

SECOND-ORDER STABILIZED SEMI-IMPLICIT ENERGY STABLE SCHEMES FOR BUBBLE ASSEMBLIES IN BINARY AND TERNARY SYSTEMS

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ABSTRACT. In this paper, we propose some second-order stabilized semi-implicit methods for solving the Allen-Cahn-Ohta-Kawasaki and the Allen-Cahn-Ohta-Nakazawa equations. In the numerical methods, some nonlocal linear stabilizing terms are introduced and treated implicitly with other linear terms, while other nonlinear and nonlocal terms are treated explicitly. We consider two different forms of such stabilizers and compare the difference regarding the energy stability. The spatial discretization is performed by the Fourier collocation method with FFT-based fast implementations. Numerically, we verify the second order temporal convergence rate of the proposed schemes. In both binary and ternary systems, the coarsening dynamics is visualized as bubble assemblies in hexagonal or square patterns.

1. Introduction. Block copolymers are macromolecules made of two or more subchains of monomers. In their thermodynamic equilibria, block copolymers form various equilibrium morphologies. These ordered structures have been studied experimentally and theoretically over the past decades [24, 18, 21, 26, 1, 2]. Diblock copolymers consist of two subchains made by species A and B , respectively, while triblock copolymers have three subchains made by species A , B , and C , respectively.

In this paper, we consider a general block copolymer system of $N + 1$ species $\{A_i\}_{i=1}^{N+1}$ with long-range interactions. Using phase field labelings $\{\phi_i\}_{i=1}^N$ to label the volume fraction of the species $\{A_i\}_{i=1}^N$ and assuming the incompressibility of the species, we can trace the species A_{N+1} by $\phi_{N+1} = 1 - \sum_{i=1}^N \phi_i$. Such a system

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can be described by the free energy functional:

$$\begin{aligned}
E^N[\phi_1, \dots, \phi_N] &= \int_{\Omega} \frac{\epsilon}{2} \sum_{\substack{i,j=1 \\ i \leq j}}^N \nabla \phi_i \cdot \nabla \phi_j + \frac{1}{2\epsilon} \left[\sum_{i=1}^N W(\phi_i) + W\left(1 - \sum_{i=1}^N \phi_i\right) \right] dx \\
&\quad + \sum_{i,j=1}^N \frac{\gamma_{ij}}{2} \int_{\Omega} \left[(-\Delta)^{-\frac{1}{2}} (f(\phi_i) - \omega_i) (-\Delta)^{-\frac{1}{2}} (f(\phi_j) - \omega_j) \right] dx.
\end{aligned} \tag{1}$$

Here $0 < \epsilon \ll 1$ is an interface parameter, and $\Omega \subset \mathbb{R}^d, d = 2, 3$, is the spatial periodic domain. The function $W(\phi) = 18(\phi^2 - \phi)^2$ is a double-well potential with two local minima at 0 and 1. Taking the sum of $W(\cdot)$ for all species, we make a potential function W_N :

$$W_N(\phi_1, \dots, \phi_N) = \frac{1}{2} \left[\sum_{i=1}^N W(\phi_i) + W\left(1 - \sum_{i=1}^N \phi_i\right) \right], \tag{2}$$

which has N local minima at $(1, 0, \dots, 0), (0, 1, 0, \dots, 0), \dots, (0, \dots, 0, 1)$. The first integral in (1) accounts for the interfacial free energy between different species which is oscillation-inhibiting, therefore it favors large domains with minimal common area between species. The parameter γ_{ij} , assuming to be symmetric $\gamma_{ij} = \gamma_{ji}$, represents the strength of the long-range repulsive interaction between the i - and j -th species. The parameter ω_i , defined as

$$\omega_i = \frac{1}{|\Omega|} \int_{\Omega} f(\phi_i) dx, \quad i = 1, \dots, N$$

represents the volume constraint for each species ϕ_i . The second term in (1) is oscillation-forcing and therefore favors micro-domains of smaller size.

In this paper, we will mainly focus on two simple cases for the system (1), the binary system ($N = 1$) and the ternary system ($N = 2$). When $N = 1$, the system (1) reduces to a binary system, which is the so-called Ohta-Kawasaki (OK) model [26] for the di-block copolymer system:

$$E^{\text{OK}}[\phi] = \int_{\Omega} \left[\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{\epsilon} W(\phi) \right] dx + \frac{\gamma}{2} \int_{\Omega} \left| (-\Delta)^{-\frac{1}{2}} (f(\phi) - \omega) \right|^2 dx, \tag{3}$$

with a volume constraint:

$$\int_{\Omega} f(\phi) dx = \omega |\Omega|. \tag{4}$$

In order to handle the volume constraint (4), we introduce a penalty term to change (3) into an unconstrained free energy functional:

$$\begin{aligned}
E^{\text{pOK}}[\phi] &= \int_{\Omega} \left[\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{\epsilon} W(\phi) \right] dx + \frac{\gamma}{2} \int_{\Omega} \left| (-\Delta)^{-\frac{1}{2}} (f(\phi) - \omega) \right|^2 dx \\
&\quad + \frac{M}{2} \left(\int_{\Omega} f(\phi) dx - \omega |\Omega| \right)^2,
\end{aligned} \tag{5}$$

with $M \gg 1$ being the penalty constant for the volume constraint. Since we are interested in the pattern formation at equilibrium for the OK system, the L^2 gradient

flow dynamics for (5) is considered, leading us to the penalized Allen-Cahn-Ohta-Kawasaki (pACOK) equation for the time evolution of $\phi(x, t)$:

$$\begin{aligned} \frac{\partial \phi}{\partial t} = & -\frac{\delta E^{\text{pOK}}[\phi]}{\delta \phi} = \epsilon \Delta \phi - \frac{1}{\epsilon} W'(\phi) - \gamma (-\Delta)^{-1} (f(\phi) - \omega) f'(\phi) \\ & - M \left(\int_{\Omega} f(\phi) dx - \omega |\Omega| \right) f'(\phi), \end{aligned} \quad (6)$$

with a given initial condition $\phi(x, t = 0) = \phi_0(x)$, and periodic boundary condition over Ω . The pACOK dynamics (6) satisfies the energy dissipative law

$$\frac{d}{dt} E^{\text{pOK}}[\phi] = -\|\phi_t\|_{L^2}^2 \leq 0.$$

When $N = 2$, the system (1) reduces to the Ohta-Nakazawa (ON) model [26] for the tri-block copolymer system:

$$\begin{aligned} & E^{\text{ON}}[\phi_1, \phi_2] \\ &= \int_{\Omega} \frac{\epsilon}{2} (|\nabla \phi_1|^2 + |\nabla \phi_2|^2 + \nabla \phi_1 \cdot \nabla \phi_2) dx + \int_{\Omega} \frac{1}{\epsilon} W_2(\phi_1, \phi_2) dx \\ &+ \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} \int_{\Omega} \left[(-\Delta)^{-\frac{1}{2}} (f(\phi_i) - \omega_i) \times (-\Delta)^{-\frac{1}{2}} (f(\phi_j) - \omega_j) \right] dx, \end{aligned} \quad (7)$$

with $W_2 = \frac{1}{2} [W(\phi_1) + W(\phi_2) + W(1 - \phi_1 - \phi_2)]$ as given in (2). The associated volume constraints for ϕ_1 and ϕ_2 are:

$$\int_{\Omega} f(\phi_i) dx = \omega_i |\Omega|, \quad i = 1, 2. \quad (8)$$

Similarly as for the binary system, we introduce penalty terms to change (7) into an unconstrained free energy functional:

$$\begin{aligned} & E^{\text{pON}}[\phi_1, \phi_2] \\ &= \int_{\Omega} \frac{\epsilon}{2} (|\nabla \phi_1|^2 + |\nabla \phi_2|^2 + \nabla \phi_1 \cdot \nabla \phi_2) dx + \int_{\Omega} \frac{1}{\epsilon} W_2(\phi_1, \phi_2) dx \\ &+ \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} \int_{\Omega} \left[(-\Delta)^{-\frac{1}{2}} (f(\phi_i) - \omega_i) \times (-\Delta)^{-\frac{1}{2}} (f(\phi_j) - \omega_j) \right] dx \\ &+ \sum_{i=1}^2 \frac{M_i}{2} \left(\int_{\Omega} f(\phi_i) dx - \omega_i |\Omega| \right)^2, \end{aligned} \quad (9)$$

with two penalty constants $M_1, M_2 \gg 1$. Then the L^2 gradient flow dynamics for the penalized Allen-Cahn-Ohta-Nakazawa (pACON) equation (9) is:

$$\begin{aligned} \frac{\partial \phi_i}{\partial t} = & -\epsilon (-\Delta) \phi_i - \frac{\epsilon}{2} (-\Delta) \phi_j - \frac{1}{\epsilon} \frac{\partial W_2}{\partial \phi_i} \\ & - \gamma_{ii} (-\Delta)^{-1} [f(\phi_i) - \omega_i] f'(\phi_i) - \gamma_{ij} (-\Delta)^{-1} [f(\phi_j) - \omega_j] f'(\phi_i) \\ & - M_i \left(\int_{\Omega} f(\phi_i) dx - \omega_i |\Omega| \right) f'(\phi_i), \quad \text{for } i, j = 1, 2, \end{aligned} \quad (10)$$

with given initial data $\phi_i(x, t = 0) = \phi_{i,0}(x)$ and periodic boundary condition over Ω . The pACON dynamics (10) satisfies the energy dissipative law

$$\frac{d}{dt} E^{\text{pON}}[\phi_1, \phi_2] = -\|\phi_{1,t}\|_{L^2}^2 - \|\phi_{2,t}\|_{L^2}^2 \leq 0.$$

The main purpose of this paper is to study some second order stabilized semi-implicit schemes that inherit the energy dissipative law in the discrete level, which are called energy stable schemes. There have been extensive studies on the energy stable methods for various gradient flow dynamics such as the standard Allen-Cahn and Cahn-Hilliard equations [27], phase field crystal model [34, 19], modified phase field crystal model [31], and epitaxial thin film growth model [29, 6], etc. One example is the convex splitting method [12] in which the double well potential $W(\phi)$ is split into the sum of a convex function and a concave one, and the convex part is treated implicitly and the concave one is treated explicitly. However, a nonlinear system usually needs to be solved at each time step which induces high computational cost. Another widely adapted method is the stabilized semi-implicit method [36, 27] in which $W(\phi)$ is treated explicitly. A linear stabilizing term is added to maintain the energy stability. Recently IEQ and SAV methods [39, 30] have become popular in which all nonlinear terms are treated semi-implicitly, the energy stability is preserved and the resulting numerical schemes lead to a symmetric positive definite linear system to be solved at each time step.

Due to the nonlinear terms $f(\phi)$ and the nonlocal interactions, we will consider a linear splitting method for the OK/ON energy functional and the resulting stabilized linear semi-implicit scheme for the pACOK equation (6) and pACON equation (10) such that all nonlocal and nonlinear terms are treated explicitly. By doing so, we can solve the fully discrete system efficiently via Fourier spectral method. In this paper, we will firstly present our linear scheme and show the energy stability in semi-discretization level. Then we will discuss the energy stability for the full discretization with spectral discretization in space. Note that recently there have been several studies on the OK and ON models. For example, an implicit midpoint spectral approximation is studied in [3] for the equilibrium of OK model. The IEQ method is adapted in [8] to study the diblock copolymer model. Recently, the SAV method is also applied to the OK and ON models [40, 7]. However, the existing works mainly focus on the Cahn-Hilliard dynamics, namely, the H^{-1} gradient flow dynamics of the OK/ON energy with $f(\phi) = \phi$. Our work is advantageous of studying the force balance in the process of phase separation and emphasizing the force localization near the interface, and could have potential applications in other complex dynamics involving interfacial structures such as cell motility [5] and implicit solvation [41]. Besides, some other nonlocal extensions of the Allen-Cahn and Cahn-Hilliard equations and the related numerical methods have been studied [15, 16, 17, 22].

In this paper, we use artificial regularization terms to control the nonlocal terms in order to stabilize the proposed numerical scheme. In fact, there have been extensive works on the artificial regularization for the energy stable numerical schemes for various gradient flows, such as artificial regularization for the no-slope-selection epitaxial thin film model [25]. For the ternary gradient flow, there has been a recent work [9] on the energy stable numerical schemes for ternary Cahn-Hilliard system, in which both the energy stability analysis and optimal rate convergence estimate have been established.

1.1. Notations. Some conventional notations adopted throughout the paper are collected in this section. For the discussion of energy stability in the rest of the paper, we revise the $W(s)$ quadratically and $f(s)$ linearly when $|s| > M_{\text{cut}} > 0$ for some M_{cut} in order to have finite upper bounds for W'' and f'' . These modifications are necessary for the stabilized semi-implicit schemes for Ginzburg-Landau type

dynamics [27]. We will take the quadratic extension $\tilde{W}(\phi)$ of $W(\phi)$ as adapted in [27] and other related citations therein. For the linear extension of $f(\phi)$, we choose:

$$\tilde{f}(\phi) = \begin{cases} 0, & \phi < 0, \\ f(\phi) = 6\phi^5 - 15\phi^4 + 10\phi^3, & 0 \leq \phi \leq 1, \\ 1, & \phi > 1. \end{cases} \quad (11)$$

Such a linear extension will guarantee that $\tilde{f}(\phi)$ is Lipschitz continuous with bounded second derivative. We denote by $L_{W''}, L_{f''}$ the upper bounds for $|\tilde{W}''(s)|$ and $|\tilde{f}''(s)|$, respectively, and $L_{\tilde{f}}$ the Lipschitz constant for $\tilde{f}$. For brevity, we will still use $f(\phi), W(\phi)$ to represent $\tilde{f}(\phi), \tilde{W}(\phi)$, respectively

. Note that for the Allen-Cahn and Cahn-Hilliard dynamics without nonlocal term, the quadratic extension for $W(s)$ guarantees that the solutions always satisfy the maximum principle [4]. Even though it is unnecessary to do the quadratic extension for the solutions to satisfy the maximum principle for the Allen-Cahn dynamics, it can avoid some technical difficulties in the analysis and approximation. The main purpose of the linear extension of $f(s)$ here is to easily perform the stability analysis. Besides, if the initial ϕ_0 takes some value beyond $[0, 1]$, the Allen-Cahn dynamics will quickly change the value of $\phi(t)$ to stay within $[0, 1]$ so that the linear extension of $f(s)$ will not affect the volume constraint (4) in practice.

