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Error estimates for the Scalar Auxiliary Variable (SAV) schemes to the modified phase field crystal equation[☆]

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ABSTRACT

We design first-order and second-order time-stepping schemes for the modified phase field crystal model based on the scalar auxiliary variable method in this work. The model is a nonlinear sixth-order damped wave equation that includes both elastic interactions and diffusive dynamics. Our schemes are linear and satisfy the unconditional energy stability with respect to pseudo energy. We also rigorously estimate the errors of the numerical schemes. Finally, some numerical tests are presented to validate our theoretical results.

1. Introduction

In this work, we consider the following modified phase field crystal (MPFC) equation

$$u_{tt} + \beta u_t = M\Delta((1+\Delta)^2 u + f(u)), \quad \text{in } \Omega \times (0, T], \tag{1.1}$$

with the following initial conditions:

$$u|_{t=0} = u_0(x), \quad u_t|_{t=0} = \psi_0(x), \quad x \in \Omega, \tag{1.2}$$

where Ω is a domain in $\mathbb{R}^d$ $(d = 1, 2, 3)$, $f(u) = u^3 - \epsilon u$, u is the atomic density field function, $M > 0$ is the mobility constant, ϵ $(0 < \epsilon < 1)$ is a positive constant with physical significance, $\beta > 0$ is a constant. Here we study the numerical schemes for the MPFC equation with periodic boundary condition since that is used very frequently in numerical or analytical works of the MPFC equation. If $\Omega = [0, L_x] \times [0, L_y]$ (L_x and L_y are two positive constants), the periodic boundary condition means

$$u(x + L_x, y, t) = u(x, y, t), \quad u(x, y + L_y, t) = u(x, y, t), \quad \forall\, (x, y) \in \Omega,\ t > 0.$$

While the periodic boundary condition is assumed herein, the theory and numerical analysis to follow also hold for the homogeneous Neumann boundary condition.

In [1,2] Elder and Grant proposed the phase field crystal (PFC) equation as a continuum model to study the dynamics of atomic-scale crystal growth on diffusive time scales. But the PFC equation does not contain a mechanism to simulating elastic interactions since it only evolves on diffusive time scales and it fails to distinguish between the diffusion time scales and elastic relaxation. To overcome the major disadvantage of the PFC model, Stefanovic et al. [3,4] introduced the modified phase field crystal (MPFC) model. The MPFC model includes both elastic interactions and diffusive dynamics,

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hence when the length scale is the same as the size of the system, the separation of the elastic relaxation and diffusion time scales can be observed. Compared with the PFC equation, there is a wave operator for elastic interaction in the MPFC equation, therefore the form of the MPFC equation is more complicated and it is more difficult to develop time-stepping schemes for the MPFC equation.

Numerical methods about the MPFC model has been studied by many researchers. In [4], Stefanovic et al. proposed a semi-implicit scheme based on finite difference method, they solved the resulting algebraic equations by multigrid algorithm, but they did not give the analysis about energy stability, unique solvability and error estimate about their algorithm. In [5], based on convex splitting method, Wang and Wise designed an energy-stable first-order nonlinear finite difference scheme for the MPFC model. In [6], Baskaran et al. designed first- and second-order unconditionally energy-stable nonlinear finite difference methods for the MPFC equation based on convex splitting scheme and they provided the convergence analysis for their second-order scheme in [7]. In [8], Lee et al. presented first-and second-order schemes for the MPFC equation based on an appropriate splitting of the energy for the PFC equation, Fourier spectral method was used for spatial discretization, moreover, they show their algorithms were unconditionally stable with respect to the energy and pseudo energy of the MPFC equation. In [9], Dehghan and Mohammadi proposed a semi-implicit scheme based on meshless methods for PFC and MPFC models. In [10], Grasselli and Pierre proposed a space semi-discrete and a fully discrete finite element scheme for the MPFC equation and their algorithm was convergent and energy-stable. In [11], Guo and Xu designed a high-order adaptive time-stepping method and local discontinuous Galerkin method for the MPFC equation. Other than the MPFC model, the square phase field crystal (SPFC) model has also attracted great attentions in the study of crystal dynamics. There has been some numerical works on the SPFC model and the energy stability and convergence estimate have been theoretically justified, such as [12–15]. Although quite a number of algorithms have been designed to solve the MPFC equation, most of them were based on convex splitting approach and were therefore nonlinear, it is generally complicated to implement nonlinear algorithm and the computational costs are expensive. Hence, linear schemes are desirable for the MPFC model.

Recent years, invariant energy quadratization (IEQ) scheme [16–20] and scalar auxiliary variable (SAV) scheme [21–23] are proposed and enable one to design unconditionally energy-stable, linear, symmetric positive definite schemes for various kinds of gradient flow problems. These approaches satisfy unconditional energy stability based on a modified energy functional and the stability of the original energy is not guaranteed. This problem has been partially addressed in [24,25]. In [26], adopting the IEQ scheme, Li et al. proposed three temporal discretization schemes based on the first-order backward Euler, the second-order Crank–Nicolson scheme and the second-order backward difference scheme, respectively, but they did not give the error analysis about their algorithm. There have been a few error estimate works for the second-order SAV numerical schemes, such as [27] for the thin film epitaxial equation and [13] for the square phase field crystal equation. Due to the nonlinear hyperbolic properties of the MPFC model, error analysis is a challenging work. As far as we know, first- and second-order error analysis for any linear schemes for the MPFC equation are lacking in the existing literature.

In this work, we design first- and second-order unconditionally energy-stable linear schemes based on the SAV approach and derive a rigorous error estimates for our schemes. We adopt the first-order backward Euler and Crank–Nicolson schemes for temporal discretization and prove they satisfy unconditional energy dissipation law with respect to pseudo energy. We also present the second-order fully discrete Crank–Nicolson scheme based on the block-centered finite difference method and its convergence analysis. In the end, several numerical experiments are given to validate the unconditional energy stability and convergence of our algorithms.

The rest of the paper is organized as follows. In Section 2, we present the governing equation for the MPFC model and give the mass conservation and energy dissipation law in the continuous case. In Section 3, we construct a first-order SAV scheme based on the backward Euler scheme and prove it is unconditionally energy-stable with respect to the pseudo energy, and we derive the error estimate for this scheme. In Section 4, we construct a second-order SAV scheme based on the Crank–Nicolson scheme and prove it is unconditionally energy-stable with respect to the pseudo energy, and we derive the error estimate for this scheme. In Section 5, based on the block-centered finite difference method, we present the second-order fully discrete Crank–Nicolson scheme and its convergence analysis. In Section 6, several numerical tests are carried out to verify the theoretical results. We conclude this paper in Section 7.

We introduce some notations which will be used in the analysis. We denote the spaces $L^p(\Omega)$ associated with the L^p norm $\|u\|_{L^p} := (\int_\Omega |u(x)|^p dx)^{1/p}$. We also introduce the space $L^\infty(\Omega)$ with $\|v\|_{L^\infty} = \sup_{x\in\Omega} |v(x)|$. $W^{k,p}(\Omega)$ stands for the standard Sobolev spaces equipped with the standard Sobolev norms $\|\cdot\|_{k,p}$. For $p = 2$, we write $H^k(\Omega)$ for $W^{k,2}(\Omega)$ and the corresponding norm is $\|\cdot\|_k$. The space $W^{k,p}(0, T; V)$ represents the $W^{k,p}$ space on the interval $(0, T)$ with values in the function space V. We denote by $(\cdot,\cdot)$ the inner product in L^2 and $\|\cdot\|$ the norm in L^2.

2. Mass conservation and energy dissipation for the MPFC model

We consider the following free energy functional

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}u(1+\Delta)^2 u + F(u)dx, \tag{2.1}$$

and introducing the following chemical potential μ

$$\mu := \frac{\delta \mathcal{E}}{\delta u} = (1+\Delta)^2 u + f(u), \tag{2.2}$$

where $\frac{\delta}{\delta u}$ denotes the variational derivative, $F(u) = \frac{1}{4}u^4 - \frac{\epsilon}{2}u^2$ and $f(u) = F'(u)$. Thus, the MPFC equation can be rewritten as follows

$$u_{tt} + \beta u_t = M\Delta\mu, \quad \text{in } \Omega \times (0, T]. \tag{2.3}$$

By setting $\int_\Omega u_t(x,0)\mathrm{d}x = 0$ and integrating (2.3) over Ω with the periodic boundary value condition for μ, we see that

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega u_t(x,t)\mathrm{d}x + \beta\int_\Omega u_t(x,t)\mathrm{d}x = M\int_{\partial\Omega} \nabla\mu\cdot\mathbf{n}\mathrm{d}s = 0, \tag{2.4}$$

where $\mathbf{n}$ is the unit outward normal vector on the boundary $\partial\Omega$, (2.4) implies that

$$\int_\Omega u_t(x,t)\mathrm{d}x = e^{-\beta t}\int_\Omega u_t(x,0)\mathrm{d}x = 0,$$

and we obtain the mass conservation

$$\int_\Omega u_t(x,t)\mathrm{d}x = \int_\Omega u_{tt}(x,t)\mathrm{d}x = 0. \tag{2.5}$$

We define the inverse Laplace operator Δ^{-1} such that $\omega = \Delta^{-1}\phi$ (with $\int_\Omega \phi\mathrm{d}x = 0$) if and only if

$$\Delta\omega = \phi, \quad \int_\Omega \omega\mathrm{d}x = 0,$$

with the periodic boundary condition for ω. With this notation, we can define the H^{-1}_{per} inner product and norm by

$$(\phi,\varphi)_{-1} := (\nabla\Delta^{-1}\phi, \nabla\Delta^{-1}\varphi), \quad \|\phi\|^2_{-1} := (\nabla\Delta^{-1}\phi, \nabla\Delta^{-1}\phi),$$

where $(\cdot,\cdot)$ is the standard L^2 inner product.

We can see from [26] that the MPFC equation satisfies the following energy dissipation law

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathcal{E}}(u) = -\frac{\beta}{M}\|u_t\|^2_{-1} \le 0, \tag{2.6}$$

where the pseudo energy $\hat{\mathcal{E}}(u)$ is defined by

$$\hat{\mathcal{E}}(u) = \int_\Omega \left(\frac{1}{2}u(1+\Delta)^2 u + F(u)\right)\mathrm{d}x + \frac{1}{2M}\|u_t\|^2_{-1}. \tag{2.7}$$

Let $N > 0$ be any positive integer and set

$$\tau = T/N, \quad t_n = n\tau, \quad \text{for } n \le N,$$

let ϕ^n be the numerical approximation of $\phi(t_n)$.

3. The stability and error analysis of the first-order SAV scheme

In this section, we develop a semi-discrete time-stepping numerical scheme to solve the MPFC equation based on the SAV method, and then we prove the scheme is energy-stable. First, we assume that for any u,

$$E(u) = \int_\Omega F(u)\mathrm{d}x > -d_0.$$

Let $D_0 > d_0$ such that $E(u) + D_0 > 0$. In the approach, we introduce two auxiliary functions as follows,

$$r(t) = \sqrt{E(u) + D_0}, \quad \psi = u_t.$$

Obviously, we have $\int_\Omega \psi\mathrm{d}x = \int_\Omega \psi_t\mathrm{d}x = 0$ from (2.5). Now, we obtain an equivalent PDE system as follows:

$$\psi_t + \beta\psi = M\Delta\mu, \tag{3.1}$$

$$\mu = (1+\Delta)^2 u + \frac{r(t)}{\sqrt{E(u)+D_0}}f(u), \tag{3.2}$$

$$r_t = \frac{1}{2\sqrt{E(u)+D_0}}\int_\Omega f(u)u_t\mathrm{d}x, \tag{3.3}$$

$$\psi = u_t. \tag{3.4}$$

The initial conditions are

$$u|_{t=0} = u_0, \quad \psi|_{t=0} = 0, \quad r|_{t=0} = \sqrt{E(u_0) + D_0}, \tag{3.5}$$

where we set the initial profile of ψ to be zero point-wise for simplicity.

The new transformed system (3.1)–(3.4) still satisfies an energy dissipation law. By applying Δ^{-1} to (3.1) and taking the L^2 inner product of it with $\frac{u_t}{M}$, of (3.2) with u_t, of (3.3) with $2r$, using (3.4) and

$$\beta(\Delta^{-1}\psi, \psi) = -\beta\|\psi\|_{-1}^2, \quad (\Delta^{-1}\psi_t, \psi) = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\psi\|_{-1}^2,$$

and summing them up, we can get the energy dissipation law of the new PDE system (3.1)–(3.4) as follows

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\mathcal{E}}(u, r, \psi) = -\frac{\beta}{M}\|\psi\|_{-1}^2 \le 0, \tag{3.6}$$

where

$$\widehat{\mathcal{E}}(u, r, \psi) = \int_\Omega \left(\frac{1}{2}u(1+\Delta)^2 u\right)\mathrm{d}x + r^2 - D_0 + \frac{1}{2M}\|\psi\|_{-1}^2.$$

We design the first-order scheme based on the backward Euler method as follows,

$$\frac{\psi^{n+1} - \psi^n}{\tau} + \beta\psi^{n+1} = M\Delta\mu^{n+1}, \tag{3.7}$$

$$\mu^{n+1} = (1+\Delta)^2 u^{n+1} + \frac{r^{n+1}}{\sqrt{E(u^n) + D_0}} f(u^n), \tag{3.8}$$

$$r^{n+1} - r^n = \frac{1}{2\sqrt{E(u^n) + D_0}}(f(u^n), u^{n+1} - u^n), \tag{3.9}$$

$$\psi^{n+1} = \frac{u^{n+1} - u^n}{\tau}. \tag{3.10}$$

From (3.7)–(3.9), we can obtain

$$\begin{aligned} \frac{\psi^{n+1} - \psi^n}{\tau} + \beta\psi^{n+1} = M\Delta&\left((1+\Delta)^2 u^{n+1} + \frac{r^n}{\sqrt{E(u^n) + D_0}} f(u^n)\right) \\ &+ M\Delta\left(\frac{f(u^n)}{2E(u^n) + 2D_0}(f(u^n), u^{n+1} - u^n)\right). \end{aligned} \tag{3.11}$$

By applying (3.10) and denoting

$$a^n = \frac{f(u^n)}{\sqrt{E(u^n) + D_0}}, \tag{3.12}$$

(3.11) can be rewritten as

$$\begin{aligned} &(1 + \beta\tau - \tau^2 M\Delta(1+\Delta)^2)u^{n+1} - \frac{\tau^2 M}{2}\Delta a^n(a^n, u^{n+1}) \\ &\qquad = (1+\beta\tau)u^n + \tau\psi^n + \tau^2 M r^n \Delta a^n - \frac{\tau^2 M}{2}\Delta a^n(a^n, u^n) := h^n. \end{aligned} \tag{3.13}$$

First, we calculate (a^n, u^{n+1}) from (3.13). Let $T^{-1} := (1 + \beta\tau - \tau^2 M\Delta(1+\Delta)^2)^{-1}$, multiplying (3.13) with T^{-1}, then taking the L^2 inner product of it with a^n, we have

$$(a^n, u^{n+1}) + \frac{\tau^2 M}{2}\theta^n(a^n, u^{n+1}) = (a^n, T^{-1}h^n) \tag{3.14}$$

where

$$\theta^n = -(a^n, T^{-1}\Delta a^n) \ge 0,$$

since $-T^{-1}\Delta$ is a positive definite operator. Then, from (3.14), we obtain that

$$(a^n, u^{n+1}) = \frac{(a^n, T^{-1}h^n)}{1 + \frac{\tau^2 M\theta^n}{2}}.$$

Thus, we can obtain u^{n+1} and ψ^{n+1} from (3.10) and (3.13), respectively.

