1) of the MPFC equation may increase in time on some time intervals. Thus, it is desirable to introduce a pseudo energy. Besides, we can observe that (2.2) does not satisfy the mass conservation due to the term  $\frac{\partial^2 \phi}{\partial t^2}$ . However, it is possible to verify that  $\int_{\Omega} \frac{\partial \phi}{\partial t} d\mathbf{x} = 0$  with a suitable initial condition for  $\frac{\partial \phi}{\partial t}$ . In what follows, similar to [1, 8], we can simply set  $\frac{\partial \phi}{\partial t}(x, 0) = 0$  point-wise so that  $\int_{\Omega} \frac{\partial \phi}{\partial t}(x, 0) d\mathbf{x} = 0$  is trivially satisfied.

To fix the idea, we consider the homogeneous Neumann boundary conditions

$$\partial_{\mathbf{n}} \phi|_{\partial\Omega} = 0, \quad \partial_{\mathbf{n}} \Delta \phi|_{\partial\Omega} = 0, \quad \partial_{\mathbf{n}} \mu|_{\partial\Omega} = 0, \quad (2.3)$$

where  $\mathbf{n}$  is the unit outward normal vector of the domain  $\Omega$ .

**Remark 2.1.** The homogeneous Neumann boundary conditions are assumed to simplify the presentation. The algorithm and its analysis also hold for the periodic boundary conditions with very little modification. One can refer to [17, Lemma 3.6] for more details about the periodic boundary conditions. While we only present the algorithm and analysis for homogeneous Neumann boundary conditions, we do present some numerical results with periodic boundary conditions in Section 5.

To introduce an appropriate pseudo energy for the MPFC equation, we need to define the  $H^{-1}$  inner-product [1]. Let  $\Omega$  be a bounded domain with the Lipschitz continuous boundary and

$$u_1, u_2 \in \left\{ f \in L^2(\Omega) \mid \int_{\Omega} f d\mathbf{x} = 0 \right\} =: L_0^2(\Omega).$$

We define  $\eta_{u_i} \in H^2(\Omega) \cap L_0^2(\Omega)$  to be the unique solution to the following problem:

$$-\Delta \eta_{u_i} = u_i \quad \text{in } \Omega, \quad \partial_{\mathbf{n}} \eta_{u_i} |_{\partial\Omega} = 0, \quad i = 1, 2. \tag{2.4}$$

Then we have  $\eta_{u_i} = -\Delta^{-1} u_i$ . Define

$$(u_1, u_2)_{H^{-1}} := (\nabla \eta_{u_1}, \nabla \eta_{u_2})_{L^2}. \tag{2.5}$$

By using the integration by parts, we can obtain

$$(u_1, u_2)_{H^{-1}} = -(\Delta^{-1} u_1, u_2)_{L^2} = -(\Delta^{-1} u_2, u_1)_{L^2} = (u_2, u_1)_{H^{-1}}. \tag{2.6}$$

Then we define  $\|u\|_{H^{-1}} = \sqrt{(u, u)_{H^{-1}}}$  for every  $u \in L_0^2(\Omega)$ .

In order to construct an efficient scheme for the MPFC equation (2.2), we first reformulate it using the so-called SAV approach [13]. Introduce two auxiliary functions as follows:

$$\psi = \frac{\partial \phi}{\partial t}, \quad r = \sqrt{E_1(\phi)} := \sqrt{\int_{\Omega} F(\phi) d\mathbf{x}}. \tag{2.7}$$

Then the MPFC equation (2.2) can be recast as the following system:

$$\frac{\partial \psi}{\partial t} + \beta \psi = M \Delta \mu, \tag{2.8a}$$

$$\mu = \Delta^2 \phi + 2\Delta \phi + \alpha \phi + \frac{r(t)}{\sqrt{E_1(\phi)}} F'(\phi), \tag{2.8b}$$

$$r_t = \frac{1}{2\sqrt{E_1(\phi)}} \int_{\Omega} F'(\phi) \phi_t d\mathbf{x}. \tag{2.8c}$$

Next, we derive that the MPFC system (2.8) is mass conserving with the initial condition  $\int_{\Omega} \psi(x, 0) d\mathbf{x} = 0$ . To prove this, integrating (2.8a) over  $\Omega$  and taking notice of (2.3) lead to

$$\frac{d}{dt} \int_{\Omega} \psi(x, t) d\mathbf{x} + \beta \int_{\Omega} \psi(x, t) d\mathbf{x} = M \int_{\partial\Omega} \nabla \mu \cdot \mathbf{n} ds = 0. \tag{2.9}$$

Since (2.9) is actually an ODE system for time, we can easily obtain the solution

$$\int_{\Omega} \psi(x, t) d\mathbf{x} = \exp(-\beta t) \int_{\Omega} \psi(x, 0) d\mathbf{x}. \tag{2.10}$$

Thus we can obtain the desired mass conservation

$$\int_{\Omega} \frac{\partial \phi}{\partial t}(x, t) d\mathbf{x} = \int_{\Omega} \psi(x, t) d\mathbf{x} = 0 \tag{2.11}$$

under the condition  $\int_{\Omega} \psi(x, 0) d\mathbf{x} = 0$ .

Define the pseudo energy

$$\mathcal{E}(\phi, r, \psi) = \int_{\Omega} \left( \frac{1}{2}(\Delta\phi)^2 - |\nabla\phi|^2 + \frac{\alpha}{2}\phi^2 \right) d\mathbf{x} + r^2 + \frac{1}{2M}\|\psi\|_{H^{-1}}^2, \quad (2.12)$$

which requires that  $\int_{\Omega} \psi = 0$  for well-posedness. As long as  $\psi = \frac{\partial\phi}{\partial t}$  is of mean zero, we can obtain the following dissipation law:

$$\begin{aligned} \frac{d}{dt}\mathcal{E}(\phi, r, \psi) &= \int_{\Omega} \mu \frac{\partial\phi}{\partial t} d\mathbf{x} - \frac{1}{M} \int_{\Omega} \Delta\eta_{\psi} \frac{\partial\eta_{\psi}}{\partial t} d\mathbf{x} \\ &= \left( \mu, \frac{\partial\phi}{\partial t} \right) - \frac{1}{M} \left( \psi, \Delta^{-1} \frac{\partial\psi}{\partial t} \right) \\ &= \frac{\beta}{M} (\psi, \Delta^{-1}\psi) = -\frac{\beta}{M} \|\psi\|_{H^{-1}}^2 \leq 0, \end{aligned} \quad (2.13)$$

where  $\eta_{\psi} = (-\Delta)^{-1}\psi$ .

## 2.2 The time discretization scheme

Let  $N > 0$  be a positive integer and  $J = (0, T]$ . Set  $\Delta t = T/N$  and  $t^n = n\Delta t$  for  $n \leq N$ , where  $T$  is the final time. The second-order semi-discrete scheme based on the Crank-Nicolson method for (2.8) is as follows:

Assuming  $\phi^n, \psi^n$  and  $r^n$  are known, we update  $\phi^{n+1}, \psi^{n+1}$  and  $r^{n+1}$  by solving

$$\begin{cases} \psi^{n+1} - \psi^n + \beta\Delta t\psi^{n+1/2} = M\Delta t\Delta\mu^{n+1/2}, & (2.14) \\ \Delta t\psi^{n+1/2} = \phi^{n+1} - \phi^n, & (2.15) \end{cases}$$

$$\begin{cases} \mu^{n+1/2} = \Delta^2\phi^{n+1/2} + 2\Delta\tilde{\phi}^{n+1/2} + \alpha\phi^{n+1/2} + \frac{r^{n+1/2}}{\sqrt{E_1(\tilde{\phi}^{n+1/2})}} F'(\tilde{\phi}^{n+1/2}), & (2.16) \end{cases}$$

$$\begin{cases} r^{n+1} - r^n = \frac{1}{2\sqrt{E_1(\tilde{\phi}^{n+1/2})}} (F'(\tilde{\phi}^{n+1/2}), \phi^{n+1} - \phi^n), & (2.17) \end{cases}$$

where  $f^{n+1/2} = (f^{n+1} + f^n)/2$  and  $\tilde{f}^{n+1/2} = (3f^n - f^{n-1})/2$  for any function  $f$ . For the case where  $n = 0$ , we can compute  $\tilde{\phi}^{1/2}$  by the first-order scheme.

**Theorem 2.2.** *The scheme (2.14)–(2.17) is mass conserving, i.e.,  $\int_{\Omega} \phi^{n+1} d\mathbf{x} = \int_{\Omega} \phi^n d\mathbf{x}$  for all  $n$ , and unconditionally stable in the sense that*

$$\tilde{\mathcal{E}}(\phi^{n+1}, r^{n+1}, \psi^{n+1}) - \tilde{\mathcal{E}}(\phi^n, r^n, \psi^n) \leq -\frac{\beta}{M} \Delta t \|\psi^{n+1/2}\|_{H^{-1}}^2, \quad (2.18)$$

where  $\tilde{\mathcal{E}}(\phi^n, r^n, \psi^n) = \mathcal{E}(\phi^n, r^n, \psi^n) + \frac{1}{2}\|\nabla\phi^n - \nabla\phi^{n-1}\|^2$ .