While we consider the penalized models in need of extensions of W and f , some recent works [11, 23] suggest maximum bound principle preserving schemes by which the phase field function ϕ can be bounded between 0 and 1 such that the extensions of W and f can be safely removed. A similar scheme is also considered in our earlier work [38], but using the penalty formulation. Another formulation using Lagrange multiplier approach [23] is also possible to handle the volume constraint, under the condition that the formulation itself possesses a variational structure.

We adopt the following notations from [37]. Let $\Omega = \prod_{i=1}^d [-X_i, X_i] \subset \mathbb{R}^d, d = 2, 3$ be a periodic domain. Denote the space consisting of periodic functions in $H^s(\Omega), s \geq 0$ as $H_{\text{per}}^s(\Omega)$. We define the subspaces

$$\dot{H}_{\text{per}}^s(\Omega) := \left\{ u \in H_{\text{per}}^s(\Omega) : \int_{\Omega} u(x) dx = 0 \right\} \quad (12)$$

consisting of all functions $u \in H_{\text{per}}^s(\Omega)$ with zero mean. We use $\|\cdot\|_{H^s}$ to represent the standard Sobolev norm. When $s = 0$, $H^s(\Omega) = L^2(\Omega)$ and we take $\langle \cdot, \cdot \rangle$ as the L^2 inner product and $\|\cdot\|_{H^s} = \|\cdot\|_{L^2}$.

We define the inverse Laplacian $(-\Delta)^{-1}: \dot{L}_{\text{per}}^2(\Omega) \rightarrow \dot{H}_{\text{per}}^1(\Omega)$ as

$$(-\Delta)^{-1}g = u \iff -\Delta u = g,$$

or in terms of Fourier series:

$$(-\Delta)^{-1}g = \sum_{k \in \mathbb{Z}^d \setminus \{0\}} |k|^{-2} \hat{g}(k) e^{ik \cdot \tilde{x}}, \quad (13)$$

where $\hat{g}(k) = \int_{\Omega} g(x) e^{-ik \cdot \tilde{x}} dx$ with $\tilde{x} = (\pi x_1/X_1, \dots, \pi x_d/X_d)$. Note that the definition (13) can be extended to any function $g \in L_{\text{per}}^2(\Omega)$ because of the removal of the zero-th mode. In other words, for any $g \in L_{\text{per}}^2(\Omega)$, $(-\Delta)^{-1}g$ can be defined as

$$(-\Delta)^{-1}g = (-\Delta)^{-1}(g - \hat{g}(0)).$$

We use $\|(-\Delta)^{-1}\|$ to denote the optimal constant such that $\|(-\Delta)^{-1}f\|_{L^\infty} \leq C\|f\|_{L^\infty}$. Namely, $\|(-\Delta)^{-1}\|$ is the norm of the operator $(-\Delta)^{-1}$ from $L^\infty(\mathbb{T}^d)$ to itself. Note that the constant C is bounded and depends on Ω which is a simple consequence of the elliptic regularity. One can also see Lemma 3.2 for the discrete counterpart. We will take $[n]$ to be the set of integers $\{1, 2, \dots, n\}$. Lastly, we denote $\tilde{\omega} = \max\{1 + \omega, 2 - \omega\}$.

The rest of the paper is organized as follows. In Section 2, we will develop the second order semi-discrete energy stable schemes, perform the energy stability analysis and conduct the corresponding error estimate analysis. In Section 3, we will present the spectral discretization in space, and show the energy stability for the fully-discrete scheme. In Section 4, we will give some numerical examples to illustrate the force localization, energy stability and the effect of the long-range repulsive force on the pattern formations.

2. Time-discrete energy stable schemes. In this section, we will propose some second order semi-discrete energy stable schemes for the pACOK equation (6) and pACON system (10), respectively. For each system, we will consider two stabilizers for the semi-discrete energy stability.

2.1. Second order time-discrete energy stable schemes for pACOK. Given a time interval $[0, T]$, we take the uniform time step size $\tau = \frac{T}{N}$, where $N > 0$ is an integer. Let $t_n = n\tau$ for $n = 0, 1, \dots, N$ and $\phi^n \approx \phi(x, t_n)$. We begin with energy stable time discretization for the pACOK system (6). The method we adopt here is a second order backward differentiation formula (BDF) scheme. For the energy stability at discrete level, two different stabilizers are introduced [27, 13]:

$$\phi^{n+1} - 2\phi^n + \phi^{n-1}, \quad (14)$$

$$\tau(\phi^{n+1} - \phi^n). \quad (15)$$

We will show that while the former stabilizer (14) restricts τ to be relatively small, the latter one (15) leads to unconditional energy stability.

Incorporating the stabilizer (14), a time-discrete semi-implicit BDF scheme for pACOK equation (6) reads: given initial data $\phi^{-1} = \phi^0 = \phi_0(x)$, we find ϕ^{n+1} for $n = 1, 2, \dots, N$, such that

$$\begin{aligned} & \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau} \\ &= \epsilon \Delta \phi^{n+1} - \frac{1}{\epsilon} [2W'(\phi^n) - W'(\phi^{n-1})] - \frac{\kappa}{\epsilon} (\phi^{n+1} - 2\phi^n + \phi^{n-1}) \\ & \quad - \gamma(-\Delta)^{-1} [2f(\phi^n) - f(\phi^{n-1}) - \omega] (2f'(\phi^n) - f'(\phi^{n-1})) \\ & \quad - \gamma\beta(-\Delta)^{-1} (\phi^{n+1} - 2\phi^n + \phi^{n-1}) \\ & \quad - M \left[\int_{\Omega} (2f(\phi^n) - f(\phi^{n-1})) dx - \omega|\Omega| \right] (2f'(\phi^n) - f'(\phi^{n-1})), \end{aligned} \quad (16)$$

where $\frac{\kappa}{\epsilon} (\phi^{n+1} - 2\phi^n + \phi^{n-1})$ is added to control the growth of W' and $\gamma\beta(-\Delta)^{-1} (\phi^{n+1} - 2\phi^n + \phi^{n-1})$ is introduced to dominate the behavior of $(-\Delta)^{-1}$. Here $\kappa \geq 0$ and $\beta \geq 0$ are stabilization constants.

If choosing the stabilizer (15), the semi-implicit BDF scheme for (6) becomes

$$\begin{aligned}
& \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau} \\
&= \epsilon \Delta \phi^{n+1} - \frac{1}{\epsilon} [2W'(\phi^n) - W'(\phi^{n-1})] - \frac{\kappa}{\epsilon} \tau (\phi^{n+1} - \phi^n) \\
&\quad - \gamma(-\Delta)^{-1} [2f(\phi^n) - f(\phi^{n-1}) - \omega] (2f'(\phi^n) - f'(\phi^{n-1})) \\
&\quad - \gamma\beta\tau(-\Delta)^{-1} (\phi^{n+1} - \phi^n) \\
&\quad - M \left[\int_{\Omega} (2f(\phi^n) - f(\phi^{n-1})) dx - \omega|\Omega| \right] (2f'(\phi^n) - f'(\phi^{n-1})).
\end{aligned} \tag{17}$$

The unique solvability of the schemes (16) and (17) is straightforward. For instance, for the scheme (17), it can be rewritten as:

$$\left(\frac{3}{2\tau} + \frac{\kappa}{\epsilon} \tau + \epsilon(-\Delta) + \gamma\beta\tau(-\Delta)^{-1} \right) \phi^{n+1} = \text{RHS},$$

in which the RHS only depends on ϕ^n and ϕ^{n-1} . Then the unique solvability of (17) can be guaranteed by realizing the positivity of the eigenvalues of the operator applying on ϕ^{n+1} .

In what follows, we show that the semi-implicit BDF schemes (16) and (17) inherit a modified energy stability at time-discrete level.

Theorem 2.1. *Let $\kappa, \beta \geq 0$ and*

$$C = \frac{L_{W''}}{2\epsilon} + \frac{1}{2}(L_{f'}^2 + L_{f''}\tilde{\omega})(\gamma\|(-\Delta)^{-1}\| + M|\Omega|).$$

Let $\{\phi^n\}_{n=1}^N$ be generated by the scheme (16). Then

$$\begin{aligned}
& E^{\text{pOK}}[\phi^{n+1}] + \left(\frac{1}{4\tau} + \frac{\kappa}{2\epsilon} + C \right) \|\phi^{n+1} - \phi^n\|_{L^2}^2 \\
& + \frac{\gamma\beta}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2 \\
& \leq E^{\text{pOK}}[\phi^n] + \left(\frac{1}{4\tau} + \frac{\kappa}{2\epsilon} + C \right) \|\phi^n - \phi^{n-1}\|_{L^2}^2 \\
& + \frac{\gamma\beta}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi^n - \phi^{n-1})\|_{L^2}^2,
\end{aligned} \tag{18}$$

provided that $\tau < \frac{1}{3C}$. If $\{\phi^n\}_{n=1}^N$ is generated by the scheme (17), then

$$\begin{aligned}
& E^{\text{pOK}}[\phi^{n+1}] + \left(\frac{1}{4\tau} + C \right) \|\phi^{n+1} - \phi^n\|_{L^2}^2 \\
& \leq E^{\text{pOK}}[\phi^n] + \left(\frac{1}{4\tau} + C \right) \|\phi^n - \phi^{n-1}\|_{L^2}^2,
\end{aligned} \tag{19}$$

provided that either

$$\kappa \geq 9C^2 \frac{\epsilon}{4}, \quad \beta \geq 0 \tag{20}$$

or

$$\kappa \geq \left(3C - \frac{\gamma L_{f'}^2}{2} \|(-\Delta)^{-1}\| \right)^2 \frac{\epsilon}{4}, \quad \beta \geq \frac{L_{f'}^2}{2\tau}. \tag{21}$$

Proof. We consider the scheme (16) first. Taking L^2 inner product on (16) with $\phi^{n+1} - \phi^n$, we have

$$\begin{aligned}
& \frac{1}{\tau} \|\phi^{n+1} - \phi^n\|_{L^2}^2 + \frac{1}{4\tau} (\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2) \\
& + \frac{1}{4\tau} \|\phi^{n+1} - 2\phi^n + \phi^{n-1}\|_{L^2}^2 \\
& = -\frac{\epsilon}{2} (\|\nabla \phi^{n+1}\|_{L^2}^2 - \|\nabla \phi^n\|_{L^2}^2) - \frac{\epsilon}{2} \|\nabla(\phi^{n+1} - \phi^n)\|_{L^2}^2 \\
& \quad - \underbrace{\frac{1}{\epsilon} \langle 2W'(\phi^n) - W'(\phi^{n-1}), \phi^{n+1} - \phi^n \rangle}_{\text{I}} \\
& \quad - \frac{\kappa}{2\epsilon} (\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2 + \|\phi^{n+1} - 2\phi^n + \phi^{n-1}\|_{L^2}^2) \quad (22) \\
& \quad - \underbrace{\gamma \langle (-\Delta)^{-1} [2f(\phi^n) - f(\phi^{n-1}) - \omega] (2f'(\phi^n) - f'(\phi^{n-1})), \phi^{n+1} - \phi^n \rangle}_{\text{II}} \\
& \quad - \frac{\gamma\beta}{2} (\|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(\phi^n - \phi^{n-1})\|_{L^2}^2) \\
& \quad - \frac{\gamma\beta}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - 2\phi^n + \phi^{n-1})\|_{L^2}^2 \\
& \quad - \underbrace{M \left[\int_{\Omega} (2f(\phi^n) - f(\phi^{n-1})) dx - \omega|\Omega| \right] \langle 2f'(\phi^n) - f'(\phi^{n-1}), \phi^{n+1} - \phi^n \rangle}_{\text{III}}.
\end{aligned}$$

Since $|W''| \leq L_{W''}$, $|f'| \leq L_{f'}$, $|f''| \leq L_{f''}$, and $\int_{\Omega} |f(\phi) - \omega| dx \leq \tilde{\omega}|\Omega|$, we further have

$$\begin{aligned}
\text{I} & \leq -\frac{1}{\epsilon} \langle W(\phi^{n+1}) - W(\phi^n), 1 \rangle + \frac{L_{W''}}{2\epsilon} (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2); \\
\text{II} & = -\frac{\gamma}{2} (\|(-\Delta)^{-\frac{1}{2}}(f(\phi^{n+1}) - \omega)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(f(\phi^n) - \omega)\|_{L^2}^2) \\
& \quad + \frac{\gamma}{2} \|(-\Delta)^{-\frac{1}{2}}(f(\phi^{n+1}) - f(\phi^n))\|_{L^2}^2 \\
& \quad - \gamma \langle (-\Delta)^{-1}(f(\phi^n) - f(\phi^{n-1})), f(\phi^{n+1}) - f(\phi^n) \rangle \\
& \quad + \frac{\gamma f''(\xi^n)}{2} \langle (-\Delta)^{-1} (2f(\phi^n) - f(\phi^{n-1}) - \omega), (\phi^{n+1} - \phi^n)^2 \rangle \\
& \quad - \gamma f''(\xi^{n-1}) \langle (-\Delta)^{-1} (2f(\phi^n) - f(\phi^{n-1}) - \omega), (\phi^n - \phi^{n-1})(\phi^{n+1} - \phi^n) \rangle \\
& \leq -\frac{\gamma}{2} (\|(-\Delta)^{-\frac{1}{2}}(f(\phi^{n+1}) - \omega)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(f(\phi^n) - \omega)\|_{L^2}^2) \\
& \quad + \frac{\gamma L_{f'}^2}{2} \|(-\Delta)^{-1} (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2) \\
& \quad + \frac{\gamma L_{f''}}{2} \tilde{\omega} \|(-\Delta)^{-1} (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2); \\
\text{III} & = -\frac{M}{2} \left(\left| \int_{\Omega} [f(\phi^{n+1}) - \omega] dx \right|^2 - \left| \int_{\Omega} [f(\phi^n) - \omega] dx \right|^2 \right) \\
& \quad + \frac{M}{2} \left| \int_{\Omega} [f(\phi^{n+1}) - f(\phi^n)] dx \right|^2
\end{aligned}$$

$$\begin{aligned}
& -M \int_{\Omega} [f(\phi^n) - f(\phi^{n-1})] dx \int_{\Omega} [f(\phi^{n+1}) - f(\phi^n)] dx \\
& + M \frac{f''(\xi^n)}{2} \int_{\Omega} (2f(\phi^n) - f(\phi^{n-1}) - \omega) dx \cdot \|\phi^{n+1} - \phi^n\|_{L^2}^2 \\
& - M f''(\xi^{n-1}) \int_{\Omega} (2f(\phi^n) - f(\phi^{n-1}) - \omega) dx \cdot \langle \phi^n - \phi^{n-1}, \phi^{n+1} - \phi^n \rangle \\
& \leq -\frac{M}{2} \left(\left| \int_{\Omega} [f(\phi^{n+1}) - \omega] dx \right|^2 - \left| \int_{\Omega} [f(\phi^n) - \omega] dx \right|^2 \right) \\
& + \frac{ML_{f'}^2}{2} |\Omega| (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2) \\
& + \frac{ML_{f''}}{2} \tilde{\omega} |\Omega| (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2).
\end{aligned}$$

Inserting the estimates of I, II and III into (22) and dropping some unnecessary terms, we get

$$\begin{aligned}
& E^{\text{pOK}}[\phi^{n+1}] - E^{\text{pOK}}[\phi^n] + \frac{1}{\tau} \|\phi^{n+1} - \phi^n\|_{L^2}^2 \\
& + \left(\frac{1}{4\tau} + \frac{\kappa}{2\epsilon} \right) (\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2) \\
& + \frac{\gamma\beta}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(\phi^n - \phi^{n-1})\|_{L^2}^2 \right) \\
& \leq C(\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2),
\end{aligned}$$

with $C = \frac{L_{W''}}{2\epsilon} + \frac{1}{2}(L_{f'}^2 + L_{f''}\tilde{\omega})(\gamma\|(-\Delta)^{-1}\| + M|\Omega|)$.

