An Efficient and Unconditionally Energy Stable Fully Discrete Scheme for the Confined Ternary Blended Polymers Model

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Abstract. In this paper, we develop a fully discrete scheme to solve the confined ternary blended polymers (TBP) model with four order parameters based on the stabilized-scalar auxiliary variable (S-SAV) approach in time and the Fourier spectral method in space. Then, theoretical analysis is given for the scheme based on the backward differentiation formula. The unconditional energy stability and mass conservation are derived. Rigorous error analysis is carried out to show that the fully discrete scheme converges with order $O(\tau^2 + h^m)$ in the sense of the $L^2$ norm, where $\tau$ is the time step, $h$ is the spatial step, and $m$ is the regularity of the exact solution. Finally, some numerical results are given to demonstrate the theoretical analysis. Moreover, the phase separation of two kinds of polymer particles, namely, Ashura and Janus core-shell particles, is presented to show the morphological structures.

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1 Introduction

Nanostructured polymer particles have attracted some experimental and theoretical studies because they have been widely applied in biological, photonic, mechanical and many other fields, such as drug delivery [6, 32], photonic materials [1, 31, 33, 34], electronic ink [2, 40] and so on [17, 18, 24, 38]. To produce various kinds of polymer blended particles, H. Yabu et al. [39] proposed a simple method called the self-organized precipitation

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The process is introduced as follows. First, two miscible solvents should be prepared: volatile (good) and nonvolatile (poor). Polymers are dissolved in the good solvent, and then, the poor solvent is mixed into the polymer emulsion. After the good solvent is completely evaporated, uniformly sized polymer blended particles will form in the poor solvent.

Using the SORP method, various kinds of nanostructured polymer particles in binary polymer blended systems can be prepared. Janus-type particles [14] and core-shell-type particles [41] can be formed from polymer blends. Lamellar, onion, screw, wheel, mushroom and tennis structures can be formed from block copolymer blends [15]. Moreover, in [37], ring, helix and multi-pod structures are prepared.

To prepare ternary polymer blended particles, Y. Hirai et al. [16] studied the relationship between the surface tensions of polymers and the phase-separated structures in binary polymer blended systems. They found that when the two polymers both have low surface tensions, Janus-type particles are formed. A combination of low and high surface tension polymers forms core-shell-type particles, in which the polymer with the lower surface tension forms the core and the polymer with the higher surface tension forms the shell. Thus, in ternary polymer blended systems, three polymers with low surface tensions form Ashura particles, and if one of the polymers has a much higher surface tension, they form Janus core-shell particles.

Here, we pay more attention to how to simulate the phase separation of different structures in ternary polymer blended systems. In [16], a model of phase separation based on Cahn-Hilliard equations with four order parameters, namely, confined ternary blended polymers (TBP) model, was constructed to describe the dynamical systems of Ashura and Janus core-shell particles. Moreover, a semi-implicit scheme was implemented to simulate the phase separation process. However, Hirai et al. only focused on the physical experiment and simulation results of the confined TBP model. It lacks of energy stable schemes and numerical analyses, which is what we concern about.

In fact, there are many numerical methods that have been applied for solving coupled Cahn-Hilliard equations, with the aim of developing energy stable schemes. Examples are the convex splitting method [12, 13], the stabilization method [29, 30, 43], the invariant energy quadratization (IEQ) approach [42], the scalar auxiliary variable (SAV) approach [27, 28] and the new Lagrange Multiplier approach [10]. These approaches provide different methods of time discretization. A. Edgar et al. [3, 4] used the linear splitting method to solve two coupled Cahn-Hilliard equations with a nonlocal term. Q. Li et al. [19] used the scalar auxiliary variable (SAV) approach to achieve two second-order, efficient, decoupled, and linear numerical schemes for the block copolymer. Using the new Lagrange Multiplier approach combined with the stabilization method, a second-order and unconditionally energy stable scheme for the coupled nonlocal Cahn-Hilliard system was proposed by Q. Cheng et al. in [10]. C. Chen et al. [7] established a ternary Cahn-Hilliard-type Nakazawa-Ohta phase-field model for the triblock copolymer and solved the model via the stabilized-SAV (S-SAV) approach.

For the confined TBP model, we have two main tasks. The first task is constructing
a fully discrete scheme that possesses the following properties: (i) unconditional energy stability and mass conservation; (ii) second-order accuracy in time and spectral accuracy in space; and (iii) efficiency. Only several linear systems must be solved at each time step since we need to solve four coupled fourth-order nonlinear parabolic partial differential equations in three dimensions. Thus, the scalar auxiliary variable (SAV) approach is used. We first introduce a scalar auxiliary variable to reformulate the free energy functional into a sum of a linear term and a nonlinear term. Treating the linear term implicitly and the nonlinear term explicitly, we develop a decoupled, linear, unconditionally energy stable and fully discrete scheme based on the backward differentiation formula in time and the Fourier spectral method in space. Stabilization terms are added to avoid blow-up when the time step is not small enough. Representative work on combining the stabilization method with other numerical methods can be seen in [8, 36]. The solving steps are given in detail, and the energy dissipation law and mass conservation are easy to prove. Moreover, some numerical experiments are carried out to show the accuracy of the scheme, the phase-separated structures of Ashura and Janus core-shell particles, the stability of the original and modified energy and the mass conservation.

Another task is to provide error estimates for the fully discrete scheme based on the Fourier spectral method in space. Recently, there has been some work on error estimates for the SAV approach. J. Shen et al. first proposed the convergence and error estimates for the semidiscrete SAV scheme in [26]. Then, error analyses were conducted for SAV schemes with the Fourier spectral method [21], block-centered finite difference method [20], and finite element method [9, 35] in space. These studies focus on first- and second-order schemes based on the Crank-Nicolson method with only one order parameter. We present the error estimates for the S-SAV/BDF2 scheme with second-order accuracy in time and spectral accuracy in space and provide a detailed proving process. We need to overcome three main difficulties in our proof: (i) There are four order parameters in the model of phase separation for the ternary polymer blended system, and thus, it is challenging for some inequalities. (ii) We can easily obtain the $H^1$ bound for the numerical solution from the energy stability; however, the $L^\infty$ bound is necessary for our proof. (iii) We do not assume the regularity of the scalar auxiliary variable $r(t)$. Instead, we derive the estimates for the derivatives of $r(t)$ based on the regularity hypothesis of the exact solution. To the best of our knowledge, this is the first such result for the schemes and analyses for the confined TBP model.

The remainder of the paper is organized as follows. In Section 2, notation and definitions are introduced. In Section 3, the confined TBP model is presented. In Section 4, we use the SAV approach combined with stabilization terms in time and the Fourier spectral method in space to construct a decoupled, linear, unconditionally energy stable and fully discrete scheme for the quaternary coupled Cahn-Hilliard system. In section 5, the error estimates for the fully discrete scheme are derived. Then, the numerical simulations in three dimensions are shown in Section 6. Our conclusions and further discussion are given in the last section.
2 Preliminaries

Before we introduce the model of phase separation and the corresponding fully discrete scheme, we introduce some notation first.

We denote $W^{s,p}(\Omega)$ as the usual Sobolev spaces for $0 \leq s \leq \infty, 1 \leq p \leq \infty$. In particular, we denote $H^s(\Omega) := W^{s,2}(\Omega)$ with the norm $\| \cdot \|_{H^s}$. The norm and the inner product of $L^2(\Omega) = H^0(\Omega)$ are denoted by $\| \cdot \|$ and $(\cdot, \cdot)$, respectively. The norms in $L^p(\Omega)$ and $L^\infty(\Omega)$ are denoted by $\|\cdot\|_{L^p}$ and $\|\cdot\|_{L^\infty}$, respectively.

We define the space $L^2_0(\Omega) = \{ \phi \in L^2(\Omega) | (\phi, 1) = 0 \}$. Suppose that $f, g \in L^2_0(\Omega)$; we define $\phi_f \in L^2_0(\Omega) \cap H^2(\Omega)$ as the unique solution to the function $-\Delta \phi_f = f$ in $\Omega$, where $\phi_f$ satisfies the boundary conditions that either (i) $\phi_f$ is periodic or (ii) $\partial_n \phi_f |_{\partial \Omega} = 0$. Thus, we can define the operator $(-\Delta)^{-1}$ as $\phi_f = (-\Delta)^{-1} f$. We denote the dual space of $H^1_0(\Omega)$ as $H^{-1}(\Omega)$, equipped with the inner product $(f, g)_{-1} = ((-\Delta)^{-1/2} f, (-\Delta)^{-1/2} g)$ and the norm $\|f\|_{-1} = (f, f)_{-1}$.

We denote $C$ as a generic positive constant that is independent of the time step $\tau$ and the space step $h$ but possibly depends on the exact solution and the initial value. We use $f \lesssim g$ to say that there exists a generic positive constant $C$ such that $f \leq Cg$.

Then, we describe the framework of the Fourier spectral method in three dimensions. We consider the domain $\Omega = [0, L_x] \times [0, L_y] \times [0, L_z]$ and the space step $h_x = L_x / N_x$, $h_y = L_y / N_y$, $h_z = L_z / N_z$, where $N_x, N_y, N_z$ are the grid numbers for the $x, y, z$ direction. The Fourier approximation space is

$$X_N = \text{span} \left\{ \sum_{l=-N/2}^{N/2-1} \sum_{\beta=0}^{N/2-1} \sum_{\gamma=0}^{N/2-1} \Phi_{l\beta\gamma} e^{i(lx\alpha_1 + \beta y_\beta + \gamma z_\gamma)} \right\},$$

where $i = \sqrt{-1}$, $\alpha_1 = 2\pi l / L_x$, $\beta_\beta = 2\pi \beta / L_y$, $\gamma_\gamma = 2\pi \gamma / L_z$. Then, any function $\phi(x, y, z) \in L^2(\Omega)$ can be approximated by

$$\phi(x, y, z) \approx \Phi(x, y, z) = \sum_{l=-N_x/2}^{N_x/2-1} \sum_{\beta=0}^{N_y/2-1} \sum_{\gamma=0}^{N_z/2-1} \Phi_{l\beta\gamma} e^{i(lx\alpha_1 + \beta y_\beta + \gamma z_\gamma)},$$

where the Fourier coefficients are denoted as follows:

$$\Phi_{l\beta\gamma} = \langle \phi, e^{i(lx\alpha_1 + \beta y_\beta + \gamma z_\gamma)} \rangle = \frac{1}{|\Omega|} \int_{\Omega} \phi \ e^{-i(lx\alpha_1 + \beta y_\beta + \gamma z_\gamma)} \ dx.$$

For simplicity, we take a cube area with the same mesh in three directions, as follows: $N = N_x = N_y = N_z$, $L = L_x = L_y = L_z$, and $h = h_x = h_y = h_z$.