The following theorem implies that the first-order scheme (3.7)–(3.10) is energy-stable.

Theorem 3.1. *The scheme (3.7)–(3.10) satisfies unconditional energy dissipation law, that is, for $n < N$,*

$$\hat{\mathcal{E}}(u^{n+1}, r^{n+1}, \psi^{n+1}) \le \hat{\mathcal{E}}(u^n, r^n, \psi^n),$$

and then, we have the following boundedness

$$\max_{0\le n\le N}\left(\frac{1}{2}\|(1+\Delta)u^n\|^2 + (r^n)^2 + \frac{1}{2M}\|\psi^n\|_{-1}^2\right) \le \frac{1}{2}\|(1+\Delta)u^0\|^2 + (r^0)^2 + \frac{1}{2M}\|\psi^0\|_{-1}^2. \tag{3.15}$$

Proof. Combining (3.7)–(3.8) together and applying Δ^{-1}, we obtain

$$\frac{1}{\tau}\Delta^{-1}(\psi^{n+1}-\psi^n) + \beta\Delta^{-1}\psi^{n+1} = M(1+\Delta)^2u^{n+1} + \frac{Mr^{n+1}}{E(u^n)+D_0}f(u^n). \tag{3.16}$$

Taking the L^2 inner product of (3.16) with $u^{n+1}-u^n$, we derive

$$\begin{aligned}
&\frac{1}{\tau}(\Delta^{-1}(\psi^{n+1}-\psi^n), u^{n+1}-u^n) + \beta(\Delta^{-1}\psi^{n+1}, u^{n+1}-u^n)\\
=&\frac{M}{2}(\|(1+\Delta)u^{n+1}\|^2 - \|(1+\Delta)u^n\|^2 + \|(1+\Delta)(u^{n+1}-u^n)\|^2)\\
&+ M\left(\frac{r^{n+1}}{\sqrt{E(u^n)+D_0}}f(u^n), u^{n+1}-u^n\right).
\end{aligned} \tag{3.17}$$

Taking the L^2 inner product of (3.9) with $2r^{n+1}$, we have

$$(r^{n+1})^2 - (r^n)^2 + (r^{n+1}-r^n)^2 = \frac{r^{n+1}}{\sqrt{E(u^n)+D_0}}(f(u^n), u^{n+1}-u^n). \tag{3.18}$$

From (3.10), we have

$$\begin{aligned}
\frac{1}{\tau}(\Delta^{-1}(\psi^{n+1}-\psi^n), u^{n+1}-u^n) &= (\Delta^{-1}(\psi^{n+1}-\psi^n), \psi^{n+1})\\
&= -(\nabla\Delta^{-1}(\psi^{n+1}-\psi^n), \nabla\Delta^{-1}\psi^{n+1})\\
&= -\frac{1}{2}(\|\psi^{n+1}\|_{-1}^2 - \|\psi^n\|_{-1}^2 + \|\psi^{n+1}-\psi^n\|_{-1}^2),
\end{aligned} \tag{3.19}$$

and

$$\begin{aligned}
\beta(\Delta^{-1}\psi, u^{n+1}-u^n) &= \beta\tau(\Delta^{-1}\psi^{n+1}, \psi^{n+1})\\
&= -\beta\tau(\nabla\Delta^{-1}\psi^{n+1}, \nabla\Delta^{-1}\psi^{n+1})\\
&= -\beta\tau\|\psi^{n+1}\|_{-1}^2.
\end{aligned} \tag{3.20}$$

In the end, we combine (3.17)–(3.20) and obtain

$$\begin{aligned}
&\frac{1}{2}(\|\psi^{n+1}\|_{-1}^2 - \|\psi^n\|_{-1}^2 + \|\psi^{n+1}-\psi^n\|_{-1}^2) + \frac{M}{2}(\|(1+\Delta)u^{n+1}\|^2 - \|(1+\Delta)u^n\|^2 + \|(1+\Delta)(u^{n+1}-u^n)\|^2)\\
&+ M((r^{n+1})^2 - (r^n)^2 + (r^{n+1}-r^n)^2) = -\beta\tau\|\psi^{n+1}\|_{-1}^2 \le 0.
\end{aligned}$$

Dividing both sides of the above equation by M and dropping some positive terms, we obtain the desired energy dissipation law and boundedness. □

Remark 3.1. There are many pioneering works about energy stability for the PFC model, the reader can refer to [28], [29] for details.

In this work, we assume that the initial data satisfies the following stability:

$$\hat{\mathcal{E}}(u^0, r^0, \psi^0) = \frac{1}{2}\|(1+\Delta)u^0\|^2 + (r^0)^2 - D_0 + \frac{1}{2M}\|\psi^0\|_{-1}^2 < C_0. \tag{3.21}$$

We now establish the uniform in time H^2 bound of the numerical solution u^n of the scheme (3.7)–(3.10).

Theorem 3.2. *Let u^n be the solution of the scheme (3.7)–(3.10), there exists a positive constant C such that*

$$\|u^n\|_{H^2} \le C.$$

Proof. Using the Hölder's inequality, we have

$$\|u^n\|^2 \le \eta_1\|u^n\|_{L^4}^4 + \frac{1}{4\eta_1}|\Omega|, \quad \|\nabla u^n\|^2 \le \eta_2\|\Delta u^n\|^2 + \frac{1}{4\eta_2}\|u^n\|^2,$$

for any $\eta_1, \eta_2 > 0$, where $|\Omega|$ is the measure of the domain Ω. Taking $\eta_1 = \frac{1}{4}$, $\eta_2 = \frac{1}{3}$, we have the following estimate

$$\begin{aligned}
\hat{\mathcal{E}}(u^n, r^n, \psi^n) &= \frac{1}{2}\|(1+\Delta)u^n\|^2 + (r^n)^2 - D_0 + \frac{1}{2M}\|\psi^n\|_{-1}^2 \\
&\geq \frac{1}{2}\|u^n\|^2 - \|\nabla u^n\|^2 + \frac{1}{2}\|\Delta u^n\|^2 + \frac{1}{4}\|u^n\|_{L^4}^4 - \frac{\epsilon}{2}\|u^n\|^2 \\
&= \frac{1}{8}(\|u^n\|^2 + \|\nabla u^n\|^2 + \|\Delta u^n\|^2) + \frac{1}{4}\|u^n\|_{L^4}^4 + \frac{3}{8}\|\Delta u^n\|^2 \\
&\quad - \frac{9}{8}\|\nabla u^n\|^2 + \frac{3-4\epsilon}{8}\|u^n\|^2 \\
&\geq \frac{1}{8}\|u^n\|_{H^2}^2 + \frac{1}{4}\|u^n\|_{L^4}^4 + \frac{3}{8}\|\Delta u^n\|^2 - \frac{9}{8}\left(\frac{1}{3}\|\Delta u^n\|^2 + \frac{3}{4}\|u^n\|^2\right) \\
&\quad + \frac{3-4\epsilon}{8}\|u^n\|^2 \\
&= \frac{1}{8}\|u^n\|_{H^2}^2 + \frac{1}{4}\|u^n\|_{L^4}^4 + \left(\frac{3-4\epsilon}{8} - \frac{27}{32}\right)\|u^n\|^2 \\
&\geq \frac{1}{8}\|u^n\|_{H^2}^2 + \frac{1}{4}\|u^n\|_{L^4}^4 - \frac{15+16\epsilon}{32}\left(\frac{1}{4}\|u^n\|_{L^4}^4 + |\Omega|\right) \\
&= \frac{1}{8}\|u^n\|_{H^2}^2 + \frac{1}{4}\|u^n\|_{L^4}^4 - \frac{1}{4}\cdot\frac{15+16\epsilon}{32}\|u^n\|_{L^4}^4 - \frac{15+16\epsilon}{32}|\Omega| \\
&\geq \frac{1}{8}\|u^n\|_{H^2}^2 - |\Omega|,
\end{aligned}$$

in the last inequality, we used the fact that

$$\frac{1}{4} - \frac{1}{4}\cdot\frac{15+16\epsilon}{32} = \frac{1}{4}\cdot\frac{27-16\epsilon}{32} > 0, \quad \frac{15+16\epsilon}{32} < 1.$$

Applying Theorem 3.1 and the initial data assumption (3.21), we have

$$\|u^n\|_{H^2}^2 \leq 8\hat{\mathcal{E}}(u^n, r^n, \psi^n) + 8|\Omega| \leq 8\hat{\mathcal{E}}(u^0, r^0, \psi^0) + 8|\Omega| \leq 8(C_0 + |\Omega|).$$

Let $C = \sqrt{8(C_0 + |\Omega|)}$, we obtain the desired result. □

We now give the error analysis for the first-order scheme (3.7)–(3.10). First, we formulate a truncation form for the MPFC system (3.7)–(3.10) as follows:

$$\frac{\psi(t_{n+1}) - \psi(t_n)}{\tau} + \beta\psi(t_{n+1}) = M\Delta\mu(t_{n+1}) + G_\psi^{n+1}, \tag{3.22}$$

$$\mu(t_{n+1}) = (1+\Delta)^2 u(t_{n+1}) + \frac{r(t_{n+1})}{\sqrt{E(u(t_n)) + D_0}} f(u(t_n)) + G_\mu^{n+1}, \tag{3.23}$$

$$r(t_{n+1}) - r(t_n) = \frac{1}{2\sqrt{E(u(t_n) + D_0)}}(f(u(t_n)), u(t_{n+1}) - u(t_n)) + \tau G_r^{n+1}, \tag{3.24}$$

$$\psi(t_{n+1}) = \frac{u(t_{n+1}) - u(t_n)}{\tau} + G_u^{n+1}, \tag{3.25}$$

where

$$\begin{aligned}
G_\psi^{n+1} &= \frac{\psi(t_{n+1}) - \psi(t_n)}{\tau} - \psi_t(t_{n+1}), \\
G_\mu^{n+1} &= r(t_{n+1})\left(\frac{f(u(t_{n+1}))}{\sqrt{E(u(t_{n+1})) + D_0}} - \frac{f(u(t_n))}{\sqrt{E(u(t_n)) + D_0}}\right), \\
G_r^{n+1} &= \frac{r(t_{n+1}) - r(t_n)}{\tau} - r_t(t_{n+1}) - \frac{1}{2}\int_\Omega \frac{f(u(t_{n+1}))}{\sqrt{E(u(t_{n+1})) + D_0}}\left(\frac{u(t_{n+1}) - u(t_n)}{\tau} - u_t(t_{n+1})\right)\mathrm{d}x \\
&\quad + \frac{1}{2}\int_\Omega \left(\frac{f(u(t_{n+1}))}{\sqrt{E(u(t_{n+1})) + D_0}} - \frac{f(u(t_n))}{\sqrt{E(u(t_n)) + D_0}}\right)\frac{u(t_{n+1}) - u(t_n)}{\tau}\mathrm{d}x, \\
G_u^{n+1} &= u_t(t_{n+1}) - \frac{u(t_{n+1}) - u(t_n)}{\tau}.
\end{aligned}$$

To give the error estimate, we assume that the analytic solution of the system (3.1)–(3.4) satisfies the following regularity conditions. The reader can refer to [30] about the global smooth solutions of the MPFC equation.

$$\zeta \in L^\infty(0, T; H^4(\Omega)) \cap L^\infty(0, T; W^{1,\infty}(\Omega)), \tag{3.26}$$

$$\zeta_t, \zeta_{tt} \in L^2(0, T; H^2(\Omega)) \cap L^\infty(0, T; L^\infty(\Omega)), \quad \zeta_{ttt} \in L^2(0, T; H^{-1}(\Omega)), \tag{3.27}$$

where $\zeta = \psi, u, \mu, r$. Let $u \lesssim v$ denote there is a positive constant C that is independent on τ and n such that $u \leq Cv$. By Taylor expansion, we can easily derive the following estimates for the truncation errors.

Lemma 3.1. *Under the regularity assumption* (3.26) and (3.27), *the truncation errors satisfy*

$$\sum_{n=0}^{N-1} \left(\|G_\psi^{n+1}\|_{-1}^2 + \|G_u^{n+1}\|_1^2 + \|G_\mu^{n+1}\|_1^2 + \|G_r^{n+1}\|^2 \right) \lesssim \tau^2. \tag{3.28}$$

Proof. Using (3.26)–(3.27) and Theorem 4.1 in [23], we can get $r_{tt} \in L^2(0, T; L^2(\Omega))$. Then we can easily derive the desired result. □

We define the error functions for $n = 0, 1, 2, \ldots, N$ as

$$e_u^n = u(t_n) - u^n, \;\; e_\mu^n = \mu(t_n) - \mu^n, \;\; e_r^n = r(t_n) - r^n, \;\; e_\psi^n = \psi(t_n) - \psi^n. \tag{3.29}$$

Subtracting (3.7)–(3.10) from (3.22)–(3.25), respectively, we get the following error equations for $n \geq 0$,

$$\frac{e_\psi^{n+1} - e_\psi^n}{\tau} + \beta e_\psi^{n+1} = M \Delta e_\mu^{n+1} + G_\psi^{n+1}, \tag{3.30}$$

$$\begin{aligned} e_\mu^{n+1} = {} & (1+\Delta)^2 e_u^{n+1} + r^{n+1} \left(\frac{f(u(t_n))}{\sqrt{E(u(t_n)) + D_0}} - \frac{f(u^n)}{\sqrt{E(u^n) + D_0}} \right) \\ & + \frac{e_r^{n+1}}{\sqrt{E(u(t_n)) + D_0}} f(u(t_n)) + G_\mu^{n+1}, \end{aligned} \tag{3.31}$$

$$\begin{aligned} e_r^{n+1} - e_r^n = {} & \left(\frac{f(u(t_n))}{2\sqrt{E(u(t_n)) + D_0}} - \frac{f(u^n)}{2\sqrt{E(u^n) + D_0}}, u(t_{n+1}) - u(t_n) \right) \\ & + \frac{1}{2\sqrt{E(u^n) + D_0}} (f(u^n), e_u^{n+1} - e_u^n) + \tau G_r^{n+1}, \end{aligned} \tag{3.32}$$

$$e_\psi^{n+1} = \frac{e_u^{n+1} - e_u^n}{\tau} + G_u^{n+1}. \tag{3.33}$$

We derive error analysis of the first-order SAV scheme by applying a mathematical induction on $\|u^n\|_{L^\infty}$ and the norm is used to control the nonlinear terms in the equations.