Adding $C(\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2)$ on both sides, it yields

$$\begin{aligned}
& E^{\text{pOK}}[\phi^{n+1}] - E^{\text{pOK}}[\phi^n] + \left(\frac{1}{4\tau} + \frac{\kappa}{2\epsilon} + C \right) (\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2) \\
& + \frac{\gamma\beta}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(\phi^n - \phi^{n-1})\|_{L^2}^2 \right) \\
& \leq \left(3C - \frac{1}{\tau} \right) \|\phi^{n+1} - \phi^n\|_{L^2}^2 \leq 0,
\end{aligned}$$

provided $\tau \leq \frac{1}{3C}$, which leads to the modified energy stability (18).

For the scheme (17), the proof is similar to the one for (16). We only point out key steps different from the proof for (18). Taking L^2 inner product on (17) with $\phi^{n+1} - \phi^n$, all the terms are identical with those obtained from (22), except for the two stabilization terms on the right hand side which become:

$$-\frac{\kappa}{\epsilon} \tau \|\phi^{n+1} - \phi^n\|_{L^2}^2, \quad -\gamma\beta\tau \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2.$$

The estimates of I and III remain the same. There are two possible estimates for II, one is the same as in the last proof:

$$\begin{aligned}
\text{II} & \leq -\frac{\gamma}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(f(\phi^{n+1}) - \omega)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(f(\phi^n) - \omega)\|_{L^2}^2 \right) \\
& + \frac{\gamma}{2} (L_{f'}^2 + L_{f''}) \|(-\Delta)^{-1}\| (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2).
\end{aligned} \tag{23}$$

The other is to use the inequality

$$\|(-\Delta)^{-\frac{1}{2}}(f(\phi^{n+1}) - f(\phi^n))\|_{L^2}^2 \leq L_{f'}^2 \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2$$

to reach:

$$\begin{aligned} \Pi \leq & -\frac{\gamma}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(f(\phi^{n+1}) - \omega)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(f(\phi^n) - \omega)\|_{L^2}^2 \right) \\ & + \frac{\gamma}{2} (L_{f'}^2 + L_{f''}) \|(-\Delta)^{-1}\| (\|\phi^n - \phi^{n-1}\|_{L^2}^2 + 2\|\phi^{n+1} - \phi^n\|_{L^2}^2) \\ & - \frac{\gamma L_{f'}^2}{2} \|(-\Delta)^{-1}\| \|\phi^{n+1} - \phi^n\|_{L^2}^2 + \frac{\gamma L_{f'}^2}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2. \end{aligned} \quad (24)$$

After inserting the estimates for I-III, dropping unnecessary terms, and adding $C(\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2)$ on two sides, we get the inequality:

$$\begin{aligned} & E^{\text{pOK}}[\phi^{n+1}] - E^{\text{pOK}}[\phi^n] + \left(\frac{1}{4\tau} + C \right) (\|\phi^{n+1} - \phi^n\|_{L^2}^2 - \|\phi^n - \phi^{n-1}\|_{L^2}^2) \\ \leq & \begin{cases} (3C - \frac{1}{\tau} - \frac{\kappa}{\epsilon}\tau) \|\phi^{n+1} - \phi^n\|_{L^2}^2 - \gamma\beta\tau \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2, & \text{if using (23),} \\ (3C - \frac{\gamma L_{f'}^2}{2} \|(-\Delta)^{-1}\| - \frac{1}{\tau} - \frac{\kappa}{\epsilon}\tau) \|\phi^{n+1} - \phi^n\|_{L^2}^2 \\ \quad + (\frac{\gamma L_{f'}^2}{2} - \gamma\beta\tau) \|(-\Delta)^{-\frac{1}{2}}(\phi^{n+1} - \phi^n)\|_{L^2}^2, & \text{if using (24).} \end{cases} \end{aligned}$$

If the condition (20) or (21) holds, the right hand side of the above inequality becomes nonpositive, leading to the desired energy stability (19). The proof is completed. $\square$

Remark 1. In theorem 2.2, the stabilizer (14) leads to a restriction on time step τ , but no condition on κ and β . Therefore one can take $\kappa = \beta = 0$ to recover the usual second order semi-implicit scheme. In practice, however, numerical examples show that the choice of positive stabilization constants $\kappa, \beta > 0$ allows much larger step size than that for the case of $\kappa = \beta = 0$.

For the stabilizer (15), one can have two conditions for the energy stability. For the condition (20), κ needs to be sufficiently large, but β is only required to be nonnegative. In this case, it is unconditionally stable as there is no restriction on τ . For the condition (21), κ still has to be sufficiently large (but not as large as κ in (20)), and β needs to be reversely proportional to τ . It is of practical interest to consider this case as τ is expected to be relatively large to expedite the numerical simulation so that β need not be too large. However, it is unwise to choose condition (21) for sufficiently small τ .

One potential issue for the stabilizer (15) is that taking sufficiently large κ (or both κ and β) might cause big error for the numerical accuracy, which can be mitigated by choosing sufficiently small τ (see Table 1 for the test of rate of convergence in which although κ is large, the error is still well controlled due to the smallness of τ). In practice, on the other hand, numerical evidences indicate that one can take a mildly large κ (or both κ and β) and still maintain the energy stability.

2.2. Second order time-discrete energy stable schemes for pACON. For the ternary system, we consider the pACON system over time interval $[0, T]$, and take uniform time step size $\tau = \frac{T}{N}$ with $t_n = n\tau$ for $n = 0, 1, \dots, N$. Let $\phi_i^n \approx \phi_i(x, t_n)$ for $i = 1, 2$. We will still adopt the second order BDF scheme for the time discretization, and consider two stabilizers similar as the ones for pACOK dynamics:

$$\phi_i^{n+1} - 2\phi_i^n + \phi_i^{n-1}, \quad i = 1, 2, \quad (25)$$

$$\tau(\phi_i^{n+1} - \phi_i^n), \quad i = 1, 2. \quad (26)$$

Using the stabilizer (25), a time-discrete semi-implicit BDF scheme for pACON system (10) becomes: given initial data $\phi_i^{-1} = \phi_i^0 = \phi_{i,0}, i = 1, 2$, we find ϕ_i^{n+1} for $n = 1, 2, \dots, N$ such that

$$\begin{aligned}
& \frac{3\phi_i^{n+1} - 4\phi_i^n + \phi_i^{n-1}}{2\tau} \\
&= \epsilon \Delta \phi_i^{n+1} + \frac{\epsilon}{2} \Delta (2\phi_j^{n+\text{mod}(i+1,2)} - \phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) \\
&\quad - \frac{1}{\epsilon} \left[2 \frac{\partial W_2}{\partial \phi_i} (\phi_1^{n+\text{mod}(i+1,2)}, \phi_2^n) - \frac{\partial W_2}{\partial \phi_i} (\phi_1^{n-1+2 \cdot \text{mod}(i+1,2)}, \phi_2^{n-1}) \right] \\
&\quad - \frac{\kappa_i}{\epsilon} (\phi_i^{n+1} - 2\phi_i^n + \phi_i^{n-1}) - \gamma_{ii} \beta_i (-\Delta)^{-1} (\phi_i^{n+1} - 2\phi_i^n + \phi_i^{n-1}) \\
&\quad - \gamma_{ii} (-\Delta)^{-1} [2f(\phi_i^n) - f(\phi_i^{n-1}) - \omega_i] [2f'(\phi_i^n) - f'(\phi_i^{n-1})] \\
&\quad - \gamma_{ij} (-\Delta)^{-1} [2f(\phi_j^{n+\text{mod}(i+1,2)}) - f(\phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) - \omega_j] \\
&\quad \quad \times [2f'(\phi_i^n) - f'(\phi_i^{n-1})] \\
&\quad - M_i \left\{ \int_{\Omega} [2f(\phi_i^n) - f(\phi_i^{n-1})] dx - \omega_i |\Omega| \right\} [2f'(\phi_i^n) - f'(\phi_i^{n-1})], \tag{27}
\end{aligned}$$

for $i = 1, 2$ and $j \neq i$, where $\kappa_1, \kappa_2, \beta_1, \beta_2 \geq 0$ are stabilization constants.

On the other hand, choosing the stabilizer (26) leads to the semi-implicit BDF scheme for (10) as follows:

$$\begin{aligned}
& \frac{3\phi_i^{n+1} - 4\phi_i^n + \phi_i^{n-1}}{2\tau} \\
&= \epsilon \Delta \phi_i^{n+1} + \frac{\epsilon}{2} \Delta (2\phi_j^{n+\text{mod}(i+1,2)} - \phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) \\
&\quad - \frac{1}{\epsilon} \left[2 \frac{\partial W_2}{\partial \phi_i} (\phi_1^{n+\text{mod}(i+1,2)}, \phi_2^n) - \frac{\partial W_2}{\partial \phi_i} (\phi_1^{n-1+2 \cdot \text{mod}(i+1,2)}, \phi_2^{n-1}) \right] \\
&\quad - \frac{\kappa_i}{\epsilon} \tau (\phi_i^{n+1} - \phi_i^n) - \gamma_{ii} \beta_i \tau (-\Delta)^{-1} (\phi_i^{n+1} - \phi_i^n) \\
&\quad - \gamma_{ii} (-\Delta)^{-1} [2f(\phi_i^n) - f(\phi_i^{n-1}) - \omega_i] [2f'(\phi_i^n) - f'(\phi_i^{n-1})] \\
&\quad - \gamma_{ij} (-\Delta)^{-1} [2f(\phi_j^{n+\text{mod}(i+1,2)}) - f(\phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) - \omega_j] \\
&\quad \quad \times [2f'(\phi_i^n) - f'(\phi_i^{n-1})] \\
&\quad - M_i \left\{ \int_{\Omega} [2f(\phi_i^n) - f(\phi_i^{n-1})] dx - \omega_i |\Omega| \right\} [2f'(\phi_i^n) - f'(\phi_i^{n-1})], \tag{28}
\end{aligned}$$

for $i = 1, 2$ and $j \neq i$.

For the BDF schemes (27) and (28), we can show that they inherit the energy stability as summarized in the following theorem.

Theorem 2.2. *Let $\kappa_i, \beta_i \geq 0$, and*

$$C_i = \frac{L_{W''}}{2\epsilon} + \frac{1}{2} (L_{f'}^2 + L_{f''} \tilde{\omega}) ((\gamma_{i1} + \gamma_{i2}) \|(-\Delta_h)^{-1}\| + M_i |\Omega|), \quad i = 1, 2.$$

If $\{(\phi_1^n, \phi_2^n)\}_{n=1}^N$ is generated by the scheme (27), then

$$\begin{aligned} & E^{\text{PON}}[\phi_1^{n+1}, \phi_2^{n+1}] + \sum_{i=1}^2 \left[\left(\frac{1}{4\tau} + \frac{\kappa_i}{2\epsilon} + C_i \right) \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 \right. \\ & \quad \left. + \frac{\gamma_{ii}\beta_i}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi_i^{n+1} - \phi_i^n)\|_{L^2}^2 \right] \\ & \leq E^{\text{PON}}[\phi_1^n, \phi_2^n] + \sum_{i=1}^2 \left[\left(\frac{1}{4\tau} + \frac{\kappa_i}{2\epsilon} + C_i \right) \|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 \right. \\ & \quad \left. + \frac{\gamma_{ii}\beta_i}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi_i^n - \phi_i^{n-1})\|_{L^2}^2 \right], \end{aligned} \quad (29)$$

provided that $\tau < \min\{\frac{1}{3C_1}, \frac{1}{3C_2}\}$; if $\{(\phi_1^n, \phi_2^n)\}_{n=1}^N$ is generated by the scheme (28), then

$$\begin{aligned} & E^{\text{PON}}[\phi_1^{n+1}, \phi_2^{n+1}] + \sum_{i=1}^2 \left(\frac{1}{4\tau} + C_i \right) \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 \\ & \leq E^{\text{PON}}[\phi_1^n, \phi_2^n] + \sum_{i=1}^2 \left(\frac{1}{4\tau} + C_i \right) \|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2, \end{aligned} \quad (30)$$

provided that either

$$\kappa_i \geq 9C_i^2 \frac{\epsilon}{4}, \quad \beta_i \geq 0, \quad i = 1, 2, \quad (31)$$

or

$$\kappa_i \geq \left(3C_i - \frac{\gamma_{ii}L_{f'}^2}{2} \|(-\Delta)^{-1}\| \right)^2 \frac{\epsilon}{4}, \quad \beta_i \geq \frac{L_{f'}^2}{2\tau}, \quad i = 1, 2. \quad (32)$$

Proof. The proof is similar to the one in the binary case (Theorem 2.2), except we need to deal with (27) for $i = 1, 2$ separately and then add them up. To show how the coupling maintains the energy stability, we still show the proof in detail.