We define the $L^2$-orthogonal projection operator $\Pi_N : L^2(\Omega) \rightarrow X_N$ by

$$\langle \Pi_N \phi - \phi, \Psi \rangle = 0, \quad \phi \in L^2(\Omega), \quad \forall \Psi \in X_N$$

(2.1)

Then, we have the error estimates for the orthogonalization [5,22,25]: for any $\phi \in H^m_{per}(\Omega)$ and any $0 \leq m \leq N$, there exists a constant $C$ that

$$\|\Pi_N \phi - \phi\|_{H^0} \lesssim N^{m} \|\phi\|_{H^m},$$

(2.2)
where

\[ H_{\text{per}}^m(\Omega) = \{ \phi \in H^m(\Omega) | \phi^{(i)} \text{ is periodic on } \partial \Omega, 0 \leq v \leq m \}. \]

### 3 Governing systems

In this section, we introduce the system that describes the Ashura and Janus core-shell particles. In [16], Y. Hirai et al. constructed the confined TBP model based on Cahn-Hilliard equations to simulate phase-separated structures of ternary blended polymers in three-dimensionally confined spaces. The free energy functional is given as follows:

\[
F(\phi_1, \phi_2, \phi_3, \phi_4) = \int_\Omega \left\{ \sum_{i=1}^{4} \frac{\epsilon_i^2}{2} |\nabla \phi_i|^2 + W(\phi_1, \phi_2, \phi_3, \phi_4) \right\},
\]

(3.1)

where \( \epsilon_i \) is proportional to the thickness of the interface of the order parameters \( \phi_i \). The order parameter \( \phi_1 \) describes the macrophase separation; i.e., the polymers are confined in a region that is generated by the solvent. The value of \( \phi_1 \) is within the interval \([-1, +1]\), where -1 represents the solvent-rich domain, and +1 represents the polymer-rich domain. The remaining order parameters \( \phi_2, \phi_3 \) and \( \phi_4 \) describe the states of the three polymers. The values of \( \phi_2, \phi_3 \) and \( \phi_4 \) are within the interval \([-1, +1]\), where +1 represents the polymer-rich domain, and -1 represents the polymer-nonrich domain. \( W(\phi_1, \phi_2, \phi_3, \phi_4) \) is given as follows:

\[
W(\phi_1, \phi_2, \phi_3, \phi_4) = \sum_{i=1}^{4} \frac{(\phi_i^2 - 1)^2}{4} + b_1 \phi_1 (\phi_2 + \phi_3 + \phi_4) + b_2 \phi_1 (\phi_2^2 + \phi_3^2 + \phi_4^2) + b_3 (\pm \phi_2 \phi_3 \pm \phi_2 \phi_4 - \phi_3 \phi_4) + b_4 \phi_2 \phi_3 \phi_4 + b_5 \phi_2 (\phi_3^2 + \phi_4^2),
\]

(3.2)

where the plus and minus signs for the \( \phi_2 \phi_3 \) and \( \phi_3 \phi_4 \) of Eq. (3.2) represent Janus core-shell and Ashura, respectively. The coupling parameters \( b_i \) are negative for \( i = 1, 2, 3, 4, 5 \). \( b_1 \) controls the affinity between the solvent \( \phi_1 \) and the three polymers \( \phi_2, \phi_3 \) and \( \phi_4 \). As \( b_1 \) increases, the affinity also increases. \( b_2 \) is a confinement parameter that confines the polymers to the polymer-rich domain (\( \phi_1 = +1 \)) and separates polymers from the solvent. Moreover, \( b_2 < 0 \) lowers the energy and promotes microphase separation when \( \phi_1 > 0 \). \( b_3 \) is related to the interfacial tension between the polymers, and the term \( b_3 (\pm \phi_2 \phi_3 \pm \phi_2 \phi_4 - \phi_3 \phi_4) \) reveals the difference between Ashura and Janus core-shell particles. For Ashura particles, the term \(-\phi_2 \phi_3 - \phi_2 \phi_4 - \phi_3 \phi_4\) means the interfacial tensions between each pair of polymers, i.e., \( \phi_2 \) and \( \phi_3 \), \( \phi_2 \) and \( \phi_4 \), \( \phi_3 \) and \( \phi_4 \), have similar intensities. For Janus core-shell particles, the term \( \phi_2 \phi_3 + \phi_2 \phi_4 - \phi_3 \phi_4 \) means that the interfacial tension between the core and the shell \( (\phi_2 \phi_3 \text{ and } \phi_2 \phi_4) \) is much larger than that of the two cores \( (\phi_3 \phi_4) \), in such a way that \( \phi_3 \) and \( \phi_4 \) can be surrounded by \( \phi_2 \). \( b_4 \) represents the triple juncture between three polymers \( \phi_2, \phi_3 \) and \( \phi_4 \). \( b_5 \) is another confinement parameter that confines polymers \( \phi_3 \) and \( \phi_4 \) to the interior of polymer \( \phi_2 \) (\( \phi_2 = -1 \)). Thus, for Ashura particles,
For Janus core-shell particles, $b_5 < 0$ lowers the energy and promotes microphase separation when $\phi_2 > 0$, which is similar to the parameter $b_2$.

The dynamical systems are based on Cahn-Hilliard equations

$$\frac{\partial \phi_i}{\partial t} = M_i \Delta \frac{\delta F}{\delta \phi_i}, \quad i = 1, 2, 3, 4, \quad (3.3)$$

where $M_i$ is the mobility parameter that controls the speed at which the order parameter $\phi_i$ moves for $i = 1, 2, 3, 4$. With the variational derivative of the free energy functional (3.1), we obtain four coupled Cahn-Hilliard equations

$$\frac{\partial \phi_i}{\partial t} = M_i \Delta \left( -\epsilon_i^2 \Delta \phi_i + \frac{\partial W}{\partial \phi_i} \right), \quad (3.4)$$

where

$$\frac{\partial W}{\partial \phi_1} = \phi_1^3 - \phi_1 + b_1 (\phi_2 + \phi_3 + \phi_4) + b_2 (\phi_2^2 + \phi_3^2 + \phi_4^2),$$

$$\frac{\partial W}{\partial \phi_2} = \phi_2^3 - \phi_2 + b_1 \phi_1 + 2b_2 \phi_1 \phi_2 + b_3 (\pm \phi_3 \pm \phi_4) + b_4 \phi_3 \phi_4 + b_5 (\phi_3^2 + \phi_4^2),$$

$$\frac{\partial W}{\partial \phi_3} = \phi_3^3 - \phi_3 + b_1 \phi_1 + 2b_2 \phi_1 \phi_3 + b_3 (\pm \phi_2 \pm \phi_4) + b_4 \phi_2 \phi_4 + 2b_5 \phi_2 \phi_3,$$

$$\frac{\partial W}{\partial \phi_4} = \phi_4^3 - \phi_4 + b_1 \phi_1 + 2b_2 \phi_1 \phi_4 + b_3 (\pm \phi_2 - \phi_3) + b_4 \phi_2 \phi_3 + 2b_5 \phi_2 \phi_4.$$

In this paper, we assume periodic boundary conditions. System (3.4) has the properties of unconditional energy stability and mass conservation. The theorems and proofs are given as follows.

**Theorem 3.1.** The system (3.4) is unconditionally energy stable, i.e.,

$$\frac{d}{dt} F[\phi_1, \phi_2, \phi_3, \phi_4] \leq 0.$$

**Proof.** Taking the $L^2$ inner product of (3.3) with $\delta F / \delta \phi_i, i = 1, 2, 3, 4$, and summing over $i$ gives

$$\frac{d}{dt} F[\phi_1, \phi_2, \phi_3, \phi_4] = \sum_{i=1}^{4} \int_{\Omega} \frac{\delta F}{\delta \phi_i} \frac{\partial \phi_i}{\partial t} d\mathbf{x} = - \sum_{i=1}^{4} M_i \int_{\Omega} \left| \nabla \frac{\delta F}{\delta \phi_i} \right|^2 d\mathbf{x} \leq 0.$$

This completes the proof.

**Theorem 3.2.** The order parameters $\phi_i, i = 1, 2, 3, 4$ in the system (3.4) are mass-conservative, i.e.,

$$\int_{\Omega} \phi_i(x,y,z,t) d\mathbf{x} = \int_{\Omega} \phi_i(x,y,z,0) d\mathbf{x} \quad \text{for all} \quad t > 0.$$
Proof. Integrating Eqs. (3.3) over \( \Omega \), using integration by parts, and with the periodic boundary conditions, we have

\[
\frac{d}{dt} \int_\Omega \phi_i \, dx = \left( \frac{\partial \phi_i}{\partial t}, 1 \right) = M_i \left( \Delta \delta F, 1 \right) = 0.
\]

This completes the proof. \( \square \)

4 Numerical schemes

In this section, we aim to construct a linear, decoupled and unconditionally energy stable scheme to solve the system (3.4). We use the SAV approach combined with stabilization terms based on the backward differentiation formula for temporal discretization and the Fourier spectral method for spatial discretization.

4.1 Equivalent system

To reformulate the quaternary Cahn-Hilliard equations (3.4) into an equivalent system, we rewrite the free energy functional as the sum of a linear term and a nonlinear term. The stabilization terms are added by extracting four quadratic terms from the nonlinear term, as follows:

\[
F[\phi_1, \phi_2, \phi_3, \phi_4] = \int_\Omega \left( \sum_{i=1}^4 \epsilon_i^2 |\nabla \phi_i|^2 + \sum_{i=1}^4 s_i \phi_i^2 \right) d\Omega + F_1[\phi_1, \phi_2, \phi_3, \phi_4],
\]

where

\[
F_1[\phi_1, \phi_2, \phi_3, \phi_4] = \int_\Omega \left( W(\phi_1, \phi_2, \phi_3, \phi_4) - \sum_{i=1}^4 s_i \phi_i^2 \right) d\Omega,
\]

and \( s_i \) is the stabilization coefficient.

Since the terms within the integral of function \( F_1 \) are polynomials and the highest order term is quartic, there exists a positive constant \( C_0 \) that satisfies \( F_1[\phi_1, \phi_2, \phi_3, \phi_4] + C_0 > 0 \). Introducing the scalar auxiliary variable \( r(t) = \sqrt{F_1[\phi_1, \phi_2, \phi_3, \phi_4] + C_0} \), the system (3.4) can be reformulated as

\[
\frac{\partial \phi_i}{\partial t} = M_i \Delta \mu_i, \quad (4.1a)
\]

\[
\mu_i = -\epsilon_i^2 \Delta \phi_i + s_i \phi_i + \frac{r}{\sqrt{F_1 + C_0}} U_i, \quad (4.1b)
\]

\[
\frac{dr}{dt} = \frac{1}{2 \sqrt{F_1 + C_0}} \int_\Omega \sum_{j=1}^4 U_j \frac{\partial \phi_j}{\partial t} \, dx, \quad (4.1c)
\]

where \( U_i = \delta F_1 / \delta \phi_i \). The equivalent system (4.1) maintains the property of unconditional energy stability, which is given as follows:
Theorem 4.1. For the modified energy,

\[
\tilde{F}[\phi_1, \phi_2, \phi_3, \phi_4, r] = \sum_{i=1}^{4} \int_{\Omega} \left( \sum_{i=1}^{4} \frac{\epsilon_i^2}{2} |\nabla \phi_i|^2 + \sum_{i=1}^{4} s_i \phi_i^2 \right) dx + r^2 - C_0.
\]

The system in (4.1) is unconditionally energy stable, i.e.,

\[
\frac{d}{dt} \tilde{F}[\phi_1, \phi_2, \phi_3, \phi_4, r] \leq 0.
\]

Proof. Taking the inner product of (4.1a) with \( \mu_i \), of (4.1b) with \( \partial \phi_i / \partial t \), multiplying (4.1c) by \( 2r \), and taking the sum over \( i \), we have

\[
\sum_{i=1}^{4} \left( \frac{\partial \phi_i}{\partial t}, \mu_i \right) = \sum_{i=1}^{4} M_i (\Delta \mu_i, \mu_i),
\]

\[
\sum_{i=1}^{4} \left( \frac{\partial \phi_i}{\partial t}, \mu_i \right) = \sum_{i=1}^{4} \left( -\epsilon_i^2 \Delta \phi_i + s_i \phi_i \frac{\partial \phi_i}{\partial t} \right) + \sum_{i=1}^{4} \left( \frac{U_i}{\sqrt{F_1 + C_0}} \frac{\partial \phi_i}{\partial t} \right),
\]

\[
2r \frac{dr}{dt} = \sum_{i=1}^{4} \left( \frac{U_i}{\sqrt{F_1 + C_0}} \frac{\partial \phi_i}{\partial t} \right).
\]

Then, the energy dissipation law is derived by adding all of the equalities together:

\[
\frac{d}{dt} \tilde{F} = \sum_{i=1}^{4} \left( -\epsilon_i^2 \Delta \phi_i + s_i \phi_i \frac{\partial \phi_i}{\partial t} \right) + 2r \frac{dr}{dt} = -\sum_{i=1}^{4} M_i ||\nabla \mu_i||^2 \leq 0.
\]

This completes the proof. \( \square \)

Remark 4.1. The equivalent system (4.1) also maintains the property of mass conservation. The form of the theorem and the proving process are similar to Theorem 3.2, and thus, we omit these for simplicity.