Theorem 3.3. *Under the regularity assumption* (3.26) and (3.27) *and let* $(\psi^n, u^n, \mu^n, r^n)$ *be the solutions of* (3.7)–(3.10), *we have the error estimate as follow*

$$\|e_u^N\| + \left(\tau \sum_{n=0}^{N-1} \|e_\psi^{n+1}\|_{-1}^2 \right)^{\frac{1}{2}} \lesssim \tau. \tag{3.34}$$

Proof. We apply Δ^{-1} to (3.30) and take the L^2 inner product with τe_ψ^{n+1}, using (3.31) and (3.33), we have

$$\begin{aligned} & \frac{1}{2M} (\|e_\psi^{n+1}\|_{-1}^2 - \|e_\psi^n\|_{-1}^2 + \|e_\psi^{n+1} - e_\psi^n\|_{-1}^2) + \frac{\beta\tau}{M} \|e_\psi^{n+1}\|_{-1}^2 \\ & + \frac{1}{2} (\|(1+\Delta) e_u^{n+1}\|^2 - \|(1+\Delta) e_u^n\|^2 + \|(1+\Delta)(e_u^{n+1} - e_u^n)\|^2) \\ = & -\frac{\tau}{M} (\Delta^{-1} G_\psi^{n+1}, e_\psi^{n+1}) - r^{n+1} \tau \left(\frac{f(u(t_n))}{\sqrt{E(u(t_n)) + D_0}} - \frac{f(u^n)}{\sqrt{E(u^n) + D_0}}, e_\psi^{n+1} \right) \\ & - \tau \left(\frac{e_r^{n+1}}{\sqrt{E(u(t_n)) + D_0}} f(u(t_n)), e_\psi^{n+1} \right) - \tau((1+\Delta)^2 e_u^{n+1}, G_u^{n+1}) - \tau(G_\mu^{n+1}, e_\psi^{n+1}). \end{aligned} \tag{3.35}$$

Taking the L^2 inner product of (3.32) with $2e_r^{n+1}$ and applying (3.33), we have

$$\begin{aligned} |e_r^{n+1}|^2 - |e_r^n|^2 + |e_r^{n+1} - e_r^n|^2 = {} & e_r^{n+1} \left(\frac{f(u(t_n))}{\sqrt{E(u(t_n)) + D_0}} - \frac{f(u^n)}{\sqrt{E(u^n) + D_0}}, u(t_{n+1}) - u(t_n) \right) \\ & + 2e_r^{n+1} \tau G_r^{n+1} + \tau \frac{e_r^{n+1}}{\sqrt{E(u^n) + D_0}} (f(u^n), e_\psi^{n+1}) - \tau \frac{e_r^{n+1}}{\sqrt{E(u^n) + D_0}} (f(u^n), G_u^{n+1}). \end{aligned} \tag{3.36}$$

Combining (3.35) and (3.36), we get

$$\frac{1}{2M}(\|e_\psi^{n+1}\|_{-1}^2-\|e_\psi^n\|_{-1}^2+\|e_\psi^{n+1}-e_\psi^n\|_{-1}^2)+|e_r^{n+1}|^2-|e_r^n|^2+|e_r^{n+1}-e_r^n|^2+\frac{\beta\tau}{M}\|e_\psi^{n+1}\|_{-1}^2$$
$$+\frac{1}{2}(\|(1+\Delta)e_u^{n+1}\|^2-\|(1+\Delta)e_u^n\|^2+\|(1+\Delta)(e_u^{n+1}-e_u^n)\|^2):=J_1+J_2,$$

where

$$\begin{aligned}J_1=&-\tau((1+\Delta)^2e_u^{n+1},G_u^{n+1})-\tau\frac{e_r^{n+1}}{\sqrt{E(u^n)+D_0}}(f(u^n),G_u^{n+1})-\tau(G_\mu^{n+1},e_\psi^{n+1})+2e_r^{n+1}\tau G_r^{n+1}\\&-\frac{\tau}{M}(\Delta^{-1}G_\psi^{n+1},e_\psi^{n+1}),\\J_2=&\,e_r^{n+1}\left(\frac{f(u(t_n))}{\sqrt{E(u(t_n))+D_0}}-\frac{f(u^n)}{E(u^n)+D_0},u(t_{n+1})-u(t_n)\right)\\&-r(t_{n+1})\tau\left(\frac{f(u(t_n))}{\sqrt{E(u(t_n))+D_0}}-\frac{f(u^n)}{E(u^n)+D_0},e_\psi^{n+1}\right).\end{aligned}$$

We now estimate J_1 and J_2. First, we try to prove that

$$\|u^n\|_{L^\infty}\le\|u\|_{L^\infty(L^\infty)}+1 \tag{3.37}$$

by mathematical induction. Because $u^0=u(t_0)$, (3.37) holds naturally for $n=0$. Hereinafter, we derive the error estimates of the numerical solution under the assumption that (3.37) holds for $0\le n\le m$, for some positive integer m. We will see that if (3.37) is true for $0\le n\le m$, it is also true for $n=m+1$. First of all, applying (3.37) and $E(\cdot)+D_0>0$, we get

$$\begin{aligned}J_1\le&\,\tau(\|e_\psi^{n+1}\|^2+|e_r^{n+1}|^2+\|e_\psi^{n+1}\|_{-1}^2+\|e_u^{n+1}\|_2^2)\\&+C\tau(\|G_\mu^{n+1}\|^2+\|G_u^{n+1}\|_2^2+\|G_r^{n+1}\|^2+\|G_\psi^{n+1}\|_{-1}^2).\end{aligned}\tag{3.38}$$

$$\begin{aligned}&\frac{\nabla f(u(t_n))}{\sqrt{E(u(t_n))+D_0}}-\frac{\nabla f(u^n)}{\sqrt{E(u^n)+D_0}}=\nabla f(u^n)\frac{E(u^n)-E(u(t_n))}{\sqrt{(E(u(t_n))+D_0)(E(u^n)+D_0)(E(u(t_n))+E(u^n)+2D_0)}}\\&+\frac{\nabla(f(u(t_n))-f(u^n))}{\sqrt{E(u(t_n))+D_0}}:=H_1+H_2,\end{aligned}\tag{3.39}$$

Because $f(\cdot)$ is Lipschitz continuous and $E(\cdot)+D_0>0$ and applying (3.26), (3.27) and (3.37), we can estimate H_1 and H_2 as follows

$$\|H_1\|\lesssim\|\nabla f(u^n)\|\|e_u^n\|\lesssim\|e_u^n\|,\tag{3.40}$$

and

$$\begin{aligned}\|H_2\|\lesssim&\,\|\nabla(f(u(t_n))-f(u^n))\|\\=&\,\|f'(u(t_n))\nabla u(t_n)-\nabla f'(u^n)\nabla u^n-f'(u^n)\nabla u(t_n)+f'(u^n)\nabla u(t_n)\|\\\lesssim&\,\|(f'(u(t_n))-f'(u^n))\nabla u(t_n)\|+\|f'(u^n)\|_{L^\infty}\|\nabla e_u^n\|\\\lesssim&\,\|e_u^n\|+\|\nabla e_u^n\|.\end{aligned}\tag{3.41}$$

Hence, combining (3.39),(3.40) and (3.41), using the Poincaré inequality, we obtain

$$\left\|\frac{\nabla f(u(t_n))}{\sqrt{E(u(t_n))+D_0}}-\frac{\nabla f(u^n)}{E(u^n)+D_0}\right\|\lesssim\|\nabla e_u^n\|,\tag{3.42}$$

together with (3.26) and (3.27), it implies that

$$J_2\lesssim\tau(|e_r^{n+1}|^2+\|\nabla e_u^n\|^2+\|e_\psi^{n+1}\|_{-1}^2).\tag{3.43}$$

Combining (3.38) and (3.43), we get

$$\begin{aligned}&\frac{1}{2M}(\|e_\psi^{n+1}\|_{-1}^2-\|e_\psi^n\|_{-1}^2+\|e_\psi^{n+1}-e_\psi^n\|_{-1}^2)+|e_r^{n+1}|^2-|e_r^n|^2+|e_r^{n+1}-e_r^n|^2+\frac{\beta\tau}{M}\|e_\psi^{n+1}\|_{-1}^2\\&+\frac{1}{2}(\|(1+\Delta)e_u^{n+1}\|^2-\|(1+\Delta)e_u^n\|^2+\|(1+\Delta)(e_u^{n+1}-e_u^n)\|^2)\\\le&\,\tau(|e_r^{n+1}|^2+\|e_\psi^{n+1}\|_{-1}^2+\|e_u^{n+1}\|_2^2)+\tau(\|G_\mu^{n+1}\|^2+\|G_u^{n+1}\|_2^2+\|G_r^{n+1}\|^2+\|G_\psi^{n+1}\|_{-1}^2).\end{aligned}\tag{3.44}$$

Summing up for n from 0 to m and then using the Grönwall's inequality, there is a number $\tau_1 > 0$ such that provided $\tau \le \tau_1$, we have the following estimate

$$\left(\frac{1}{2M}\|e_\psi^{m+1}\|_{-1}^2 + |e_r^{m+1}|^2 + \frac{1}{2}\|(1+\Delta)e_u^{m+1}\|^2\right) + \sum_{n=0}^{m}\left(\|e_\psi^{n+1} - e_\psi^n\|_{-1}^2 + |e_r^{n+1} - e_r^n|^2 + \|(1+\Delta)(e_u^{n+1} - e_u^n)\|^2 + \frac{\beta\tau}{M}\|e_\psi^{n+1}\|_{-1}^2\right) \le C_1\tau^2. \tag{3.45}$$

Applying the H^2 elliptic regularity of (3.8) and $\|\cdot\|_{-2} \le \|\cdot\|$, there is a number $C_2 > 0$ which is independent of n such that

$$\begin{aligned}
\|u^{m+1}\|_2 &\lesssim \|\mu^{m+1}\| + \|f(u^m)\| + \|\psi^{m+1}\| \\
&\lesssim \left\|\frac{\Delta^{-1}\psi^{m+1} - \Delta^{-1}\psi^m}{\tau}\right\| + \|\Delta^{-1}\psi^{m+1}\| + \|f(u^m)\| + \|\psi^{m+1}\| \\
&\lesssim \left\|\frac{\Delta^{-1}(\psi(t_{m+1}) - \psi(t_m))}{\tau}\right\| + \left\|\frac{e_\psi^{m+1} - e_\psi^m}{\tau}\right\|_{-1} + \|f(u^m)\| + \|e_\psi^{m+1}\| + \|\psi(t_{m+1})\| \\
&\le C_2.
\end{aligned} \tag{3.46}$$

From (3.26), (3.27) and (3.46), it holds that

$$\|e_u^{m+1}\|_2 \le \|u^{m+1}\|_2 + \|u(t_{m+1})\|_2 \le C_3. \tag{3.47}$$

Moreover, according to (3.45) and (3.47), we get

$$\begin{aligned}
\|u^{m+1}\|_{L^\infty} &= \|e_u^{m+1}\|_{L^\infty} + \|u(t_{m+1})\|_{L^\infty} \\
&\le C_\Omega\|e_u^{m+1}\|_1^{\frac{1}{2}}\|e_u^{m+1}\|_2^{\frac{1}{2}} + \|u(t_{m+1})\|_{L^\infty} \\
&\le C_\Omega\sqrt[4]{C_1}\sqrt{\tau}\sqrt{C_3} + \|u(t_{m+1})\|_{L^\infty},
\end{aligned} \tag{3.48}$$

in which C_Ω is a positive constant depends on Ω. Hence, we can find a $\tau_2 > 0$ ($\tau_2 < \tau_1$), such that provided $\tau < \tau_2$,

$$\|u^{m+1}\|_{L^\infty} \le \|u(t)\|_{L^\infty(L^\infty)} + 1, \tag{3.49}$$

and we complete the induction on (3.37) in the case $\tau < \tau_2$. Hence (3.45) is true when $m = N-1$ if $\tau < \tau_2$.

In the case $\tau \ge \tau_2$, according to (3.15), (3.26) and (3.27), we have

$$\begin{aligned}
&\max_{0\le n\le N-1}\left(\|e_\psi^{n+1}\|_{-1}^2 + |e_r^{n+1}|^2 + \|(1+\Delta)e_u^{n+1}\|^2\right) \\
&+ \sum_{n=0}^{N-1}\left(\|e_\psi^{n+1} - e_\psi^n\|_{-1}^2 + |e_r^{n+1} - e_r^n|^2 + \tau\|e_\psi^{n+1}\|_{-1}^2 + \|(1+\Delta)(e_u^{n+1} - e_u^n)\|^2\right) \\
&\le C_4 \le C_4(\tau_2^{-2})\tau^2,
\end{aligned} \tag{3.50}$$

for some $C_4 > 0$.