We begin by taking the L^2 inner product on (27) with $\phi_i^{n+1} - \phi_i^n$ for $i = 1, 2$. Then the two equations become

$$\begin{aligned} & \frac{1}{\tau} \|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2 + \frac{1}{4\tau} (\|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2 - \|\phi_1^n - \phi_1^{n-1}\|_{L^2}^2) \\ & + \frac{1}{4\tau} \|\phi_1^{n+1} - 2\phi_1^n + \phi_1^{n-1}\|_{L^2}^2 \\ & = -\frac{\epsilon}{2} (\|\nabla \phi_1^{n+1}\|_{L^2}^2 - \|\nabla \phi_1^n\|_{L^2}^2) + \nabla(\phi_1^{n+1} - \phi_1^n) \cdot \nabla(\phi_1^{n+1} - \phi_1^n) \\ & - \frac{\epsilon}{2} \langle \nabla \phi_2^n + \nabla(\phi_2^n - \phi_2^{n-1}), \nabla(\phi_1^{n+1} - \phi_1^n) \rangle \\ & - \frac{1}{\epsilon} \underbrace{\left\langle 2 \frac{\partial W_2}{\partial \phi_1}(\phi_1^n, \phi_2^n) - \frac{\partial W_2}{\partial \phi_1}(\phi_1^{n-1}, \phi_2^{n-1}), \phi_1^{n+1} - \phi_1^n \right\rangle}_{\mathbf{II}} \\ & - \frac{\kappa_1}{2\epsilon} (\|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2 - \|\phi_1^n - \phi_1^{n-1}\|_{L^2}^2 + \|\phi_1^{n+1} - 2\phi_1^n + \phi_1^{n-1}\|_{L^2}^2) \\ & - \frac{\gamma_{11}\beta_1}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(\phi_1^{n+1} - \phi_1^n)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(\phi_1^n - \phi_1^{n-1})\|_{L^2}^2 \right) \end{aligned} \quad (33)$$

$$\begin{aligned}
& -\frac{\gamma_{11}\beta_1}{2}\|(-\Delta)^{-\frac{1}{2}}(\phi_1^{n+1}-2\phi_1^n+\phi_1^{n-1})\|_{L^2}^2 \\
& \underbrace{-\gamma_{11}\langle(-\Delta)^{-1}[2f(\phi_1^n)-f(\phi_1^{n-1})-\omega_1][2f'(\phi_1^n)-f'(\phi_1^{n-1})],\phi_1^{n+1}-\phi_1^n\rangle}_{\text{II1}} \\
& \underbrace{-\gamma_{12}\langle(-\Delta)^{-1}[2f(\phi_2^n)-f(\phi_2^{n-1})-\omega_2][2f'(\phi_1^n)-f'(\phi_1^{n-1})],\phi_1^{n+1}-\phi_1^n\rangle}_{\text{III1}} \\
& \underbrace{-M_1\left\{\int_{\Omega}[2f(\phi_1^n)-f(\phi_1^{n-1})]dx-\omega_1|\Omega|\right\}\langle 2f'(\phi_1^n)-f'(\phi_1^{n-1}),\phi_1^{n+1}-\phi_1^n\rangle}_{\text{IV1}}; \\
& \frac{1}{\tau}\|\phi_2^{n+1}-\phi_2^n\|_{L^2}^2+\frac{1}{4\tau}(\|\phi_2^{n+1}-\phi_2^n\|_{L^2}^2-\|\phi_2^n-\phi_2^{n-1}\|_{L^2}^2) \\
& +\frac{1}{4\tau}\|\phi_2^{n+1}-2\phi_2^n+\phi_2^{n-1}\|_{L^2}^2 \\
& =-\frac{\epsilon}{2}(\|\nabla\phi_2^{n+1}\|_{L^2}^2-\|\nabla\phi_2^n\|_{L^2}^2+\|\nabla(\phi_2^{n+1}-\phi_2^n)\|_{L^2}^2) \\
& -\frac{\epsilon}{2}\langle\nabla\phi_1^{n+1},\nabla(\phi_2^{n+1}-\phi_2^n)\rangle \\
& \underbrace{-\frac{1}{\epsilon}\left\langle 2\frac{\partial W_2}{\partial\phi_2}(\phi_1^{n+1},\phi_2^n)-\frac{\partial W_2}{\partial\phi_2}(\phi_1^{n+1},\phi_2^{n-1}),\phi_2^{n+1}-\phi_2^n\right\rangle}_{\text{I2}} \\
& -\frac{\kappa_2}{2\epsilon}(\|\phi_2^{n+1}-\phi_2^n\|_{L^2}^2-\|\phi_2^n-\phi_2^{n-1}\|_{L^2}^2+\|\phi_2^{n+1}-2\phi_2^n+\phi_2^{n-1}\|_{L^2}^2) \tag{34} \\
& -\frac{\gamma_{22}\beta_2}{2}\left(\|(-\Delta)^{-\frac{1}{2}}(\phi_2^{n+1}-\phi_2^n)\|_{L^2}^2-\|(-\Delta)^{-\frac{1}{2}}(\phi_2^n-\phi_2^{n-1})\|_{L^2}^2\right) \\
& -\frac{\gamma_{22}\beta_2}{2}\|(-\Delta)^{-\frac{1}{2}}(\phi_2^{n+1}-2\phi_2^n+\phi_2^{n-1})\|_{L^2}^2 \\
& \underbrace{-\gamma_{22}\langle(-\Delta)^{-1}[2f(\phi_2^n)-f(\phi_2^{n-1})-\omega_2][2f'(\phi_2^n)-f'(\phi_2^{n-1})],\phi_2^{n+1}-\phi_2^n\rangle}_{\text{II2}} \\
& \underbrace{-\gamma_{21}\langle(-\Delta)^{-1}[f(\phi_1^{n+1})-\omega_1][2f'(\phi_2^n)-f'(\phi_2^{n-1})],\phi_2^{n+1}-\phi_2^n\rangle}_{\text{III2}} \\
& \underbrace{-M_2\left\{\int_{\Omega}[2f(\phi_2^n)-f(\phi_2^{n-1})]dx-\omega_2|\Omega|\right\}\langle 2f'(\phi_2^n)-f'(\phi_2^{n-1}),\phi_2^{n+1}-\phi_2^n\rangle}_{\text{IV2}}.
\end{aligned}$$

Now we add the above two equations term by term. Note that I1+I2 and III1+III2 are the coupling terms between ϕ_1 and ϕ_2 , and the detailed estimates are shown below; while II1+II2, IV1+IV2 are decoupled terms, we can directly follow the estimates of II and III in the proof of theorem 2.1. All the estimates are given as:

I1 + I2

$$\begin{aligned}
& =-\frac{1}{2\epsilon}\langle W(\phi_1^{n+1})-W(\phi_1^n),1\rangle-\frac{1}{2\epsilon}\langle W(\phi_2^{n+1})-W(\phi_2^n),1\rangle \\
& -\frac{1}{2\epsilon}\langle W(1-\phi_1^{n+1}-\phi_2^n)-W(1-\phi_1^n-\phi_2^n),1\rangle \\
& -\frac{1}{2\epsilon}\langle W(1-\phi_1^{n+1}-\phi_2^{n+1})-W(1-\phi_1^{n+1}-\phi_2^n),1\rangle
\end{aligned}$$

$$\begin{aligned}
& + \frac{W''(\xi_1^n) + W''(\eta_1^n)}{4\epsilon} \|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2 + \frac{W''(\xi_2^n) + W''(\eta_2^n)}{4\epsilon} \|\phi_2^{n+1} - \phi_2^n\|_{L^2}^2 \\
& - \frac{W''(\xi_1^{n-1}) + W''(\eta_1^{n-1})}{2\epsilon} \langle \phi_1^n - \phi_1^{n-1}, \phi_1^{n+1} - \phi_1^n \rangle \\
& - \frac{W''(\xi_2^{n-1}) + W''(\eta_2^{n-1})}{2\epsilon} \langle \phi_2^n - \phi_2^{n-1}, \phi_2^{n+1} - \phi_2^n \rangle \\
\leq & - \frac{1}{\epsilon} \langle W_2(\phi_1^{n+1} - \phi_2^{n+1}) - W_2(\phi_1^n - \phi_2^n), 1 \rangle \\
& + \frac{L_{W''}}{2\epsilon} \sum_{i=1}^2 (\|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 + 2\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2);
\end{aligned}$$

III1 + III2

$$\begin{aligned}
\leq & - \sum_{i=1}^2 \frac{\gamma_{ii}}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(f(\phi_i^{n+1}) - \omega_i)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(f(\phi_i^n) - \omega_i)\|_{L^2}^2 \right) \quad (35) \\
& + \sum_{i=1}^2 \frac{\gamma_{ii}}{2} (L_{f'}^2 + L_{f''}\tilde{\omega}) \|(-\Delta)^{-1}\| (\|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 + 2\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2);
\end{aligned}$$

III1 + III2

$$\begin{aligned}
= & - \gamma_{12} \langle (-\Delta)^{-1}(f(\phi_2^n)), f(\phi_1^{n+1}) - f(\phi_1^n) \rangle \\
& - \gamma_{21} \langle (-\Delta)^{-1}(f(\phi_1^{n+1})), f(\phi_2^{n+1}) - f(\phi_2^n) \rangle \\
& - \gamma_{12} \langle (-\Delta)^{-1}(f(\phi_2^n) - f(\phi_2^{n-1})), f(\phi_1^{n+1}) - f(\phi_1^n) \rangle \\
& + \frac{\gamma_{12}f''(\xi_1^n)}{2} \langle (-\Delta)^{-1}(2f(\phi_2^n) - f(\phi_2^{n-1}) - \omega_2), (\phi_1^{n+1} - \phi_1^n)^2 \rangle \\
& + \frac{\gamma_{21}f''(\xi_2^n)}{2} \langle (-\Delta)^{-1}(2f(\phi_1^n) - f(\phi_1^{n-1}) - \omega_1), (\phi_2^{n+1} - \phi_2^n)^2 \rangle \\
& - \gamma_{12}f''(\xi_1^{n-1}) \langle (-\Delta)^{-1}(2f(\phi_2^n) - f(\phi_2^{n-1}) - \omega_2), (\phi_1^n - \phi_1^{n-1})(\phi_1^{n+1} - \phi_1^n) \rangle \\
& - \gamma_{21}f''(\xi_2^{n-1}) \langle (-\Delta)^{-1}(2f(\phi_1^n) - f(\phi_1^{n-1}) - \omega_1), (\phi_2^n - \phi_2^{n-1})(\phi_2^{n+1} - \phi_2^n) \rangle \\
\leq & - \gamma_{12} \langle (-\Delta)^{-1}(f(\phi_1^{n+1})), f(\phi_2^{n+1}) \rangle + \gamma_{21} \langle (-\Delta)^{-1}(f(\phi_1^n)), f(\phi_2^n) \rangle \\
& + \frac{\gamma_{12}}{2} L_{f''}\tilde{\omega} \|(-\Delta)^{-1}\| (\|\phi_1^n - \phi_1^{n-1}\|_{L^2}^2 + 2\|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2) \\
& + \frac{\gamma_{12}}{2} L_{f'}^2 \|(-\Delta)^{-1}\| (\|\phi_2^n - \phi_2^{n-1}\|_{L^2}^2 + \|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2) \\
& + \frac{\gamma_{21}}{2} L_{f''}(\tilde{\omega} - 1) \|(-\Delta)^{-1}\| (\|\phi_2^n - \phi_2^{n-1}\|_{L^2}^2 + 2\|\phi_2^{n+1} - \phi_2^n\|_{L^2}^2);
\end{aligned}$$

IV1 + IV2

$$\begin{aligned}
\leq & - \sum_{i=1}^2 \frac{M_i}{2} \left(\left| \int_{\Omega} [f(\phi_i^{n+1}) - \omega_i] dx \right|^2 - \left| \int_{\Omega} [f(\phi_i^n) - \omega_i] dx \right|^2 \right) \\
& + \sum_{i=1}^2 \frac{M_i}{2} (L_{f'}^2 + L_{f''}\tilde{\omega}) |\Omega| (\|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 + 2\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2).
\end{aligned}$$

Using the above estimates and dropping unnecessary terms, we find that

$$\begin{aligned}
& E^{\text{PON}}[\phi_1^{n+1}, \phi_2^{n+1}] - E^{\text{PON}}[\phi_1^n, \phi_2^n] \\
& + \sum_{i=1}^2 \left(\frac{1}{4\tau} + \frac{\kappa_i}{2\epsilon} \right) (\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 - \|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2) \\
& + \sum_{i=1}^2 \frac{\gamma_{ii}\beta_i}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(\phi_i^{n+1} - \phi_i^n)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(\phi_i^n - \phi_i^{n-1})\|_{L^2}^2 \right) \\
& \leq \sum_{\substack{i=1 \\ j \neq i}}^2 \left[\frac{L_{W''}}{2\epsilon} + \frac{1}{2}(L_{f'}^2 + L_{f''}\tilde{\omega})(\gamma_{ii}\|(-\Delta)^{-1}\|) + M_i|\Omega| \right] \\
& \quad + \frac{\gamma_{ij}}{2} L_{f''} (\tilde{\omega} - \text{mod}(i+1, 2)) \|(-\Delta)^{-1}\| \\
& \quad \times (\|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 + 2\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2) \\
& \quad + \frac{1}{2} L_{f'}^2 \|(-\Delta)^{-1}\| (\gamma_{12}\|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2 + \gamma_{21}\|\phi_2^n - \phi_2^{n-1}\|_{L^2}^2) \\
& \quad - \frac{1}{\tau} \|\phi_1^{n+1} - \phi_1^n\|_{L^2}^2 - \frac{1}{\tau} \|\phi_2^{n+1} - \phi_2^n\|_{L^2}^2 \\
& \leq \sum_{i=1}^2 \left(C_i (\|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 + 2\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2) - \frac{1}{\tau} \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 \right)
\end{aligned}$$

where

$$C_i = \frac{L_{W''}}{2\epsilon} + \frac{1}{2}(L_{f'}^2 + L_{f''}\tilde{\omega}) ((\gamma_{i1} + \gamma_{i2})\|(-\Delta)^{-1}\|) + M_i|\Omega|, \quad i = 1, 2.$$

Adding $\sum_{i=1}^2 C_i (\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 - \|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2)$ on both sides of the above inequality, the resulting right hand side becomes nonpositive provided

$$\tau \leq \min \{ (3C_1)^{-1}, (3C_2)^{-1} \}.$$

Hence, we obtain the modified energy stability (18).