*Proof.* Taking the inner products of (2.14) with 1 leads to

$$(\psi^{n+1} - \psi^n, 1) + \beta\Delta t(\psi^{n+1/2}, 1) = M\Delta t(\Delta\mu^{n+1/2}, 1). \quad (2.19)$$

Similarly, by taking the inner products of (2.15) with 1, we can obtain

$$(\phi^{n+1} - \phi^n, 1) = \Delta t(\psi^{n+1/2}, 1). \quad (2.20)$$

By using the integration by parts, the term on the right-hand side of (2.19) can be transformed into

$$M\Delta t(\Delta\mu^{n+1/2}, 1) = -M\Delta t(\nabla\mu^{n+1/2}, \nabla 1) = 0. \quad (2.21)$$

Then (2.19) can be recast as follows:

$$\left( 1 + \frac{\beta}{2}\Delta t \right) (\psi^{n+1}, 1) = \left( 1 - \frac{\beta}{2}\Delta t \right) (\psi^n, 1). \quad (2.22)$$

Combining (2.22) with the condition on the initial condition  $(\psi^0, 1) = 0$  leads to  $(\psi^{n+1}, 1) = 0$  for all  $n \geq 0$ . Recalling (2.20), we have  $(\phi^{n+1}, 1) = (\phi^n, 1)$ .

Next, we prove (2.18). Taking the inner products of (2.15) with  $\mu^{n+1/2}$  gives

$$\Delta t(\psi^{n+1/2}, \mu^{n+1/2}) = (\phi^{n+1} - \phi^n, \mu^{n+1/2}). \tag{2.23}$$

Taking the inner products of (2.16) with  $\phi^{n+1} - \phi^n$ , we have

$$\begin{aligned} (\mu^{n+1/2}, \phi^{n+1} - \phi^n) &= (\Delta^2 \phi^{n+1/2}, \phi^{n+1} - \phi^n) + 2(\Delta \tilde{\phi}^{n+1/2}, \phi^{n+1} - \phi^n) \\ &\quad + \alpha(\phi^{n+1/2}, \phi^{n+1} - \phi^n) + \left( \frac{r^{n+1/2}}{\sqrt{E_1(\tilde{\phi}^{n+1/2})}} F'(\tilde{\phi}^{n+1/2}), \phi^{n+1} - \phi^n \right). \end{aligned} \tag{2.24}$$

The first three terms on the right-hand side of (2.24) can be estimated with the help of the integration by parts:

$$(\Delta^2 \phi^{n+1/2}, \phi^{n+1} - \phi^n) = \frac{1}{2}(\|\Delta \phi^{n+1}\|^2 - \|\Delta \phi^n\|^2), \tag{2.25}$$

$$\begin{aligned} 2(\Delta \tilde{\phi}^{n+1/2}, \phi^{n+1} - \phi^n) &= -\|\nabla \phi^{n+1}\|^2 + \|\nabla \phi^n\|^2 + \frac{1}{2}(\|\nabla \phi^{n+1} - \nabla \phi^n\|^2 - \|\nabla \phi^n - \nabla \phi^{n-1}\|^2) \\ &\quad + \frac{1}{2}\|\nabla \phi^{n+1} - 2\nabla \phi^n + \nabla \phi^{n-1}\|^2 \end{aligned} \tag{2.26}$$

and

$$\alpha(\phi^{n+1/2}, \phi^{n+1} - \phi^n) = \frac{\alpha}{2}(\|\phi^{n+1}\|^2 - \|\phi^n\|^2). \tag{2.27}$$

Multiplying (2.17) by  $(r^{n+1} + r^n)$  leads to

$$(r^{n+1})^2 - (r^n)^2 = \left( \frac{r^{n+1/2}}{\sqrt{E_1(\tilde{\phi}^{n+1/2})}} F'(\tilde{\phi}^{n+1/2}), \phi^{n+1} - \phi^n \right). \tag{2.28}$$

Combining (2.24) with (2.23) and (2.25)–(2.28), we have

$$\begin{aligned} &\frac{1}{2}(\|\Delta \phi^{n+1}\|^2 - \|\Delta \phi^n\|^2) - \|\nabla \phi^{n+1}\|^2 + \|\nabla \phi^n\|^2 + |r^{n+1}|^2 - |r^n|^2 \\ &\quad + \frac{1}{2}(\|\nabla \phi^{n+1} - \nabla \phi^n\|^2 - \|\nabla \phi^n - \nabla \phi^{n-1}\|^2) \\ &\quad + \frac{1}{2}\|\nabla \phi^{n+1} - 2\nabla \phi^n + \nabla \phi^{n-1}\|^2 + \frac{\alpha}{2}(\|\phi^{n+1}\|^2 - \|\phi^n\|^2) \\ &= \Delta t(\psi^{n+1/2}, \mu^{n+1/2}). \end{aligned} \tag{2.29}$$

Recalling (2.14), we can derive

$$\begin{aligned} \frac{1}{2M}(\|\psi^{n+1}\|_{H^{-1}}^2 - \|\psi^n\|_{H^{-1}}^2) &= \frac{1}{M}(\psi^{n+1} - \psi^n, \psi^{n+1/2})_{-1} \\ &= -\frac{1}{M}(\psi^{n+1} - \psi^n, \Delta^{-1} \psi^{n+1/2}) \\ &= -\frac{\beta}{M} \Delta t \|\psi^{n+1/2}\|_{H^{-1}}^2 - \Delta t(\mu^{n+1/2}, \psi^{n+1/2}). \end{aligned} \tag{2.30}$$

Finally, combining (2.29) with (2.30) gives the desired result. □

Since the scheme (2.14)–(2.17) is linear, one can also show that it admits a unique solution, and can be efficiently implemented. For the sake of brevity, we shall provide the details only for the fully discrete scheme presented in the next section.

### 3 Fully discrete schemes and their properties

In this section, we construct two linear SAV block-centered finite difference schemes for the SAV reformulated MPFC equation (2.8).

#### 3.1 Fully discrete schemes based on the block-centered finite difference method

First, we describe briefly the block-centered finite difference framework that we will employ to define and analyze our schemes. To fix the idea, we set  $\Omega = (0, L_x) \times (0, L_y)$ , although the algorithm and analysis presented below can be also applied to the one- and three-dimensional rectangular domains.

We begin with the definitions of grid points and difference operators. Let  $L_x = N_x h_x$  and  $L_y = N_y h_y$ , where  $h_x$  and  $h_y$  are grid spacings in  $x$  and  $y$  directions, and  $N_x$  and  $N_y$  are the number of grids along the  $x$  and  $y$  coordinates, respectively. The grid points are denoted by

$$(x_{i+1/2}, y_{j+1/2}), \quad i = 0, \dots, N_x, \quad j = 0, \dots, N_y$$

and

$$\begin{aligned} x_i &= (x_{i-\frac{1}{2}} + x_{i+\frac{1}{2}})/2, \quad i = 1, \dots, N_x, \\ y_j &= (y_{j-\frac{1}{2}} + y_{j+\frac{1}{2}})/2, \quad j = 1, \dots, N_y. \end{aligned}$$

Define

$$\begin{aligned} [d_x g]_{i+\frac{1}{2},j} &= (g_{i+1,j} - g_{i,j})/h_x, \\ [d_y g]_{i,j+\frac{1}{2}} &= (g_{i,j+1} - g_{i,j})/h_y, \\ [D_x g]_{i,j} &= (g_{i+\frac{1}{2},j} - g_{i-\frac{1}{2},j})/h_x, \\ [D_y g]_{i,j} &= (g_{i,j+\frac{1}{2}} - g_{i,j-\frac{1}{2}})/h_y, \\ [\Delta_h g]_{i,j} &= D_x(d_x g)_{i,j} + D_y(d_y g)_{i,j}. \end{aligned}$$

Define the discrete inner products and norms as follows:

$$\begin{aligned} (f, g)_m &= \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} h_x h_y f_{i,j} g_{i,j}, \\ (f, g)_x &= \sum_{i=1}^{N_x-1} \sum_{j=1}^{N_y} h_x h_y f_{i+\frac{1}{2},j} g_{i+\frac{1}{2},j}, \\ (f, g)_y &= \sum_{i=1}^{N_x} \sum_{j=1}^{N_y-1} h_x h_y f_{i,j+\frac{1}{2}} g_{i,j+\frac{1}{2}}. \end{aligned}$$

**Lemma 3.1.** *Let  $q_{i,j}, w_{1,i+1/2,j}$  and  $w_{2,i,j+1/2}$  be any values such that  $w_{1,1/2,j} = w_{1,N_x+1/2,j} = w_{2,i,1/2} = w_{2,i,N_y+1/2} = 0$ . Then*

$$(q, D_x w_1)_m = -(d_x q, w_1)_x, \quad (q, D_y w_2)_m = -(d_y q, w_2)_y.$$

Next, we define the discrete  $H^{-1}$  inner product. Suppose  $\eta_{\phi_i} \in \{f \mid (f, 1)_m = 0\} =: \mathcal{H}$  to be the unique solution to the following problem:

$$-\Delta_h \eta_{\phi_i} = \phi_i, \tag{3.1}$$

where  $\eta_{\phi_i}$  satisfies the discrete homogenous Neumann boundary condition

$$\begin{cases} (\eta_{\phi_i})_{0,j} = (\eta_{\phi_i})_{1,j}, & (\eta_{\phi_i})_{N_x+1,j} = (\eta_{\phi_i})_{N_x,j}, & j = 1, 2, \dots, N_y, \\ (\eta_{\phi_i})_{k,0} = (\eta_{\phi_i})_{k,1}, & (\eta_{\phi_i})_{k,N_y+1} = (\eta_{\phi_i})_{k,N_y}, & k = 1, 2, \dots, N_x. \end{cases} \tag{3.2}$$

We define the bilinear form

$$(\phi_1, \phi_2)_{-1} = (d_x \eta_{\phi_1}, d_x \eta_{\phi_2})_x + (d_y \eta_{\phi_1}, d_y \eta_{\phi_2})_y$$

for any  $\phi_1, \phi_2 \in \mathcal{H}$ . Then we can obtain that  $(\phi_1, \phi_2)_{-1}$  is an inner product on the space  $\mathcal{H}$ . Moreover, we have

$$(\phi_1, \phi_2)_{-1} = -(\phi_1, \Delta_h^{-1} \phi_2)_m = -(\Delta_h^{-1} \phi_1, \phi_2)_m.$$

Then we can define the discrete  $H^{-1}$  norm  $\|\phi\|_{-1} = \sqrt{(\phi, \phi)_{-1}}$ .