4.2 Fully discrete scheme

With the Fourier spectral method, we now develop a fully discrete scheme based on the backward differentiation formula. We consider the initial value

\[
\Phi_i^0 = \Pi_N \phi_i(0) \in X_N, \quad i = 1, 2, 3, 4,
\]

\[
R^0 = \sqrt{F_1[\Phi_1^0, \Phi_2^0, \Phi_3^0, \Phi_4^0] + C_0},
\]

where \( \phi_i(0), i = 1, 2, 3, 4 \) are the initial values of the equivalent system (4.1). Then, the fully discrete S-SAV/BDF2 scheme is given as follows:
Scheme 4.1 (Fully discrete S-SAV/BDF2 scheme). Let $i = 1, 2, 3, 4$. Having computed $\Phi_{i}^{k-1}, \Phi_{i}^{k} \in \mathbb{X}_{i}, R_{i}^{k-1}$ and $R_{i}^{k}$, we can derive $\Phi_{i}^{k+1} \in \mathbb{X}_{i}$ and $R_{i}^{k+1}$ by solving

$$
\frac{3\Phi_{i}^{k+1} - 4\Phi_{i}^{k} + \Phi_{i}^{k-1}}{2\tau} = M_{i} \Delta \Lambda_{i}^{k+1}, \tag{4.2a}
$$

$$
\Lambda_{i}^{k+1} = -\epsilon_{i}^{2} \Delta \Phi_{i}^{k+1} + s_{i} \Phi_{i}^{k+1} + \frac{R_{i}^{k+1}}{\sqrt{F_{i}^{k+1} + C_{0}}}, \tag{4.2b}
$$

$$
3R_{i}^{k+1} - 4R_{i}^{k} + R_{i}^{k-1} = \frac{1}{2} \sum_{i=1}^{4} \left( \frac{U_{i}^{k+1}}{\sqrt{F_{i}^{k+1} + C_{0}}}, 3\Phi_{i}^{k+1} - 4\Phi_{i}^{k} + \Phi_{i}^{k-1} \right), \tag{4.2c}
$$

where

$$
U_{i}^{k+1} = U_{i}[\Phi_{i}^{k+1}, \Phi_{i}^{k+1}, \Phi_{i}^{k+1}, \Phi_{i}^{k+1}],
$$

$$
F_{i}^{k+1} = F_{i}^{k} = \Phi_{i}^{k+1}, \Phi_{i}^{k+1}, \Phi_{i}^{k+1}, \Phi_{i}^{k+1}],
$$

$$
\Phi_{i}^{k+1} = 2\Phi_{i}^{k} - \Phi_{i}^{k-1}.
$$

Remark 4.2. $\Phi_{i}^{k} \in \mathbb{X}_{i}, i = 1, 2, 3, 4$ and $R_{i}^{k}$ can be obtained by the first-order S-SAV scheme based on the backward Euler method

$$
\frac{\Phi_{i}^{1} - \Phi_{i}^{0}}{\tau} = M_{i} \Delta \Lambda_{i}^{1}, \tag{4.3a}
$$

$$
\Lambda_{i}^{1} = -\epsilon_{i}^{2} \Delta \Phi_{i}^{1} + s_{i} \Phi_{i}^{1} + \frac{R_{i}^{1}}{\sqrt{F_{i}^{0} + C_{0}}}, \tag{4.3b}
$$

$$
R_{i}^{1} - R_{i}^{0} = \frac{1}{2} \sum_{i=1}^{4} \left( \frac{U_{i}^{0}}{\sqrt{F_{i}^{0} + C_{0}}} \Phi_{i}^{1} - \Phi_{i}^{0} \right). \tag{4.3c}
$$

To solve scheme (4.2), we first substitute (4.2b) and (4.2c) into (4.2a) and obtain

$$
A_{i} \Phi_{i}^{k+1} = \frac{2}{\tau M_{i}} \Phi_{i}^{k} - \frac{1}{2 \tau M_{i}} \Phi_{i}^{k-1} + (R_{i}^{k} + b_{i}^{k+1}) \Delta \zeta_{i}^{s+1}, \tag{4.4}
$$

where

$$
\zeta_{i}^{s+1} = \frac{U_{i}^{k+1}}{\sqrt{F_{i}^{k+1} + C_{0}}},
$$

$$
A_{i} = \epsilon_{i}^{2} \Delta^{2} - s_{i} \Delta + \frac{3}{2 \tau M_{i}^{2}},
$$

$$
R_{i}^{k} = \frac{4}{3} R_{i}^{k} - \frac{1}{3} R_{i}^{k-1} + \frac{1}{6} \sum_{i=1}^{4} \left( \zeta_{i}^{s+1}, \Phi_{i}^{k-1} - 4\Phi_{i}^{k} \right),
$$

$$
b_{i}^{k+1} = \frac{1}{2} \sum_{i=1}^{4} \left( \zeta_{i}^{s+1}, \Phi_{i}^{k+1} \right). \tag{4.5}
$$
Eq. (4.4) yields
\[
\Phi_{i}^{k+1} = \Psi_{i}^{k} + \frac{1}{2}(R_{g}^{k} + b^{k+1})\eta_{i}^{s, k+1},
\] (4.6)
where
\[
\Psi_{i}^{k} = A_{i}^{-1}\left(2\tau M_{i}\Phi_{i}^{k} - \frac{1}{2\tau M_{i}}\Phi_{i}^{k-1}\right), \quad \eta_{i}^{s, k+1} = A_{i}^{-1}(\Delta \xi_{i}^{s, k+1}).
\] (4.7)
To update \(\Phi_{i}^{k+1}\) by (4.6), we must update \(b^{k+1}\) first. Taking the inner products of (4.6) with \(\xi_{i}^{s, k+1}, i = 1, 2, 3, 4\) and summing them together, we obtain
\[
2b^{k+1} = c^{k} + (R_{g}^{k} + b^{k+1})d^{k},
\]
where
\[
c^{k} = \sum_{i=1}^{4} (\Psi_{i}^{k} \xi_{i}^{s, k+1}), \quad d^{k} = \sum_{i=1}^{4} (\eta_{i}^{s, k+1} \xi_{i}^{s, k+1}).
\] (4.8)
Subsequently, \(b^{k+1}\) is updated as
\[
b^{k+1} = \frac{c^{k} + R_{g}^{k}d^{k}}{2 - d^{k}}.
\] (4.9)
Substituting \(b^{k+1}\) into (4.6), we obtain \(\Phi_{i}^{k+1}\).

To summarize, the term \(\Phi_{i}^{k+1}\) is updated by Algorithm 1:

**Algorithm 1**

1: Solve eight symmetric positive definite linear equations to obtain \(\Psi_{i}^{k}\) and \(\eta_{i}^{s, k+1}\) from (4.7), \(i = 1, 2, 3, 4\).
2: Compute \(R_{g}^{k}\) from (4.5), \(c^{k}\) and \(d^{k}\) from (4.8).
3: Compute \(b^{k+1}\) from (4.9).
4: Compute \(\Phi_{i}^{k+1}\) from (4.6), \(i = 1, 2, 3, 4\).

### 4.3 Energy stability and mass conservation

Furthermore, the unconditional energy stability and mass conservation for the fully discrete S-SAV/BDF2 scheme can be proved. The same results can be established for the semidiscrete versions.

**Theorem 4.2.** For the modified energy
\[
\mathcal{E}_{bd/2}^{k+1} = \sum_{i=1}^{4} \frac{c_{i}^{2}}{4} \left(\|\nabla \Phi_{i}^{k+1}\|^{2} + \|\nabla (2\Phi_{i}^{k+1} - \Phi_{i}^{k})\|^{2}\right) + \sum_{i=1}^{4} S_{i}^{*} \left(\|\Phi_{i}^{k+1}\|^{2} + \|2\Phi_{i}^{k+1} - \Phi_{i}^{k}\|^{2}\right) + \frac{1}{2} \left[(R^{k+1})^{2} + (2R^{k+1} - R^{k})^{2}\right] - C_{0},
\]
the scheme (4.2) is unconditionally energy stable, i.e.,
\[ \tilde{F}^{k+1}_{bd/2} - \tilde{F}^{k-1}_{bd/2} \leq 0. \]

**Proof.** Considering the \( L^2 \) inner product of the functions (4.2a) with \( 2\tau \Lambda^{k+1}_i \), of (4.2b) with \( 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1} \), and taking the sum over \( i \), we obtain

\[
\sum_{i=1}^{4} \left( 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1}, \Lambda_i^{k+1} \right) = 2\tau \sum_{i=1}^{4} M_i \left( \Delta \Lambda_i^{k+1}, \Lambda_i^{k+1} \right),
\]

\[
\sum_{i=1}^{4} \left( 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1}, \Lambda_i^{k+1} \right) = -\frac{4}{4} \sum_{i=1}^{4} \epsilon_i^2 \left( \Delta \Phi_i^{k+1}, 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1} \right) + \frac{4}{4} \sum_{i=1}^{4} s_i \left( \Phi_i^{k+1}, 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1} \right) + R^{k+1} \sum_{i=1}^{4} \left( \zeta_i^{k+1}, 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1} \right).
\]

Then, by multiplying (4.2c) with \( 2R^{k+1} \), we obtain

\[ 2R^{k+1} (3R^{k+1} - 4R_k + R^{k-1}) = R^{k+1} \sum_{i=1}^{4} \left( \zeta_i^{k+1}, 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi_i^{k-1} \right). \]

Combining the above three equations and with the following identity

\[ 2a(3a - 4b + c) = a^2 - b^2 + (2a - b)^2 - (2b - c)^2 + (a - 2b + c)^2, \]

we have

\[
0 \geq -2\tau \sum_{i=1}^{2} M_i \|
\sum_{i=1}^{4} \frac{\epsilon_i^2}{2} \left( \| \nabla \Phi_i^{k+1} \|^2 - \| \nabla \Phi_i^k \|^2 + \| \nabla (2\Phi_i^{k+1} - \Phi_i^k) \|^2 - \| \nabla (2\Phi_i^k - \Phi_i^{k-1}) \|^2 \right) + \frac{4}{4} \sum_{i=1}^{4} s_i \left( \| \Phi_i^{k+1} \|^2 - \| \Phi_i^k \|^2 + \| 2\Phi_i^{k+1} - \Phi_i^k \|^2 - \| 2\Phi_i^k - \Phi_i^{k-1} \|^2 \right) + (R^{k+1})^2 - (R^k)^2 + (2R^{k+1} - R^k)^2 - (2R^k - R^{k-1})^2 \\
+ \frac{4}{4} \sum_{i=1}^{4} \frac{\epsilon_i^2}{2} \left( \sum_{i=1}^{4} \frac{\sum_{i=1}^{4} s_i}{2} \| \Phi_i^{k+1} - 2\Phi_i^k + \Phi_i^{k-1} \|^2 \right)^2 + \frac{4}{4} \sum_{i=1}^{4} \frac{\sum_{i=1}^{4} s_i}{2} \| \Phi_i^{k+1} - 2\Phi_i^k + \Phi_i^{k-1} \|^2 \\
+ (R^{k+1} - 2R^k + R^{k-1})^2. \]

Then, the energy dissipation law can be obtained after dropping some positive terms. \( \square \)
Theorem 4.3. The order parameters $\Phi_i$, $i = 1, 2, 3, 4$ in the S-SAV/BDF2 scheme (4.2) are mass-conservative, i.e.,
\[
\int_{\Omega} \Phi_i^k dx = \int_{\Omega} \Phi_i^0 dx \quad \text{for all } k > 0.
\]

Proof. Integrating Eq. (4.2a) over $\Omega$, we have
\[
\int_{\Omega} \Phi_i^{k+1} dx = \frac{2}{3} \int_{\Omega} \Delta \Lambda_i^{k+1} dx + \frac{1}{3} \int_{\Omega} (4\Phi_i^k - \Phi_i^{k-1}) dx
\]
where the first term on the right hand side vanishes due to the divergence theorem and the periodic boundary conditions. Then, applying the same process to (4.3a), we can obtain
\[
\int_{\Omega} \Phi_i^k dx = \int_{\Omega} \Phi_i^0 dx.
\]
Finally we can deduce the mass conservation with the mathematical induction.