In the end, Combining (3.45) and (3.50), we derive for any τ,

$$\begin{aligned}
&\max_{0\le n\le N-1}\left(\|e_\psi^{n+1}\|_{-1}^2 + |e_r^{n+1}|^2 + \|(1+\Delta)e_u^{n+1}\|^2\right) \\
&+ \sum_{n=0}^{N-1}\left(\|e_\psi^{n+1} - e_\psi^n\|_{-1}^2 + |e_r^{n+1} - e_r^n|^2 + \tau\|e_\psi^{n+1}\|_{-1}^2 + \|(1+\Delta)(e_u^{n+1} - e_u^n)\|^2\right) \\
&\le (C_1 + C_4\tau_2^{-2})\tau^2.
\end{aligned}$$

which implies (3.34). □

4. The stability and error analysis of the second-order SAV scheme

In this section, we construct a second-order scheme based on Crank–Nicolson method as follows: for $n \ge 1$,

$$\frac{\psi^{n+1} - \psi^n}{\tau} + \beta\frac{\psi^{n+1} + \psi^n}{2} = M\Delta\mu^{n+1/2}, \tag{4.1}$$

$$\mu^{n+1/2} = (1+\Delta)^2\frac{u^{n+1} + u^n}{2} + \frac{r^{n+1} + r^n}{2\sqrt{E(\bar{u}^n) + D_0}}f(\bar{u}^n), \tag{4.2}$$

$$r^{n+1}-r^n=\frac{1}{2\sqrt{E(\bar{u}^n)+D_0}}(f(\bar{u}^n),u^{n+1}-u^n), \tag{4.3}$$
$$\frac{\psi^{n+1}+\psi^n}{2}=\frac{u^{n+1}-u^n}{\tau}, \tag{4.4}$$

in which

$$\bar{u}^n=\frac{3}{2}u^n-\frac{1}{2}u^{n-1}. \tag{4.5}$$

Remark 4.1. Since the second-order scheme involves three time levels, it requires an initialization step. Here, (u^0,ψ^0,r^0) is determined by the initial conditions. In order to obtain the second-order time accuracy of the main scheme, we calculate (u^1,ψ^1,r^1) by a predictor–corrector scheme. We first predict $(\tilde{u}^1,\tilde{\psi}^1,\tilde{r}^1)$ by the following first-order backward Euler scheme

$$\begin{aligned}
&\frac{\tilde{\psi}^1-\psi^0}{\tau}+\beta\tilde{\psi}^1=M\Delta\mu^1,\\
&\mu^1=(1+\Delta)^2\tilde{u}^1+\frac{\tilde{r}^1}{\sqrt{E(u^0)+D_0}}f(u^0),\\
&\tilde{r}^1-r^0=\frac{1}{2\sqrt{E(u^0)+D_0}}(f(u^0),\tilde{u}^1-u^0),\\
&\tilde{\psi}^1=\frac{\tilde{u}^1-u^0}{\tau}.
\end{aligned}$$

Then we use the following second-order corrector scheme to obtain (u^1,ψ^1,r^1)

$$\begin{aligned}
&\frac{\psi^1-\psi^0}{\tau}+\beta\frac{\psi^1+\psi^0}{2}=M\Delta\mu^{1/2},\\
&\mu^{1/2}=(1+\Delta)^2\frac{u^1+u^0}{2}+\frac{r^1+r^0}{2\sqrt{E(\tilde{u}^1)+D_0}}f(\tilde{u}^1),\\
&r^1-r^0=\frac{1}{2\sqrt{E(\tilde{u}^1)+D_0}}(f(\tilde{u}^1),u^1-u^0),\\
&\frac{\psi^1+\psi^0}{2}=\frac{u^1-u^0}{\tau}.
\end{aligned}$$

From (4.1) and (4.2), we have

$$\begin{aligned}
\frac{\psi^{n+1}-\psi^n}{\tau}+\beta\frac{\psi^{n+1}+\psi^n}{2}&=M\Delta\left((1+\Delta)^2\frac{u^{n+1}+u^n}{2}+\frac{r^n}{\sqrt{E(\bar{u}^n)+D_0}}f(\bar{u}^n)\right)\\
&\quad+M\Delta\left(\frac{f(\bar{u}^n)}{4(E(\bar{u}^n)+D_0)}(f(\bar{u}^n),u^{n+1}-u^n)\right).
\end{aligned} \tag{4.6}$$

Applying (4.4) and let

$$\hat{a}^n=\frac{f(\bar{u}^n)}{\sqrt{E(\bar{u}^n)+D_0}}, \tag{4.7}$$

Eq. (4.6) can be rewritten as

$$\begin{aligned}
&(2+\beta\tau-\frac{\tau^2}{2}M\Delta(1+\Delta)^2)u^{n+1}-\frac{\tau^2}{4}M\Delta\hat{a}^n(\hat{a}^n,u^{n+1})\\
&\qquad=(2+\beta\tau)u^n+2\tau\psi^n+\frac{\tau^2}{2}M\Delta(1+\triangle)^2u^n+\tau^2M\Delta\hat{a}^nr^n-\frac{\tau^2}{4}M\Delta\hat{a}^n(\hat{a}^n,u^n):=\hat{h}^n.
\end{aligned} \tag{4.8}$$

From (4.4), we have

$$\psi^{n+1}=\frac{2u^{n+1}-2u^n}{\tau}-\psi^n. \tag{4.9}$$

Let $\hat{T}^{-1}:=(2+\beta\tau-\frac{\tau^2}{2}M\Delta(1+\Delta)^2)^{-1}$, applying $\hat{T}^{-1}$ to (4.8) and then taking the inner product with $\hat{a}^n$, we get

$$(\hat{a}^n,u^{n+1})+\frac{\tau^2}{4}\hat{\theta}^n(\hat{a}^n,u^{n+1})=(\hat{a}^n,\hat{T}^{-1}\hat{h}^n), \tag{4.10}$$

in which

$$\hat{\theta}^n = -(\hat{a}^n, \hat{T}^{-1} M \Delta \hat{a}^n) \geq 0,$$

because $-\hat{T}^{-1}\Delta$ is a positive definite operator. Then from (4.10), we have

$$(\hat{a}^n, u^{n+1}) = \frac{(\hat{a}^n, \hat{T}^{-1}\hat{h}^n)}{1 + \frac{\tau^2}{4}\hat{\theta}^n}. \tag{4.11}$$

Thus, we can obtain u^{n+1} and ψ^{n+1} from (4.8) and (4.9), respectively.

The following theorem implies that the second-order scheme (4.1)–(4.5) is energy-stable.

Theorem 4.1. *The scheme (4.1)–(4.5) satisfies unconditional energy dissipation law, that is, for $n < T/\tau$,*

$$\hat{\mathcal{E}}(u^{n+1}, r^{n+1}, \psi^{n+1}) \leq \hat{\mathcal{E}}(u^n, r^n, \psi^n), \tag{4.12}$$

and then, we have the following boundedness

$$\max_{0 \leq n \leq N} (\frac{1}{2}\|(1+\Delta)u^n\|^2 + (r^n)^2 + \frac{1}{2M}\|\psi^n\|_{-1}^2) \leq \frac{1}{2}\|(1+\Delta)u^0\|^2 + (r^0)^2 + \frac{1}{2M}\|\psi^0\|_{-1}^2.$$

Proof. Combining (4.1) and (4.2) together and applying Δ^{-1}, we obtain

$$\frac{1}{\tau}\Delta^{-1}(\psi^{n+1} - \psi^n) + \frac{\beta}{2}\Delta^{-1}(\psi^{n+1} + \psi^n) = M(1+\Delta)^2 \frac{u^{n+1} + u^n}{2} + M\frac{r^{n+1} + r^n}{2\sqrt{E(\bar{u}^n) + D_0}} f(\bar{u}^n). \tag{4.13}$$

Taking the L^2 inner product of (4.13) with $u^{n+1} - u^n$, we obtain

$$\begin{aligned} &\frac{1}{\tau}(\Delta^{-1}(\psi^{n+1} - \psi^n), u^{n+1} - u^n) + \frac{\beta}{2}(\Delta^{-1}(\psi^{n+1} + \psi^n), u^{n+1} - u^n) \\ &\quad = \frac{M}{2}\left(\|(1+\Delta)u^{n+1}\|^2 - \|(1+\Delta)u^n\|^2\right) + M\left(\frac{r^{n+1} + r^n}{2\sqrt{E(\bar{u}^n) + D_0}} f(\bar{u}^n), u^{n+1} - u^n\right). \end{aligned} \tag{4.14}$$

Taking the L^2 inner product of (4.3) with $r^{n+1} + r^n$, we have

$$(r^{n+1})^2 - (r^n)^2 = \frac{r^{n+1} + r^n}{2\sqrt{E(\bar{u}^n) + D_0}}(f(\bar{u}^n), u^{n+1} - u^n). \tag{4.15}$$

From (4.4), we have

$$\begin{aligned} \frac{1}{\tau}(\Delta^{-1}(\psi^{n+1} - \psi^n), u^{n+1} - u^n) &= \frac{1}{\tau}(\Delta^{-1}(\psi^{n+1} - \psi^n), \frac{\tau}{2}(\psi^{n+1} + \psi^n)) \\ &\quad - \frac{1}{2}(\nabla\Delta^{-1}(\psi^{n+1} - \psi^n), \nabla\Delta^{-1}(\psi^{n+1} + \psi^n)) \\ &\quad - \frac{1}{2}(\|\psi^{n+1}\|_{-1}^2 - \|\psi^n\|_{-1}^2), \end{aligned} \tag{4.16}$$

and

$$\begin{aligned} \frac{\beta}{2}(\Delta^{-1}(\psi^{n+1} + \psi^n), u^{n+1} - u^n) &= \frac{\beta}{2}(\Delta^{-1}(\psi^{n+1} + \psi^n), \frac{\tau}{2}(\psi^{n+1} + \psi^n)) \\ &\quad - \frac{\beta\tau}{4}(\nabla\Delta^{-1}(\psi^{n+1} + \psi^n), \nabla\Delta^{-1}(\psi^{n+1} + \psi^n)) \\ &\quad - \frac{\beta\tau}{4}\|\psi^{n+1} + \psi^n\|_{-1}^2. \end{aligned} \tag{4.17}$$

In the end, we combine (4.14)–(4.17) and obtain

$$\begin{aligned} &\frac{M}{2}(\|(1+\Delta)u^{n+1}\|^2 - \|(1+\Delta)u^n\|^2) + M((r^{n+1})^2 - (r^n)^2) + \frac{1}{2}(\|\psi^{n+1}\|_{-1}^2 - \|\psi^n\|_{-1}^2) \\ &= -\frac{\beta\tau}{4}\|\psi^{n+1} + \psi^n\|_{-1}^2. \end{aligned}$$

Dividing both sides of the above equation by M and we obtain the desired energy dissipation law and boundedness. □

Now we consider the error estimates for the second-order scheme. Let $t_{n+1/2} = (t_{n+1} + t_n)/2$. We write the MPFC system (4.1)–(4.5) as a truncation form as follows:

$$\frac{\psi(t_{n+1}) - \psi(t_n)}{\tau} + \beta\frac{\psi(t_{n+1}) + \psi(t_n)}{2} = M\Delta\mu(t_{n+1/2}) + \hat{G}_\psi^{n+1}, \tag{4.18}$$

$$\mu(t_{n+1/2}) = (1+\Delta)^2 u(t_{n+1/2}) + \frac{r(t_{n+1/2})}{\sqrt{E(\bar{u}(t_n))+D_0}} f(\bar{u}(t_n)) + \hat{G}_\mu^{n+1}, \tag{4.19}$$

$$r(t_{n+1}) - r(t_n) = \frac{1}{2\sqrt{E(\bar{u}(t_n))+D_0}} (f(\bar{u}(t_n)), u(t_{n+1}) - u(t_n)) + \tau \hat{G}_r^{n+1}, \tag{4.20}$$

$$\frac{\psi(t_{n+1}) + \psi(t_n)}{2} = \frac{u(t_{n+1}) - u(t_n)}{\tau} + \hat{G}_u^{n+1}, \tag{4.21}$$

in which

$$\begin{aligned}
\bar{u}(t_n) &= \frac{3}{2}u(t_n) - \frac{1}{2}u(t_{n-1}),\\
\hat{G}_\psi^{n+1} &= \frac{\psi(t_{n+1}) - \psi(t_n)}{\tau} - \psi_t(t_{n+1/2}) + \beta\frac{\psi(t_{n+1}) + \psi(t_n)}{2} - \beta\psi(t_{n+1/2}),\\
\hat{G}_\mu^{n+1} &= r(t_{n+1/2})\left(\frac{f(u(t_{n+1/2}))}{2\sqrt{E(u(t_{n+1/2}))+D_0}} - \frac{f(\bar{u}(t_n))}{2\sqrt{E(\bar{u}(t_n))+D_0}}\right),\\
\hat{G}_r^{n+1} &= \frac{r(t_{n+1}) - r(t_n)}{\tau} - r_t(t_{n+1/2}) - \frac{1}{2}\int_\Omega \frac{f(u(t_{n+1/2}))}{2\sqrt{E(u(t_{n+1/2}))+D_0}}\left(\frac{u(t_{n+1}) - u(t_n)}{\tau} - u_t(t_{n+1/2})\right)\mathrm{d}x\\
&\quad + \frac{1}{2}\int_\Omega \left(\frac{f(u(t_{n+1/2}))}{2\sqrt{E(u(t_{n+1/2}))+D_0}} - \frac{f(\bar{u}(t_n))}{2\sqrt{E(\bar{u}(t_n))+D_0}}\right)\frac{u(t_{n+1}) - u(t_n)}{\tau}\mathrm{d}x,\\
\hat{G}_u^{n+1} &= u_t(t_{n+1/2}) - \frac{u(t_{n+1}) - u(t_n)}{\tau} + \frac{\psi(t_{n+1}) + \psi(t_n)}{2} - \psi(t_{n+1/2}).
\end{aligned}$$

To prove the error estimate, we assume that the analytic solution of the system (3.7)–(3.10) satisfies the following regularity conditions

$$\zeta \in L^\infty(0,T;H^5(\Omega)) \cap L^\infty(0,T;W^{1,\infty}(\Omega)), \tag{4.22}$$

$$\zeta_t, \zeta_{tt}, \zeta_{ttt} \in L^2(0,T;H^5(\Omega)) \cap L^\infty(0,T;L^\infty(\Omega)), \quad \zeta_{tttt} \in L^2(0,T;H^{-1}(\Omega)), \tag{4.23}$$

where $\zeta = \psi, u, \mu, r$. By Taylor expansion, we can easily derive the following estimates for the truncation errors.

Lemma 4.1. *Under the regularity assumption (4.22)–(4.23), the truncation errors satisfy, for any $N \le T/\tau$,*

$$\sum_{n=0}^{N-1}\left(\|\hat{G}_\psi^{n+1}\|_{-1}^2 + \|\hat{G}_u^{n+1}\|_2^2 + \|\hat{G}_\mu^{n+1}\|_1^2 + \|\hat{G}_r^{n+1}\|^2\right) \lesssim \tau^4. \tag{4.24}$$

Subtracting (4.1)–(4.4) from (4.18)–(4.21) and with the error functions we defined in (3.29), we get the following error equations for $n \ge 0$,

$$\frac{e_\psi^{n+1} - e_\psi^n}{\tau} + \beta\frac{e_\psi^{n+1} + e_\psi^n}{2} = M\Delta e_\mu^{n+1/2} + \hat{G}_\psi^{n+1}, \tag{4.25}$$

$$\begin{aligned}
e_\mu^{n+1/2} &= (1+\Delta)^2\left(u(t_{n+1/2}) - \frac{u(t_{n+1}) + u(t_n)}{2}\right) + (1+\Delta)^2\left(\frac{e_u^{n+1} + e_u^n}{2}\right) + \hat{G}_\mu^{n+1}\\
&\quad + \frac{r(t_{n+1/2}) - (r(t_{n+1}) + r(t_n))/2}{\sqrt{E(\bar{u}(t_n))+D_0}} f(\bar{u}(t_n)) + \frac{r(t_{n+1}) + r(t_n)}{2}\left(\frac{f(\bar{u}(t_n))}{\sqrt{E(\bar{u}(t_n))+D_0}} - \frac{f(\bar{u}^n)}{\sqrt{E(\bar{u}^n)+D_0}}\right)\\
&\quad + \frac{e_r^{n+1} + e_r^n}{2\sqrt{E(\bar{u}^n)+D_0}} f(\bar{u}^n),
\end{aligned} \tag{4.26}$$

$$\begin{aligned}
e_r^{n+1} - e_r^n &= \left(\frac{f(\bar{u}(t_n))}{2\sqrt{E(\bar{u}(t_n))+D_0}} - \frac{f(\bar{u}^n)}{2\sqrt{E(\bar{u}^n)+D_0}}, u(t_{n+1}) - u(t_n)\right)\\
&\quad + \frac{1}{2\sqrt{E(\bar{u}^n)+D_0}}(f(\bar{u}^n), e_u^{n+1} - e_u^n) + \tau\hat{G}_r^{n+1},
\end{aligned} \tag{4.27}$$

$$\frac{e_\psi^{n+1} + e_\psi^n}{2} = \frac{e_u^{n+1} - e_u^n}{\tau} + \hat{G}_u^{n+1}, \tag{4.28}$$

in which we define $e_\mu^{n+1/2} = \mu(t_{n+1/2}) - \mu^{n+1/2}$.