The proof for the energy stability (19) is similar, except for the terms involving stabilization constants κ_i , and β_i . We only point out the key difference. After taking L^2 inner product on (28) with $\phi_i^{n+1} - \phi_i^n$ for $i = 1, 2$, respectively, we obtain the two resulting equations similar to those in the last proof, except that the stabilization terms become:

$$-\frac{\kappa_i}{\epsilon} \tau \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2, \quad -\gamma_{ii}\beta_i \tau \|(-\Delta)^{-\frac{1}{2}}(\phi_{ii}^{n+1} - \phi_{ii}^n)\|_{L^2}^2, \quad i = 1, 2.$$

The estimates of I1+I2, III1+ III2, IV1+IV2 are identical to those for the proof of (18). To estimate II1+II2, we can either follow the inequality (35) exactly, or we

can perform:

$$\begin{aligned}
& \text{II1} + \text{II2} \\
& \leq - \sum_{i=1}^2 \frac{\gamma_{ii}}{2} \left(\|(-\Delta)^{-\frac{1}{2}}(f(\phi_i^{n+1}) - \omega_i)\|_{L^2}^2 - \|(-\Delta)^{-\frac{1}{2}}(f(\phi_i^n) - \omega_i)\|_{L^2}^2 \right) \\
& \quad + \sum_{i=1}^2 \frac{\gamma_{ii}}{2} (L_{f'}^2 + L_{f''}\tilde{\omega}) \|(-\Delta)^{-1}\| (\|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2 + 2\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2) \\
& \quad + \sum_{i=1}^2 \left(-\frac{\gamma_{ii}L_{f'}^2}{2} \|(-\Delta)^{-1}\| \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 \right) \\
& \quad + \sum_{i=1}^2 \frac{\gamma_{ii}L_{f'}^2}{2} \|(-\Delta)^{-\frac{1}{2}}(\phi_i^{n+1} - \phi_i^n)\|_{L^2}^2.
\end{aligned} \tag{36}$$

After summing all the estimates for I1+I2, II1+II2, III1+III2 and IV1+IV2, and adding

$$\sum_{i=1}^2 C_i (\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 - \|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2)$$

on both sides of resulting inequality, we have

$$\begin{aligned}
& E^{\text{pON}}[\phi_1^{n+1}, \phi_2^{n+1}] - E^{\text{pON}}[\phi_1^n, \phi_2^n] \\
& \quad + \sum_{i=1}^2 \left(\frac{1}{4\tau} + C_i \right) (\|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 - \|\phi_i^n - \phi_i^{n-1}\|_{L^2}^2) \\
& \leq \begin{cases} \sum_{i=1}^2 (3C_i - \frac{1}{\tau} - \frac{\kappa_i}{\epsilon}\tau) \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 + (-\gamma_{ii}\beta_i\tau) \|(-\Delta)^{-\frac{1}{2}}(\phi_i^{n+1} - \phi_i^n)\|_{L^2}^2, \\ \sum_{i=1}^2 \left(3C_i - \frac{\gamma_{ii}L_{f'}^2}{2} \|(-\Delta)^{-1}\| - \frac{1}{\tau} - \frac{\kappa_i}{\epsilon}\tau \right) \|\phi_i^{n+1} - \phi_i^n\|_{L^2}^2 \\ \quad + \left(\frac{\gamma_{ii}L_{f'}^2}{2} - \gamma_{ii}\beta_i\tau \right) \|(-\Delta)^{-\frac{1}{2}}(\phi_i^{n+1} - \phi_i^n)\|_{L^2}^2, \end{cases}
\end{aligned}$$

by using the estimates (35) and (36), respectively. Using the conditions (31) and (32), respectively, leads to the desired inequality for the energy stability. $\square$

2.3. Error analysis of time-discrete schemes. Now we perform an error estimate for the time-discrete scheme (16) for the pACOK dynamics. We begin with a lemma which provides an estimate for the time-discrete local truncation error and will be applied on the error estimate in Theorem 2.5 later.

Lemma 2.3 (Time-discrete LTE). *Let $\phi = \phi(t)$ be the solution to the pACOK dynamics (6) with initial data ϕ_0 . Then the time-discrete local truncation error Γ^n for the scheme (16), defined by*

$$\begin{aligned}
& \frac{3\phi(t_{n+1}) - 4\phi(t_n) + \phi(t_{n-1}))}{2\tau} \\
& = \epsilon \Delta \phi(t_{n+1}) - \frac{1}{\epsilon} [2W'(\phi(t_n)) - W'(\phi(t_{n-1}))] - \frac{\kappa}{\epsilon} (\phi(t_{n+1}) - 2\phi(t_n) + \phi(t_{n-1})) \\
& \quad - \gamma(-\Delta)^{-1} (2f(\phi(t_n)) - f(\phi(t_{n-1}))) \cdot [2f'(\phi(t_n)) - f'(\phi(t_{n-1}))] \\
& \quad - \gamma\beta(-\Delta)^{-1} (\phi(t_{n+1}) - 2\phi(t_n) + \phi(t_{n-1})) \\
& \quad - M \left[\int_{\Omega} (2f(\phi(t_n)) - f(\phi(t_{n-1}))) dx - \omega|\Omega| \right] \cdot [2f'(\phi(t_n)) - f'(\phi(t_{n-1}))]
\end{aligned} \tag{37}$$

$$+ \Gamma^n,$$

has estimates

$$\begin{aligned} \|\Gamma^n\|_{L^2}^2 &\leq C\tau^3 \left[\int_{t_{n-1}}^{t_{n+1}} (\|\partial_{tt} W'(\phi)\|_{L^2}^2 + \|\partial_{tt}\phi\|_{L^\infty}^2) dt \right. \\ &\quad \left. + \int_{t_{n-1}}^{t_{n+1}} (\|\partial_{tt} f(\phi)\|_{L^\infty}^2 + \|\partial_{tt} f'(\phi)\|_{L^\infty}^2 + \|\partial_{ttt}\phi\|_{L^2}^2) dt \right], \end{aligned}$$

and

$$\begin{aligned} \tau \sum_{j=1}^{n-1} \|\Gamma^j\|_{L^2}^2 &\leq C\tau^4 \left[\int_0^{t_n} (\|\partial_{tt} W'(\phi)\|_{L^2}^2 + \|\partial_{tt}\phi\|_{L^\infty}^2 + \|\partial_{tt} f(\phi)\|_{L^\infty}^2) dt \right. \\ &\quad \left. + \int_0^{t_n} (\|\partial_{tt} f'(\phi)\|_{L^\infty}^2 + \|\partial_{ttt}\phi\|_{L^2}^2) dt \right], \end{aligned}$$

where C is a generic constant which might change the value but only depends on $\epsilon, \gamma, M, \|(-\Delta)^{-1}\|, |\Omega|, L_{f'}, \tilde{\omega}, \kappa, \beta$.

Proof. Applying the Taylor expansion with integral residual

$$g(t_1) = g(t_0) + g'(t_0)(t_1 - t_0) + \frac{1}{2}g''(t_0)(t_1 - t_0)^2 + \frac{1}{2} \int_{t_0}^{t_1} g'''(t)(t - t_1)^2 dt$$

to the solution $\phi(t)$, we have

$$\begin{aligned} \phi(t_n) &= \phi(t_{n+1}) - \partial_t \phi(t_{n+1})\tau + \frac{1}{2}\partial_{tt}\phi(t_{n+1})\tau^2 + \frac{1}{2} \int_{t_{n+1}}^{t_n} \partial_{ttt}\phi(t)(t - t_n)^2 dt, \\ \phi(t_{n-1}) &= \phi(t_{n+1}) - \partial_t \phi(t_{n+1}) \cdot 2\tau + \partial_{tt}\phi(t_{n+1}) \cdot 2\tau^2 \\ &\quad + \frac{1}{2} \int_{t_{n+1}}^{t_{n-1}} \partial_{ttt}\phi(t)(t - t_{n-1})^2 dt, \end{aligned}$$

which implies that

$$\begin{aligned} &\frac{3\phi(t_{n+1}) - 4\phi(t_n) + \phi(t_{n-1}))}{2\tau} \\ &= \partial_t \phi(t_{n+1}) + \frac{1}{\tau} \int_{t_n}^{t_{n+1}} \partial_{ttt}\phi(t)(t - t_n)^2 dt - \frac{1}{4\tau} \int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}\phi(t)(t - t_{n-1})^2 dt \\ &= \epsilon \Delta \phi(t_{n+1}) - \frac{1}{\epsilon} W'(\phi(t_{n+1})) - \gamma(-\Delta)^{-1}(f(\phi(t_{n+1}))) \cdot f'(\phi(t_{n+1})) \\ &\quad - M \int_{\Omega} (f(\phi(t_{n+1})) - \omega|\Omega|) dx \cdot f'(\phi(t_{n+1})) \\ &\quad + \frac{1}{\tau} \int_{t_n}^{t_{n+1}} \partial_{ttt}\phi(t)(t - t_n)^2 dt - \frac{1}{4\tau} \int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}\phi(t)(t - t_{n-1})^2 dt. \end{aligned}$$

Subtracting the above equation from (37) leads to the explicit form of Γ^n

$$\begin{aligned} \Gamma^n &= -\frac{1}{\epsilon} [W'(\phi(t_{n+1})) - 2W'(\phi(t_n)) + W'(\phi(t_{n-1}))] \\ &\quad + \frac{\kappa}{\epsilon} (\phi(t_{n+1}) - 2\phi(t_n) + \phi(t_{n-1})) - \gamma(-\Delta)^{-1}(f(\phi(t_{n+1}))) \cdot f'(\phi(t_{n+1})) \\ &\quad + \gamma(-\Delta)^{-1}(2f(\phi(t_n)) - f(\phi(t_{n-1}))) \cdot [2f'(\phi(t_n)) - f'(\phi(t_{n-1}))] \\ &\quad + \gamma\beta(-\Delta)^{-1}(\phi(t_{n+1}) - 2\phi(t_n) + \phi(t_{n-1})) \end{aligned}$$

$$\begin{aligned}
& -M \int_{\Omega} (f(\phi(t_{n+1})) - \omega|\Omega|) dx \cdot f'(\phi(t_{n+1})) \\
& + M \left[\int_{\Omega} (2f(\phi(t_n)) - f(\phi(t_{n-1}))) dx - \omega|\Omega| \right] \cdot [2f'(\phi(t_n)) - f'(\phi(t_{n-1}))] \\
& + \frac{1}{\tau} \int_{t_n}^{t_{n+1}} \partial_{ttt}\phi(t)(t-t_n)^2 dt - \frac{1}{4\tau} \int_{t_{n-1}}^{t_{n+1}} \partial_{ttt}\phi(t)(t-t_{n-1})^2 dt \\
& =: \text{I}(a) + \text{I}(b) + \text{II}(a) + \text{II}(b) + \text{II}(c) + \text{III}(a) + \text{III}(b) + \text{IV}(a) + \text{IV}(b).
\end{aligned}$$

Now we estimate each term individually. For the terms $\text{I}(a)$ and $\text{I}(b)$, we use again the Taylor expansion with integral residual

$$g(t_1) = g(t_0) + g'(t_0)(t_1 - t_0) - \int_{t_0}^{t_1} g''(t)(t - t_1) dt$$

and apply it to $(h \circ \phi)(t)$

$$\begin{aligned}
h(\phi(t_n)) &= h(\phi(t_{n+1})) - \partial_t h(\phi)(t_{n+1})\tau + \int_{t_n}^{t_{n+1}} \partial_{tt} h(\phi)(t)(t - t_n) dt, \\
h(\phi(t_{n-1})) &= h(\phi(t_{n+1})) - \partial_t h(\phi)(t_{n+1}) \cdot 2\tau + \int_{t_{n-1}}^{t_{n+1}} \partial_{tt} h(\phi)(t)(t - t_{n-1}) dt,
\end{aligned}$$

which imply that

$$\begin{aligned}
& h(\phi(t_{n+1})) - 2h(\phi(t_n)) + h(\phi(t_{n-1})) \\
& = -2 \int_{t_n}^{t_{n+1}} \partial_{tt} h(\phi)(t)(t - t_n) dt + \int_{t_{n-1}}^{t_{n+1}} \partial_{tt} h(\phi)(t)(t - t_{n-1}) dt.
\end{aligned}$$

We then obtain

$$\|h(\phi(t_{n+1})) - 2h(\phi(t_n)) + h(\phi(t_{n-1}))\|_{L^2}^2 \leq 8\tau^3 \|\partial_{tt} h(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^2(\Omega))}^2, \quad (38)$$

$$\|h(\phi(t_{n+1})) - 2h(\phi(t_n)) + h(\phi(t_{n-1}))\|_{L^\infty}^2 \leq 8\tau^3 \|\partial_{tt} h(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^\infty(\Omega))}^2. \quad (39)$$

Taking $h = W'$ and $h = I$ in (38) yields

$$\begin{aligned}
\|\text{I}(a)\|_{L^2}^2 &\leq \frac{8}{\epsilon^2} \tau^3 \|\partial_{tt} W'(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^2(\Omega))}^2, \\
\|\text{I}(b)\|_{L^2}^2 &\leq \frac{8\kappa^2}{\epsilon^2} \tau^3 \|\partial_{tt} \phi\|_{L^2(t_{n-1}, t_{n+1}; L^2(\Omega))}^2.
\end{aligned}$$

For the terms $\text{II}(a)$ and $\text{II}(b)$, we have

$$\begin{aligned}
\text{II}(a) + \text{II}(b) &= -\gamma(-\Delta)^{-1} [f(\phi(t_{n+1})) - 2f(\phi(t_n)) + f(\phi(t_{n-1}))] \cdot f'(\phi(t_{n+1})) \\
&\quad - \gamma(-\Delta)^{-1} [2f(\phi(t_n)) - f(\phi(t_{n-1}))] \\
&\quad \times [f'(\phi(t_{n+1})) - 2f'(\phi(t_n)) + f'(\phi(t_{n-1}))],
\end{aligned}$$

which, by estimate (39), implies that

$$\begin{aligned}
\|\text{II}(a) + \text{II}(b)\|_{L^2}^2 &\leq |\Omega|^2 \|\text{II}(a) + \text{II}(b)\|_{L^\infty}^2 \\
&\leq |\Omega|^2 \gamma^2 L_{f'}^2 \|(-\Delta)^{-1}\|^2 8\tau^3 \|\partial_{tt} f(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^\infty(\Omega))}^2 \\
&\quad + |\Omega|^2 \gamma^2 \tilde{\omega}^2 \|(-\Delta)^{-1}\|^2 8\tau^3 \|\partial_{tt} f'(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^\infty(\Omega))}^2.
\end{aligned}$$