Hereafter, we use  $C$  with or without a subscript to define a positive constant, which could have different values at different appearances.

Let us denote by  $\{Z^n, W^n, R^n, \Psi^n\}_{n=0}^N$  the finite difference approximations to  $\{\phi^n, \mu^n, r^n, \psi^n\}_{n=0}^N$ . The second-order scheme defined by the Crank-Nicolson method for (2.8) is as follows:

Set the boundary condition as

$$\begin{cases} Z_{0,j} = Z_{1,j}, & Z_{N_x+1,j} = Z_{N_x,j}, & j = 1, 2, \dots, N_y, \\ Z_{i,0} = Z_{i,1}, & Z_{i,N_y+1} = Z_{i,N_y}, & i = 1, 2, \dots, N_x, \\ W_{0,j} = W_{1,j}, & W_{N_x+1,j} = W_{N_x,j}, & j = 1, 2, \dots, N_y, \\ W_{i,0} = W_{i,1}, & W_{i,N_y+1} = W_{i,N_y}, & i = 1, 2, \dots, N_x, \\ \Delta_h Z_{0,j} = \Delta_h Z_{1,j}, & \Delta_h Z_{N_x+1,j} = \Delta_h Z_{N_x,j}, & j = 1, 2, \dots, N_y, \\ \Delta_h Z_{i,0} = \Delta_h Z_{i,1}, & \Delta_h Z_{i,N_y+1} = \Delta_h Z_{i,N_y}, & i = 1, 2, \dots, N_x. \end{cases} \quad (3.3)$$

We find  $\{Z^{n+1}, W^{n+1}, R^{n+1}, \Psi^{n+1}\}_{n=0}^{N-1}$  such that

$$\begin{cases} \Psi^{n+1} - \Psi^n + \beta \Delta t \Psi^{n+1/2} = M \Delta t \Delta_h W^{n+1/2}, & (3.4) \\ \Delta t \Psi^{n+1/2} = Z^{n+1} - Z^n, & (3.5) \end{cases}$$

$$\begin{cases} W^{n+1/2} = \Delta_h^2 Z^{n+1/2} + 2\Delta_h \tilde{Z}^{n+1/2} + \alpha Z^{n+1/2} \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} F'(\tilde{Z}^{n+1/2}), & (3.6) \end{cases}$$

$$\begin{cases} R^{n+1} - R^n = \frac{1}{2\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} (F'(\tilde{Z}^{n+1/2}), Z^{n+1} - Z^n)_m, & (3.7) \end{cases}$$

where  $f^{n+1/2} = (f^{n+1} + f^n)/2$ ,  $f = W, \Psi, R$ ,  $\tilde{Z}^{n+1/2} = (3Z^n - Z^{n-1})/2$ , and the discrete form of  $E_1(\tilde{Z}^{n+1/2})$  is defined as follows:

$$E_1^h(\tilde{Z}^{n+1/2}) = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} h_x h_y F(\tilde{Z}_{i,j}^{n+1/2}).$$

### 3.2 Efficient implementation

A remarkable property about the above schemes is that it can be solved very efficiently. We demonstrate the detailed procedure to solve the second-order SAV scheme (3.4)–(3.7). Indeed, we can eliminate  $\Psi^{n+1}$ ,  $W^{n+1}$  and  $R^{n+1}$  from (3.4)–(3.7) to obtain

$$\begin{aligned} & \left(\frac{2}{\Delta t} + \beta\right) \frac{Z^{n+1} - Z^n}{\Delta t} - \frac{2}{\Delta t} \Psi^n \\ &= M \left( \frac{1}{2} \Delta_h^3 Z^{n+1} + \frac{1}{2} \Delta_h^3 Z^n + 2\Delta_h^2 \tilde{Z}^{n+1/2} + \frac{\alpha}{2} \Delta_h Z^{n+1} + \frac{\alpha}{2} \Delta_h Z^n \right) \\ &+ M \frac{\Delta_h F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} \left( R^n + \left( \frac{F'(\tilde{Z}^{n+1/2})}{4\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}, Z^{n+1} - Z^n \right)_m \right). \end{aligned} \quad (3.8)$$

Let  $b^n = \frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}$ . Then the above equation can be transformed into the following:

$$\mathcal{A}Z^{n+1} - \frac{M}{4} (b^n, Z^{n+1})_m \Delta_h b^n = f^n, \quad (3.9)$$

where  $\mathcal{A} = (\frac{2}{\Delta t^2} + \frac{\beta}{\Delta t})I - \frac{M}{2}\Delta_h^3 - \frac{M}{2}\alpha\Delta_h$  and the term on the right-hand side satisfies

$$f^n = \frac{2}{\Delta t}\Psi^n + \left( \left( \frac{2}{\Delta t^2} + \frac{\beta}{\Delta t} \right)I + \frac{M}{2}\Delta_h^3 + \frac{M}{2}\alpha\Delta_h \right) Z^n + 2M\Delta_h^2\tilde{Z}^{n+1/2} + M\left( R^n - \frac{1}{4}(b^n, Z^n)_m \right)\Delta_h b^n.$$

In order to solve the above equation, we should determine  $(b^n, Z^{n+1})_m$  first. To this end, multiplying (3.9) by  $\mathcal{A}^{-1}$  leads to

$$Z^{n+1} - \frac{M}{4}(b^n, Z^{n+1})_m\mathcal{A}^{-1}\Delta_h b^n = \mathcal{A}^{-1}f^n. \tag{3.10}$$

Multiplying (3.10) by  $b_{i,j}^n h_x h_y$  and making summation on  $i$  and  $j$  for  $1 \leq i \leq N_x$  and  $1 \leq j \leq N_y$ , we have

$$(b^n, Z^{n+1})_m = \frac{(b^n, \mathcal{A}^{-1}f^n)_m}{1 - \frac{M}{4}(\mathcal{A}^{-1}\Delta_h b^n, b^n)_m}. \tag{3.11}$$

Since  $M > 0$  and for  $\alpha, \beta \geq 0$ ,  $\mathcal{A}^{-1}\Delta_h$  is negative definite,  $(b^n, Z^{n+1})_m$  can be uniquely determined from above. Finally, we can get  $Z^{n+1}$  by (3.10). Since the scheme is linear, the above procedure shows that it admits a unique solution.

In conclusion, the second-order SAV scheme (3.4)–(3.7) can be effectively implemented in the following algorithm:

---

**Give**  $\Psi^n, Z^n, R^n$  and  $b^n$ .

Step 1. Compute  $(\mathcal{A}^{-1}\Delta_h b^n, b^n)_m$ . This can be accomplished by solving a sixth-order equation with constant coefficients.

Step 2. Calculate  $(b^n, Z^{n+1})_m$  using (3.11), which requires solving another sixth-order equation  $\mathcal{A}^{-1}f^n$  with constant coefficients.

Step 3. Update  $Z^{n+1}$  by  $Z^{n+1} = \frac{M}{4}(b^n, Z^{n+1})_m\mathcal{A}^{-1}\Delta_h b^n + \mathcal{A}^{-1}f^n$ .

---

While the second-order scheme above is suitable in most situations, there are cases, e.g., when only steady state solutions are desired, where a first-order scheme is preferred. For the readers' convenience, we list the first-order SAV scheme below:

We find  $\{Z^{n+1}, W^{n+1}, R^{n+1}, \Psi^{n+1}\}_{n=0}^{N-1}$  such that

$$\Psi^{n+1} - \Psi^n + \beta\Delta t\Psi^{n+1} = M\Delta t\Delta_h W^{n+1}, \tag{3.12}$$

$$\Delta t\Psi^{n+1} = Z^{n+1} - Z^n, \tag{3.13}$$

$$W^{n+1} = \Delta_h^2 Z^{n+1} + 2\Delta_h Z^n + \alpha Z^{n+1} + \frac{R^{n+1}}{\sqrt{E_1^h(Z^n)}}F'(Z^n), \tag{3.14}$$

$$R^{n+1} - R^n = \frac{1}{2\sqrt{E_1^h(Z^n)}}(F'(Z^n), Z^{n+1} - Z^n)_m. \tag{3.15}$$

### 3.3 The mass conservation and unconditional energy stability

Define the discrete pseudo energy

$$\mathcal{E}_d(Z^n, R^n, \Psi^n) = \frac{1}{2}\|\Delta_h Z^n\|_m^2 - \|\nabla_h Z^n\|^2 + \frac{\alpha}{2}\|Z^{n+1}\|_m^2 + R^2 + \frac{1}{2M}\|\Psi^n\|_{H^{-1}}^2, \tag{3.16}$$

where  $\|\nabla_h Z\| = \sqrt{(d_x Z, d_x Z)_x + (d_y Z, d_y Z)_y}$ .