Theorem 4.2. *Under the regularity assumption* (4.22) and (4.23) *and let* $(\psi^n, u^n, \mu^n, r^n)$ *be the solution of* (4.1)–(4.4), *we have the error estimate as follows*

$$\|e_u^N\| + \left(\tau \sum_{n=0}^{N-1} \|e_\psi^{n+1} + e_\psi^n\|_{-1}^2\right)^{\frac{1}{2}} \lesssim \tau^2. \tag{4.29}$$

Proof. We prove the theorem by using the mathematical induction. Because (u^0, ψ^0, r^0) is given as (3.5) and we calculate (u^1, ψ^1, r^1) by setting $(u^{-1}, \psi^{-1}, r^{-1}) = (u^0, \psi^0, r^0)$, (3.37) holds for the case $n = -1, 0$. Hereinafter, we derive the error estimates of the numerical solution under the assumption that (3.37) holds for $0 \le n \le m$, for some positive integer m. We will see that if (3.37) is true for $0 \le n \le m$, it is also true for $n = m + 1$.

We apply Δ^{-1} to (4.25) and taking its L^2 inner product with $-\tau(e_\psi^{n+1} + e_\psi^n)$, using (4.26) and (4.28), we have

$$\begin{aligned}
&\|e_\psi^{n+1}\|_{-1}^2 - \|e_\psi^n\|_{-1}^2 + \frac{\beta\tau}{2}\|e_\psi^{n+1} + e_\psi^n\|_{-1}^2 \\
=& -\tau(\Delta^{-1}\hat{G}_\psi^{n+1}, e_\psi^{n+1} + e_\psi^n) - M\tau\left((1+\Delta)^2(u(t_{n+1/2}) - \frac{u(t_{n+1}) + u(t_n)}{2}), e_\psi^{n+1} + e_\psi^n\right) \\
&- M(\|(1+\Delta)e_u^{n+1}\|^2 - \|(1+\Delta)e_u^n\|^2) - M\tau\left(\frac{r(t_{n+1/2}) - (r(t_{n+1}) + r(t_n))/2}{\sqrt{E(\bar{u}(t_n)) + D_0}} f(\bar{u}(t_n)), e_\psi^{n+1} + e_\psi^n\right) \\
&- M\tau\frac{r(t_{n+1}) + r(t_n)}{2}\left(\frac{f(\bar{u}(t_n))}{\sqrt{E(\bar{u}(t_n)) + D_0}} - \frac{f(\bar{u}^n)}{\sqrt{E(\bar{u}^n) + D_0}}, e_\psi^{n+1} + e_\psi^n\right) \\
&- M\tau\left(\frac{e_r^{n+1} + e_r^n}{2\sqrt{E(\bar{u}^n) + D_0}} f(\bar{u}^n), e_\psi^{n+1} + e_\psi^n\right) - M\tau(\hat{G}_\mu^{n+1}, e_\psi^{n+1} + e_\psi^n) - M\tau((1+\Delta)^2(e_u^{n+1} + e_u^n), \hat{G}_u^{n+1}).
\end{aligned} \tag{4.30}$$

Taking the L^2 inner product of (4.27) with $2M(e_r^{n+1} + e_r^n)$ and applying (4.28), we have

$$\begin{aligned}
&2M|e_r^{n+1}|^2 - 2M|e_r^n|^2 = 2M(e_r^{n+1} + e_r^n)\left(\frac{f(\bar{u}(t_n))}{2\sqrt{E(\bar{u}(t_n)) + D_0}} - \frac{f(\bar{u}^n)}{2\sqrt{E(\bar{u}^n) + D_0}}, u(t_{n+1}) - u(t_n)\right) \\
&+ M\frac{e_r^{n+1} + e_r^n}{\sqrt{E(\bar{u}^n) + D_0}}(f(\bar{u}^n), e_u^{n+1} - e_u^n) + 2M\tau\hat{G}_r^{n+1}(e_r^{n+1} + e_r^n) \\
&= 2M(e_r^{n+1} + e_r^n)\left(\frac{f(\bar{u}(t_n))}{2\sqrt{E(\bar{u}(t_n)) + D_0}} - \frac{f(\bar{u}^n)}{2\sqrt{E(\bar{u}^n) + D_0}}, u(t_{n+1}) - u(t_n)\right) \\
&+ M\tau\frac{e_r^{n+1} + e_r^n}{2\sqrt{E(\bar{u}^n) + D_0}}(f(\bar{u}^n), e_\psi^{n+1} - e_\psi^n) - M\tau\frac{e_r^{n+1} + e_r^n}{\sqrt{E(\bar{u}^n) + D_0}}(f(\bar{u}^n), \hat{G}_u^{n+1}) + 2M\tau\hat{G}_r^{n+1}(e_r^{n+1} + e_r^n).
\end{aligned} \tag{4.31}$$

Combining (4.30) and (4.31), we get

$$\begin{aligned}
&\|e_\psi^{n+1}\|_{-1}^2 - \|e_\psi^n\|_{-1}^2 + \frac{\beta\tau}{2}\|e_\psi^{n+1} + e_\psi^n\|_{-1}^2 + 2|e_r^{n+1}|^2 - 2|e_r^n|^2 \\
&+ M(\|(1+\Delta)e_u^{n+1}\|^2 - \|(1+\Delta)e_u^n\|^2) \le K_1 + K_2,
\end{aligned} \tag{4.32}$$

where

$$\begin{aligned}
K_1 =& -\tau(\Delta^{-1}\hat{G}_\psi^{n+1}, e_\psi^{n+1} + e_\psi^n) - M\tau\left((1+\Delta)^2(u(t_{n+1/2}) - \frac{u(t_{n+1}) + u(t_n)}{2}), e_\psi^{n+1} + e_\psi^n\right) \\
&- M\tau(\hat{G}_\mu^{n+1}, e_\psi^{n+1} + e_\psi^n) - M\tau((1+\Delta)^2(e_u^{n+1} + e_u^n), \hat{G}_u^{n+1}) + 2M\tau\hat{G}_r^{n+1}(e_r^{n+1} + e_r^n), \\
K_2 =& -M\tau\left(\frac{r(t_{n+1/2}) - (r(t_{n+1}) + r(t_n))/2}{\sqrt{E(\bar{u}(t_n)) + D_0}} f(\bar{u}(t_n)), e_\psi^{n+1} + e_\psi^n\right) \\
&- M\tau\frac{r(t_{n+1}) + r(t_n)}{2}\left(\frac{f(\bar{u}(t_n))}{\sqrt{E(\bar{u}(t_n)) + D_0}} - \frac{f(\bar{u}^n)}{\sqrt{E(\bar{u}^n) + D_0}}, e_\psi^{n+1} + e_\psi^n\right) \\
&+ 2M(e_r^{n+1} + e_r^n)\left(\frac{f(\bar{u}(t_n))}{2\sqrt{E(\bar{u}(t_n)) + D_0}} - \frac{f(\bar{u}^n)}{2\sqrt{E(\bar{u}^n) + D_0}}, u(t_{n+1}) - u(t_n)\right) \\
&- M\tau\frac{e_r^{n+1} + e_r^n}{\sqrt{E(\bar{u}^n) + D_0}}(f(\bar{u}^n), \hat{G}_u^{n+1}).
\end{aligned}$$

By applying (4.22) and (4.23), we derive

$$K_1 \le C\tau(\|(1+\Delta)e_u^{n+1}\|^2 + \|(1+\Delta)e_u^n\|^2 + |e_r^{n+1}|^2 + |e_r^n|^2) + \frac{1}{8}\tau\|e_\psi^{n+1}+e_\psi^n\|^2$$
$$+ C\tau(\|\Delta^{-1}\hat{G}_\psi^{n+1}\|^2 + \|\hat{G}_\mu^{n+1}\|^2 + \|\hat{G}_u^{n+1}\|_2^2 + \|\hat{G}_r^{n+1}\|^2) + C\tau^5. \tag{4.33}$$

$$\frac{f(\bar{u}(t_n))}{\sqrt{E(\bar{u}(t_n))+D_0}} - \frac{f(\bar{u}^n)}{\sqrt{E(\bar{u}^n)+D_0}} = f(\bar{u}^n)\frac{E(\bar{u}^n)-E(\bar{u}(t_n))}{\sqrt{(E(\bar{u}(t_n))+D_0)(E(\bar{u}^n)+D_0)}(\sqrt{E(\bar{u}(t_n))+D_0}+\sqrt{E(\bar{u}^n)+D_0})}$$
$$+\frac{f(\bar{u}(t_n))-f(\bar{u}^n)}{\sqrt{E(\bar{u}(t_n))+D_0}} := O_1 + O_2, \tag{4.34}$$

Because $f(\cdot)$ is Lipschitz continuous and $E(\cdot)+D_0>0$ and applying (4.22), (3.37) and (4.23), we can estimate O_1 and O_2 as follows

$$\|O_1\|, \|O_2\| \lesssim \|f\|_{W^{1,\infty}}(\|e_u^n\| + \|e_u^{n-1}\|) \lesssim \|e_u^n\| + \|e_u^{n-1}\|. \tag{4.35}$$

Hence, combining (4.34) and (4.35), we have

$$\left\|\frac{f(\bar{u}(t_n))}{\sqrt{E(\bar{u}(t_n))+D_0}} - \frac{f(\bar{u}^n)}{\sqrt{E(\bar{u}^n)+D_0}}\right\| \lesssim \|e_u^n\| + \|e_u^{n-1}\|, \tag{4.36}$$

together with (4.22) and (4.23), it implies that

$$K_2 \le C\tau(\|e_u^n\|^2 + \|e_u^{n-1}\|^2 + |e_r^{n+1}|^2 + |e_r^n|^2 + \|\hat{G}_u^{n+1}\|^2)$$
$$+\frac{1}{8}\tau\|e_\psi^{n+1}+e_\psi^n\|^2 + C\tau^5. \tag{4.37}$$

Combining (4.33) and (4.37), summing up for n from 0 to m and then using Lemma 4.1, the Poincaré inequality and the Grönwall's inequality, there is a number $\hat{\tau}_1>0$ such that provided $\tau\le\hat{\tau}_1$, we have the following estimate

$$\|e_\psi^{m+1}\|_{-1}^2 + |e_r^{m+1}|^2 + \|(1+\Delta)e_u^{m+1}\|^2 + \tau\sum_{n=0}^{m}\|e_\psi^{n+1}+e_\psi^n\|_{-1}^2 \lesssim \hat{C}_1\tau^4. \tag{4.38}$$

From (4.22), (4.23) and (4.38), it holds that

$$\|u^{m+1}\|_{L^\infty} \le \|e_u^{m+1}\|_{L^\infty} + \|u(t_{m+1})\|_{L^\infty}$$
$$\le C_\Omega\|e_u^{m+1}\|_1^{\frac12}\|e_u^{m+1}\|_2^{\frac12} + \|u(t_{m+1})\|_{L^\infty}$$
$$\lesssim C_\Omega\sqrt{\hat{C}_1}\tau^2 + \|u(t_{m+1})\|_{L^\infty}. \tag{4.39}$$

Hence, we can find a $\hat{\tau}_2>0$ ($\hat{\tau}_2<\hat{\tau}_1$), such that provided $\tau<\hat{\tau}_2$,

$$\|u^{m+1}\|_{L^\infty} \le \|u(t)\|_{L^\infty(L^\infty)} + 1, \tag{4.40}$$

and we complete the induction on (3.37) in the case $\tau<\hat{\tau}_2$. Hence (4.38) is true when $m=N-1$ if $\tau<\hat{\tau}_2$.

In the case $\tau>\hat{\tau}_2$, according to (4.12), (4.22) and (4.23), we have

$$\max_{0\le n\le N-1}\left(\|e_\psi^{n+1}\|_{-1}^2 + |e_r^{n+1}|^2 + \|(1+\Delta)e_u^{n+1}\|^2\right) + \tau\sum_{n=0}^{N-1}\|e_\psi^{n+1}+e_\psi^n\|_{-1}^2 \le \hat{C}_2 \le \hat{C}_2(\tau_2)^{-4}\tau^4, \tag{4.41}$$

for some $\hat{C}_2>0$.

In the end, Combining (4.38) and (4.41), we derive for any τ,

$$\max_{0\le n\le N-1}\left(\|e_\psi^{n+1}\|_{-1}^2 + |e_r^{n+1}|^2 + \|(1+\Delta)e_u^{n+1}\|^2\right) + \tau\sum_{n=0}^{N-1}\|e_\psi^{n+1}+e_\psi^n\|_{-1}^2 \le (\hat{C}_1 + \hat{C}_2(\tau_2)^{-4})\tau^4,$$

which implies (4.29). □

5. Fully discrete scheme and its error estimate

In this section, we present the fully discrete scheme based on the block-centered finite difference method. Here we consider the system with the homogeneous Neumann boundary condition. Since the proof for the first-order scheme is essentially the same as for the second-order scheme, for the sake of brevity, we shall provide the details only for the second-order Crank–Nicolson scheme. We first describe the block-centered finite difference framework. To fix the idea, we set the two-dimensional domain $\Omega=(0,L_x)\times(0,L_y)$. Let $L_x=N_xh_x$ and $L_y=N_yh_y$, 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

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

and

$$x_i = (x_{i-1/2} + x_{i+1/2})/2, \quad i = 0, 1, \ldots, N_x,$$
$$y_j = (y_{j-1/2} + y_{j+1/2})/2, \quad j = 0, 1, \ldots, N_y.$$

Define difference operators

$$[d_x u]_{i+1/2,j} = (u_{i+1,j} - u_{i,j})/h_x,$$
$$[d_y u]_{i,j+1/2} = (u_{i,j+1} - u_{i,j})/h_y,$$
$$[D_x u]_{i,j} = (u_{i+1/2,j} - u_{i-1/2,j})/h_x,$$
$$[D_y u]_{i,j} = (u_{i,j+1/2} - u_{i,j-1/2})/h_y,$$
$$[\Delta_h u]_{i,j} = D_x(d_x u)_{i,j} + D_y(d_y u)_{i,j}.$$

Define the discrete inner products as follows:

$$(u, v)_m = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} h_x h_y u_{i,j} v_{i,j},$$
$$(u, v)_x = \sum_{i=1}^{N_x-1} \sum_{j=1}^{N_y} h_x h_y u_{i+1/2,j} v_{i+1/2,j},$$
$$(u, v)_y = \sum_{i=1}^{N_x} \sum_{j=1}^{N_y-1} h_x h_y u_{i,j+1/2} v_{i,j+1/2}.$$

Lemma 5.1. *Let $u_{i,j}$, $v_{1,i+1/2,j}$ and $v_{2,i,j+1/2}$ be any values such that $v_{1,1/2,j} = v_{1,N_x+1/2,j} = v_{2,i,1/2} = v_{2,i,N_y+1/2} = 0$. Then*

$$(u, D_x v_1)_m = -(d_x u, v_1)_x, \quad (u, D_y v_2)_m = -(d_y u, v_2)_y.$$

Next, we define the discrete H^{-1} inner product. Let $S = \{\phi | (\phi, 1)_m = 0\}$ and suppose $\eta_{\phi_i} \in S$ to be the unique solution to the following problem:

$$-\Delta_h \eta_{\phi_i} = \phi_i, \tag{5.1}$$

where η_{ϕ_i} satisfies the discrete homogeneous Neumann boundary condition

$$\begin{cases} (\eta_{\phi_i})_{0,j} = (\eta_{\phi_i})_{1,j}, \ (\eta_{\phi_i})_{N_x+1,j} = (\eta_{\phi_i})_{N_x,j}, \ j = 1, 2, \ldots, N_y, \\ (\eta_{\phi_i})_{k,0} = (\eta_{\phi_i})_{k,1}, \ (\eta_{\phi_i})_{k,N_y+1} = (\eta_{\phi_i})_{k,N_y}, \ k = 1, 2, \ldots, N_x. \end{cases} \tag{5.2}$$

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 $\phi_1, \phi_2 \in S$. Then we can obtain that $(\phi_1, \phi_2)_{-1}$ is an inner product on the space S. 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 $\|\phi\|_{-1} = \sqrt{(\phi, \phi)_{-1}}$.