The estimate of term $\text{II}(c)$ is similar as that of $\text{I}(b)$, which reads

$$\begin{aligned}
\|\text{II}(c)\|_{L^2}^2 &\leq |\Omega|^2 \|\text{II}(c)\|_{L^\infty}^2 \\
&\leq |\Omega|^2 \gamma^2 \beta^2 \|(-\Delta)^{-1}\|^2 8\tau^3 \|\partial_{tt} \phi\|_{L^2(t_{n-1}, t_{n+1}; L^\infty(\Omega))}^2.
\end{aligned}$$

The estimate of term $\text{III}(a) + \text{III}(b)$ is similar as that of $\text{II}(a) + \text{II}(b)$, which reads

$$\begin{aligned} \|\text{III}(a) + \text{III}(b)\|_{L^2}^2 &\leq M^2 L_{f'}^2 |\Omega|^2 8\tau^3 \|\partial_{tt} f(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^\infty(\Omega))}^2 \\ &\quad + M^2 \tilde{\omega}^2 |\Omega|^2 8\tau^3 \|\partial_{tt} f'(\phi)\|_{L^2(t_{n-1}, t_{n+1}; L^\infty(\Omega))}^2. \end{aligned}$$

Finally, the estimate of term $\text{IV}(a) + \text{IV}(b)$ gives

$$\begin{aligned} \|\text{IV}(a) + \text{IV}(b)\|_{L^2}^2 &\leq 2\|\text{IV}(a)\|_{L^2}^2 + 2\|\text{IV}(b)\|_{L^2}^2 \\ &\leq \frac{2}{5}\tau^3 \|\partial_{ttt}\phi\|_{L^2(t_n, t_{n+1}; L^2(\Omega))}^2 + \frac{4}{5}\tau^3 \|\partial_{ttt}\phi\|_{L^2(t_{n-1}, t_{n+1}; L^2(\Omega))}^2 \\ &\leq \frac{6}{5}\tau^3 \|\partial_{ttt}\phi\|_{L^2(t_{n-1}, t_{n+1}; L^2(\Omega))}^2. \end{aligned}$$

Combining all the above estimates together yields

$$\begin{aligned} \|\Gamma^n\|_{L^2}^2 &\leq 48\tau^3 \left\{ \frac{1}{\epsilon^2} \int_{t_{n-1}}^{t_{n+1}} \|\partial_{tt} W'(\phi)\|_{L^2}^2 dt + \int_{t_{n-1}}^{t_{n+1}} \frac{\kappa^2}{\epsilon^2} \|\partial_{tt}\phi\|_{L^2}^2 dt \right. \\ &\quad + \int_{t_{n-1}}^{t_{n+1}} |\Omega|^2 \gamma^2 \beta^2 \|(-\Delta)^{-1}\|^2 \|\partial_{tt}\phi\|_{L^\infty}^2 dt \\ &\quad + |\Omega|^2 \gamma^2 \|(-\Delta)^{-1}\|^2 \int_{t_{n-1}}^{t_{n+1}} (L_{f'}^2 \|\partial_{tt} f(\phi)\|_{L^\infty}^2 + \tilde{\omega}^2 \|\partial_{tt} f'(\phi)\|_{L^\infty}^2) dt \\ &\quad + |\Omega|^2 M^2 \int_{t_{n-1}}^{t_{n+1}} (L_{f'}^2 \|\partial_{tt} f(\phi)\|_{L^\infty}^2 + \tilde{\omega}^2 \|\partial_{tt} f'(\phi)\|_{L^\infty}^2) dt \\ &\quad \left. + \frac{6}{5} \int_{t_{n-1}}^{t_{n+1}} \|\partial_{ttt}\phi\|_{L^2}^2 dt \right\} \\ &\leq C\tau^3 \left[\int_{t_{n-1}}^{t_{n+1}} (\|\partial_{tt} W'(\phi)\|_{L^2}^2 + \|\partial_{tt}\phi\|_{L^\infty}^2 + \|\partial_{tt} f(\phi)\|_{L^\infty}^2) dt \right. \\ &\quad \left. + \int_{t_{n-1}}^{t_{n+1}} (\|\partial_{tt} f'(\phi)\|_{L^\infty}^2 + \|\partial_{ttt}\phi\|_{L^2}^2) dt \right], \end{aligned}$$

and

$$\begin{aligned} \tau \sum_{j=1}^{n-1} \|\Gamma^j\|_{L^2}^2 &\leq C\tau^4 \left[\int_0^{t_n} (\|\partial_{tt} W'(\phi)\|_{L^2}^2 + \|\partial_{tt}\phi\|_{L^\infty}^2 + \|\partial_{tt} f(\phi)\|_{L^\infty}^2) dt \right. \\ &\quad \left. + \int_0^{t_n} (\|\partial_{tt} f'(\phi)\|_{L^\infty}^2 + \|\partial_{ttt}\phi\|_{L^2}^2) dt \right], \end{aligned}$$

which completes the proof. $\square$

We also need the following lemma for the estimate of terms involving $(-\Delta)^{-1}$.

Lemma 2.4. *The following inequalities hold under periodic boundary conditions for a generic constant C :*

$$\begin{aligned} \langle (-\Delta)^{-1} u, v \rangle &\leq \|(-\Delta)^{-\frac{1}{2}} u\|_{L^2}^2 \|(-\Delta)^{-\frac{1}{2}} v\|_{L^2}^2, \\ \langle (-\Delta)^{-1} u, u \rangle &\leq C \|u\|_{L^2}^2, \\ \langle (-\Delta)^{-1} u, v \rangle &\leq C \|u\|_{L^2}^2 \|v\|_{L^2}^2. \end{aligned}$$

Proof. Let $(-\Delta)^{-1}u = U, (-\Delta)^{-1}v = V$. Then

$$\begin{aligned} \int_{\Omega} U(-\Delta)V dx &= \int_{\Omega} \nabla U \cdot \nabla V dx \\ &\leq \|\nabla U\|_{L^2}^2 \|\nabla V\|_{L^2}^2 = \|(-\Delta)^{-\frac{1}{2}}u\|_{L^2}^2 \|(-\Delta)^{-\frac{1}{2}}v\|_{L^2}^2, \end{aligned}$$

which proves the first inequality. For the second inequality, we have

$$\|\nabla U\|_{L^2}^2 = \int_{\Omega} U u dx \leq \|U\|_{L^6} \|u\|_{L^{6/5}} \leq C \|U\|_{H^1} \|u\|_{L^{6/5}} \leq C \|\nabla U\|_{L^2} \|u\|_{L^2},$$

canceling $\|\nabla U\|_{L^2}$ from both sides leads to the desired result. The last inequality is the combination of the first two. The proof is completed. $\square$

Now we are ready to present the error estimate for the numerical solution of the scheme (16) for the pACOK dynamics.

Theorem 2.5. *Given $T > 0$ and an integer $N > 0$ such that $\tau = \frac{T}{N}$ and $t_n = n\tau$ for $n = 0, 1, \dots, N$. Assume that*

$$\begin{aligned} (W'(\phi))_{tt}, \phi_{ttt} &\in L^2(0, T; L^2(\Omega)), \\ (f(\phi))_{tt}, (f'(\phi))_{tt}, \phi_{tt} &\in L^2(0, T; L^\infty(\Omega)). \end{aligned}$$

Let $\{\phi^n\}$ be the numerical solution for the scheme (16), then for sufficiently small time step τ , we have

$$\|\phi(t_n) - \phi^n\|_{L^2} \leq C\tau^2, n = 1, 2, \dots, N, \quad (40)$$

where C is a generic constant which depends on $\epsilon, \gamma, M, \|(-\Delta)^{-1}\|, |\Omega|, L_{f'}, \tilde{\omega}, \kappa, \beta$, the $L^2(0, T; L^2(\Omega))$ -norm of $(W'(\phi))_{tt}, \phi_{ttt}$, and the $L^2(0, T; L^\infty(\Omega))$ -norm of $(f(\phi))_{tt}, (f'(\phi))_{tt}, \phi_{tt}$.

Proof. In the proof, we will denote by C a generic constant whose value may vary. Denote $e^n = \phi(t_n) - \phi^n$. Subtracting the scheme (16) from the equation (37), we have

$$\begin{aligned} &\frac{3e^{n+1} - 4e^n + e^{n-1}}{2\tau} \\ &= \underbrace{\epsilon \Delta e^{n+1} - \frac{1}{\epsilon} [2W'(\phi(t_n)) - 2W'(\phi^n) - W'(\phi(t_{n-1})) + W'(\phi^{n-1})]}_{\text{I}} \\ &\quad - \frac{\kappa}{\epsilon} (e^{n+1} - 2e^n + e^{n-1}) \\ &\quad - \underbrace{\gamma(-\Delta)^{-1} (2f(\phi(t_n)) - f(\phi(t_{n-1}))) \cdot [2f'(\phi(t_n)) - f'(\phi(t_{n-1}))]}_{\text{II(a)}} \\ &\quad + \underbrace{\gamma(-\Delta)^{-1} (2f(\phi^n) - f(\phi^{n-1})) \cdot [2f'(\phi^n) - f'(\phi^{n-1})]}_{\text{II(b)}} \\ &\quad - \gamma\beta(-\Delta)^{-1} (e^{n+1} - 2e^n + e^{n-1}) \\ &\quad - \underbrace{M \left[\int_{\Omega} (2f(\phi(t_n)) - f(\phi(t_{n-1}))) dx - \omega|\Omega| \right] \cdot [2f'(\phi(t_n)) - f'(\phi(t_{n-1}))]}_{\text{III(a)}} \end{aligned}$$

$$+ M \underbrace{\left[\int_{\Omega} (2f(\phi^n) - f(\phi^{n-1})) dx - \omega|\Omega| \right] \cdot [2f'(\phi^n) - f'(\phi^{n-1})]}_{\text{III}(b)} + \Gamma^n.$$

Taking L^2 inner product with e^{n+1} on both sides, we get

$$\begin{aligned} & \frac{1}{2\tau} \langle 3e^{n+1} - 4e^n + e^{n-1}, e^{n+1} \rangle + \epsilon \|\nabla e^{n+1}\|_{L^2}^2 \\ &= \langle \text{I}, e^{n+1} \rangle - \frac{\kappa}{\epsilon} \langle e^{n+1} - 2e^n + e^{n-1}, e^{n+1} \rangle \\ & \quad + \langle \text{II}(a) + \text{II}(b), e^{n+1} \rangle - \gamma\beta \langle (-\Delta)^{-1}(e^{n+1} - 2e^n + e^{n-1}), e^{n+1} \rangle \\ & \quad + \langle \text{III}(a) + \text{III}(b), e^{n+1} \rangle + \langle \Gamma^n, e^{n+1} \rangle. \end{aligned} \quad (41)$$

For terms in the above equation (41), we can estimate them as

$$\langle 3e^{n+1} - 4e^n + e^{n-1}, e^{n+1} \rangle = X^{n+1} - X^n + \frac{1}{2} \|e^{n+1} - 2e^n + e^{n-1}\|_{L^2}^2; \quad (42)$$

$$\langle \text{I}, e^{n+1} \rangle \leq \frac{L_{W''}}{\epsilon} (4\|e^n\|_{L^2}^2 + \|e^{n-1}\|_{L^2}^2) + \frac{L_{W''}}{2\epsilon} \|e^{n+1}\|_{L^2}^2; \quad (43)$$

$$-\langle e^{n+1} - 2e^n + e^{n-1}, e^{n+1} \rangle \leq \frac{5}{2} \|e^{n+1}\|_{L^2}^2 + \|e^n\|_{L^2}^2 + \frac{1}{2} \|e^{n-1}\|_{L^2}^2; \quad (44)$$

$$\begin{aligned} & -\langle (-\Delta)^{-1}(e^{n+1} - 2e^n + e^{n-1}), e^{n+1} \rangle \\ & \leq C \left(\frac{5}{2} \|e^{n+1}\|_{L^2}^2 + \|e^n\|_{L^2}^2 + \frac{1}{2} \|e^{n-1}\|_{L^2}^2 \right), \end{aligned} \quad (45)$$

in which $X^n = \frac{3}{2} \|e^n\|_{L^2}^2 - \frac{1}{2} \|e^{n-1}\|_{L^2}^2 + \|e^n - e^{n-1}\|_{L^2}^2$, and the last inequality (45) is due to Lemma 2.4. Additionally,

$$\begin{aligned} & \langle \text{II}(a) + \text{II}(b), e^{n+1} \rangle \\ &= -\gamma \langle (-\Delta)^{-1} [2f(\phi(t_n)) - f(\phi(t_{n-1}))] \\ & \quad \times (2f'(\phi(t_n)) - 2f'(\phi^n) - f'(\phi(t_{n-1})) + f'(\phi^{n-1})), e^{n+1} \rangle \\ & \quad - \gamma \langle (-\Delta)^{-1} [2f(\phi(t_n)) - 2f(\phi^n) - f(\phi(t_{n-1})) + f(\phi^{n-1})] \\ & \quad \times (2f'(\phi^n) - f'(\phi^{n-1})), e^{n+1} \rangle \\ & \leq \gamma \|(-\Delta)^{-1}\| \tilde{\omega} L_{f''} (4\|e^n\|_{L^2}^2 + \|e^{n-1}\|_{L^2}^2) \\ & \quad + \gamma C(3L_{f'}) L_{f'} (4\|e^n\|_{L^2}^2 + \|e^{n-1}\|_{L^2}^2) \\ & \quad + \frac{\gamma}{2} \|(-\Delta)^{-1}\| \tilde{\omega} L_{f''} \|e^{n+1}\|_{L^2}^2 + \frac{\gamma}{2} C(3L_{f'}) L_{f'} \|e^{n+1}\|_{L^2}^2 \\ & = \gamma (\|(-\Delta)^{-1}\| \tilde{\omega} L_{f''} + 3CL_{f'}^2) \left(\frac{1}{2} \|e^{n+1}\|_{L^2}^2 + 4\|e^n\|_{L^2}^2 + \|e^{n-1}\|_{L^2}^2 \right), \end{aligned} \quad (46)$$

and

$$\begin{aligned} & \langle \text{III}(a) + \text{III}(b), e^{n+1} \rangle \\ & \leq M|\Omega| (\tilde{\omega} L_{f''} + 3L_{f'}^2) \left(\frac{1}{2} \|e^{n+1}\|_{L^2}^2 + 4\|e^n\|_{L^2}^2 + \|e^{n-1}\|_{L^2}^2 \right). \end{aligned} \quad (47)$$