**Theorem 3.2.** *The scheme (3.4)–(3.7) admits a unique solution, which is mass conserving, i.e.,  $(Z^{n+1}, 1)_m = (Z^n, 1)_m$  for all  $n$ , and unconditionally stable in the sense that*

$$\tilde{\mathcal{E}}_d(Z^{n+1}, R^{n+1}, \Psi^{n+1}) - \tilde{\mathcal{E}}_d(Z^n, R^n, \Psi^n) \leq -\frac{\beta}{M}\Delta t\|\Psi^{n+1/2}\|_{H^{-1}}^2, \tag{3.17}$$

where  $\tilde{\mathcal{E}}_d(Z^n, R^n, \Psi^n) = \mathcal{E}_d(Z^n, R^n, \Psi^n) + \frac{1}{2}\|\nabla_h Z^n - \nabla_h Z^{n-1}\|^2$ .



*Proof.* Since the scheme (3.4)–(3.7) is linear, the algorithm described in Subsection 3.2 indicates that it admits a unique solution. The proof for the mass conservation and energy dissipation is essentially the same as that for the semi-discrete case. For the readers’ convenience, we still provide the details below.

Summing (3.4) on  $i$  and  $j$  for  $1 \leq i \leq N_x$  and  $1 \leq j \leq N_y$  leads to

$$(\Psi^{n+1} - \Psi^n, 1)_m + \beta \Delta t (\Psi^{n+1/2}, 1)_m = M \Delta t (\Delta_h W^{n+1/2}, 1)_m. \tag{3.18}$$

Similarly, by summing (3.5), we can obtain

$$(Z^{n+1} - Z^n, 1)_m = \Delta t (\Psi^{n+1/2}, 1)_m. \tag{3.19}$$

By noticing Lemma 3.1 and the boundary condition (3.3), the term on the right-hand side of (3.18) can be transformed into

$$M \Delta t (\Delta_h W^{n+1/2}, 1)_m = -M \Delta t ((d_x W^{n+1/2}, d_x 1)_x + (d_y W^{n+1/2}, d_y 1)_y) = 0. \tag{3.20}$$

Then (3.18) can be estimated as follows:

$$\left(1 + \frac{\beta}{2} \Delta t\right) (\Psi^{n+1}, 1)_m = \left(1 - \frac{\beta}{2} \Delta t\right) (\Psi^n, 1)_m. \tag{3.21}$$

Combining (3.21) and  $(\Psi^0, 1) = 0$  leads to  $(\Psi^{n+1}, 1)_m = 0$  for all  $n \geq 0$ . Recalling (3.19), we have  $(Z^{n+1}, 1)_m = (Z^n, 1)_m$ .

Next, we prove (3.17). Multiplying (3.5) by  $W_{i,j}^{n+1/2} h_x h_y$  and making summation on  $i$  and  $j$  for  $1 \leq i \leq N_x$  and  $1 \leq j \leq N_y$ , we have

$$\Delta t (\Psi^{n+1/2}, W^{n+1/2})_m = (Z^{n+1} - Z^n, W^{n+1/2})_m. \tag{3.22}$$

Multiplying (3.6) by  $(Z_{i,j}^{n+1} - Z_{i,j}^n) h_x h_y$  and making summation on  $i$  and  $j$  for  $1 \leq i \leq N_x$  and  $1 \leq j \leq N_y$ , we have

$$\begin{aligned} & (W^{n+1/2}, Z^{n+1} - Z^n)_m \\ &= (\Delta_h^2 Z^{n+1/2}, Z^{n+1} - Z^n)_m + 2(\Delta_h \tilde{Z}^{n+1/2}, Z^{n+1} - Z^n)_m \\ &+ \alpha (Z^{n+1/2}, Z^{n+1} - Z^n)_m + \left( \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} F'(\tilde{Z}^{n+1/2}), Z^{n+1} - Z^n \right)_m. \end{aligned} \tag{3.23}$$

The first three terms on the right-hand side of (3.23) can be dealt with the help of Lemma 3.1 and the boundary condition (3.3), i.e.,

$$(\Delta_h^2 Z^{n+1/2}, Z^{n+1} - Z^n)_m = \frac{1}{2} (\|\Delta_h Z^{n+1}\|_m^2 - \|\Delta_h Z^n\|_m^2), \tag{3.24}$$

$$\begin{aligned} & 2(\Delta_h \tilde{Z}^{n+1/2}, Z^{n+1} - Z^n)_m \\ &= -\|\nabla_h Z^{n+1}\|^2 + \|\nabla_h Z^n\|^2 + \frac{1}{2} (\|\nabla_h Z^{n+1} - \nabla_h Z^n\|^2 - \|\nabla_h Z^n - \nabla_h Z^{n-1}\|^2) \\ &+ \frac{1}{2} \|\nabla_h Z^{n+1} - 2\nabla_h Z^n + \nabla_h Z^{n-1}\|^2, \end{aligned} \tag{3.25}$$

$$\alpha (Z^{n+1/2}, Z^{n+1} - Z^n)_m = \frac{\alpha}{2} (\|Z^{n+1}\|_m^2 - \|Z^n\|_m^2). \tag{3.26}$$

Multiplying (3.7) by  $(R^{n+1} + R^n)$  leads to

$$(R^{n+1})^2 - (R^n)^2 = \left( \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} F'(\tilde{Z}^{n+1/2}), Z^{n+1} - Z^n \right)_m. \tag{3.27}$$

Combining (3.23) with (3.22) and (3.24)–(3.27), we have

$$\frac{1}{2} (\|\Delta_h Z^{n+1}\|_m^2 - \|\Delta_h Z^n\|_m^2) - \|\nabla_h Z^{n+1}\|^2 + \|\nabla_h Z^n\|^2 + (R^{n+1})^2 - (R^n)^2$$

$$\begin{aligned}
 & + \frac{1}{2}(\|\nabla_h Z^{n+1} - \nabla_h Z^n\|^2 - \|\nabla_h Z^n - \nabla_h Z^{n-1}\|^2) \\
 & + \frac{1}{2}\|\nabla_h Z^{n+1} - 2\nabla_h Z^n + \nabla_h Z^{n-1}\|^2 + \frac{\alpha}{2}(\|Z^{n+1}\|_m^2 - \|Z^n\|_m^2) \\
 & = \Delta t(\Psi^{n+1/2}, W^{n+1/2})_m.
 \end{aligned} \tag{3.28}$$

Recalling (3.4), we can derive

$$\begin{aligned}
 \frac{1}{2M}(\|\Psi^{n+1}\|_{H^{-1}}^2 - \|\Psi^n\|_{H^{-1}}^2) & = \frac{1}{M}(\Psi^{n+1} - \Psi^n, \Psi^{n+1/2})_{-1} \\
 & = -\frac{1}{M}(\Psi^{n+1} - \Psi^n, \Delta_h^{-1}\Psi^{n+1/2})_m \\
 & = -\frac{\beta}{M}\Delta t\|\Psi^{n+1/2}\|_{H^{-1}}^2 - \Delta t(W^{n+1/2}, \Psi^{n+1/2})_m.
 \end{aligned} \tag{3.29}$$

Finally, combining (3.28) with (3.29) gives the desired result. □

### 4 An error analysis

In this section, we carry out a rigorous error analysis for the second-order scheme (3.4)–(3.7).

Set

$$\begin{aligned}
 e_\phi^n & = Z^n - \phi(t^n), & e_\psi^n & = \Psi^n - \psi(t^n), \\
 e_\mu^n & = W^n - \mu(t^n), & e_r^n & = R^n - r(t^n).
 \end{aligned}$$

We start by proving the following lemma which will be used to control the backward diffusion term in the error analysis.

**Lemma 4.1.** *Suppose that  $\phi$  and  $\Delta_h\phi$  satisfy the homogeneous Neumann boundary conditions. Then we have*

$$\|\Delta_h\phi\|_m^2 \leq \frac{1}{3\epsilon^2}\|\phi\|_m^2 + \frac{2\epsilon}{3}\|\nabla_h(\Delta_h\phi)\|^2. \tag{4.1}$$

*Proof.* The proof for the homogeneous Neumann boundary condition is essentially the same as that for the periodic boundary condition. One can refer to [18, Lemma 3.10] for more detail. □

**Theorem 4.2.** *Assume that*

$$\phi \in L^\infty(J; W^{8,\infty}(\Omega)) \cap W^{2,\infty}(J; W^{4,\infty}(\Omega)) \cap W^{3,\infty}(J; W^{3,\infty}(\Omega)) \cap W^{4,\infty}(J; L^\infty(\Omega)).$$

*Let  $\Delta t \leq C(h_x + h_y)$ . Then for the discrete scheme (3.4)–(3.7), there exists a positive constant  $C$  independent of  $h_x, h_y$  and  $\Delta t$  such that*

$$\begin{aligned}
 & \|Z^{k+1} - \phi(t^{k+1})\|_m + \|\nabla_h(\Delta_h Z^{k+1}) - \nabla_h(\Delta_h\phi(t^{k+1}))\| + \|\Delta_h Z^{k+1} - \Delta_h\phi(t^{k+1})\|_m + |R^{k+1} - r(t^{k+1})| \\
 & \leq C(\|\phi\|_{W^{4,\infty}(J;L^\infty(\Omega))} + \|\phi\|_{W^{2,\infty}(J;W^{4,\infty}(\Omega))} + \|\phi\|_{W^{3,\infty}(J;W^{3,\infty}(\Omega))})\Delta t^2 \\
 & + C\|\phi\|_{L^\infty(J;W^{8,\infty}(\Omega))}(h_x^2 + h_y^2), \quad \forall 0 \leq k \leq N - 1.
 \end{aligned} \tag{4.2}$$