Remark 4.3. We can also easily develop another fully discrete scheme based on the Crank-Nicolson method (S-SAV/CN scheme). The solving steps are similar to Algorithm 1, and the unconditional energy stability can be proven in a similar way as in Theorem 4.2 with the modified energy $\tilde{F}_{cn} = \sum_{i=1}^4 \epsilon_i^2 \|\nabla \Phi_i^k\|^2 + \sum_{i=1}^4 s_i^2 \|\Phi_i^k\|^2 + (R_k)^2 - C_0$. The S-SAV/CN scheme also maintains the property of mass conservation.

5 Error estimates

In this section, we provide error estimates for the fully discrete S-SAV/BDF2 scheme (4.2), which is presented in Theorem 5.1. The most important and difficult thing in proving Theorem 5.1 is to obtain $L^\infty$ boundedness of the discrete solutions. So we couple the proof of $L^\infty$ boundedness and error estimates, and use mathematical induction to derive the results. Three steps are carried out in the whole proof. Firstly, the regularity of the scalar auxiliary variable $r(t)$ is derived based on the regularity of the exact solutions $\phi_i$. Secondly, $L^\infty$ boundedness of the discrete solutions $\Phi_i$ is proved by mathematical induction, so that the derivatives of the nonlinear term $F_i$ can be simplified. Finally, the error estimates are obtained.

We denote that
\[
\begin{align*}
\epsilon_i^k &= \Phi_i^k - \Pi_N \phi_i(t^k) + \Pi_N \phi_i(t^k) - \phi_i(t^k) := \tilde{\epsilon}_i^k + \hat{\epsilon}_i^k, \\
\mu_i^k &= \mu_i^k - \Pi_N \mu_i(t^k) + \Pi_N \mu_i(t^k) - \mu_i(t^k) := \tilde{\mu}_i^k + \hat{\mu}_i^k, \\
R_k &= R - r(t^k).
\end{align*}
\]

Theorems 4.1 and 4.2 imply that the functions $\phi_i$, $r$, $\Phi_i^k$ and $R$ in (4.1) and (4.2) are bounded as follows:
\[
\|\phi_i\|_{H^1}, \|\Phi_i^k\|_{H^1}, |r|, |R| \leq C, \quad i = 1, 2, 3, 4, \quad k \leq T_{\text{max}} / \tau,
\]

(5.1)
where $C$ depends on $\Omega$, $\phi_i(0)$ and $\Phi_i^0$.

We suppose that the exact solutions $\phi_i$, $i=1,2,3,4$ for the system (4.1) possess the following regularity:

$$
\begin{align*}
\phi_i & \in L^\infty(0,T;H^{m+1}_\text{per}(\Omega)); \\
\frac{\partial \phi_i}{\partial t} & \in L^\infty(0,T;H^{-1}_\text{per}) \cap L^\infty(0,T;H^{1}_\text{per}(\Omega)); \\
\frac{\partial^2 \phi_i}{\partial t^2} & \in L^\infty(0,T;L^2(\Omega)) \cap L^2(0,T;H^{1}_\text{per}(\Omega)); \\
\frac{\partial^3 \phi_i}{\partial t^3} & \in L^2(0,T;H^{-1}_\text{per}(\Omega)); \\
\|\nabla \phi_i\|_{L^\infty((0,T) \times \Omega)} & \leq C.
\end{align*}
$$

(5.2)

The regularity hypotheses for the scalar auxiliary variable $r(t)$ are not necessary. Instead, we can obtain through the regularity of the exact solutions (5.2).

**Lemma 5.1.** Under the regularity hypotheses (5.2), we have $r_{tt}, r_{ttt} \in L^2(0,T)$.

**Proof.** By direct calculation,

$$
\begin{align*}
r_{tt} &= \frac{1}{4} \sqrt{F^3_1} \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial \phi_i}{\partial t} \, dx \right)^2 + \frac{1}{2} \sqrt{F^3_1} \sum_{i=1}^{4} \int_{\Omega} \left( \frac{\partial \phi_i}{\partial t} \sum_{j=1}^{4} \frac{\partial U_i}{\partial \phi_j} \frac{\partial \phi_j}{\partial t} + U_i \frac{\partial^2 \phi_i}{\partial t^2} \right) \, dx, \\
r_{ttt} &= \frac{3}{8} \sqrt{F^5_1} \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial \phi_i}{\partial t} \, dx \right)^3 \\
& \quad \quad - \frac{3}{4} \sqrt{F^3_1} \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial \phi_i}{\partial t} \, dx \right) \sum_{i=1}^{4} \int_{\Omega} \left( \frac{\partial \phi_i}{\partial t} \sum_{j=1}^{4} \frac{\partial U_i}{\partial \phi_j} \frac{\partial \phi_j}{\partial t} + U_i \frac{\partial^2 \phi_i}{\partial t^2} \right) \, dx \\
& \quad \quad + \frac{1}{2} \sqrt{F^3_1} \sum_{i=1}^{4} \int_{\Omega} \left( 2 \frac{\partial^2 \phi_i}{\partial t^2} \sum_{j=1}^{4} \frac{\partial U_i}{\partial \phi_j} \frac{\partial \phi_j}{\partial t} + \frac{\partial \phi_i}{\partial t} \sum_{j=1}^{4} \frac{\partial U_i}{\partial \phi_j} \frac{\partial^2 \phi_j}{\partial t^2} + U_i \frac{\partial^3 \phi_i}{\partial t^3} \right) \, dx.
\end{align*}
$$

By using Hölder’s inequality and Sobolev’s embedding theorem, we have

$$
\begin{align*}
|r_{tt}|^2 & \lesssim \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial \phi_i}{\partial t} \, dx \right)^4 + \left( \sum_{i=1}^{4} \int_{\Omega} \frac{\partial \phi_i}{\partial t} \sum_{j=1}^{4} \frac{\partial U_i}{\partial \phi_j} \frac{\partial \phi_j}{\partial t} \, dx \right)^2 + \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial^2 \phi_i}{\partial t^2} \, dx \right)^2 \\
& \lesssim \sum_{i=1}^{4} \left( \|\frac{\partial \phi_i}{\partial t}\|_4^4 + \|\frac{\partial^2 \phi_i}{\partial t^2}\|^2 \right) \\
& \lesssim \sum_{i=1}^{4} \left( \|\frac{\partial \phi_i}{\partial t}\|_{H^1}^4 + \|\frac{\partial^2 \phi_i}{\partial t^2}\|^2 \right). 
\end{align*}
$$

(5.3)
For the term
\[ |r_{iii}|^2 \lesssim \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial \phi_i}{\partial t} \, dx \right)^6 \quad (\text{:= } A_1) \]
\[ + C \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial \phi_i}{\partial t} \, dx \right)^2 \left( \sum_{i=1}^{4} \int_{\Omega} \left( \frac{\partial \phi_i}{\partial t} + \sum_{j=1}^{4} U_i \frac{\partial \phi_j}{\partial t} \right) \, dx \right)^2 \quad (\text{:= } A_2) \]
\[ + C \left( \sum_{i=1}^{4} \int_{\Omega} \frac{\partial^2 \phi_i}{\partial t^2} \sum_{j=1}^{4} \frac{\partial U_i}{\partial t} \frac{\partial \phi_j}{\partial t} \, dx \right)^2 \quad (\text{:= } A_3) \]
\[ + C \left( \sum_{i=1}^{4} \int_{\Omega} \frac{\partial \phi_i}{\partial t} \left( \sum_{j=1}^{4} \frac{\partial U_i}{\partial t} \frac{\partial \phi_j}{\partial t} \right) \, dx \right)^2 \quad (\text{:= } A_4) \]
\[ + C \left( \sum_{i=1}^{4} \int_{\Omega} \frac{\partial^2 \phi_i}{\partial t^2} \left( \sum_{j=1}^{4} \frac{\partial U_i}{\partial t} \frac{\partial \phi_j}{\partial t} \right) \, dx \right)^2 \quad (\text{:= } A_5) \]
\[ + C \left( \sum_{i=1}^{4} \int_{\Omega} U_i \frac{\partial^2 \phi_i}{\partial t^2} \, dx \right)^2 \quad (\text{:= } A_6) \]

we can estimate in a similar way with (5.3) as follows:

\[ A_1 \lesssim \sum_{i=1}^{4} \left\| \frac{\partial \phi_i}{\partial t} \right\|_{L^6}^6 \lesssim \sum_{i=1}^{4} \left\| \frac{\partial \phi_i}{\partial t} \right\|_{H^1}^6, \quad (5.4) \]

\[ A_2 \lesssim \left( \sum_{i=1}^{4} \int_{\Omega} \left\| \frac{\partial \phi_i}{\partial t} \right\|_{L^6}^2 \, dx \right)^2 \left( \sum_{i=1}^{4} \int_{\Omega} \left\| \frac{\partial \phi_i}{\partial t} \right\|_{L^6}^2 \, dx + \sum_{i=1}^{4} \int_{\Omega} \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{L^6}^2 \, dx \right) \]
\[ \lesssim \left( \sum_{i=1}^{4} \left\| \frac{\partial \phi_i}{\partial t} \right\|_{L^6}^2 \right) \left( \sum_{i=1}^{4} \left\| \frac{\partial \phi_i}{\partial t} \right\|_{L^6}^4 + \sum_{i=1}^{4} \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{L^6}^4 \right) \]
\[ \lesssim \sum_{i=1}^{4} \left( \left\| \frac{\partial \phi_i}{\partial t} \right\|_{H^1}^6 + \left\| \frac{\partial \phi_i}{\partial t} \right\|_{H^1}^4 + \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{H^1}^4 \right), \quad (5.5) \]

\[ A_3 \text{ and } A_4 \text{ can be estimated in a similar way:} \]

\[ A_3 \lesssim \sum_{i=1}^{4} \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{L^6}^2 \left\| \frac{\partial \phi_i}{\partial t} \right\|_{L^6}^2 \lesssim \sum_{i=1}^{4} \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{L^6}^2 \left\| \frac{\partial \phi_i}{\partial t} \right\|_{H^1}^2 \lesssim \sum_{i=1}^{4} \left( \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{H^1}^4 + \left\| \frac{\partial \phi_i}{\partial t} \right\|_{H^1}^4 \right), \quad (5.6) \]
\[ A_4 \lesssim \sum_{i=1}^{4} \left( \left\| \frac{\partial^2 \phi_i}{\partial t^2} \right\|_{H^1}^4 + \left\| \frac{\partial \phi_i}{\partial t} \right\|_{H^1}^4 \right), \quad (5.7) \]
Thus, Lemma 5.1 can be proved by (5.3)-(5.9).

The estimates for the truncation errors are given as follows.