Inserting the estimates (42)-(47) back to (41), and dropping the unnecessary terms $\epsilon \|\nabla e^{n+1}\|_{L^2}^2$ and $\frac{1}{2} \|e^{n+1} - 2e^n + e^{n-1}\|_{L^2}^2$, we arrive at

$$\frac{1}{2\tau} (X^{n+1} - X^n)$$

$$\begin{aligned}
&\leq (1+C) \left(\frac{5}{2} \|e^{n+1}\|_{L^2}^2 + \|e^n\|_{L^2}^2 + \frac{1}{2} \|e^{n-1}\|_{L^2}^2 \right) \\
&\quad + \left[\frac{L_{W''}}{\epsilon} + (\gamma \|(-\Delta)^{-1}\| + M|\Omega|) (\tilde{\omega} L_{f''} + 3CL_{f'}^2) \right] \\
&\quad \times \left(\frac{1}{2} \|e^{n+1}\|_{L^2}^2 + 4\|e^n\|_{L^2}^2 + \|e^{n-1}\|_{L^2}^2 \right) \\
&\quad + \frac{1}{2} \|\Gamma^n\|_{L^2}^2 + \frac{1}{2} \|e^{n+1}\|_{L^2}^2.
\end{aligned}$$

Let D, E, F be generic constants depending on $\epsilon, \gamma, M, \|(-\Delta)^{-1}\|, |\Omega|, L_{f'}, \tilde{\omega}, \kappa$, and β . Then the above inequality becomes

$$X^{n+1} - X^n \leq D\tau \|e^{n+1}\|_{L^2}^2 + E\tau \|e^n\|_{L^2}^2 + F\tau \|e^{n-1}\|_{L^2}^2 + \tau \|\Gamma^n\|_{L^2}^2. \quad (48)$$

Summing from 0 to $n-1$ and noting that $e^{-1} = e^0 = 0$, we have

$$X^n \leq D\tau \|e^n\|_{L^2}^2 + (E+F)\tau \sum_{j=1}^{n-1} \|e^j\|_{L^2}^2 + \tau \sum_{j=1}^{n-1} \|\Gamma^n\|_{L^2}^2.$$

Note that $X^n = \frac{1}{2} \|e^n\|_{L^2}^2 + \frac{1}{2} \|2e^n - e^{n-1}\|_{L^2}^2 \geq \frac{1}{2} \|e^n\|_{L^2}^2$. Then

$$\left(\frac{1}{2} - D\tau \right) \|e^n\|_{L^2}^2 \leq (E+F)\tau \sum_{j=1}^{n-1} \|e^j\|_{L^2}^2 + \tau \sum_{j=1}^{n-1} \|\Gamma^n\|_{L^2}^2.$$

If $\tau \leq \frac{1}{4D}$, we have

$$\|e^n\|_{L^2}^2 \leq 4(E+F)\tau \sum_{j=1}^{n-1} \|e^j\|_{L^2}^2 + 4\tau \sum_{j=1}^{n-1} \|\Gamma^n\|_{L^2}^2.$$

The discrete Gronwall inequality leads to

$$\|e^n\|_{L^2}^2 \leq e^{4(E+F)\tau} \cdot 4\tau \sum_{j=1}^{n-1} \|\Gamma^n\|_{L^2}^2 \leq C\tau^4$$

in which the last inequality is due to Lemma 2.3. Therefore the desired error estimate holds. $\square$

Remark 2. The error analysis for the time-discrete scheme (17) of pACOK is similar, and we omit the details. However, for the error analysis of the time-discrete schemes (27)-(28) of pACON, we have a technical issue with the crossing term $\frac{\epsilon}{2} \Delta(2\phi_j^{n+\text{mod}(i+1,2)} - \phi_j^{n-1+2 \cdot \text{mod}(i+1,2)})$ that needs to be addressed in the future work.

3. Fully-discrete schemes for pACOK and pACON. In this section, we will use spectral approximation in space to construct the fully discrete schemes for pACOK (6) and pACON (10), and analyze the corresponding energy stabilities.

3.1. Spectral collocation approximation for spatial discretization. We discretize the spatial operators using the spectral collocation approximation. To this end, we adopt some notations for the spectral approximation as in [20, 10, 37].

We consider $\Omega = [-X, X] \times [-Y, Y] \subset \mathbb{R}^2$. For the three-dimensional case, the notations can be defined in similar manner. Let N_x and N_y be two positive even

integers. We take $h_x = \frac{2X}{N_x}$ and $h_y = \frac{2Y}{N_y}$ and define $\Omega_h = \Omega \cap (h_x\mathbb{Z} \otimes h_y\mathbb{Z})$. We define the index sets:

$$S_h = \{(i, j) \in \mathbb{Z}^2 | 1 \leq i \leq N_x, 1 \leq j \leq N_y\},$$

$$\hat{S}_h = \left\{ (k, l) \in \mathbb{Z}^2 | -\frac{N_x}{2} + 1 \leq k \leq \frac{N_x}{2}, -\frac{N_y}{2} + 1 \leq l \leq \frac{N_y}{2} \right\}.$$

Denote by $\mathcal{M}_h$ the collection of periodic grid functions on Ω_h :

$$\mathcal{M}_h = \{f : \Omega_h \rightarrow \Omega | f_{i+mN_x, j+nN_y} = f_{ij}, \forall (i, j) \in S_h, \forall (m, n) \in \mathbb{Z}^2\}.$$

For any $f, g \in \mathcal{M}_h$ and $\mathbf{f} = (f^1, f^2)^T, \mathbf{g} = (g^1, g^2)^T \in \mathcal{M}_h \times \mathcal{M}_h$, we define the discrete L^2 inner product $\langle \cdot, \cdot \rangle_h$, discrete L^2 norm $\|\cdot\|_{h, L^2}$, and discrete L^∞ norm $\|\cdot\|_{h, L^\infty}$ as follows:

$$\langle f, g \rangle_h = h_x h_y \sum_{(i, j) \in S_h} f_{ij} g_{ij}, \quad \|f\|_{h, L^2} = \sqrt{\langle f, f \rangle_h}, \quad \|f\|_{h, L^\infty} = \max_{(i, j) \in S_h} |f_{ij}|;$$

$$\langle \mathbf{f}, \mathbf{g} \rangle_h = h_x h_y \sum_{(i, j) \in S_h} (f_{ij}^1 g_{ij}^1 + f_{ij}^2 g_{ij}^2), \quad \|\mathbf{f}\|_{h, L^2} = \sqrt{\langle \mathbf{f}, \mathbf{f} \rangle_h}.$$

For a function $f \in \mathcal{M}_h$, the 2D discrete Fourier transform (DFT) $\hat{f} = Pf$ is defined as:

$$\hat{f}_{kl} = \frac{1}{N_x N_y} \sum_{(i, j) \in S_h} f_{ij} \exp\left(-i \frac{k\pi}{X} x_i\right) \exp\left(-i \frac{l\pi}{Y} y_j\right), \quad (k, l) \in \hat{S}_h,$$

where 'i' is the complex unity, and $x_i = -X + ih_x, y_j = -Y + jh_y, 1 \leq i \leq N_x, 1 \leq j \leq N_y$. The corresponding inverse DFT (iDFT) is given as:

$$f_{ij} = \sum_{(k, l) \in \hat{S}_h} \hat{f}_{kl} \exp\left(i \frac{k\pi}{X} x_i\right) \exp\left(i \frac{l\pi}{Y} y_j\right), \quad (i, j) \in S_h.$$

Let $\widehat{\mathcal{M}}_h = \{Pf | f \in \mathcal{M}_h\}$ and define the operators $\hat{D}_x, \hat{D}_y$ on $\widehat{\mathcal{M}}_h$ as

$$(\hat{D}_x \hat{f})_{kl} = \left(\frac{ik\pi}{X}\right) \hat{f}_{kl}, \quad (\hat{D}_y \hat{f})_{kl} = \left(\frac{il\pi}{Y}\right) \hat{f}_{kl}, \quad (k, l) \in \hat{S}_h,$$

then the Fourier spectral approximations to the spatial operators $\partial_x, \partial_{xx}$ can be written as

$$D_x = P^{-1} \hat{D}_x P, \quad D_y = P^{-1} \hat{D}_y P, \quad D_x^2 = P^{-1} \hat{D}_x^2 P, \quad D_y^2 = P^{-1} \hat{D}_y^2 P.$$

For any $f \in \mathcal{M}_h$ and $\mathbf{f} = (f^1, f^2)^T \in \mathcal{M}_h \times \mathcal{M}_h$, the discrete gradient, divergence and Laplace operators are given respectively by

$$\nabla_h f = (D_x f, D_y f)^T, \quad \nabla_h \cdot \mathbf{f} = D_x f^1 + D_y f^2,$$

$$\Delta_h f = D_x^2 f + D_y^2 f = P^{-1} (\hat{D}_x^2 + \hat{D}_y^2) P f.$$

Let $\mathring{\mathcal{M}}_h = \{f \in \mathcal{M}_h | \langle f, 1 \rangle_h = 0\}$ be the collection of all periodic grid functions with zero mean, we define $(-\Delta_h)^{-1} : \mathring{\mathcal{M}}_h \rightarrow \mathring{\mathcal{M}}_h$ as

$$(-\Delta_h)^{-1} f = u \iff -\Delta_h u = f.$$

More precisely in terms of DFT and iDFT, we define it as

$$(-\Delta_h)^{-1} f = -P^{-1} (\hat{D}_x^2 + \hat{D}_y^2)^{-1} P f$$

$$= -P^{-1} \begin{cases} \left[\left(\frac{k\pi}{X} \right)^2 + \left(\frac{l\pi}{Y} \right)^2 \right]^{-1} \hat{f}_{kl}, & (k, l) \neq (0, 0) \\ 0, & (k, l) = (0, 0) \end{cases}$$

Note that $(-\Delta_h)^{-1}$ can be defined for $g \in \mathcal{M}_h \setminus \mathring{\mathcal{M}}_h$ by simply removing the $(0, 0)$ -mode $\hat{g}_{00}$, namely, $(-\Delta_h)^{-1}g := (-\Delta_h)^{-1}(g - \hat{g}_{00})$ if $g \in \mathcal{M}_h \setminus \mathring{\mathcal{M}}_h$. Furthermore, we define $(-\Delta_h)^{-\frac{1}{2}}$ as follows:

$$\|(-\Delta_h)^{-\frac{1}{2}}f\|_{h,L^2}^2 = \left\langle (-\Delta_h)^{-\frac{1}{2}}f, (-\Delta_h)^{-\frac{1}{2}}f \right\rangle_h = \left\langle (-\Delta_h)^{-1}f, f \right\rangle_h.$$

We denote by $\|(-\Delta_h)^{-1}\|$ the optimal constant such that $\|(-\Delta_h)^{-1}f\|_{h,L^\infty} \leq C\|f\|_{h,L^\infty}$, namely the norm of the operator $(-\Delta_h)^{-1}$ from $L^\infty(\mathring{\mathcal{M}}_h)$ to itself.

Note that an aliasing error will appear in the pseudo-spectral approximation. An aliasing error control technique was developed recently and applied for the 3-D viscous Burgers' equation [14], 3-D incompressible Navier-Stokes equation [33] and 'Good' Boussinesq equation [35]. We will take this technique into our consideration in the future work.

3.2. Estimate of $\|(-\Delta_h)^{-1}\|$. As the energy stability for the fully-discrete schemes depends on $\|(-\Delta_h)^{-1}\|$, we will provide an explicit L^∞ bound of the operator $(-\Delta_h)^{-1}$. To this end, we need two lemmas, the first one is the discrete analogy of a Sobolev embedding inequality, and the second one is regarding the stability of the spectrally discrete Laplacian operator $-\Delta_h$. Noting that the first lemma is a consequence of the standard Sobolev embedding theory, and the second lemma is due to the elliptic regularity, we will not repeat the detailed proofs.

Lemma 3.1. *Define the discrete H^s norm for $f \in \mathcal{M}_h$ as:*

$$\|f\|_{h,H^s}^2 = \sum_{(k,l) \in \hat{\mathcal{S}}_h} (1 + (k^2 + l^2)^s) |\hat{f}_{kl}|^2$$

Then for any function $f \in \mathcal{M}_h$, we have

$$\|f\|_{h,L^\infty} \leq C_s \|f\|_{h,H^s} \quad (49)$$

provided $s > d/2$, $d = 2, 3$, where C_s is a constant only depending on s and is independent of h .

Remark 3. Taking $s = 2$ in the Lemma 3.1, we can have an estimate on C_2 :

$$\begin{aligned} C_2^2 &= \sum_{(k,l) \in \mathbb{Z}^2} \frac{1}{1 + (k^2 + l^2)^2} \leq 1 + 4 \sum_{k=1}^{\infty} \frac{1}{1 + k^2} + \int_{\mathbb{R}^2} \frac{1}{1 + (x^2 + y^2)^2} dx dy \\ &\leq 1 + 4 \cdot \frac{\pi^2}{6} + \frac{\pi^2}{2}. \end{aligned}$$

We also have a uniform L^∞ bound for the operator $(-\Delta_h)^{-1}$.

Lemma 3.2. *Let any $u, f \in \mathcal{M}_h$ be such that $-\Delta_h u = f$, then we have*

$$\|u\|_{h,L^\infty} \leq C_2 \sqrt{(1 + C_p^4)|\Omega|} \|f\|_{h,L^\infty}, \quad (50)$$

where $C_p \leq \frac{\max\{X,Y\}}{\pi}$ is the discrete Poincare constant. In other words, $\|(-\Delta_h)^{-1}\|$ is uniformly bounded as:

$$\|(-\Delta_h)^{-1}\| \leq C_2 \sqrt{(1 + C_p^4)|\Omega|}.$$

Now we will use the estimate of $\|(-\Delta_h)^{-1}\|$ to obtain the conditions of energy stability for the fully-discrete schemes of pACOK (6) and pACON (10) given in the next subsection.