*Proof.* Subtracting (2.8a) from (3.4), we obtain

$$\frac{e_\psi^{n+1} - e_\psi^n}{\Delta t} + \beta e_\psi^{n+1/2} = M\Delta_h e_\mu^{n+1/2} + T_1^{n+1/2}, \tag{4.3}$$

where

$$\begin{aligned}
 T_1^{n+1/2} & = \frac{\partial\psi}{\partial t} \Big|_{t=n+1/2} - \frac{\psi(t^{n+1}) - \psi(t^n)}{\Delta t} + M(\Delta_h - \Delta)\mu^{n+1/2} \\
 & \leq C\|\psi\|_{W^{3,\infty}(J;L^\infty(\Omega))}\Delta t^2 + \|\mu\|_{L^\infty(J;W^{4,\infty}(\Omega))}(h_x^2 + h_y^2).
 \end{aligned} \tag{4.4}$$

Recalling (2.7) and (3.5), we have

$$e_\psi^{n+1/2} = \frac{e_\phi^{n+1} - e_\phi^n}{\Delta t} + T_2^{n+1/2}, \tag{4.5}$$

where

$$T_2^{n+1/2} = \frac{\phi(t^{n+1}) - \phi(t^n)}{\Delta t} - \frac{\partial \phi}{\partial t} \Big|_{t=n+1/2} \leq C \|\phi\|_{W^{3,\infty}(J;L^\infty(\Omega))} \Delta t^2. \tag{4.6}$$

Subtracting (2.8b) from (3.6) leads to

$$\begin{aligned} e_\mu^{n+1/2} &= \Delta_h^2 e_\phi^{n+1/2} + 2\Delta_h \tilde{e}_\phi^{n+1/2} + \alpha e_\phi^{n+1/2} + \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} F'(\tilde{Z}^{n+1/2}) \\ &\quad - \frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}} F'(\phi^{n+1/2}) + T_3^{n+1/2}, \end{aligned} \tag{4.7}$$

where

$$\begin{aligned} T_3^{n+1/2} &= \Delta_h^2 \phi(t^{n+1/2}) - \Delta^2 \phi(t^{n+1/2}) + 2\Delta_h \tilde{\phi}(t^{n+1/2}) - 2\Delta \phi(t^{n+1/2}) \\ &\leq C(\|\phi\|_{L^\infty(J;W^{6,\infty}(\Omega))} + \|\phi\|_{L^\infty(J;W^{4,\infty}(\Omega))})(h_x^2 + h_y^2) \\ &\quad + C\|\phi\|_{W^{2,\infty}(J;W^{2,\infty}(\Omega))} \Delta t^2. \end{aligned} \tag{4.8}$$

Subtracting (2.8c) from (3.7) gives that

$$\begin{aligned} \frac{e_r^{n+1} - e_r^n}{\Delta t} &= \frac{1}{2\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} \left( F'(\tilde{Z}^{n+1/2}), \frac{Z^{n+1} - Z^n}{\Delta t} \right)_m \\ &\quad - \frac{1}{2\sqrt{E_1(\phi^{n+1/2})}} \int_\Omega F'(\phi^{n+1/2}) \phi_t^{n+1/2} d\mathbf{x} + T_4^{n+1/2}, \end{aligned} \tag{4.9}$$

where

$$T_4^{n+1/2} = r_t^{n+1/2} - \frac{r(t^{n+1}) - r(t^n)}{\Delta t} \leq C\|r\|_{W^{3,\infty}(J)} \Delta t^2. \tag{4.10}$$

Multiplying (4.3) by  $e_{\psi,i,j}^{n+1/2} h_x h_y$  and making summation on  $i$  and  $j$  for  $1 \leq i \leq N_x$  and  $1 \leq j \leq N_y$ , we have

$$\left( \frac{e_\psi^{n+1} - e_\psi^n}{\Delta t}, e_\psi^{n+1/2} \right)_m + \beta \|e_\psi^{n+1/2}\|_m^2 = M(\Delta_h e_\mu^{n+1/2}, e_\psi^{n+1/2})_m + (T_1^{n+1/2}, e_\psi^{n+1/2})_m. \tag{4.11}$$

The first term on the left-hand side of (4.11) can be transformed into the following:

$$\left( \frac{e_\psi^{n+1} - e_\psi^n}{\Delta t}, e_\psi^{n+1/2} \right)_m = \frac{\|e_\psi^{n+1}\|_m^2 - \|e_\psi^n\|_m^2}{2\Delta t}. \tag{4.12}$$

Noticing (4.7), we can write the first term on the right-hand side of (4.11) as

$$\begin{aligned} M(\Delta_h e_\mu^{n+1/2}, e_\psi^{n+1/2})_m &= M(\Delta_h^3 e_\phi^{n+1/2}, e_\psi^{n+1/2})_m + 2M(\Delta_h^2 \tilde{e}_\phi^{n+1/2}, e_\psi^{n+1/2})_m \\ &\quad + M\left( \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} \Delta_h F'(\tilde{Z}^{n+1/2}) - \frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}} \Delta_h F'(\phi^{n+1/2}), e_\psi^{n+1/2} \right)_m \\ &\quad + M\alpha(\Delta_h e_\phi^{n+1/2}, e_\psi^{n+1/2})_m + M(\Delta_h T_3^{n+1/2}, e_\psi^{n+1/2})_m. \end{aligned} \tag{4.13}$$

Using Lemma 3.1, the boundary condition (3.3) and (4.5), we can write the first and second terms on the right-hand side of (4.13) as

$$M(\Delta_h^3 e_\phi^{n+1/2}, e_\psi^{n+1/2})_m$$

$$\begin{aligned}
&= -M(\nabla_h(\Delta_h e_\phi^{n+1/2}), \nabla_h(\Delta_h e_\psi^{n+1/2})) \\
&= -M \frac{\|\nabla_h(\Delta_h e_\phi^{n+1/2})\|^2 - \|\nabla_h(\Delta_h e_\phi^n)\|^2}{2\Delta t} - M(\nabla_h(\Delta_h e_\phi^{n+1/2}), \nabla_h(\Delta_h T_2^{n+1/2})) \\
&\leq -M \frac{\|\nabla_h(\Delta_h e_\phi^{n+1/2})\|^2 - \|\nabla_h(\Delta_h e_\phi^n)\|^2}{2\Delta t} + C\|\nabla_h(\Delta_h e_\phi^{n+1/2})\|^2 \\
&\quad + C\|\phi\|_{W^{3,\infty}(J;W^{3,\infty}(\Omega))}^2 \Delta t^4, \tag{4.14} \\
2M(\Delta_h^2 \tilde{e}_\phi^{n+1/2}, e_\psi^{n+1/2})_m \\
&= M(\Delta_h(3e_\phi^n - e_\phi^{n-1}), \Delta_h e_\psi^{n+1/2})_m \\
&= \frac{M}{\Delta t} \left( \|\Delta_h e_\phi^{n+1}\|_m^2 - \|\Delta_h e_\phi^n\|_m^2 - \frac{1}{2}(\|\Delta_h e_\phi^{n+1} - \Delta_h e_\phi^n\|_m^2 - \|\Delta_h e_\phi^n - \Delta_h e_\phi^{n-1}\|_m^2) \right) \\
&\quad - \frac{M}{2\Delta t} \|\Delta_h e_\phi^{n+1} - 2\Delta_h e_\phi^n + \Delta_h e_\phi^{n-1}\|_m^2 + M(\Delta_h(3e_\phi^n - e_\phi^{n-1}), \Delta_h T_2^{n+1/2})_m. \tag{4.15}
\end{aligned}$$

The third term on the right-hand side of (4.13) can be estimated by

$$\begin{aligned}
&M \left( \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} \Delta_h F'(\tilde{Z}^{n+1/2}) - \frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}} \Delta_h F'(\phi^{n+1/2}), e_\psi^{n+1/2} \right)_m \\
&= Mr^{n+1/2} \left( \frac{\Delta_h F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{\Delta_h F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, e_\psi^{n+1/2} \right)_m \\
&\quad + Mr^{n+1/2} \left( \frac{\Delta_h F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}} - \frac{\Delta_h F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}}, e_\psi^{n+1/2} \right)_m \\
&\quad + Me_r^{n+1/2} \left( \frac{\Delta_h F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}, e_\psi^{n+1/2} \right)_m. \tag{4.16}
\end{aligned}$$

Below we shall first assume that there exist three positive constants  $C_1$ ,  $C_2$  and  $C_3$  such that

$$\|Z^n\|_{L^\infty(\Omega)} \leq C_1, \quad \|\nabla_h Z^n\|_{L^\infty(\Omega)} \leq C_2, \quad \|\Delta_h Z^n\|_{L^\infty(\Omega)} \leq C_3, \quad \forall 0 \leq n \leq N, \tag{4.17}$$

which will be verified later in the proof.

Applying Lemma 4.1, the first term on the right-hand side of (4.16) can be controlled similar to the estimates in [17] by

$$\begin{aligned}
&Mr^{n+1/2} \left( \frac{\Delta_h F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{\Delta_h F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, e_\psi^{n+1/2} \right)_m \\
&\leq C(\|e_\phi^n\|_m^2 + \|\Delta_h e_\phi^n\|_m^2) + C(\|e_\phi^{n-1}\|_m^2 + \|\Delta_h e_\phi^{n-1}\|_m^2) + C\|e_\psi^{n+1/2}\|_m^2 \\
&\leq C(\|e_\phi^n\|_m^2 + \|\nabla_h(\Delta_h e_\phi^n)\|^2) + C(\|e_\phi^{n-1}\|_m^2 + \|\nabla_h(\Delta_h e_\phi^{n-1})\|^2) + C\|e_\psi^{n+1/2}\|_m^2, \tag{4.18}
\end{aligned}$$

where  $C$  is dependent on  $\|r\|_{L^\infty(J)}$ ,  $\|Z^n\|_{L^\infty(\Omega)}$  and  $\|\nabla_h Z^n\|_{L^\infty(\Omega)}$ .