**Lemma 5.2.** Denote that

\[
\hat{T}_{1,f}^{k+1} = \tau \frac{d}{dt} \left( (k+1) - f(t^k) + f(t^k) \right),
\]

(5.10)

\[
T_0^k = \frac{1}{2} (f(t^{k+1}) + f(t^{k-1})) - f(t^k),
\]

(5.11)

\[
T_{1,f}^{k+1} = 2 \tau \frac{d}{dt} (t^{k+1}) - 3 f(t^{k+1}) + 4 f(t^k) - f(t^{k-1}).
\]

(5.12)

Then, the following estimates hold:

\[
|T_{0,f}^k|^2 \lesssim \tau^2,
\]

\[
|T_{1,f}^{k+1}|^2 \lesssim \tau^2 \int_{t^{k-1}}^{t^{k+1}} \left| \frac{d^2 f}{dt^2} (s) \right|^2 ds,
\]

\[
|T_{1,f}^{k+1}|^2 \lesssim \tau^5 \int_{t^{k-1}}^{t^{k+1}} \left| \frac{d^3 f}{dt^3} (s) \right|^2 ds.
\]

**Proof.** (5.10) can be derived by the Taylor formula. (5.11) and (5.12) can be written as the following integral forms:

\[
T_0^k = \frac{1}{2} \int_{t^k}^{t^{k+1}} (t^{k+1} - s) \frac{d^2 f}{dt^2} (s) ds - \frac{1}{2} \int_{t^k}^{t^{k-1}} (t^{k-1} - s) \frac{d^2 f}{dt^2} (s) ds,
\]

\[
T_{1,f}^{k+1} = \frac{3}{2} \int_{t^k}^{t^{k+1}} (s - t^{k+1}) \frac{d^3 f}{dt^3} (s) ds + \frac{1}{2} \int_{t^k}^{t^{k-1}} (s - t^{k-1}) \frac{d^3 f}{dt^3} (s) ds - 2 \tau \int_{t^k}^{t^{k+1}} (s - t^{k+1}) \frac{d^3 f}{dt^3} (s) ds.
\]

Then, the proof is easy to conclude.

**Lemma 5.3.** Supposing that the exact solutions of system (4.1) satisfy the regularity hypothesis (5.2), then there exists positive constants \( \tau_0 \) and \( h_0 \), and for any \( \tau < \tau_0 \) and \( h < h_0 \), the solutions \( \Phi_i^k \) of Eq. (4.2) satisfy

\[
\|\Phi_i^k\|_{L^\infty} \leq C = \max_{0 \leq t \leq T, 1 \leq i \leq 4} \|\phi_i(t)\|_{L^\infty} + 2,
\]

(5.13)

where \( i = 1,2,3,4 \) and \( k = 0,1,2,\ldots,[T_{\text{max}}/\tau]. \)
Proof. We prove this lemma with mathematical induction.

When $k = 0$, with Sobolev embedding theorem and the inequality (2.2), we have

$$
\left\| \Phi^i_t \right\|_{L^\infty} = \left\| \Pi_N \phi_i(0) \right\|_{L^\infty} \leq \left\| \Pi_N \phi_i(0) - \phi_i(0) \right\|_{L^\infty} + \left\| \phi_i(0) \right\|_{L^\infty}
\lesssim \left\| \Pi_N \phi_i(0) - \phi_i(0) \right\|_{H^1} + \left\| \phi_i(0) \right\|_{L^\infty}
\leq C_1 h^{m-1} \left\| \phi_i(0) \right\|_{H^m} + \left\| \phi_i(0) \right\|_{L^\infty} \leq C, \quad \text{for } d = 2,
$$

$$
\left\| \Phi^i_t \right\|_{L^\infty} \lesssim \left\| \Pi_N \phi_i(0) - \phi_i(0) \right\|_{H^2} + \left\| \phi_i(0) \right\|_{L^\infty}
\lesssim C_1 h^{m-2} \left\| \phi_i(0) \right\|_{H^m} + \left\| \phi_i(0) \right\|_{L^\infty} \leq C, \quad \text{for } d = 3,
$$

where \( h \leq h_1 = \frac{\sqrt{2}}{2\|C_1 \| \| \phi_i(0) \|_{H^m}} \). Supposing that \( \| \Phi^i_t \|_{L^\infty} \leq C \) is valid for \( k = 0, 1, 2, \ldots, n \), we prove \( \| \Phi^{n+1}_t \|_{L^\infty} \leq C \) is also valid in 4 steps.

**Step 1: Deriving the error functions.**

Subtracting (4.1) from (4.2) at \( t^{k+1} \), we can obtain the error equations as follows:

$$
3\epsilon^k_{i+1} - 4\epsilon^k_i + \epsilon^{k-1}_i = 2\tau M_i \Delta \omega^k_i + T^{k+1}_i, \quad \text{(5.14)}
$$

$$
\omega^k_{i+1} = -\epsilon^2_i \Delta \omega^k_{i+1} + s_i \epsilon^{k+1}_i + R^{k+1} \frac{U^*_{i,k+1}}{F^{*k+1}_i} - r(t^{k+1}) \frac{U_i}{\sqrt{F_i}}(t^{k+1}), \quad \text{(5.15)}
$$

$$
3\epsilon^k_r - 4\epsilon^k_i + \epsilon^{k-1}_i = \frac{1}{2\sqrt{F^*_1(t^{k+1})}} \sum_{i=1}^4 \left( U^*_i(t^{k+1}), 3\Phi^k_i - 4\Phi^k_i \right) \frac{\Delta \omega^k_{i+1}}{\sqrt{F^*_1(t^{k+1})}} + T^{k+1}_i, \quad \text{(5.16)}
$$

Taking the $L^2$ inner product of (5.14) with \( \omega^{k+1}_i \), of (5.15) with \( 3\epsilon^{k+1}_i - 4\epsilon^k_i + \epsilon^{k-1}_i \), taking the sum over \( i \), and with the property of the orthogonal projection (2.1), we have

$$
\sum_{i=1}^4 (3\epsilon^{k+1}_i - 4\epsilon^k_i + \epsilon^{k-1}_i, \omega^{k+1}_i) = \sum_{i=1}^4 2\tau M_i \Delta \omega^{k+1}_i, \omega^{k+1}_i + \sum_{i=1}^4 (T^{k+1}_i, \omega^{k+1}_i),
$$

$$
\sum_{i=1}^4 (3\epsilon^{k+1}_i - 4\epsilon^k_i + \epsilon^{k-1}_i, \omega^{k+1}_i) = \sum_{i=1}^4 (-\epsilon^2_i \Delta \omega^{k+1}_i + s_i \epsilon^{k+1}_i, 3\epsilon^{k+1}_i - 4\epsilon^k_i + \epsilon^{k-1}_i)
+ \frac{R^{k+1}}{\sqrt{F^*_1(t^{k+1})}} \sum_{i=1}^4 (U^*_i(t^{k+1}), 3\epsilon^{k+1}_i - 4\epsilon^k_i + \epsilon^{k-1}_i)
- r(t^{k+1}) \sum_{i=1}^4 (U_i(t^{k+1}), 3\epsilon^{k+1}_i - 4\epsilon^k_i + \epsilon^{k-1}_i).$$
Then, multiplying (5.16) with $2e_r^{k+1}$, we have
\[
2e_r^{k+1}(3e_r^{k+1} - 4e_r^k + e_r^{k-1}) = 2e_r^{k+1}T_{1,r} + \frac{e_r^{k+1}}{\sqrt{F_1^{k+1}}} \sum_{i=1}^{4} \left( U_i^{k+1}, 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi^{k+1} \right) \\
- 2\tau \frac{e_r^{k+1}}{\sqrt{F_1^{(k+1)}}} \sum_{i=1}^{4} \left( U_i(t^{k+1}), \frac{\partial \phi_i}{\partial t}(t^{k+1}) \right).
\]

Combining the above three equations and dropping some positive terms, we obtain
\[
\sum_{i=1}^{4} \frac{e_i^2}{2} (\|\nabla \epsilon_i^{k+1}\|^2 - \|\nabla \epsilon_i^k\|^2 + \|\nabla (2\epsilon_i^{k+1} - \epsilon_i^k)\|^2 - \|\nabla (2\epsilon_i^k - \epsilon_i^{k-1})\|^2) \\
+ \sum_{i=1}^{4} S_i (\|\epsilon_i^{k+1}\|^2 - \|\epsilon_i^k\|^2 + \|\epsilon_i^{k+1} - \epsilon_i^k\|^2 - \|2\epsilon_i^k - \epsilon_i^{k-1}\|^2) \\
+ (\epsilon_i^{k+1})^2 - (\epsilon_i^k)^2 + (\epsilon_i^k - \epsilon_i^{k-1})^2 - (\epsilon_i^k - \epsilon_i^{k-1})^2 + \sum_{i=1}^{4} 2\tau M_i \|\nabla \bar{u}_i^{k+1}\|^2 \leq \frac{r(t^{k+1})}{\sqrt{F_1^{(k+1)}}} \sum_{i=1}^{4} \left( U_i(t^{k+1}), 3\epsilon_i^{k+1} - 4\epsilon_i^k + \epsilon_i^{k-1} \right) \quad (:= B_1) \\
- \frac{R^{k+1}}{\sqrt{F_1^{k+1}}} \sum_{i=1}^{4} \left( U_i^{k+1}, 3\epsilon_i^{k+1} - 4\epsilon_i^k + \epsilon_i^{k-1} \right) \quad (:= B_2) \\
+ \frac{e_r^{k+1}}{\sqrt{F_1^{k+1}}} \sum_{i=1}^{4} \left( U_i^{k+1}, 3\Phi_i^{k+1} - 4\Phi_i^k + \Phi^{k+1} \right) \quad (:= B_3) \\
- 2\tau \frac{e_r^{k+1}}{\sqrt{F_1^{(k+1)}}} \sum_{i=1}^{4} \left( U_i(t^{k+1}), \frac{\partial \phi_i}{\partial t}(t^{k+1}) \right) \quad (:= B_4) \\
- \sum_{i=1}^{4} (T_{1,i}^{k+1}, \bar{u}_i^{k+1}) \quad (:= B_5) \\
+ 2e_r^{k+1}T_{1,r}^{k+1} \quad (:= B_6) \quad (5.17)
\]

**Step 2:** Estimating $B_1 + B_2, B_3 + B_4, B_5$ and $B_6$.

The term $B_1 + B_2$ can be transformed into
\[
B_1 + B_2 = r(t^{k+1}) \sum_{i=1}^{4} \left( \frac{U_i}{\sqrt{F_1}}(t^{k+1}) - \frac{U_i^{k+1}}{\sqrt{F_1^{k+1}}}, 3\epsilon_i^{k+1} - 4\epsilon_i^k + \epsilon_i^{k-1} \right) \\
- \frac{e_r^{k+1}}{\sqrt{F_1^{k+1}}} \sum_{i=1}^{4} \left( U_i^{k+1}, 3\epsilon_i^{k+1} - 4\epsilon_i^k + \epsilon_i^{k-1} \right). \quad (5.18)
\]
We can know from (5.1) that $|r| \leq C$. Then, the first term on the right-hand side of (5.18) can be estimated by

$$r(t^{k+1}) \left( \frac{U_i}{\sqrt{F_1}}(t^{k+1}) - \frac{U_i^{*,k+1}}{\sqrt{F_1}} \right) \leq \left( \frac{U_i}{\sqrt{F_1}}(t^{k+1}) - \frac{U_i^{*,k+1}}{\sqrt{F_1}} \right)$$

$$\leq \frac{\tau M_i}{2} \left\| \nabla u_i^{k+1} \right\|^2 + C \left\| \frac{\nabla U_i}{\sqrt{F_1}}(t^{k+1}) - \frac{\nabla U_i^{*,k+1}}{\sqrt{F_1}} \right\|^2 + \frac{C}{\tau} \left\| (-\Delta)^{-1/2} T_{1,i}^{k+1} \right\|^2.$$ (5.19)

Note that $T_{1,i}^{k+1} \in L^2(\Omega)$ since we have the mass-conservation theorem 3.2.