Let us denote by $\{U^n, W^n, R^n, \Psi^n\}_{n=0}^N$ the finite difference approximations to $\{u^n, \mu^n, r^n, \psi^n\}_{n=0}^N$. Set the boundary condition as

$$\begin{cases} U_{0,j} = U_{1,j}, \ U_{N_x+1,j} = U_{N_x,j}, \ j = 1, 2, \ldots, N_y, \\ U_{i,0} = U_{i,1}, \ U_{i,N_y+1} = U_{i,N_y}, \ i = 1, 2, \ldots, N_x, \\ W_{0,j} = W_{1,j}, \ W_{N_x+1,j} = W_{N_x,j}, \ j = 1, 2, \ldots, N_y, \\ W_{i,0} = W_{i,1}, \ W_{i,N_y+1} = W_{i,N_y}, \ i = 1, 2, \ldots, N_x, \\ \Delta_h U_{0,j} = \Delta_h U_{1,j}, \ \Delta_h U_{N_x+1,j} = \Delta_h U_{N_x,j}, \ j = 1, 2, \ldots, N_y, \\ \Delta_h U_{i,0} = \Delta_h U_{i,1}, \ \Delta_h U_{i,N_y+1} = \Delta_h U_{i,N_y}, \ i = 1, 2, \ldots, N_x. \end{cases} \tag{5.3}$$

The second-order fully discrete Crank–Nicolson scheme is as follows: we find $\{U^{n+1}, W^{n+1}, R^{n+1}, \Psi^{n+1}\}_{n=0}^{N-1}$ such that

$$\frac{\Psi^{n+1} - \Psi^n}{\tau} + \beta \Psi^{n+1/2} = M \Delta_h W^{n+1/2}, \tag{5.4}$$

$$\Psi^{n+1/2}=\frac{U^{n+1}-U^{n}}{\tau}, \tag{5.5}$$

$$W^{n+1/2}=\Delta_h^2U^{n+1/2}+2\Delta_hU^{n+1/2}+U^{n+1/2}+\frac{R^{n+1/2}}{E_h(\bar{U}^n)+D_0}f(\bar{U}^n), \tag{5.6}$$

$$R^{n+1}-R^{n}=\frac{1}{2\sqrt{E_h(\bar{U}^n)+D_0}}(f(\bar{U}^n),U^{n+1}-U^{n})_m, \tag{5.7}$$

where $\phi^{n+1/2}=(\phi^{n+1}+\phi^n)/2$, $\phi=\Psi,W,R,U$, $\bar{U}^n=(3U^n-U^{n-1})/2$ and the discrete form of energy $E(\bar{U}^n)$ is defined as follows:

$$E_h(\bar{U}^n)=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}h_xh_yF(\bar{U}^n).$$

Next, we carry out a rigorous error analysis for the second-order fully discrete scheme (5.4)–(5.7). Set

$$\varepsilon_u^n=U^n-u(t_n),\ \ \varepsilon_\psi^n=\Psi^n-\psi(t_n),$$
$$\varepsilon_\mu^n=W^n-\mu(t_n),\ \ \varepsilon_r^n=R^n-r(t_n).$$

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

Lemma 5.2. *Suppose that u and Δ_hu satisfy the homogeneous Neumann boundary conditions. Then we have*

$$\|\Delta_hu\|_m^2\le\frac{1}{3\epsilon^2}\|u\|_m^2+\frac{2\epsilon}{3}\|\nabla_h(\Delta_hu)\|^2. \tag{5.8}$$

Proof. The proof for the homogeneous Neumann boundary condition is essentially the same as that for the periodic boundary condition. One can refer to [28] for more details. □

Theorem 5.1. *Suppose that*

$$u\in L^\infty(0,T;W^{8,\infty}(\Omega))\cap W^{2,\infty}(0,T;W^{4,\infty}(\Omega))\cap W^{3,\infty}(0,T;W^{3,\infty}(\Omega))\cap W^{4,\infty}(0,T;L^\infty(\Omega)).$$

Let $\tau\le C(h_x+h_y)$. Then for the discrete scheme (5.4)–(5.7), there exists a positive constant C independent of h_x, h_y and τ such that

$$\begin{aligned}\|U^{k+1}-u(t_{k+1})\|_m^2\le{}&C(\|u\|^2_{W^{4,\infty}(0,T;L^\infty(\Omega))}+\|u\|^2_{W^{2,\infty}(0,T;W^{4,\infty}(\Omega))}+\|u\|^2_{W^{3,\infty}(0,T;W^{3,\infty}(\Omega))})\tau^4\\&+C\|u\|^2_{L^\infty(0,T;W^{8,\infty}(\Omega))}(h_x^4+h_y^4),\quad\forall\,0\le k\le N-1.\end{aligned} \tag{5.9}$$

Proof. Subtracting (3.1) from (5.4), we get

$$\frac{\varepsilon_\psi^{n+1}-\varepsilon_\psi^n}{\tau}+\beta\varepsilon_\psi^{n+1/2}=M\Delta_h\varepsilon_\mu^{n+1/2}+T_1^{n+1/2}, \tag{5.10}$$

where

$$T_1^{n+1/2}=\psi_t(t_{n+1/2})-\frac{\psi(t_{n+1})-\psi(t_n)}{\tau}+M(\Delta_h-\Delta)\mu(t_{n+1/2}) \tag{5.11}$$

$$=C\|\psi\|_{W^{3,\infty}(0,T;L^\infty(\Omega))}\tau^2+\|\mu\|_{L^\infty(0,T;W^{4,\infty}(\Omega))}(h_x^2+h_y^2). \tag{5.12}$$

Subtracting (3.4) from (5.5), we have

$$\varepsilon_\psi^{n+1/2}=\frac{\varepsilon_u^{n+1}-\varepsilon_u^n}{\tau}+T_2^{n+1/2}, \tag{5.13}$$

where

$$T_2^{n+1/2}=\frac{u(t_{n+1})-u(t_n)}{\tau}-u_t(t_{n+1/2})\le C\|u\|_{W^{3,\infty}(0,T;L^\infty(\Omega))}\tau^2. \tag{5.14}$$

Subtracting (3.2) from (5.6), we obtain

$$\begin{aligned}\varepsilon_\mu^{n+1/2}={}&\Delta_h^2\varepsilon_u^{n+1/2}+2\Delta_h\varepsilon_u^{n+1/2}+\varepsilon_u^{n+1/2}+\frac{R^{n+1/2}}{\sqrt{E_h(\bar{U}^n)+D_0}}f(\bar{U}^n)\\&-\frac{r(t_{n+1/2})}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}f(u(t_{n+1/2}))+T_3^{n+1/2},\end{aligned} \tag{5.15}$$

where

$$T_3^{n+1/2} = \Delta_h^2 u(t_{n+1/2}) - \Delta^2 u(t_{n+1/2}) + 2\Delta_h u(t_{n+1/2}) - 2\Delta u(t_{n+1/2})$$
$$\leq C(\|u\|_{L^\infty(0,T;W^{6,\infty}(\Omega))} + \|u\|_{L^\infty(0,T;W^{4,\infty}(\Omega))})(h_x^2 + h_y^2). \tag{5.16}$$

Subtracting (3.3) from (5.7) gives that

$$\frac{\varepsilon_r^{n+1} - \varepsilon_r^n}{\tau} = \frac{1}{2\sqrt{E_h(\bar{U}^n) + D_0}}\left(f(\bar{U}^n), \frac{U^{n+1} - U^n}{\tau}\right)_m - \frac{1}{2\sqrt{E(u(t_{n+1/2})) + D_0}}(f(u(t_{n+1/2})), u_t(t_{n+1/2}))$$
$$+ T_4^{n+1/2}, \tag{5.17}$$

where

$$T_4^{n+1/2} = r_t(t_{n+1/2}) - \frac{r(t_{n+1}) - r(t_n)}{\tau} \leq C\|r\|_{W^{3,\infty}(0,T)}\tau^2. \tag{5.18}$$

Multiplying (5.10) by $\varepsilon_{\psi,i,j}^{n+1/2} h_x h_y$ and making summation on i and j for $1 \leq i \leq N_x$ and $1 \leq j \leq N_y$, we have

$$\left(\frac{\varepsilon_\psi^{n+1} - \varepsilon_\psi^n}{\tau}, \varepsilon_\psi^{n+1/2}\right)_m + \beta\|\varepsilon_\psi^{n+1/2}\|_m^2 = M(\Delta_h \varepsilon_\mu^{n+1/2}, \varepsilon_\psi^{n+1/2})_m + (T_1^{n+1/2}, \varepsilon_\psi^{n+1/2})_m. \tag{5.19}$$

The first term on the left-hand side of (5.19) can be transformed into

$$\left(\frac{\varepsilon_\psi^{n+1} - \varepsilon_\psi^n}{\tau}, \varepsilon_\psi^{n+1/2}\right)_m = \frac{\|\varepsilon_\psi^{n+1}\|_m^2 - \|\varepsilon_\psi^n\|_m^2}{2\tau}. \tag{5.20}$$

Using (5.15), we can write the first term on the right-hand side of (5.19) as

$$M(\Delta_h \varepsilon_\mu^{n+1/2}, \varepsilon_\psi^{n+1/2})_m = M(\Delta_h^3 \varepsilon_u^{n+1/2}, \varepsilon_\psi^{n+1/2})_m + 2M(\Delta_h^2 \varepsilon_u^{n+1/2}, \varepsilon_\psi^{n+1/2})_m$$
$$+ M\left(\frac{R^{n+1/2}}{\sqrt{E_h(\bar{U}^n) + D_0}}\Delta_h f(\bar{U}^n) - \frac{r(t_{n+1/2})}{\sqrt{E_h(u(t_{n+1/2})) + D_0}}\Delta_h f(u(t_{n+1/2})), \varepsilon_\psi^{n+1/2}\right)_m$$
$$+ M(\Delta_h \varepsilon_u^{n+1/2}, \varepsilon_\psi^{n+1/2})_m + M(\Delta_h T_3^{n+1/2}, \varepsilon_\psi^{n+1/2})_m. \tag{5.21}$$

Applying Lemma 5.1, the boundary condition (5.3) and (5.13), we can write the first and second terms on the right-hand side of (5.21) as

$$\begin{aligned}
&M(\Delta_h^3 \varepsilon_u^{n+1/2}, \varepsilon_\psi^{n+1/2})_m \\
=& -M(\nabla_h(\Delta_h \varepsilon_u^{n+1/2}), \nabla_h(\Delta_h \varepsilon_\psi^{n+1/2})) \\
=& -M\frac{\|\nabla_h(\Delta_h \varepsilon_u^{n+1})\|^2 - \|\nabla_h(\Delta_h \varepsilon_u^n)\|^2}{2\tau} - M(\nabla_h(\Delta_h \varepsilon_u^{n+1/2}), \nabla_h(\Delta_h T_2^{n+1/2})) \\
\leq& -M\frac{\|\nabla_h(\Delta_h \varepsilon_u^{n+1})\|^2 - \|\nabla_h(\Delta_h \varepsilon_u^n)\|^2}{2\tau} + C\|\nabla_h(\Delta_h \varepsilon_u^{n+1/2})\|^2 + C\|u\|_{W^{3,\infty}(0,T;W^{3,\infty}(\Omega))}^2\tau^4,
\end{aligned} \tag{5.22}$$

$$\begin{aligned}
&2M(\Delta_h^2 \varepsilon_u^{n+1/2}, \varepsilon_\psi^{n+1/2})_m \\
=& 2M(\Delta_h \varepsilon_u^{n+1/2}, \Delta_h \varepsilon_\psi^{n+1/2})_m \\
=& 2M\frac{\|\Delta_h \varepsilon_u^{n+1}\|_m^2 - \|\Delta_h \varepsilon_u^n\|_m^2}{2\tau} + 2M(\Delta_h \varepsilon_u^{n+1/2}, \Delta_h T_2^{n+1/2}) \\
=& \frac{M}{\tau}(\|\Delta_h \varepsilon_u^{n+1}\|_m^2 - \|\Delta_h \varepsilon_u^n\|_m^2) + C\|\Delta_h \varepsilon_u^{n+1/2}\|_m^2 + C\|u\|_{W^{3,\infty}(0,T;W^{2,\infty}(\Omega))}^2\tau^4.
\end{aligned} \tag{5.23}$$

The third term on the right-hand side of (5.21) can be estimated as follow

$$\begin{aligned}
&M\left(\frac{R^{n+1/2}}{\sqrt{E_h(\bar{U}^n) + D_0}}\Delta_h f(\bar{U}^n) - \frac{r(t_{n+1/2})}{\sqrt{E_h(u(t_{n+1/2})) + D_0}}\Delta_h f(u(t_{n+1/2})), \varepsilon_\psi^{n+1/2}\right)_m \\
=& MR^{n+1/2}\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n) + D_0}}, \varepsilon_\psi^{n+1/2}\right)_m - Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n) + D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&+ Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n) + D_0}}, \varepsilon_\psi^{n+1/2}\right)_m - Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n)) + D_0}}, \varepsilon_\psi^{n+1/2}\right)_m
\end{aligned}$$

$$
\begin{aligned}
&+ Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m - Mr(t_{n+1/2})\left(\frac{\Delta_h f(u(t_{n+1/2}))}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&= Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n)+D_0}} - \frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&+ Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n))+D_0}} - \frac{\Delta_h f(u(t_{n+1/2}))}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&+ M\varepsilon_r^{n+1/2}\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n)+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m .
\end{aligned} \tag{5.24}
$$

Next, we shall first assume that there exist three positive constants C_5, C_6 and C_7 such that

$$
\|U^n\|_{L^\infty(\Omega)} \le C_5,\ \ \|\nabla_h U^n\|_{L^\infty(\Omega)} \le C_6,\ \ \|\Delta_h U^n\|_{L^\infty(\Omega)} \le C_7,\ \ \forall\ 0 \le n \le N, \tag{5.25}
$$

which will be verified later.