The second term on the right-hand side of (4.16) can be handled by

$$\begin{aligned}
&Mr^{n+1/2} \left( \frac{\Delta_h F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}} - \frac{\Delta_h F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}}, e_\psi^{n+1/2} \right)_m \\
&= Mr^{n+1/2} \left( \frac{\Delta_h F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}} - \frac{\Delta_h F'(\phi^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, e_\psi^{n+1/2} \right)_m \\
&\quad + Mr^{n+1/2} \left( \frac{\Delta_h F'(\phi^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}} - \frac{\Delta_h F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}}, e_\psi^{n+1/2} \right)_m
\end{aligned}$$

$$\leq C\|e_\psi^{n+1/2}\|_m^2 + C\|\phi\|_{W^{2,\infty}(J;W^{2,\infty}(\Omega))}^2\Delta t^4 + C\|\phi\|_{L^\infty(J;W^{3,\infty}(\Omega))}^2(h_x^4 + h_y^4). \tag{4.19}$$

The last term on the right-hand side of (4.16) can be directly controlled by the Cauchy-Schwarz inequality

$$Me_r^{n+1/2}\left(\frac{\Delta_h F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}, e_\psi^{n+1/2}\right)_m \leq C\|e_\psi^{n+1/2}\|_m^2 + C|e_r^{n+1/2}|^2, \tag{4.20}$$

where  $C$  is dependent on  $\|Z^n\|_{L^\infty(\Omega)}$ ,  $\|\nabla_h Z^n\|_{L^\infty(\Omega)}$  and  $\|\Delta_h Z^n\|_{L^\infty(\Omega)}$ . Applying the estimates (4.18)–(4.20) yields

$$\begin{aligned} & M\left(\frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}\Delta_h F'(\tilde{Z}^{n+1/2}) - \frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\Delta_h F'(\phi^{n+1/2}), e_\psi^{n+1/2}\right)_m \\ & \leq C(\|e_\phi^n\|_m^2 + \|\nabla_h(\Delta_h e_\phi^n)\|^2) + C(\|e_\phi^{n-1}\|_m^2 + \|\nabla_h(\Delta_h e_\phi^{n-1})\|^2) \\ & \quad + C\|e_\psi^{n+1/2}\|_m^2 + C(e_r^{n+1/2})^2 + C\|\phi\|_{W^{2,\infty}(J;W^{2,\infty}(\Omega))}^2\Delta t^4 \\ & \quad + C\|\phi\|_{L^\infty(J;W^{3,\infty}(\Omega))}^2(h_x^4 + h_y^4). \end{aligned} \tag{4.21}$$

By recalling Lemma 4.1, the fourth term on the right-hand side of (4.13) can be transformed into

$$\begin{aligned} & M\alpha(\Delta_h e_\phi^{n+1/2}, e_\psi^{n+1/2})_m \\ & \leq C\|e_\psi^{n+1/2}\|_m^2 + C\|\Delta_h e_\phi^{n+1/2}\|_m^2 \\ & \leq C\|e_\phi^{n+1}\|_m^2 + C\|\nabla_h(\Delta_h e_\phi^{n+1})\|^2 + C\|e_\phi^n\|_m^2 + C\|\nabla_h(\Delta_h e_\phi^n)\|^2 + C\|e_\psi^{n+1/2}\|_m^2. \end{aligned} \tag{4.22}$$

The last term on the right-hand side of (4.13) can be estimated by

$$\begin{aligned} M(\Delta_h T_3^{n+1/2}, e_\psi^{n+1/2})_m & \leq C\|e_\psi^{n+1/2}\|_m^2 + C\|\phi\|_{W^{2,\infty}(J;W^{4,\infty}(\Omega))}^2\Delta t^4 \\ & \quad + C(\|\phi\|_{L^\infty(J;W^{8,\infty}(\Omega))}^2 + \|\phi\|_{L^\infty(J;W^{6,\infty}(\Omega))}^2)(h_x^4 + h_y^4). \end{aligned} \tag{4.23}$$

Combining (4.11) with (4.12)–(4.23) leads to

$$\begin{aligned} & \frac{\|e_\psi^{n+1}\|_m^2 - \|e_\psi^n\|_m^2}{2\Delta t} + \beta\|e_\psi^{n+1/2}\|_m^2 + M\frac{\|\nabla_h(\Delta_h e_\phi^{n+1})\|^2 - \|\nabla_h(\Delta_h e_\phi^n)\|^2}{2\Delta t} \\ & \quad + \frac{M}{2\Delta t}(\|\Delta_h e_\phi^{n+1} - \Delta_h e_\phi^n\|_m^2 - \|\Delta_h e_\phi^n - \Delta_h e_\phi^{n-1}\|_m^2) \\ & \leq C(\|e_\phi^{n+1}\|_m^2 + \|\nabla_h(\Delta_h e_\phi^{n+1})\|^2) + C(\|e_\phi^n\|_m^2 + \|\nabla_h(\Delta_h e_\phi^n)\|^2) \\ & \quad + C(\|e_\phi^{n-1}\|_m^2 + \|\nabla_h(\Delta_h e_\phi^{n-1})\|^2) + C\|e_\psi^{n+1/2}\|_m^2 + C|e_r^{n+1/2}|^2 \\ & \quad + \frac{M}{\Delta t}(\|\Delta_h e_\phi^{n+1}\|_m^2 - \|\Delta_h e_\phi^n\|_m^2) + C\|\phi\|_{L^\infty(J;W^{8,\infty}(\Omega))}^2(h_x^4 + h_y^4) \\ & \quad + C(\|\phi\|_{W^{4,\infty}(J;L^\infty(\Omega))}^2 + \|\phi\|_{W^{2,\infty}(J;W^{4,\infty}(\Omega))}^2 + \|\phi\|_{W^{3,\infty}(J;W^{3,\infty}(\Omega))}^2)\Delta t^4. \end{aligned} \tag{4.24}$$

Next, we give the error estimate of the auxiliary function  $r$ . Multiplying (4.9) by  $e_r^{n+1} + e_r^n$  leads to

$$\begin{aligned} \frac{|e_r^{n+1}|^2 - |e_r^n|^2}{\Delta t} & = \frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m \\ & \quad - \frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2} d\mathbf{x} + T_4^{n+1/2} \cdot (e_r^{n+1} + e_r^n). \end{aligned} \tag{4.25}$$

The first two terms on the right-hand side of (4.25) can be transformed into

$$\frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m - \frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2} d\mathbf{x}$$

$$\begin{aligned}
 &= \frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}} \left( (F'(\phi^{n+1/2}), d_t \phi^{n+1})_m - \int_{\Omega} F'(\phi^{n+1/2}) \phi_t^{n+1/2} d\mathbf{x} \right) \\
 &+ e_r^{n+1/2} \left( \frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}} , d_t \phi^{n+1} \right)_m \\
 &+ \frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} (F'(\tilde{Z}^{n+1/2}), d_t e_{\phi}^{n+1})_m, \tag{4.26}
 \end{aligned}$$

which can be handled in a similar way to that in [11]. Thus we have

$$\begin{aligned}
 &\frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} (F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m - \frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}} \int_{\Omega} F'(\phi^{n+1/2}) \phi_t^{n+1/2} d\mathbf{x} \\
 &\leq C|e_r^{n+1/2}|^2 + C\|\phi\|_{W^{1,\infty}(J;L^\infty(\Omega))}^2 (\|e_{\phi}^n\|_m^2 + \|e_{\phi}^{n-1}\|_m^2) \\
 &+ C\|e_{\psi}^{n+1/2}\|_m^2 + C\|\phi\|_{W^{1,\infty}(J;W^{2,\infty}(\Omega))}^2 (h_x^4 + h_y^4). \tag{4.27}
 \end{aligned}$$

Substituting (4.27) into (4.25) and applying the Cauchy-Schwarz inequality, we can obtain

$$\begin{aligned}
 \frac{|e_r^{n+1}|^2 - |e_r^n|^2}{\Delta t} &\leq C|e_r^{n+1/2}|^2 + C\|\phi\|_{W^{1,\infty}(J;L^\infty(\Omega))}^2 (\|e_{\phi}^n\|_m^2 + \|e_{\phi}^{n-1}\|_m^2) \\
 &+ C\|e_{\psi}^{n+1/2}\|_m^2 + C\|\phi\|_{W^{1,\infty}(J;W^{2,\infty}(\Omega))}^2 (h_x^4 + h_y^4) + C\|r\|_{W^{3,\infty}(J)}^2 \Delta t^4. \tag{4.28}
 \end{aligned}$$

Combining (4.24) with (4.28) and multiplying by  $2\Delta t$ , summing over  $n$  ( $n = 0, 1, \dots, k$ ), we have

$$\begin{aligned}
 &\|e_{\psi}^{k+1}\|_m^2 + \beta \sum_{n=0}^k \Delta t \|e_{\psi}^{n+1/2}\|_m^2 + M\|\nabla_h(\Delta_h e_{\phi}^{k+1})\|^2 + 2|e_r^{k+1}|^2 \\
 &\leq 2M\|\Delta_h e_{\phi}^{k+1}\|_m^2 + C \sum_{n=0}^{k+1} \Delta t \|e_{\phi}^n\|_m^2 + C \sum_{n=0}^{k+1} \Delta t \|\nabla_h(\Delta_h e_{\phi}^n)\|_m^2 + C \sum_{n=0}^{k+1} \Delta t \|e_{\psi}^n\|_m^2 \\
 &+ C \sum_{n=0}^{k+1} \Delta t |e_r^n|^2 + C(\|\phi\|_{L^\infty(J;W^{8,\infty}(\Omega))}^2 + \|\phi\|_{L^\infty(J;W^{6,\infty}(\Omega))}^2)(h_x^4 + h_y^4) \\
 &+ C(\|\phi\|_{W^{4,\infty}(J;L^\infty(\Omega))}^2 + \|\phi\|_{W^{2,\infty}(J;W^{4,\infty}(\Omega))}^2 + \|\phi\|_{W^{3,\infty}(J;W^{3,\infty}(\Omega))}^2) \Delta t^4. \tag{4.29}
 \end{aligned}$$