For the second term on the right-hand side of (5.19), we use the triangle inequality first:

$$\left\| \nabla U_i(t^{k+1}) - \nabla U_i^{*,k+1} \right\| \leq \left\| \nabla U_i(t^{k+1}) - \nabla U_i^{*,k+1} \right\| + \left\| \nabla U_i^{*,k+1} - \nabla U_i^{*,k+1} \right\|,$$ (5.20)

where

$$U_i^{*,k+1} = U_i[\phi_1^{*,k+1}, \phi_2^{*,k+1}, \phi_3^{*,k+1}, \phi_4^{*,k+1}],$$

$$F_i^{*,k+1} = F_i[\phi_1^{*,k+1}, \phi_2^{*,k+1}, \phi_3^{*,k+1}, \phi_4^{*,k+1}],$$

$$\phi_i^{*,k+1} = 2\phi_i^k - \phi_i^{k-1}.$$ 

The two terms on the right-hand side of (5.20) can be estimated in a similar way. Therefore, we only estimate the second term in detail as an example, which can be transformed into

$$\frac{\nabla U_i^{*,k+1}}{\sqrt{F_i^{*,k+1}}} - \frac{\nabla U_i^{*,k+1}}{\sqrt{F_i^{*,k+1}}} = \nabla U_i^{*,k+1} - \frac{F_i^{*,k+1} - F_i^{*,k+1}}{\sqrt{F_i^{*,k+1} + F_i^{*,k+1}}} + \frac{\nabla U_i^{*,k+1} - \nabla U_i^{*,k+1}}{\sqrt{F_i^{*,k+1}}}.$$ (5.21)
For the first term on the right-hand side of (5.21), (5.1) is used:

\[
\left\| \nabla U_{t}^{s,k+1} - \frac{F_{1}^{s,k+1} - F_{1}^{t,k+1}}{\sqrt{F_{1}^{s,k+1} F_{1}^{t,k+1}} (\sqrt{F_{1}^{s,k+1}} + \sqrt{F_{1}^{t,k+1}})} \right\|
\]

\[
\lesssim \left\| \nabla U_{t}^{s,k+1} \right\| \cdot \sum_{i=1}^{4} \| 2e_{i}^{k} - e_{i}^{k-1} \| \nabla \sum_{i=1}^{4} \| 2e_{i}^{k} - e_{i}^{k-1} \| \nabla (2\Phi_{j}(t^{k}) - \Phi_{j}(t^{k-1})) \| \sum_{i=1}^{4} \| (2e_{i}^{k} - e_{i}^{k-1}) \| + \| 2e_{i}^{k} - e_{i}^{k-1} \| \}
\]

\[
\lesssim \sum_{i=1}^{4} \| \| e_{i}^{k} \| + \| e_{i}^{k-1} \| + h^{m} \| 2\Phi_{j}(t^{k}) - \Phi_{j}(t^{k-1}) \|_{m} \). (5.22)
\]

By the Sobolev embedding theorem, we have $H_{1} \subseteq L^{3}$ and $H_{1} \subseteq L^{6}$. Together with Hölder’s inequality, the second term on the right-hand side of (5.21) can be estimated by

\[
\left\| \nabla U_{t}^{s,k+1} - \frac{\nabla U_{t}^{s,k+1}}{\sqrt{F_{1}^{s,k+1}}} \right\|
\]

\[
\lesssim \left( \sum_{j=1}^{4} \left( \left\| \frac{\partial U_{t}^{s,k+1}}{\partial \phi_{j}} - \frac{\partial U_{t}^{s,k+1}}{\partial \phi_{j}} \right\| \nabla \phi_{j}^{s,k+1} \right) \right) + \left\| \frac{\partial U_{t}^{s,k+1}}{\partial \phi_{j}} \right\| \left( \Phi_{j}^{s,k+1} - \phi_{j}^{s,k+1} \right)
\]

\[
\lesssim \sum_{i=1}^{4} \left( \sum_{i=1}^{4} \| (2e_{i}^{k} - e_{i}^{k-1}) \| \nabla \phi_{j}^{s,k+1} \| + \| \nabla (2e_{i}^{k} - e_{i}^{k-1}) \| \right)
\]

\[
\lesssim \sum_{i=1}^{4} \left( \sum_{i=1}^{4} \| 2e_{i}^{k} - e_{i}^{k-1} \| \| \phi_{j}^{s,k+1} \|_{L^{3}} + \| \nabla (2e_{i}^{k} - e_{i}^{k-1}) \| \right)
\]

\[
\lesssim \sum_{i=1}^{4} \left( \sum_{i=1}^{4} \| 2e_{i}^{k} - e_{i}^{k-1} \| \| \phi_{j}^{s,k+1} \|_{H^{1}} + \| \nabla (2e_{i}^{k} - e_{i}^{k-1}) \| \right)
\]

\[
\lesssim \sum_{i=1}^{4} \left( \| \nabla e_{i}^{k} \| + \| \nabla e_{i}^{k-1} \| + \| \phi_{i}^{s,k+1} \| + \| e_{i}^{k-1} \| + \| e_{i}^{k} \| + h^{m} \| 2\phi_{i}(t^{k}) - \phi_{i}(t^{k-1}) \|_{m+1} \right). (5.23)
\]

Combining (5.21)-(5.23), we have

\[
\left\| \nabla U_{t}^{s,k+1} - \frac{\nabla U_{t}^{s,k+1}}{\sqrt{F_{1}^{s,k+1}}} \right\|
\]

\[
\lesssim \left( \| \nabla e_{i}^{k} \| + \| \nabla e_{i}^{k-1} \| + \| \phi_{i}^{s,k+1} \| + \| e_{i}^{k-1} \| + h^{m} \| 2\phi_{i}(t^{k}) - \phi_{i}(t^{k-1}) \|_{m+1} \right), (5.24)
\]

With Lemma 5.2, the first term in (5.20) can be estimated similarly to (5.24):

\[
\left\| \nabla U_{t}^{s,k+1} - \frac{\nabla U_{t}^{s,k+1}}{\sqrt{F_{1}^{s,k+1}}} \right\|
\]

\[
\lesssim 3 \int_{t^{k-1}}^{t^{k+1}} \left\| \frac{\partial \phi_{i}}{\partial t^{2}} (s) \right\|^{2} ds. (5.25)
\]
Combining (5.18)-(5.20), (5.24) and (5.25), we obtain the estimation of the term $B_1 + B_2$

$$B_1 + B_2 \leq \sum_{i=1}^{4} \frac{\tau M_1}{4} \left( \| \nabla \theta_i^{k+1} \|^2 + C \tau \sum_{i=1}^{4} \left( \| \nabla \theta_i^{k} \| + \| \nabla \theta_i^{k-1} \| + \| \theta_i^{k} \| + \| \theta_i^{k-1} \| \right) 
+ C \tau^4 \sum_{i=1}^{4} \int_{t_i}^{t_{i+1}} \left( \| \frac{\partial^2 \phi_i^l}{\partial t^2} (s) \|_{H^2}^2 + \| \frac{\partial^3 \phi_i^l}{\partial t^3} (s) \|_{H^{-1}}^2 \right) ds 
+ C \tau h^{2m} \sum_{i=1}^{4} \int_{t_i}^{t_{i+1}} \left( \| \sum_{s \in [t_i, t_{i+1}]} \nabla U_i^{s,k+1} \|_{m+1} + \sum_{s \in [t_i, t_{i+1}]} \nabla U_i^{s,k+1} \|_{m+1} \right) \right)$$

(5.26)

The term $B_3 + B_4$ can be transformed into

$$B_3 + B_4 = -\frac{\epsilon_r^{k+1}}{F_1(t^{k+1})} \sum_{i=1}^{4} \left( U_i^{s,k+1} \theta_i^{3k+1} - 4 \epsilon_r^{k+1} \right) - \frac{\epsilon_r^{k+1}}{F_1(t^{k+1})} \sum_{i=1}^{4} \left( U_i^{s,k+1}, T_{i,j}^{k+1} \right) - \frac{\epsilon_r^{k+1}}{F_1(t^{k+1})} \sum_{i=1}^{4} \left( U_i^{s,k+1}, T_{i,j}^{k+1} \right) \right).$$

(5.27)

The second and third terms on the right-hand side of (5.27) can be estimated by (5.28) and (5.29), respectively:

$$-\frac{\epsilon_r^{k+1}}{F_1(t^{k+1})} \sum_{i=1}^{4} \left( U_i^{s,k+1}, T_{i,j}^{k+1} \right) \leq \tau (\epsilon_r^{k+1})^2 + \frac{1}{\tau} \sum_{i=1}^{4} \left( \| (-\Delta)^{-1/2} T_{i,j}^{k+1} \|_{H^2}^2 \right),$$

(5.28)

$$\epsilon_r^{k+1} \sum_{i=1}^{4} \left( \frac{U_i^{s,k+1}}{F_1(t^{k+1})} - \frac{U_i}{F_1(t^{k+1})} (t^{k+1}), 3 \phi_i(t^{k+1}) - 4 \phi_i(t^k) + \phi_i(t^{k-1}) \right) \right) \leq \tau \sum_{i=1}^{4} \left( \| \phi_i(t^{k+1}) \|_{L^\infty(0,T;H^1)} \left( (\epsilon_r^{k+1})^2 + \sum_{i=1}^{4} \| \frac{\nabla U_i^{s,k+1}}{F_1(t^{k+1})} \|_{m+1} \right) \right).$$

(5.29)

Combining (5.27)-(5.29), we have

$$B_3 + B_4 \leq \tau (\epsilon_r^{k+1})^2 + \tau \sum_{i=1}^{4} \left( \| \nabla \theta_i^{k} \| + \| \nabla \theta_i^{k-1} \| + \| \theta_i^{k} \| + \| \theta_i^{k-1} \| \right)$$

$$+ \tau^4 \sum_{i=1}^{4} \int_{t_i}^{t_{i+1}} \left( \| \frac{\partial^2 \phi_i^l}{\partial t^2} (s) \|_{H^2}^2 + \| \frac{\partial^3 \phi_i^l}{\partial t^3} (s) \|_{H^{-1}}^2 \right) ds 
+ \tau h^{2m} \sum_{i=1}^{4} \int_{t_i}^{t_{i+1}} \left( 2 \phi_i(t^k) - \phi_i(t^{k-1}) \right) \right) + \epsilon_r^{k+1} \sum_{i=1}^{4} \sum_{s \in [t_i, t_{i+1}]} \left( U_i^{s,k+1}, 3 \theta_i^{k+1} - 4 \theta_i^{k} + \theta_i^{k-1} \right).$$

(5.30)
Using Lemma 5.2, the terms $B_5$ and $B_6$ are estimated as follows:

$$B_5 \leq \frac{4}{2} \sum_{i=1}^{4} \tau M_i \| \nabla \bar{w}_i^{k+1} \|^2 + \frac{2}{\tau} \sum_{i=1}^{4} \|(-\Delta)^{-1/2} \ell_{1,i}^{k+1} \|^2,$$

$$B_6 \leq \tau (\epsilon_r^{k+1})^2 + \frac{1}{\tau} |T_{1,r}^{k+1}|^2.$$  \hspace{1cm} (5.31) \hspace{1cm} (5.32)

By combining (5.17), (5.26), (5.30) and (5.31)-(5.32), then summing over $k$ from 1 to $n$, we have

$$\sum_{i=1}^{4} (\epsilon_i^2 \| \nabla \bar{e}_i^{n+1} \|^2 + s_i \| \bar{e}_i^n \|^2) + |\epsilon_i^2| + \sum_{k=0}^{n+1} \tau M_i \| \nabla \bar{w}_i^{k} \|^2$$

$$\lesssim \sum_{i=1}^{4} (\epsilon_i^2 \| \nabla \bar{e}_i^1 \|^2 + s_i \| \bar{e}_i^1 \|^2) + |\epsilon_i^1|^2$$

$$+ \tau \sum_{k=0}^{n} \sum_{i=1}^{4} (\epsilon_i^2 \| \nabla \bar{e}_i^k \|^2 + s_i \| \bar{e}_i^k \|^2) + \tau \sum_{k=0}^{n+1} |\epsilon_r^k|^2 + \tau^4 + \gamma^2.$$  \hspace{1cm} (5.33)