Using Lemma 5.2, the first term on the right-hand side of (5.24) can be controlled similar to the estimates in [5] by

$$
\begin{aligned}
&Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n)+D_0}} - \frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&\le C(\|\varepsilon_u^n\|_m^2 + \|\Delta_h \varepsilon_u^n\|_m^2) + C(\|\varepsilon_u^{n-1}\|_m^2 + \|\Delta_h \varepsilon_u^{n-1}\|_m^2) + C\|\varepsilon_\psi^{n+1/2}\|_m^2 \\
&\le C(\|\varepsilon_u^n\|_m^2 + \|\nabla_h(\Delta_h \varepsilon_u^n)\|^2) + C(\|\varepsilon_u^{n-1}\|_m^2 + \|\nabla_h(\Delta_h \varepsilon_u^{n-1})\|^2) + C\|\varepsilon_\psi^{n+1/2}\|_m^2,
\end{aligned} \tag{5.26}
$$

where C is dependent on $\|r\|_{L^\infty(0,T)}$, $\|U^n\|_{L^\infty(\Omega)}$ and $\|\nabla_h U^n\|_{L^\infty(\Omega)}$.

The second term on the right-hand side of (5.24) can be handled by

$$
\begin{aligned}
&Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n))+D_0}} - \frac{\Delta_h f(u(t_{n+1/2}))}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&= Mr(t_{n+1/2})\left(\frac{\Delta_h f(\bar{u}(t_n))}{\sqrt{E_h(\bar{u}(t_n))+D_0}} - \frac{\Delta_h f(u(t_{n+1/2}))}{\sqrt{E_h(\bar{u}(t_n))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&+ Mr(t_{n+1/2})\left(\frac{\Delta_h f(u(t_{n+1/2}))}{\sqrt{E_h(\bar{u}(t_n))+D_0}} - \frac{\Delta_h f(u(t_{n+1/2}))}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \\
&\le C\|\varepsilon_\psi^{n+1/2}\|_m^2 + C\|u\|^2_{W^{2,\infty}(0,T;W^{2,\infty}(\Omega))}\tau^4 + C\|u\|^2_{L^\infty(0,T;W^{3,\infty}(\Omega))}(h_x^4 + h_y^4).
\end{aligned} \tag{5.27}
$$

The last term on the right-hand side of (5.24) can be directly estimated by the Cauchy–Schwarz inequality

$$
M\varepsilon_r^{n+1/2}\left(\frac{\Delta_h f(\bar{U}^n)}{\sqrt{E_h(\bar{U}^n)+D_0}}, \varepsilon_\psi^{n+1/2}\right)_m \le C\|\varepsilon_\psi^{n+1/2}\|_m^2 + C|\varepsilon_r^{n+1/2}|^2, \tag{5.28}
$$

where C is dependent on $\|U^n\|_{L^\infty(\Omega)}$, $\|\nabla_h U^n\|_{L^\infty(\Omega)}$ and $\|\Delta_h U^n\|_{L^\infty(\Omega)}$. Using (5.26)–(5.28), we have

$$
\begin{aligned}
&M\left(\frac{R^{n+1/2}}{\sqrt{E_h(\bar{U}^n)+D_0}}\Delta_h f(\bar{U}^n) - \frac{r(t_{n+1/2})}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}\Delta_h f(u(t_{n+1/2})), \varepsilon_\psi^{n+1/2}\right)_m \\
&\le C(\|\varepsilon_u^n\|_m^2 + \|\nabla_h(\Delta_h \varepsilon_u^n)\|^2) + C(\|\varepsilon_u^{n-1}\|_m^2 + \|\nabla_h(\Delta_h \varepsilon_u^{n-1})\|^2) + C\|\varepsilon_\psi^{n+1/2}\|_m^2 \\
&+ C|\varepsilon_r^{n+1/2}|^2 + C\|u\|^2_{W^{2,\infty}(0,T;W^{2,\infty}(\Omega))}\tau^4 + C\|u\|^2_{L^\infty(0,T;W^{3,\infty}(\Omega))}(h_x^4 + h_y^4).
\end{aligned} \tag{5.29}
$$

Using Lemma 5.2, the fourth term on the right-hand side of (5.21) can be transformed into

$$
\begin{aligned}
&M(\Delta_h \varepsilon_u^{n+1/2}, \varepsilon_\psi^{n+1/2})_m \\
&\le C\|\varepsilon_\psi^{n+1/2}\|_m^2 + C\|\Delta_h \varepsilon_u^{n+1/2}\|_m^2 \\
&\le C\|\varepsilon_\psi^{n+1/2}\|_m^2 + C\|\varepsilon_u^{n+1}\|_m^2 + C\|\nabla_h(\Delta_h \varepsilon_u^{n+1})\|^2 + C\|\varepsilon_u^n\|_m^2 + C\|\nabla_h(\Delta_h \varepsilon_u^n)\|^2.
\end{aligned} \tag{5.30}
$$

The last term on the right-hand side of (5.21) can be estimated by

$$
\begin{aligned}
M(\Delta_h T_3^{n+1/2}, \varepsilon_\psi^{n+1/2})_m \le\ & C\|\varepsilon_\psi^{n+1/2}\|_m^2 + C\|u\|^2_{W^{2,\infty}(0,T;W^{4,\infty}(\Omega))}\tau^4 \\
&+ C(\|u\|^2_{L^\infty(0,T;W^{8,\infty}(\Omega))} + \|u\|^2_{L^\infty(0,T;W^{6,\infty}(\Omega))})(h_x^4 + h_y^4).
\end{aligned} \tag{5.31}
$$

Combining (5.19) with (5.20)–(5.31) leads to

$$\begin{aligned}
&\frac{\|\varepsilon_\psi^{n+1}\|_m^2-\|\varepsilon_\psi^{n}\|_m^2}{2\tau}+\beta\|\varepsilon_\psi^{n+1/2}\|_m^2+M\frac{\|\nabla_h(\Delta_h\varepsilon_u^{n+1})\|^2-\|\nabla_h(\Delta_h\varepsilon_u^{n})\|^2}{2\tau}\\
&\le C(\|\varepsilon_u^{n+1}\|_m^2+\|\nabla_h(\Delta_h\varepsilon_u^{n+1})\|^2)+C(\|\varepsilon_u^{n}\|_m^2+\|\nabla_h(\Delta_h\varepsilon_u^{n})\|^2)\\
&\quad+C(\|\varepsilon_u^{n-1}\|_m^2+\|\nabla_h(\Delta_h\varepsilon_u^{n-1})\|^2)+C\|\varepsilon_\psi^{n+1/2}\|_m^2+C|\varepsilon_r^{n+1}|^2\\
&\quad+\frac{M}{\tau}(\|\Delta_h\varepsilon_u^{n+1}\|_m^2-\|\Delta_h\varepsilon_u^{n}\|_m^2)+C\|u\|^2_{L^\infty(0,T;W^{8,\infty}(\Omega))}(h_x^4+h_y^4)\\
&\quad+C(\|u\|^2_{W^{4,\infty}(0,T;L^\infty(\Omega))}+\|u\|^2_{W^{2,\infty}(0,T;W^{4,\infty}(\Omega))}+\|u\|^2_{W^{3,\infty}(0,T;W^{3,\infty}(\Omega))})\tau^4.
\end{aligned}\tag{5.32}$$

Next, we give the error estimate of the auxiliary function r. Multiplying (5.17) by $\varepsilon_r^{n+1}+\varepsilon_r^n$ leads to

$$\begin{aligned}
\frac{|\varepsilon_r^{n+1}|^2-|\varepsilon_r^{n}|^2}{\tau}&=\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(\bar U^n)+D_0}}\left(f(\bar U^n),\frac{U^{n+1}-U^n}{\tau}\right)_m\\
&\quad-\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}(f(u(t_{n+1/2})),u_t(t_{n+1/2}))+T_4^{n+1/2}(\varepsilon_r^{n+1}-\varepsilon_r^n).
\end{aligned}\tag{5.33}$$

The first two terms on the right-hand side of (5.33) can be transformed into

$$\begin{aligned}
&\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(\bar U^n)+D_0}}\left(f(\bar U^n),\frac{U^{n+1}-U^n}{\tau}\right)_m-\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}(f(u(t_{n+1/2})),u_t(t_{n+1/2}))\\
&=\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(u(t_{n+1/2}))+D_0}}\left[\left(f(u(t_{n+1/2})),\frac{u(t_{n+1})-u(t_n)}{\tau}\right)_m-(f(u(t_{n+1/2})),u_t(t_{n+1/2}))\right]\\
&\quad+\varepsilon_r^{n+1/2}\left(\frac{f(\bar U^n)}{\sqrt{E_h(\bar U^n)+D_0}}-\frac{f(u(t_{n+1/2}))}{\sqrt{E_h(u(t_{n+1/2}))+D_0}},\frac{u(t_{n+1})-u(t_n)}{\tau}\right)_m\\
&\quad+\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(\bar U^n)+D_0}}\left(f(\bar U^n),\frac{\varepsilon_u^{n+1}-\varepsilon_u^n}{\tau}\right)_m,
\end{aligned}\tag{5.34}$$

which can be handled in a similar way to that in [31]. Thus we have

$$\begin{aligned}
&\frac{\varepsilon_r^{n+1/2}}{\sqrt{E_h(\bar U^n)+D_0}}\left(f(\bar U^n),\frac{U^{n+1}-U^n}{\tau}\right)_m-\frac{\varepsilon_r^{n+1/2}}{\sqrt{E(u(t_{n+1/2}))+D_0}}(f(u(t_{n+1/2})),u_t(t_{n+1/2}))\\
&\le C|\varepsilon_r^{n+1/2}|^2+C\|u\|^2_{W^{1,\infty}(0,T;L^\infty(\Omega))}(\|\varepsilon_u^n\|_m^2+\|\varepsilon_u^{n-1}\|_m^2)+C\|\varepsilon_\psi^{n+1/2}\|_m^2\\
&\quad+C\|u\|^2_{W^{1,\infty}(0,T;W^{2,\infty}(\Omega))}(h_x^4+h_y^4).
\end{aligned}\tag{5.35}$$

Substituting (5.35) into (5.33) and using the Cauchy–Schwarz inequality, we can obtain

$$\begin{aligned}
\frac{|\varepsilon_r^{n+1}|^2-|\varepsilon_r^{n}|^2}{\tau}&\le C|\varepsilon_r^{n+1/2}|^2+C\|u\|^2_{W^{1,\infty}(0,T;L^\infty(\Omega))}(\|\varepsilon_u^n\|_m^2+\|\varepsilon_u^{n-1}\|_m^2)+C\|\varepsilon_\psi^{n+1/2}\|_m^2\\
&\quad+C\|u\|^2_{W^{1,\infty}(0,T;W^{2,\infty}(\Omega))}(h_x^4+h_y^4)+C\|r\|^2_{W^{3,\infty}(0,T)}\tau^4.
\end{aligned}\tag{5.36}$$

Combining (5.32) with (5.36) and multiplying by 2τ, summing over n ($n=0,1,\dots,k$), we have

$$\|\varepsilon_\psi^{k+1}\|_m^2+\beta\sum_{n=0}^{k}\tau\|\varepsilon_\psi^{n+1/2}\|_m^2+M\|\nabla_h(\Delta_h\varepsilon_u^{k+1})\|^2+2|\varepsilon_r^{k+1}|^2\tag{5.37}$$

$$\begin{aligned}
&\le 2M\|\Delta_h\varepsilon_u^{k+1}\|_m^2+C\sum_{n=0}^{k+1}\tau\|\varepsilon_u^n\|_m^2+C\sum_{n=0}^{k+1}\tau\|\nabla_h(\Delta_h\varepsilon_u^n)\|_m^2+C\sum_{n=0}^{k+1}\tau\|\varepsilon_\psi^n\|^2\\
&\quad+C\sum_{n=0}^{k+1}\tau|\varepsilon_r^n|^2+C(\|u\|^2_{L^\infty(0,T;W^{8,\infty}(\Omega))}+\|u\|^2_{L^\infty(0,T;W^{6,\infty}(\Omega))})(h_x^4+h_y^4)\\
&\quad+C(\|u\|^2_{W^{4,\infty}(0,T;L^\infty(\Omega))}+\|u\|^2_{W^{2,\infty}(0,T;W^{4,\infty}(\Omega))}+\|u\|^2_{W^{3,\infty}(0,T;W^{3,\infty}(\Omega))})\tau^4.
\end{aligned}\tag{5.38}$$

To carry out further analysis, we should give the following inequality first. Recalling (5.13), we have

$$\varepsilon_u^{k+1}=\varepsilon_u^0+\sum_{l=0}^{k}\tau\varepsilon_\psi^{l+1/2}+\sum_{l=0}^{k}\tau T_2^{l+1/2},$$

and using the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}\|\varepsilon_u^{k+1}\|_m^2 &\le 2\|\varepsilon_u^0\|_m^2 + 2\left\|\sum_{l=0}^{k}\tau\varepsilon_\psi^{l+1/2}\right\|_m^2 + 2\left\|\sum_{l=0}^{k}\tau T_2^{l+1/2}\right\|_m^2\\ &\le 2\|\varepsilon_u^0\|_m^2 + 2T\sum_{l=0}^{k}\tau\|\varepsilon_\psi^{l+1/2}\|_m^2 + 2T\sum_{l=0}^{k}\tau\|T_2^{l+1/2}\|_m^2. \end{aligned} \tag{5.39}$$

Using Lemma 5.2 and (5.39), the first term on the right-hand side of (5.37) can be transformed into

$$\begin{aligned}2M\|\Delta_h\varepsilon_u^{k+1}\|_m^2 &\le C\|\varepsilon_u^{k+1}\|_m^2 + \frac{M}{2}\|\nabla_h(\Delta_h\varepsilon_u^{k+1})\|^2\\ &\le C\sum_{l=0}^{k+1}\tau\|\varepsilon_\psi^{l}\|_m^2 + C\sum_{l=0}^{k+1}\tau\|T_2^{l}\|_m^2 + \frac{M}{2}\|\nabla_h(\Delta_h\varepsilon_u^{k+1})\|^2. \end{aligned} \tag{5.40}$$