To carry out further analysis, we should give the following inequality first. Recalling (4.5), we have

$$e_{\phi}^{k+1} = e_{\phi}^0 + \sum_{l=0}^k \Delta t e_{\psi}^{l+1/2} + \sum_{l=0}^k \Delta t T_2^{l+1/2},$$

and using the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}
 \|e_{\phi}^{k+1}\|_m^2 &\leq 2\|e_{\phi}^0\|_m^2 + 2\left\| \sum_{l=0}^k \Delta t e_{\psi}^{l+1/2} \right\|_m^2 + 2\left\| \sum_{l=0}^k \Delta t T_2^{l+1/2} \right\|_m^2 \\
 &\leq 2\|e_{\phi}^0\|_m^2 + 2T \sum_{l=0}^k \Delta t \|e_{\psi}^{l+1/2}\|_m^2 + 2T \sum_{l=0}^k \Delta t \|T_2^{l+1/2}\|_m^2. \tag{4.30}
 \end{aligned}$$

By applying Lemma 4.1 and (4.30), the first term on the right-hand side of (4.29) can be transformed into

$$\begin{aligned}
 2M\|\Delta_h e_{\phi}^{k+1}\|_m^2 &\leq C\|e_{\phi}^{k+1}\|_m^2 + \frac{M}{2}\|\nabla_h(\Delta_h e_{\phi}^{k+1})\|^2 \\
 &\leq C \sum_{l=0}^{k+1} \Delta t \|e_{\psi}^l\|_m^2 + C \sum_{l=0}^{k+1} \Delta t \|T_2^l\|_m^2 + \frac{M}{2}\|\nabla_h(\Delta_h e_{\phi}^{k+1})\|^2. \tag{4.31}
 \end{aligned}$$

Then by using the discrete Gronwall inequality and Lemma 4.1, (4.29) can be estimated as follows:

$$\begin{aligned} & \|e_\psi^{k+1}\|_m^2 + \|e_\phi^{k+1}\|_m^2 + \|\Delta_h e_\phi^{k+1}\|_m^2 + \|\nabla_h(\Delta_h e_\phi^{k+1})\|^2 + |e_r^{k+1}|^2 \\ & \leq C(\|\phi\|_{W^{4,\infty}(J;L^\infty(\Omega))}^2 + \|\phi\|_{W^{2,\infty}(J;W^{4,\infty}(\Omega))}^2 + \|\phi\|_{W^{3,\infty}(J;W^{3,\infty}(\Omega))}^2)\Delta t^4 \\ & \quad + C\|\phi\|_{L^\infty(J;W^{8,\infty}(\Omega))}^2(h_x^4 + h_y^4), \quad \forall 0 \leq k \leq N-1. \end{aligned} \tag{4.32}$$

It remains to verify the hypothesis (4.17). Actually, this part of the proof follows a similar procedure to that in our previous works [9, 11]. For the readers' convenience, we still provide a detailed proof for  $\|Z^n\|_{L^\infty(\Omega)} \leq C_1$  in the following two steps by using the mathematical induction.

**Step 1** (Definition of  $C_1$ ). Using the scheme (3.4)–(3.7) for  $n = 0$  and applying the inverse assumption, we can get the approximation  $Z^1$  with the following property:

$$\begin{aligned} \|Z^1\|_{L^\infty(\Omega)} & \leq \|Z^1 - \phi^1\|_{L^\infty(\Omega)} + \|\phi^1\|_{L^\infty(\Omega)} \\ & \leq \|Z^1 - \Pi_h \phi^1\|_{L^\infty(\Omega)} + \|\Pi_h \phi^1 - \phi^1\|_{L^\infty(\Omega)} + \|\phi^1\|_{L^\infty(\Omega)} \\ & \leq Ch^{-1}(\|Z^1 - \phi^1\|_m + \|\phi^1 - \Pi_h \phi^1\|_m) + \|\Pi_h \phi^1 - \phi^1\|_{L^\infty(\Omega)} + \|\phi^1\|_{L^\infty(\Omega)} \\ & \leq C(h + h^{-1}\Delta t^2) + \|\phi^1\|_{L^\infty(\Omega)} \leq C, \end{aligned}$$

where  $h = \max\{h_x, h_y\}$  and  $\Pi_h$  is a bilinear interpolant operator with the following estimate:

$$\|\Pi_h \phi^1 - \phi^1\|_{L^\infty(\Omega)} \leq Ch^2. \tag{4.33}$$

Thus we can choose the positive constant  $C_1$  independent of  $h$  and  $\Delta t$  such that

$$C_1 \geq \max\{\|Z^1\|_{L^\infty(\Omega)}, 2\|\phi^1\|_{L^\infty(\Omega)}\}.$$

**Step 2** (Induction). By the definition of  $C_1$ , it is trivial that the hypothesis  $\|Z^l\|_{L^\infty(\Omega)} \leq C_1$  holds true for  $l = 1$ . Supposing that  $\|Z^{l-1}\|_{L^\infty(\Omega)} \leq C_1$  holds true for an integer  $l = 1, \dots, k+1$  with the aid of the estimate (4.32), we have  $\|Z^l - \phi^l\|_m \leq C(\Delta t^2 + h^2)$ . Next, we prove that  $\|Z^l\|_{L^\infty(\Omega)} \leq C_1$  holds true. Since

$$\begin{aligned} \|Z^l\|_{L^\infty(\Omega)} & \leq \|Z^l - \phi^l\|_{L^\infty(\Omega)} + \|\phi^l\|_{L^\infty(\Omega)} \\ & \leq \|Z^l - \Pi_h \phi^l\|_{L^\infty(\Omega)} + \|\Pi_h \phi^l - \phi^l\|_{L^\infty(\Omega)} + \|\phi^l\|_{L^\infty(\Omega)} \\ & \leq Ch^{-1}(\|Z^l - \phi^l\|_m + \|\phi^l - \Pi_h \phi^l\|_m) + \|\Pi_h \phi^l - \phi^l\|_{L^\infty(\Omega)} + \|\phi^l\|_{L^\infty(\Omega)} \\ & \leq C_4(h + h^{-1}\Delta t^2) + \|\phi^l\|_{L^\infty(\Omega)}. \end{aligned} \tag{4.34}$$

Let  $\Delta t \leq C_5 h$  and a positive constant  $h_1$  be small enough to satisfy  $C_4(1 + C_5^2)h_1 \leq \frac{C_1}{2}$ . Then for  $h \in (0, h_1]$ , we derive from (4.34) that

$$\|Z^l\|_{L^\infty(\Omega)} \leq C_4(h + h^{-1}\Delta t^2) + \|\phi^l\|_{L^\infty(\Omega)} \leq C_4(h_1 + C_5^2 h_1) + \frac{C_1}{2} \leq C_1.$$

This indicates that  $\|Z^n\|_{L^\infty(\Omega)} \leq C_1$  for all  $n$ . The proof for the other two inequalities in (4.17) is essentially identical with the above procedure so we skip it for the sake of brevity.  $\square$

### 5 Numerical results and discussions

In this section, we carry out some numerical experiments with the proposed scheme for the MPFC equation. We first verify the order of convergence. Then we plot evolutions of the original energy as well as the pseudo energy to show that the pseudo energy is indeed dissipative while the original energy is not. Finally, we conclude this section by applying our constructed scheme to the problem of long time simulation.

**5.1 Accuracy test**

We take  $\Omega = (0, 1) \times (0, 1)$ ,  $T = 0.5$ ,  $\epsilon = 0.25$ ,  $M = 0.001$  and the initial solution  $\phi_0 = \cos(2\pi x) \cos(2\pi y)$  with the homogenous Neumann boundary conditions. We use the second-order scheme (3.4)–(3.7) and measure the Cauchy error since we do not know the exact solution. Specifically, the error between two different grid spacings  $h$  and  $\frac{h}{2}$  is calculated by  $\|e_\zeta\| = \|\zeta_h - \zeta_{h/2}\|$ . We take the time step to be  $\Delta t = \frac{T}{N}$  with  $N = N_x = N_y$ , and list the results in Tables 1 and 2 with different  $\beta$ . For simplicity, we define  $\|e_f\|_\infty = \max_{0 \leq l \leq k} \|e_f^l\|$ . We observe a solid second-order convergence rate, which are consistent with the error estimates in Theorem 4.2. It can be easily obtained that our constructed scheme (3.4)–(3.7) is robust with respect to  $\beta$ , in particular, as  $\beta \rightarrow 0$ .