**Step 3. Estimating the errors of the first step.**

Since there are errors of the first step on the right hand of (5.33), we give the estimates as follows. Note that $\bar{e}_i^0 = \Phi_i^0 - \Pi_N \phi_i(0) = 0$. For Eq. (4.3), we use the same method described in **Step 1** and obtain the error functions for the first step:

$$\sum_{i=1}^{4} (\epsilon_i^2 \| \nabla \bar{e}_i^1 \|^2 + s_i \| \bar{e}_i^1 \|^2) + |\epsilon_i^1|^2 + \sum_{i=1}^{4} \tau M_i \| \nabla \bar{w}_i^1 \|^2$$

$$= \frac{r(\tau)}{\sqrt{F_1(\tau)}} \sum_{i=1}^{4} (U_i(\tau), \bar{e}_i^1) - \frac{R_1}{\sqrt{F_1^0(\tau)}} \sum_{i=1}^{4} (U_i^0, \bar{e}_i^1)$$

$$+ \frac{e_1^1}{\sqrt{F_1^0(\tau)}} \sum_{i=1}^{4} (U_i^0, \Phi_i^1 - \Phi_i^0) - \tau \frac{e_1^1}{\sqrt{F_1(\tau)}} \left( U_i(\tau), \frac{\partial \phi_i}{\partial t}(\tau) \right)$$

$$+ 2e_1^1 \tilde{T}_{1,r}^1$$

$$- \frac{4}{\tau} (\tilde{T}_{1,r}^1, \bar{w}_i^1).$$  \hspace{1cm} (5.34)

Then, the estimates for the terms $D_1, D_2, D_3$ can be derived by using similar methods as
Step 2:

\[
D_1 \leq \frac{1}{2} \sum_{i=1}^{4} \tau M_i \|\nabla \bar{w}_1^i\|^2 + C \tau^4 + Ch^{2m} - \frac{\epsilon_1^i}{\sqrt{F_1^0}} \sum_{i=1}^{4} (U_i^0, e_i^1), \tag{5.35}
\]

\[
D_2 \leq \frac{\epsilon_1^i}{\sqrt{F_1^0}} \sum_{i=1}^{4} (U_i^0, e_i^1) + C \tau (e_1^i)^2 + \frac{1}{6} (e_1^i)^2 + C \tau^4 + Ch^{2m}, \tag{5.36}
\]

\[
D_3 \leq \frac{1}{6} (e_1^i)^2 + C |\hat{T}_{1,i}|^2 \leq \frac{1}{6} (e_1^i)^2 + C \tau^4. \tag{5.37}
\]

Note that

\[
\bar{w}_1^i = \Lambda_1^i - \Pi_N \mu_i (\tau) = -\epsilon_1^i \Delta \hat{e}_1^i + s_i \hat{e}_1^i + R_1 \frac{U_i^0}{\sqrt{F_1^0}} - r(\tau) \Pi_N U_i (\tau),
\]

Then, we have

\[
(\hat{T}_{1,i,\nu}^1, \bar{w}_1^i) \leq \frac{\epsilon_1^i}{2} \|\nabla \hat{e}_1^i\|^2 + C \|\nabla \hat{T}_{1,i}^1\|^2 + \frac{s_i}{4} \|\hat{e}_1^i\|^2 + C \|\hat{T}_{1,i}^1\|^2 + \frac{R_1}{\sqrt{F_1^0}} (\hat{T}_{1,i}^1, U_i^0) - \frac{r(\tau)}{\sqrt{F_1(\tau)}} (\hat{T}_{1,i}^1, \Pi_N U_i^0). \tag{5.38}
\]

The last two terms in (5.38) can be transformed into

\[
\frac{R_1}{\sqrt{F_1^0}} (\hat{T}_{1,i}^1, U_i^0) - \frac{r(\tau)}{\sqrt{F_1(\tau)}} (\hat{T}_{1,i}^1, \Pi_N U_i^0)
\]

\[
= \left( \frac{R_1}{\sqrt{F_1^0}} - \frac{r(\tau)}{\sqrt{F_1(\tau)}} \right) (\hat{T}_{1,i}^1, U_i^0) + \frac{r(\tau)}{\sqrt{F_1(\tau)}} (\hat{T}_{1,i}^1, U_i^0 - \Pi_N U_i (\tau))
\]

\[
\leq \frac{1}{2} \left| \frac{R_1}{\sqrt{F_1^0}} - \frac{r(\tau)}{\sqrt{F_1(\tau)}} \right|^2 + \frac{1}{2} \|\hat{T}_{1,i}^1, U_i^0\|^2 + C \|\nabla U_i^0 - \Pi_N \nabla U_i (\tau)\|^2 + C \|(-\Delta)^{1/2} \hat{T}_{1,i}^1\|^2. \tag{5.39}
\]

Since \(\sqrt{F_1^0} \geq 3\) can be satisfied by increasing \(C_0\), the first term in (5.39) can be estimated
by
\[
\left\| \frac{R_1}{\sqrt{F_0}} - \frac{r(\tau)}{\sqrt{F_1(\tau)}} \right\|^2 \lesssim \left| r(\tau) \frac{F_1(\tau) - F_0}{\sqrt{F_0} \sqrt{F_1(\tau)} \left( \sqrt{F_1(\tau)} + \sqrt{F_0} \right)} \right|^2 + \left\| \frac{R_1 - r(\tau)}{\sqrt{F_1}} \right\|^2 \leq C \sum_{i=1}^{4} \| \phi_i(\tau) - \phi_i(0) \|^2 + C \sum_{i=1}^{4} \| e^0_i \|^2 + \frac{1}{3} (e_0^1)^2
\]
\[
\leq \frac{1}{3} (e_0^1)^2 + C (h^{2m} + \tau^4). \tag{5.40}
\]

For the third term in (5.39), we have the estimates as follows:
\[
\| \nabla U_0^i - \Pi N \nabla U_i(\tau) \|^2 \leq \| \nabla U_0^i - \nabla U_i(0) \|^2 + \| \nabla U_i(0) - \nabla U_i(\tau) \|^2 + \| \nabla U_i(\tau) - \Pi N \nabla U_i(\tau) \|^2
\]
\[
\leq C \sum_{j=1}^{4} \| \nabla e^0_j \|^2 + C \sum_{j=1}^{4} \| \nabla (\phi_j(0) - \phi_j(\tau)) \|^2 + C h^{2m} \| \nabla U_i(\tau) \|^2_m
\]
\[
\lesssim \tau^4 + h^{2m}. \tag{5.41}
\]

Combining (5.34)-(5.41), the error estimates of the first step can be obtained:
\[
\sum_{i=1}^{4} \left( e_i^2 \| \nabla \tilde{e}_i^1 \|^2 + s_i \| \tilde{e}_i^1 \|^2 \right) + |e_0^1|^2 + \sum_{i=1}^{4} \tau M_i \| \nabla \tilde{w}_i^1 \|^2 \lesssim \tau^4 + h^{2m}. \tag{5.42}
\]

Taking (5.42) into (5.33) and using discrete Gronwall inequality, there exists a positive constant \( \tau_1 \) such that
\[
\sum_{i=1}^{4} \left( e_i^2 \| \nabla \tilde{e}_i^{n+1} \|^2 + s_i \| \tilde{e}_i^{n+1} \|^2 \right) + \| e_0^{n+1} \|^2 + \sum_{i=1}^{n+4} \sum_{k=0}^{4} \tau M_i \| \nabla \tilde{w}_i^k \|^2 \lesssim \tau^4 + h^{2m}, \tag{5.43}
\]

where \( \tau < \tau_1 \) and \( n = 0, 1, 2, \ldots, [T_{\text{max}} / \tau] - 1 \).

**Step 4. Prove** \( \| \Phi_k^{n+1} \|_{L^\infty} \leq C. \)

To give the proof of \( \| \Phi_i^{n+1} \|_{L^\infty} \leq C \), we need \( H^2 \) boundedness of \( e^i_{n+1} \). With the \( H^2 \) regularity results for elliptic equation, Eq. (5.15), Poincaré inequality, the estimates in
Step 2 and (5.43), we can obtain
\[
\|e_i^{n+1}\|_{H^2} \lesssim \|e_i^{n+1}\| + \|\Delta e_i^{n+1}\|
\]
\[
= \|e_i^{n+1}\| + \left| -w_i^{n+1} + s_i e_i^{n+1} + R_i^{n+1} \frac{U_i^{n+1}}{\sqrt{F_i^{n+1}}} - r(t_i^{n+1}) \frac{U_i}{\sqrt{F_i}} (t_i^{n+1}) \right|
\]
\[
\lesssim \|e_i^{n+1}\| + \|\Delta e_i^{n+1}\| + \left| R_i^{n+1} \frac{U_i^{n+1}}{\sqrt{F_i^{n+1}}} - r(t_i^{n+1}) \frac{U_i}{\sqrt{F_i}} (t_i^{n+1}) \right|
\]
\[
\lesssim \|e_i^{n+1}\| + \|\nabla w_i^{n+1}\| + \left| \frac{U_i^{n+1}}{\sqrt{F_i^{n+1}}} - \frac{U_i}{\sqrt{F_i}} (t_i^{n+1}) \right| + |e_i^{n+1}|
\]
\[
\lesssim \tau^2 + h^m. \tag{5.44}
\]
Then we can derive
\[
\|\Phi_i^{n+1}\|_{L^\infty} \lesssim \|e_i^{n+1}\|_{L^\infty} + \|\Phi(t_i^{n+1})\|_{L^\infty} \lesssim \|e_i^{n+1}\|_{H^2} + \|\Phi(t_i^{n+1})\|_{L^\infty}
\]
\[
\leq C_3 \tau^2 + C_3 h^m + \|\Phi(t_i^{n+1})\|_{L^\infty} \leq C, \tag{5.45a}
\]
\[
\|\Phi_i^{n+1}\|_{L^\infty} \lesssim \|e_i^{n+1}\|_{L^\infty} + \|\Phi(t_i^{n+1})\|_{L^\infty} \lesssim \|e_i^{n+1}\|_{H^2} + \|\Phi(t_i^{n+1})\|_{L^\infty}
\]
\[
\leq C_3 \tau^2 + C_3 h^m + \|\Phi(t_i^{n+1})\|_{L^\infty} \leq C, \tag{5.45b}
\]
where \(\tau \leq \tau_2 = \max\{\sqrt{1/C_2}, \sqrt{1/C_3}\}, h \leq h_2 = \max\{\sqrt{1/C_2}, \sqrt{1/C_3}\}\). Thus, we obtain the conclusion (5.13) for \(\tau < \tau_0 = \min\{\tau_1, \tau_2\}\) and \(h < h_0 = \min\{h_1, h_2\}\).

**Theorem 5.1.** Supposing that the exact solutions of system (4.1) satisfy the regularity hypothesis (5.2), then the scheme (4.2) has the following error estimates:
\[
\sum_{i=1}^{4} (e_i^2 \|\nabla e_i^n\|^2 + s_i \|e_i^n\|^2) + |e_i^n|^2 \lesssim \tau^4 + h^{2m}, \tag{5.46}
\]
where \(n = 0, 1, 2, \ldots, \lfloor T_{\max} / \tau \rfloor\).

**Proof.** Denote \(I_n = \sum_{i=1}^{4} (e_i^2 \|\nabla e_i^n\|^2 + s_i \|e_i^n\|^2) + |e_i^n|^2\), then by the proof of Lemma 5.3, we can obtain
\(I_n \lesssim \tau^4 + h^{2m}\) for \(\tau < \tau_0\) and \(h < h_0\). For the other cases, by the energy stability Theorem 4.1 and 4.2, we can obtain
\[
I_n \leq C \frac{C}{h_0^{1/2}} h^{2m} \lesssim \tau^4 + h^{2m}, \quad \text{for} \quad \tau < \tau_0, \ h \geq h_0,
\]
\[
I_n \leq C \frac{C}{\tau^{1/2}} \tau^4 \lesssim \tau^4 + h^{2m}, \quad \text{for} \quad \tau \geq \tau_0, \ h < h_0,
\]
\[
I_n \leq C \frac{C}{2\tau^{1/2}} \tau^4 + C \frac{C}{2h_0^{1/2}} h^{2m} \lesssim \tau^4 + h^{2m}, \quad \text{for} \quad \tau \geq \tau_0, \ h \geq h_0.
\]
Finally the proof can be concluded.
Moreover, the error estimates are also derived for the fully discrete S-SAV/CN scheme as follows:

**Theorem 5.2.** Suppose that the exact solutions \( \phi_i, i = 1,2,3,4 \) for the system (4.1) possess the following regularity:

\[
\begin{align*}
  \phi_i & \in L^\infty(0,T;H^m_{\text{per}}(\Omega)); \\
  \frac{\partial \phi_i}{\partial t} & \in L^\infty(0,T;H^{-1}_{\text{per}}(\Omega)) \cap L^\infty(0,T;H^1_{\text{per}}(\Omega)); \\
  \frac{\partial^2 \phi_i}{\partial t^2} & \in L^\infty(0,T;H^1_{\text{per}}(\Omega)) \cap L^2(0,T;H^3_{\text{per}}(\Omega)); \\
  \|
\n\|
\n\n|\n\| \in L^\infty((0,T) \times \Omega) \leq C,
\end{align*}
\]

(5.47)

then the S-SAV/CN scheme has the following error estimates:

\[
\sum_{i=1}^{4} \left( \frac{e_i^2}{2} + \frac{e_i^2}{2} \right) + |e_i^n|^2 \lesssim \tau^4 + h^{2m},
\]

(5.48)

where \( n = 0,1,2,\cdots, \lfloor T_{\text{max}} / \tau \rfloor \).