Then using the discrete Grönwall inequality and Lemma 5.2, (5.37) can be estimated as follows:

$$\begin{aligned}&\|\varepsilon_\psi^{k+1}\|_m^2 + \|\varepsilon_u^{k+1}\|_m^2 + \|\Delta_h\varepsilon_u^{k+1}\|_m^2 + M\|\nabla_h(\Delta_h\varepsilon_u^{k+1})\|^2 + |\varepsilon_r^{k+1}|^2\\ &\le C(\|u\|^2_{W^{4,\infty}(0,T;L^\infty(\Omega))} + \|u\|^2_{W^{2,\infty}(0,T;W^{4,\infty}(\Omega))} + \|u\|^2_{W^{3,\infty}(0,T;W^{3,\infty}(\Omega))})\tau^4\\ &\quad + C\|u\|^2_{L^\infty(0,T;W^{8,\infty}(\Omega))}(h_x^4 + h_y^4), \quad \forall\, 0\le k\le N-1. \end{aligned} \tag{5.41}$$

We now verify the hypothesis (5.25). This proof follows a similar procedure to that in [31,32]. We first give a detailed proof for $\|U^n\|_{L^\infty(\Omega)} \le C_5$ in the following two steps by using the mathematical induction. Using the scheme (5.4)–(5.7) for $n=0$ and applying the inverse assumption, we can get the approximation U^1 with the following property:

$$\begin{aligned}\|U^1\|_{L^\infty(\Omega)} &\le \|U^1 - u(t_1)\|_{L^\infty(\Omega)} + \|u(t_1)\|_{L^\infty(\Omega)}\\ &\le \|U^1 - \Pi_h u(t_1)\|_{L^\infty(\Omega)} + \|\Pi_h u(t_1) - u(t_1)\|_{L^\infty(\Omega)} + \|u(t_1)\|_{L^\infty(\Omega)}\\ &\le Ch^{-1}(\|U^1 - u(t_1)\|_m + \|u(t_1) - \Pi_h u(t_1)\|_m) + \|\Pi_h u(t_1) - u(t_1)\|_{L^\infty(\Omega)} + \|u(t_1)\|_{L^\infty(\Omega)}\\ &\le C(h + h^{-1}\tau^2) + \|u(t_1)\|_{L^\infty(\Omega)} \le C, \end{aligned}$$

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

$$\|\Pi_h u(t_1) - u(t_1)\|_{L^\infty(\Omega)} \le Ch^2. \tag{5.42}$$

Thus we can choose the positive constant C_5 independent of h and τ such that

$$C_5 \ge \max\{\|U^1\|_{L^\infty(\Omega)}, 2\|u(t_n)\|_{L^\infty(\Omega)}\}.$$

By the definition of C_5, it is trivial that the hypothesis $\|U^l\|_{L^\infty(\Omega)} \le C_5$ holds true for $l=1$. Supposing that $\|U^{l-1}\|_{L^\infty(\Omega)} \le C_5$ holds true for an integer $l = 1, 2, \dots, k+1$ with the aid of the estimate (5.41), we have $\|U^l - u(t_l)\|_m \le C(\tau^2 + h^2)$. Next, we prove that $\|U^l\|_{L^\infty(\Omega)} \le C_5$ holds true. Since

$$\begin{aligned}\|U^l\|_{L^\infty(\Omega)} &\le \|U^l - u(t_l)\|_{L^\infty(\Omega)} + \|u(t_l)\|_{L^\infty(\Omega)}\\ &\le \|U^l - \Pi_h u(t_l)\|_{L^\infty(\Omega)} + \|\Pi_h u(t_l) - u(t_l)\|_{L^\infty(\Omega)} + \|u(t_l)\|_{L^\infty(\Omega)}\\ &\le Ch^{-1}(\|U^l - u(t_l)\|_m + \|u(t_l) - \Pi_h u(t_l)\|_m) + \|\Pi_h u(t_l) - u(t_l)\|_{L^\infty(\Omega)} + \|u(t_l)\|_{L^\infty(\Omega)}\\ &\le C_8(h + h^{-1}\tau^2) + \|u(t_l)\|_{L^\infty(\Omega)}. \end{aligned} \tag{5.43}$$

Let $\tau \le C_9 h$ and a positive constant h_1 be small enough to satisfy $C_8(1 + C_9^2)h_1 \le \frac{C_5}{2}$. Then for $h \in (0, h_1]$, we derive from (5.43) that

$$\|U^l\|_{L^\infty(\Omega)} \le C_9(h + h^{-1}\tau^2) + \|u(t_l)\|_{L^\infty(\Omega)} \le C_8(h_1 + C_9^2 h_1) + \frac{C_5}{2} \le C_5.$$

This indicates that $\|U^n\|_{L^\infty(\Omega)} \le C_5$ for all n. The proof for the other two inequalities in (5.25) is essentially identical with the above procedure so we skip it for the sake of brevity. □

Remark 5.1. The numerical idea and the theoretical analysis can also be applied to the SPFC model, the reader can refer to [13], in which a second-order backward differentiation formula is proposed and analyzed for the SPFC model based on the SAV approach. Moreover, an optimal rate convergence analysis is provided for the proposed scheme.

6. Numerical experiments

In this section, we give several numerical experiments for the MPFC equation to verify the accuracy and energy stability of the proposed schemes.

Table 1
The errors and rate of convergence at $T = 10$ for the phase variable u with different time step size.

	τ	$\|\varepsilon_u\|_m$	Rate		τ	$\|\varepsilon_u\|_m$	Rate
The first-order scheme	1/8	3.3056e−01	–	the CN scheme	1/8	1.8364e−03	–
	1/16	1.6706e−01	0.98		1/16	4.0970e−04	2.16
	1/32	8.4211e−02	0.99		1/32	9.8583e−05	2.06
	1/64	4.2287e−02	0.99		1/64	2.4357e−05	2.02
	1/128	2.1190e−02	1.00		1/128	6.0664e−06	2.01
	1/256	1.0607e−02	1.00		1/256	1.5146e−06	2.00

Table 2
The errors and rate of convergence at $T = 10$ for the phase variable u with different spatial mesh size.

$N_x \times N_y$	$\|\varepsilon_u\|_m$	Rate
20 × 20	1.1486e−01	–
40 × 40	3.1432e−02	1.87
80 × 80	8.0201e−03	1.97
160 × 160	2.0010e−03	2.00

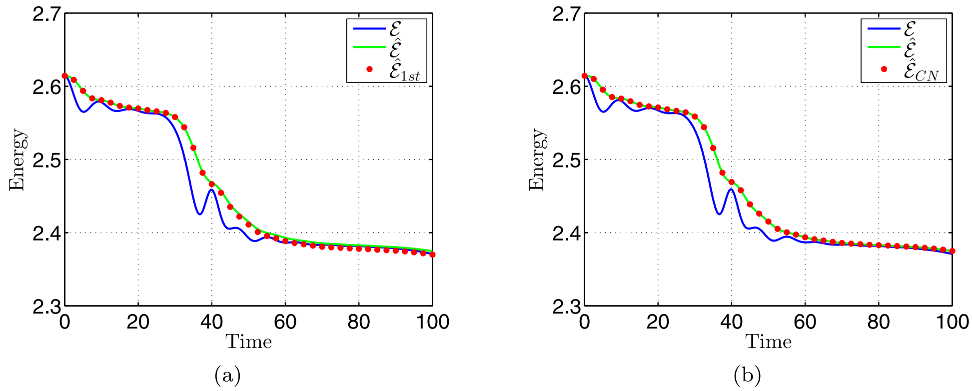


Fig. 1. Evolution of the original energy and pseudo energy using the first-order scheme (a) and the second-order Crank–Nicolson scheme (b).

6.1. Accuracy test

To verify the temporal convergence rate, we set $\Omega = [0, 128] \times [0, 128]$, the parameters are set as $M = 5$, $\epsilon = 0.025$, $\beta = 0.9$, $T = 10$. We choose a source term to the equation such that the exact solution is given by

$$u(x, y, t) = \sin(\frac{2\pi x}{64})\cos(\frac{2\pi y}{64})\cos(t).$$

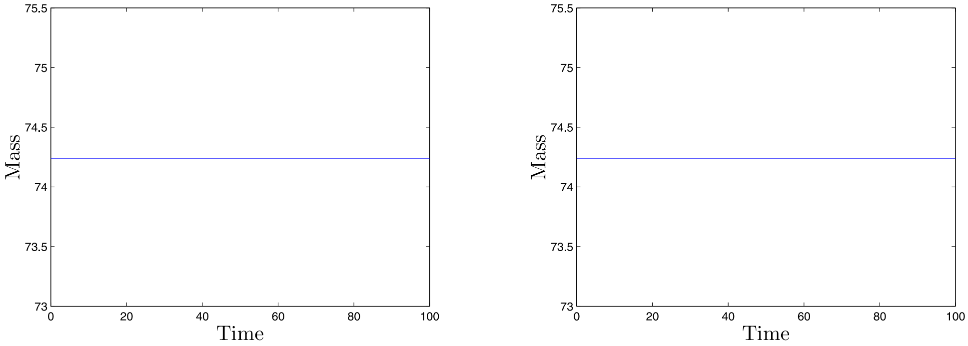
We set $N_x = N_y = 128$ so that the spatial discretization errors are negligible compared with the temporal discretization errors. The errors and convergence rate at $T = 10$ for the first-order and second-order SAV schemes are presented in Table 1 and we can observe that our schemes give desired rate of accuracy in time. To verify the spatial convergence rate, we set $\tau = 1/128$. The errors and convergence rate at $T = 10$ for the second-order Crank–Nicolson scheme are given in Table 2, which are consistent with our theoretical analysis.

6.2. Energy stability and mass conservation test

To test the energy stability, we set the initial condition as

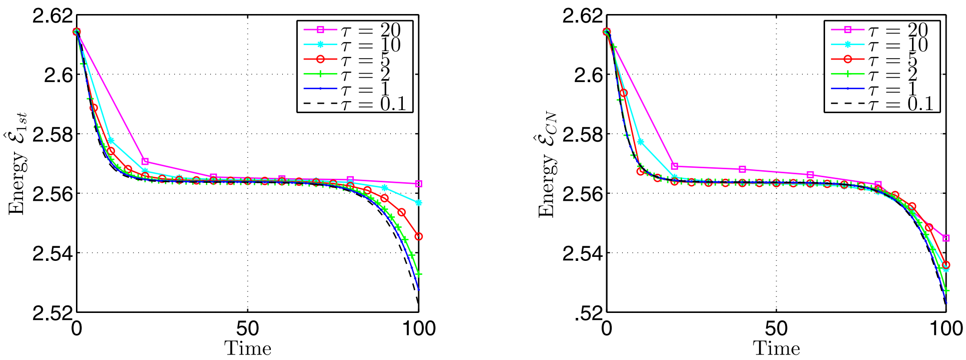
$$\begin{aligned} u(x, y) =& 0.07 - 0.02\cos\left(\frac{2\pi(x-12)}{32}\right)\sin\left(\frac{2\pi(y-1)}{32}\right) + 0.02\cos^2\left(\frac{\pi(x+10)}{32}\right)\cos^2\left(\frac{\pi(y+3)}{32}\right) \\ & - 0.01\sin^2\left(\frac{4\pi x}{32}\right)\sin^2\left(\frac{4\pi(y-6)}{32}\right). \end{aligned}$$

$M = 2$, $\epsilon = 0.05$, $\beta = 0.1$, $\Omega = [0, 32] \times [0, 32]$, $T = 100$, $\tau = 0.1$, $N_x = N_y = 128$. Fig. 1 shows that our schemes are energy-stable with respect to the pseudo energy. Fig. 2 shows the mass conservation. Let $\beta = 0.9$, Fig. 3 shows that our schemes are energy-stable with different time step size.



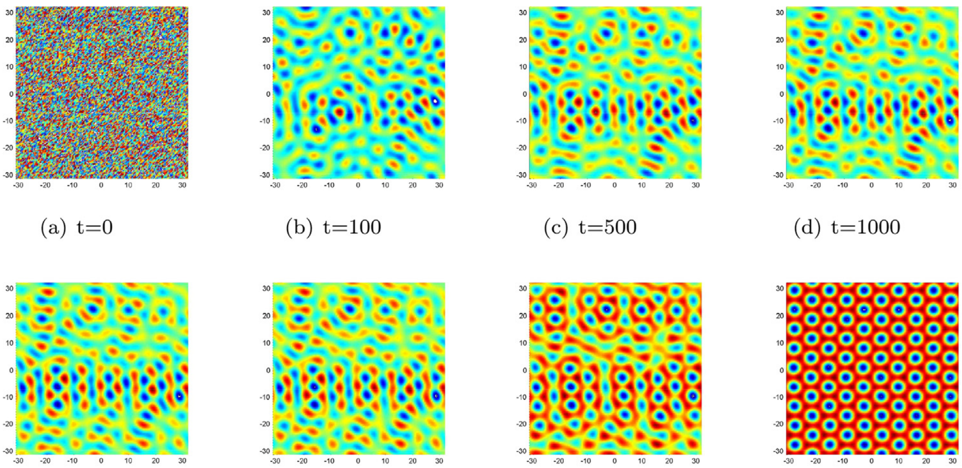
(a) (b)

Fig. 2. Evolution of the total mass using the first-order scheme (a) and the second-order Crank–Nicolson scheme (b).



(a) (b)

Fig. 3. Evolution of the pseudo energy using the first-order scheme (a) and the second-order Crank–Nicolson scheme (b) with different time step size.



(a) t=0 (b) t=100 (c) t=500 (d) t=1000

(e) t=1500 (f) t=2000 (g) t=2800 (h) t=3300

Fig. 4. The evolution of the phase transition behavior. The computational domain is $[-32, 32] \times [-32, 32]$. The parameters are $\epsilon = 0.025$, $M = 1$, $\beta = 0.2$, $\tau = 1$.

6.3. Phase transition behaviors

In this subsection, we apply the second-order Crank–Nicolson scheme to check the evolution from a randomly perturbed nonequilibrium state to a steady state. Since the first-order scheme provide similar numerical results, for simplicity, we only consider the Crank–Nicolson scheme in the following simulation. With the initial condition $u(x, y) = 0.07 + \text{rand}$, rand is a randomly chosen number between -0.001 and 0.001 at the grid points, we set $N_x = N_y = 128$ to discrete the domain $\Omega = [-32, 32] \times [-32, 32]$. Let $\epsilon = 0.025$, $M = 1$, $\beta = 0.2$, $\tau = 1$. Fig. 4 shows the time evolution of the phase transition behavior, which validates that the Crank–Nicolson scheme does lead to the expected states.

7. Conclusions

In this work, we design the first-order scheme and Crank–Nicolson scheme for the MPFC equation based on the SAV method. Rigorous results about unconditional energy stability, convergence and error estimates are derived. Several numerical experiments are presented to verify our theoretical results and demonstrate the accuracy, energy stability and mass conservation.

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