**5.2 Energy stability test**

In this example, we set  $\Omega = (0, 128) \times (0, 128)$ ,  $M = 1$ ,  $\epsilon = 0.025$ ,  $\beta = 0.1$ , and consider the MPFC model with the periodic boundary conditions. The initial condition is taken as follows [1, 7]:

$$\begin{aligned} \phi_0(x, y) = & 0.07 - 0.02 \cos\left(\frac{2\pi(x-12)}{32}\right) \sin\left(\frac{2\pi(y-1)}{32}\right) + 0.02 \cos^2\left(\frac{\pi(x+10)}{32}\right) \\ & \times \cos^2\left(\frac{\pi(y+3)}{32}\right) - 0.01 \sin^2\left(\frac{4\pi x}{32}\right) \sin^2\left(\frac{4\pi(y-6)}{32}\right). \end{aligned} \tag{5.1}$$

We evolve the system to the final time  $T = 100$ . The evolutions of the discrete original energy and the pseudo energy using the second-order scheme with  $\Delta t = 0.05$  are plotted in Figure 1(a). We observe that the discrete original energy may increase on some time intervals, while the pseudo energy is non-increasing at all times, which is consistent with our analysis. To demonstrate the robustness of our constructed second-order scheme (3.4)–(3.7), we present the modified SAV pseudo energy evolutions for different time sizes  $\Delta t$  equaling 0.1, 1, 2, 5 and 10 (see Figure 1(b)), which indicates that the constructed second-order scheme (3.4)–(3.7) is energy stable even for large time steps.

**5.3 Long time simulation**

As a final example, following Baskaran et al. [1], we show a long time simulation of the MPFC model with the homogenous Neumann boundary conditions. We set  $\Omega = (0, 128) \times (0, 128)$  with a random initial data  $\phi_{i,j} = \phi_0 + \eta_{i,j}$ , where  $\phi_0 = 0.1$  and  $\eta_{i,j}$  is a uniformly distributed random number satisfying  $|\eta_{i,j}| \leq 0.1$ . The other parameters are  $M = 1$ ,  $\epsilon = 0.025$ ,  $\beta = 0.5$  and  $h = 1$ . We present the evolutions of the density field  $\phi$  using the second-order scheme with different  $\Delta t$  equaling 0.5, 1, 4 and 10 in Figure 2, where we compare numerical results using different time steps at the same discrete modified pseudo energy, rather than at the same time, i.e., we have the same pseudo energy associated with each column in Figure 2.

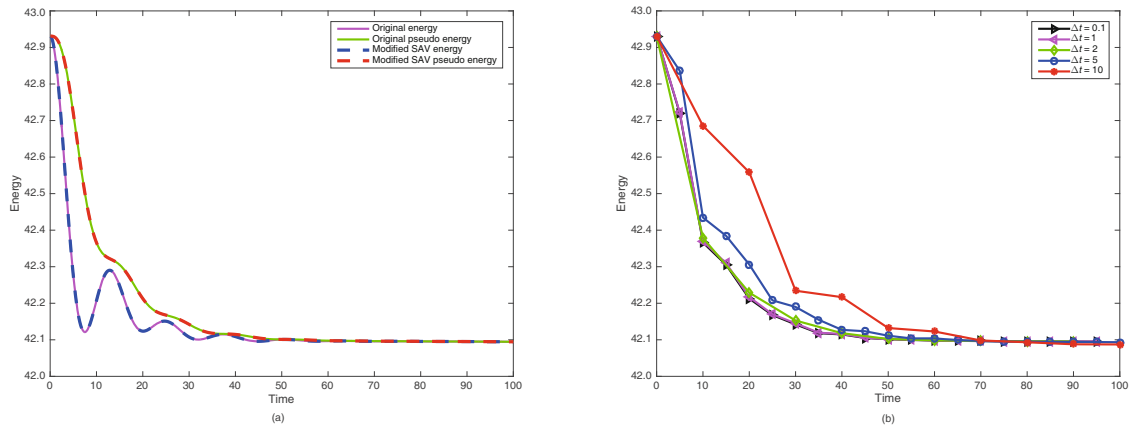
**Table 1** Errors and convergence rates for the scheme (3.4)–(3.7) with  $\beta = 0.9$

$N_x \times N_y$	$\ e_\phi\ _{\infty, m}$	Rate	$\ \nabla_h(\Delta_h e_\phi)\ _\infty$	Rate	$\ e_r\ _\infty$	Rate
20 × 20	1.15E−1	–	79.6E−0	–	2.15E−2	–
40 × 40	3.15E−2	1.87	22.0E−0	1.85	6.62E−3	1.70
80 × 80	8.02E−3	1.97	5.62E−0	1.97	1.28E−3	2.38
160 × 160	2.11E−3	1.93	1.48E−0	1.93	2.32E−4	2.46

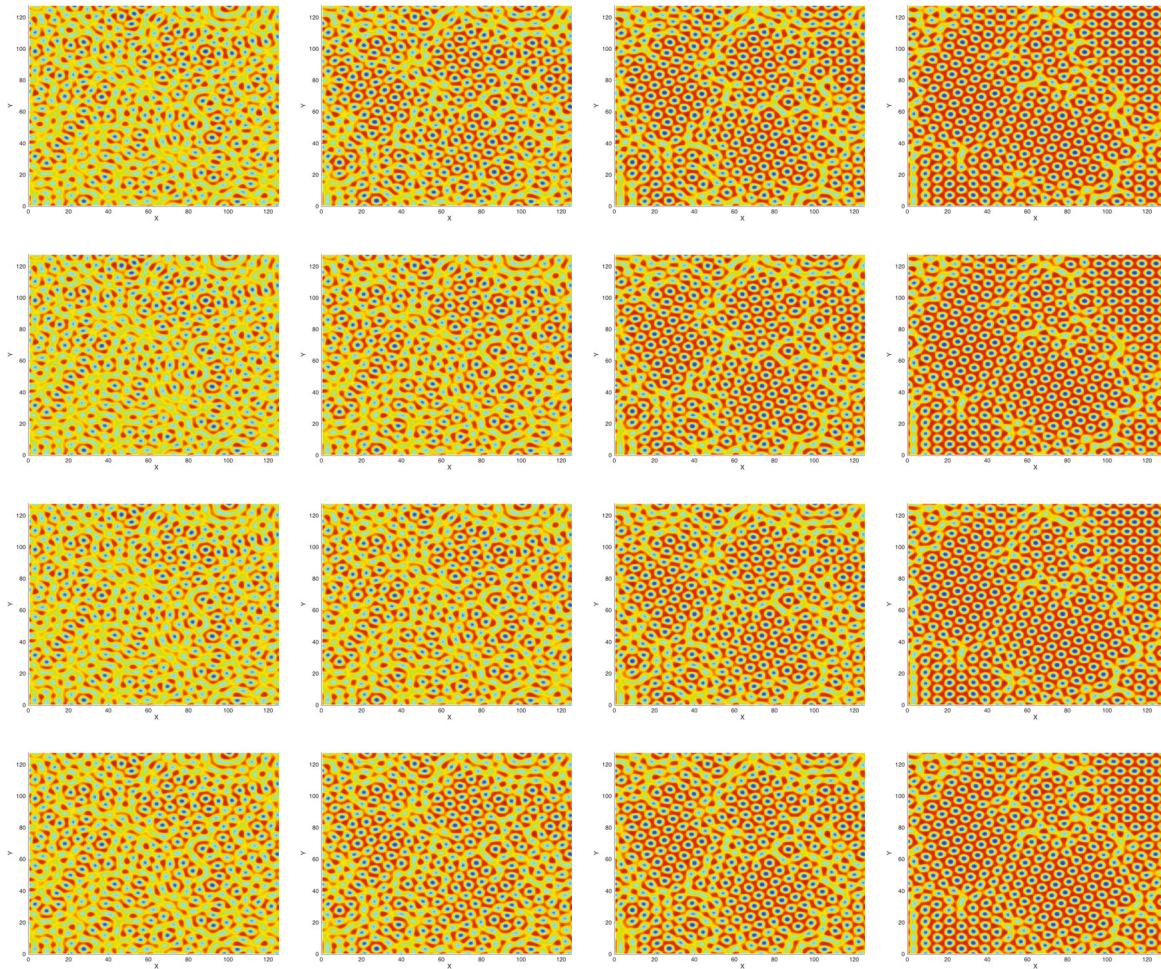
**Table 2** Errors and convergence rates for the scheme (3.4)–(3.7) with  $\beta = 0.01$

$N_x \times N_y$	$\ e_\phi\ _{\infty, m}$	Rate	$\ \nabla_h(\Delta_h e_\phi)\ _\infty$	Rate	$\ e_r\ _\infty$	Rate
20 × 20	1.41E−1	–	97.8E−0	–	2.61E−2	–
40 × 40	3.91E−2	1.85	27.4E−0	1.84	9.19E−3	1.51
80 × 80	9.99E−3	1.97	7.01E−0	1.96	1.90E−3	2.28
160 × 160	2.63E−3	1.93	1.85E−0	1.93	3.72E−4	2.35





**Figure 1** (Color online) (a) The discrete original energy and the pseudo energy plotted as functions of time; (b) Modified SAV pseudo energy evolutions for different time sizes



**Figure 2** (Color online) Snapshots of the phase function  $\phi$  using the second-order scheme with different  $\Delta t$  equaling 0.5, 1, 4 and 10 in each row, respectively in Subsection 5.3. The plots in the same column have the same modified pseudo energy

## 6 Summary

We construct in this paper two efficient schemes for the MPFC model based on the SAV approach and block-centered finite difference method. Since the original energy of the MPFC equation may increase in time on some time intervals, we introduce a pseudo energy that is dissipative for all times. It is shown that our schemes conserve mass and are unconditionally energy stable with respect to the pseudo energy. We also establish rigorously second-order error estimates in both time and space for our second-order SAV block-centered finite difference method. Finally, some numerical experiments are presented to validate our theoretical results.

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