**Proof.** Since the proving process is similar to the proof of Theorem 5.1, we leave it to the interested readers. \qed

6 Simulations

In this section, we present the results of numerical experiments. The parameters are given as follows. The mobility coefficients are set as \( M_1 = M_2 = M_3 = M_4 = 1 \), and the stabilizer coefficients are set as \( s_1 = s_2 = s_3 = s_4 = 30 \). For Ashura particles, the parameters are set as \( L = 1.28, N = 64, \epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 = 0.04, b_1 = -0.08, b_2 = -0.8, b_3 = -0.4, b_4 = -0.5, b_5 = 0 \). For Janus core-shell particles, the parameters are set as \( L = 2, N = 100, \epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon_4 = 0.04, b_1 = -0.1, b_2 = -0.8, b_3 = -0.05, b_4 = -0.2, b_5 = -0.05 \).

6.1 Accuracy test

We first test the time and space accuracy of the S-SAV/BDF2 scheme and S-SAV/CN scheme. To accomplish this goal, we use the parameters of Ashura particles, and the
10-6
10-5
10-4
10-3
10-2
10-1
10
10
10
10
(a) S-SAV/BDF2
10
10
10
10
(b) S-SAV/CN

Figure 1: The $L^2$ errors of $\phi_i$, $i=1,2,3,4$ and $r$ at $T_{\text{max}}=0.01$ for the S-SAV/BDF2 and S-SAV/CN schemes with the time step $\tau=2.5 \times 10^{-5}/2^k$, $k=0,1,2,3,4,5$.

results of Janus core-shell particles are similar. We consider the initial conditions

$$
\phi_1^0(x,y,z) = \tanh\left(\frac{0.28L - \sqrt{(x - \frac{L}{2})^2 + (y - \frac{L}{2})^2 + (z - \frac{L}{2})^2}}{0.053L}\right),
$$

$$
\phi_2^0(x,y,z) = 0.01\cos(4\pi x/L)\cos(4\pi y/L)\cos(4\pi z/L),
$$

$$
\phi_3^0(x,y,z) = 0.01\sin(4\pi x/L)\sin(4\pi y/L)\cos(4\pi z/L),
$$

$$
\phi_4^0(x,y,z) = 0.01\cos(4\pi x/L)\sin(4\pi y/L)\cos(4\pi z/L).
$$

For the time accuracy, the space step $h=0.02$ is taken. We choose the numerical solution computed with a very small time step $\tau=1 \times 10^{-7}$ as the “exact” solution. Then, numerical solutions are computed with the time step $\tau=2.5 \times 10^{-5}/2^k$, $k=0,1,2,3,4,5$ at $T_{\text{max}}=0.01$. Fig. 1 shows the $L^2$ errors of $\phi_i$, $i=1,2,3,4$ and $r$ between the numerical solution and the “exact” solution for the S-SAV/BDF2 and S-SAV/CN schemes.

For the space accuracy, the time step $\tau$ is fixed at $2 \times 10^{-5}$. We choose the numerical solution computed with the grid number $N=512$ as the “exact” solution. Then, we compute the numerical solutions with the grid number $N=8 \cdot 2^k$, $k=0,1,2,3,4$ at $T_{\text{max}}=0.01$. Fig. 2 shows the $L^2$ errors of $\phi_i$, $i=1,2,3,4$ between the numerical solution and the “exact” solution for the S-SAV/BDF2 scheme and S-SAV/CN scheme.

It can be seen from Figs. 1 and 2 that for the S-SAV/BDF2 and S-SAV/CN schemes, the convergence rates in time reach second-order accuracy, and the spatial errors converge exponentially. Since the two schemes provide similar numerical results, without loss of generality, we only use the S-SAV/BDF2 scheme to present the results of the numerical experiments in the following discussion.
6.2 Phase separation

Here, we consider the random initial conditions

$$
\begin{align*}
\phi_1^0(x,y,z) &= \tanh \left( \frac{0.28L - \sqrt{(x - \frac{L}{2})^2 + (y - \frac{L}{2})^2 + (z - \frac{L}{2})^2}}{0.053L} \right), \\
\phi_2^0(x,y,z) &= 0.01 \text{rand}(x,y,z), \\
\phi_3^0(x,y,z) &= 0.01 \text{rand}(x,y,z), \\
\phi_4^0(x,y,z) &= 0.01 \text{rand}(x,y,z).
\end{align*}
$$

First, we show how we choose the stabilizer coefficients in Fig. 3. It can be seen in Fig. 3(a) that if the stabilizers are removed, that is, $s_i = 0$, then the numerical solutions can be computed by using a very small time step $\tau = 5 \times 10^{-7}$. The time steps that are larger than $5 \times 10^{-7}$ will cause blow-up, which is shown by the yellow line. For the case $s_i = 10$, $\tau = 1 \times 10^{-5}$, and for the case $s_i = 20$, $\tau = 2 \times 10^{-5}$, the phenomenon of blow-up still exists. When the stabilizer coefficients are added to 30, the numerical solutions can be computed under large time steps, as shown in Fig. 3(b). Thus, we choose the stabilizer coefficients $s_i = 30$, which causes use to compute efficiently by using a larger time step.

Though the stabilizer coefficients can provide efficiency, accuracy cannot be guaranteed when the time step is large. Fig. 3(b) shows that the time evolution curves of the modified energy $\tilde{F}_{bdf2}$ differ greatly when the time steps are larger than $1 \times 10^{-4}$. Therefore, we compare the modified energy for smaller time steps in Fig. 4. It can be observed that for time steps $\tau = 1 \times 10^{-4}$ and $5 \times 10^{-5}$, there are large gaps between the curves. However, for time steps $\tau = 2 \times 10^{-5}, 1 \times 10^{-5}$ and $5 \times 10^{-6}$, the curves coincide. Although the S-SAV/BDF2 scheme is unconditionally energy stable for large time steps, we should...
choose the time step $\tau \leq 2e^{-5}$ to ensure the accuracy for numerical solutions. Thus, we choose the time step $\tau = 2 \times 10^{-5}$ for the later simulations.

The phases of the steady states for Ashura and Janus core-shell particles are shown in Fig. 5 and Fig. 6, respectively. The legends of the two figures are the same and are introduced as follows. The snapshots are taken at $T_{\text{max}} = 1$. The yellow surface in Fig. (a)
represents the isosurface of \( \{ \phi_2 = 0.9 \} \), the blue surface in Fig. (b) represents the isosurface of \( \{ \phi_3 = 0.9 \} \), and the green surface in Fig. (c) represents the isosurface of \( \{ \phi_4 = 0.9 \} \). We combine the three phases of polymers together and obtain the morphology of the polymer particles, as shown in Fig. (e). The gray surface in Fig. (d) represents the isosurface of \( \{ \phi_1 = -0.5 \} \). It also represents the confinement and demonstrates the boundary between the solvent and the polymers. We combine the phase of the solvent and the phase of the three polymers together and then obtain the morphology of confined ternary polymer blended particles, as shown in Fig. (f).

It can be observed in Figs. 5 and 6 that \( \phi_1 \) separates the solvent-rich domain and the polymer-rich domain; in other words, the macrophase separation and the confinement are described by \( \phi_1 \). \( \phi_2 \), \( \phi_3 \) and \( \phi_4 \) reveal the microphase separation. For Ashura particles in Fig. 5, three polymers form fan-type domains inside the particles. Since the three polymers have the same interfacial tensions, they have the same interactions, and each polymer occupies one-third of the confined domain. For Janus core-shell particles in Fig. 6, \( \phi_3 \) and \( \phi_4 \) occupy half of the domain surrounded by \( \phi_2 \) since the interfacial tension of \( \phi_2 \) is larger than that of \( \phi_3 \) and \( \phi_4 \). These results are consistent with [16].

It is worth mentioning that the initial value has an impact on forming structures of the steady state. We choose the initial value (6.1) for Ashura particles, but only parts of
the random numbers can ultimately form fan-type structures. To compute the structure of Janus core-shell particles, as shown in Fig. 6, Janus structures for $\phi_3$ and $\phi_4$ are chosen to be the initial value.

6.3 The evolution of energy and total mass

The comparison of the original and modified energies is demonstrated in Fig. 7, where (a) and (b) represent the energy evolution of Ashura and Janus core-shell particles, respectively. It can be observed that the curves of the two energies coincide together. All curves show a downward tendency; i.e., the original and modified energies both decrease with time.

To numerically verify the mass conservation of the fully discrete scheme in Theorem 4.3, we transform the integral $\int_\Omega \Phi_i^k dx$ into the discrete form $\sum_{l,p,q=1}^N \Phi_{l,p,q}^k h^3$. We plot the mass evolution curves of four order parameters for Ashura and Janus core-shell particles in Fig. 8 and Fig. 9, respectively, where (a) demonstrates $\Phi_1$ and (b) demonstrates $\Phi_2, \Phi_3, \Phi_4$. The points lie on horizontal lines, which implies that the fully discrete scheme maintains the property of mass conservation.
6.4 Influence of the stabilizer $s_i$

The influence of the stabilizers $s_i$ is shown here. We compare the numerical results when $s_i = 30, 100, 500$ for $i = 1, 2, 3, 4$, and find there is only some invisible differences in the morphology structures, that is, the steady states are still Ashura and Janus core-shell particles. Besides, as the stabilizers increases, the original and modified energy both decrease faster, as shown in Fig. 10. We only present the modified energy for Ashura particles here, since the results are similar in other cases.
Figure 9: Evolution of the total mass for Janus core-shell particles.

Figure 10: Evolution of the modified energy for Ashura particles when $s_i = 30, 100, 500$. (a) shows the evolution in the time range $[0, 1]$, and (b) enlarges part of (a).

7 Conclusions

For the confined TBP model based on the quaternary Cahn-Hilliard equations, a fully discrete scheme is developed based on the S-SAV approach in time and the Fourier spectral method in space. The fully discrete S-SAV/BDF2 scheme maintains the properties of energy stability and mass conservation, which are proved in detail. Rigorous error estimates are derived for the scheme, which has second-order accuracy in time and spectral accuracy in space. Some numerical simulations are presented to numerically prove the properties of the scheme, including the time and spatial accuracy, the original and modified energy stability, and the mass conservation. The morphological structures of Ashura
and Janus-core shell particles are also shown. We believe that this is the first study on developing unconditionally energy stable schemes and providing numerically analyses for the confined TBP model.

There are few structures for ternary blended polymers since the absence of chemical bonds between these polymers results in weak interactions [16]. Thus, we can focus on simulating homopolymer/diblock copolymer blends or triblock copolymers, to determine more structures. Moreover, the effect of the temperature on forming the structures has not yet been studied. We can also simulate the morphological transformation by annealing ternary polymer blended particles. Similar work can be seen in [4]. In conclusion, other sophisticated morphologies of nanostructured polymer particles can be studied by the confined TBP model or other similar models with an efficient and unconditionally energy stable scheme in the future.

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