3.3. Fully-discrete schemes for pACOK and pACON. Given the discrete Laplacian operator $-\Delta_h$ and its inverse $(-\Delta_h)^{-1}$ defined in the preceding subsection, and denote by

$$\Phi^n \approx \phi(x, t_n)|_{\Omega_h}, \quad \Phi_1^n \approx \phi_1(x, t_n)|_{\Omega_h}, \quad \Phi_2^n \approx \phi_2(x, t_n)|_{\Omega_h},$$

the numerical solutions of pACOK (6) and pACON (10), we arrive at the following second order fully-discrete semi-implicit schemes for the pACOK equation (6): given initial data $\Phi^{-1} = \Phi^0 = \phi_0(x)|_{\Omega_h}$, for $n \in [N]$, find $\Phi^{n+1} = (\Phi_{ij}^{n+1}) \in \mathcal{M}_h$ such that

$$\begin{aligned} & \frac{3\Phi^{n+1} - 4\Phi^n + \Phi^{n-1}}{2\tau} \\ &= \epsilon \Delta_h \Phi^{n+1} - \frac{1}{\epsilon} [2W'(\Phi^n) - W'(\Phi^{n-1})] - \frac{\kappa_h}{\epsilon} (\Phi^{n+1} - 2\Phi^n + \Phi^{n-1}) \\ & \quad - \gamma(-\Delta_h)^{-1} [2f(\Phi^n) - f(\Phi^{n-1}) - \omega] \odot (2f'(\Phi^n) - f'(\Phi^{n-1})) \\ & \quad - \gamma\beta_h(-\Delta_h)^{-1} (\Phi^{n+1} - 2\Phi^n + \Phi^{n-1}) \\ & \quad - M [\langle 2f(\Phi^n) - f(\Phi^{n-1}), 1 \rangle_h - \omega|\Omega|] (2f'(\Phi^n) - f'(\Phi^{n-1})), \end{aligned} \quad (51)$$

by using stabilizer (14); or

$$\begin{aligned} & \frac{3\Phi^{n+1} - 4\Phi^n + \Phi^{n-1}}{2\tau} \\ &= \epsilon \Delta_h \Phi^{n+1} - \frac{1}{\epsilon} [2W'(\Phi^n) - W'(\Phi^{n-1})] - \frac{\kappa_h}{\epsilon} \tau (\Phi^{n+1} - \Phi^n) \\ & \quad - \gamma(-\Delta_h)^{-1} [2f(\Phi^n) - f(\Phi^{n-1}) - \omega] \odot (2f'(\Phi^n) - f'(\Phi^{n-1})) \\ & \quad - \gamma\beta_h \tau (-\Delta_h)^{-1} (\Phi^{n+1} - \Phi^n) \\ & \quad - M [\langle 2f(\Phi^n) - f(\Phi^{n-1}), 1 \rangle_h - \omega|\Omega|] (2f'(\Phi^n) - f'(\Phi^{n-1})), \end{aligned} \quad (52)$$

by using stabilizer (15), with $\kappa_h, \beta_h \geq 0$ being the stabilization constants. The notation $\odot$ represents pointwise multiplication.

Similarly the fully-discrete semi-implicit schemes for the pACON equations (10) read: given initial data $\Phi_i^{-1} = \Phi_i^0 = \phi_{0,i}(x)|_{\Omega_h}, i = 1, 2$, we find $(\Phi_1^{n+1}, \Phi_2^{n+1}) = ((\Phi_{1,ij}^{n+1}), (\Phi_{2,ij}^{n+1})) \in \mathcal{M}_h \times \mathcal{M}_h, n \in [N]$ such that

$$\begin{aligned} & \frac{3\Phi_i^{n+1} - 4\Phi_i^n + \Phi_i^{n-1}}{2\tau} \\ &= \epsilon \Delta_h \Phi_i^{n+1} + \frac{\epsilon}{2} \Delta_h (2\Phi_j^{n+\text{mod}(i+1,2)} - \Phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) \\ & \quad - \frac{1}{\epsilon} \left[2 \frac{\partial W_2}{\partial \phi_i} (\Phi_1^{n+\text{mod}(i+1,2)}, \Phi_2^n) - \frac{\partial W_2}{\partial \phi_i} (\Phi_1^{n-1+2 \cdot \text{mod}(i+1,2)}, \Phi_2^{n-1}) \right] \\ & \quad - \frac{\kappa_{i,h}}{\epsilon} (\Phi_i^{n+1} - 2\Phi_i^n + \Phi_i^{n-1}) - \gamma_{ii} \beta_{i,h} (-\Delta_h)^{-1} (\Phi_i^{n+1} - 2\Phi_i^n + \Phi_i^{n-1}) \\ & \quad - \gamma_{ii} (-\Delta_h)^{-1} [2f(\Phi_i^n) - f(\Phi_i^{n-1}) - \omega_i] \odot [2f'(\Phi_i^n) - f'(\Phi_i^{n-1})] \\ & \quad - \gamma_{ij} (-\Delta_h)^{-1} [2f(\Phi_j^{n+\text{mod}(i+1,2)}) - f(\Phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) - \omega_j] \\ & \quad \odot [2f'(\Phi_i^n) - f'(\Phi_i^{n-1})] \end{aligned} \quad (53)$$

$$-M_i (\langle 2f(\Phi_i^n) - f(\Phi_i^{n-1}), 1 \rangle - \omega_i |\Omega|) [2f'(\Phi_i^n) - f'(\Phi_i^{n-1})],$$

for $i = 1, 2$, $j \neq i$ if choosing stabilizer (25); or

$$\begin{aligned} & \frac{3\Phi_i^{n+1} - 4\Phi_i^n + \Phi_i^{n-1}}{2\tau} \\ &= \epsilon \Delta_h \Phi_i^{n+1} + \frac{\epsilon}{2} \Delta_h (2\Phi_j^{n+\text{mod}(i+1,2)} - \Phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) \\ & \quad - \frac{1}{\epsilon} \left[2 \frac{\partial W_2}{\partial \phi_i}(\Phi_1^{n+\text{mod}(i+1,2)}, \Phi_2^n) - \frac{\partial W_2}{\partial \phi_i}(\Phi_1^{n-1+2 \cdot \text{mod}(i+1,2)}, \Phi_2^{n-1}) \right] \\ & \quad - \frac{\kappa_{i,h}}{\epsilon} \tau (\Phi_i^{n+1} - \Phi_i^n) - \gamma_{ii} \beta_{i,h} \tau (-\Delta_h)^{-1} (\Phi_i^{n+1} - \Phi_i^n) \\ & \quad - \gamma_{ii} (-\Delta_h)^{-1} [2f(\Phi_i^n) - f(\Phi_i^{n-1}) - \omega_i] \odot [2f'(\Phi_i^n) - f'(\Phi_i^{n-1})] \\ & \quad - \gamma_{ij} (-\Delta_h)^{-1} [2f(\Phi_j^{n+\text{mod}(i+1,2)}) - f(\Phi_j^{n-1+2 \cdot \text{mod}(i+1,2)}) - \omega_j] \\ & \quad \odot [2f'(\Phi_i^n) - f'(\Phi_i^{n-1})] \\ & \quad - M_i (\langle 2f(\Phi_i^n) - f(\Phi_i^{n-1}), 1 \rangle - \omega_i |\Omega|) [2f'(\Phi_i^n) - f'(\Phi_i^{n-1})], \end{aligned} \quad (54)$$

for $i = 1, 2$, $j \neq i$ if choosing stabilizer (26), with $\kappa_{i,h}, \beta_{i,h} \geq 0$ for $i = 1, 2$ being the stabilization constants.

The unique solvability of the schemes (51) and (52) for pACOK, and the schemes (53) and (54) for pACON, can be guaranteed by the following theorem.

Theorem 3.3. *The schemes (51) and (52) for pACOK, and the schemes (53) and (54) for pACON are uniquely solvable.*

Proof. We only need to show the proof for one scheme. Others are similar. Take the scheme (52) as an example. Since it is semi-implicit with nonlinear terms treated explicitly, we only need to check that the operator applying to Φ^{n+1} is invertible. Indeed, the scheme (52) can be rewritten as

$$\left(\frac{3}{2\tau} + \frac{\kappa_h}{\epsilon} \tau + \epsilon(-\Delta_h) + \gamma \beta_h \tau (-\Delta_h)^{-1} \right) \Phi^{n+1} = F_h^n,$$

and the operator in front of Φ^{n+1} is invertible as all its eigenvalues are positive. $\square$

To consider the energy stabilities for the pACOK schemes (51) and (52), we define a discrete analogy of the energy (5):

$$\begin{aligned} E_h^{\text{pOK}}[\Phi^n] &= \frac{\epsilon}{2} \|\nabla_h \Phi^n\|_{h,L^2}^2 + \frac{1}{\epsilon} \langle W(\Phi^n), 1 \rangle_h + \frac{\gamma}{2} \|(-\Delta_h)^{-\frac{1}{2}}(f(\Phi^n))\|_{h,L^2}^2 \\ & \quad + \frac{M}{2} (\langle f(\Phi^n), 1 \rangle_h - \omega |\Omega|)^2. \end{aligned} \quad (55)$$

Similarly, we also define a discrete analogy of the energy (9) for the energy stability of the pACON schemes (53) and (54):

$$\begin{aligned} & E_h^{\text{pON}}[\Phi_1^n, \Phi_2^n] \\ &= \frac{\epsilon}{2} (\|\nabla_h \Phi_1^n\|_{h,L^2}^2 + \|\nabla_h \Phi_2^n\|_{h,L^2}^2 + \langle \nabla_h \Phi_1^n, \nabla_h \Phi_2^n \rangle_h) + \frac{1}{\epsilon} \langle W_2(\Phi_1^n, \Phi_2^n), 1 \rangle \\ & \quad + \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} \langle (-\Delta_h)^{-1}(f(\Phi_i^n)) \cdot f(\Phi_j^n), 1 \rangle + \sum_{i=1}^2 \frac{M_i}{2} (\langle f(\Phi_i^n), 1 \rangle_h - \omega_i |\Omega|)^2. \end{aligned} \quad (56)$$

Then we have the following energy stability for the pACOK/pACON schemes:

Theorem 3.4. *Let $\kappa_h, \beta_h \geq 0$, and*

$$C_h = \frac{L_{W''}}{2\epsilon} + \frac{1}{2}(L_{f'}^2 + L_{f''}\tilde{\omega})(\gamma\|(-\Delta_h)^{-1}\| + M|\Omega|).$$

If $\{\Phi^n\}_{n=1}^N$ is generated by the scheme (51), then

$$\begin{aligned} & E_h^{\text{pOK}}[\Phi^{n+1}] + \left(\frac{1}{4\tau} + \frac{\kappa_h}{2\epsilon} + C_h\right) \|\Phi^{n+1} - \Phi^n\|_{h,L^2}^2 \\ & \quad + \frac{\gamma\beta_h}{2} \|(-\Delta_h)^{-\frac{1}{2}}(\Phi^{n+1} - \Phi^n)\|_{h,L^2}^2 \\ & \leq E_h^{\text{pOK}}[\Phi^n] + \left(\frac{1}{4\tau} + \frac{\kappa_h}{2\epsilon} + C_h\right) \|\Phi^n - \Phi^{n-1}\|_{h,L^2}^2 \\ & \quad + \frac{\gamma\beta_h}{2} \|(-\Delta_h)^{-\frac{1}{2}}(\Phi^n - \Phi^{n-1})\|_{h,L^2}^2, \end{aligned}$$

provided that $\tau < \frac{1}{3C_h}$; If $\{\Phi^n\}_{n=1}^N$ is generated by the scheme (52), then

$$\begin{aligned} & E_h^{\text{pOK}}[\Phi^{n+1}] + \left(\frac{1}{4\tau} + C_h\right) \|\Phi^{n+1} - \Phi^n\|_{h,L^2}^2 \\ & \leq E_h^{\text{pOK}}[\Phi^n] + \left(\frac{1}{4\tau} + C_h\right) \|\Phi^n - \Phi^{n-1}\|_{h,L^2}^2, \end{aligned}$$

provided that either

$$\kappa_h \geq 9C_h^2 \frac{\epsilon}{4}, \quad (57)$$

or

$$\kappa_h \geq \left(3C_h - \frac{\gamma L_{f'}^2}{2} \|(-\Delta_h)^{-1}\|\right)^2 \frac{\epsilon}{4}, \quad \beta_h \geq \frac{L_{f'}^2}{2\tau}. \quad (58)$$

Theorem 3.5. *Let $\kappa_{i,h}, \beta_{i,h} \geq 0$, and*

$$C_{i,h} = \frac{L_{W''}}{2\epsilon} + \frac{1}{2}(L_{f'}^2 + L_{f''}\tilde{\omega})((\gamma_{i1} + \gamma_{i2})\|(-\Delta_h)^{-1}\| + M_i|\Omega|), \quad i = 1, 2.$$

If $\{(\Phi_1^n, \Phi_2^n)\}_{n=1}^N$ is generated by the scheme (53), then

$$\begin{aligned} & E_h^{\text{pON}}[\Phi_1^{n+1}, \Phi_2^{n+1}] + \sum_{i=1}^2 \left(\frac{1}{4\tau} + \frac{\kappa_{i,h}}{2\epsilon} + C_{i,h}\right) \|\Phi_i^{n+1} - \Phi_i^n\|_{h,L^2}^2 \\ & \quad + \sum_{i=1}^2 \frac{\gamma_{ii}\beta_i}{2} \|(-\Delta_h)^{-\frac{1}{2}}(\Phi_i^{n+1} - \Phi_i^n)\|_{h,L^2}^2 \\ & \leq E_h^{\text{pON}}[\Phi_1^n, \Phi_2^n] + \sum_{i=1}^2 \left(\frac{1}{4\tau} + \frac{\kappa_{i,h}}{2\epsilon} + C_{i,h}\right) \|\Phi_i^n - \Phi_i^{n-1}\|_{h,L^2}^2 \\ & \quad + \sum_{i=1}^2 \frac{\gamma_{ii}\beta_i}{2} \|(-\Delta_h)^{-\frac{1}{2}}(\Phi_i^n - \Phi_i^{n-1})\|_{h,L^2}^2 \end{aligned}$$

provided that $\tau < \min\{\frac{1}{3C_{1,h}}, \frac{1}{3C_{2,h}}\}$; if $\{(\Phi_1^n, \Phi_2^n)\}_{n=1}^N$ is generated by the scheme (54),

$$E_h^{\text{pON}}[\Phi_1^{n+1}, \Phi_2^{n+1}] + \sum_{i=1}^2 \left(\frac{1}{4\tau} + C_{i,h}\right) \|\Phi_i^{n+1} - \Phi_i^n\|_{h,L^2}^2$$

$$\leq E_h^{\text{pON}}[\Phi_1^n, \Phi_2^n] + \sum_{i=1}^2 \left(\frac{1}{4\tau} + C_{i,h} \right) \|\Phi_i^n - \Phi_i^{n-1}\|_{h,L^2}^2,$$

provided that either

$$\kappa_{i,h} \geq 9C_{i,h}^2 \frac{\epsilon}{4}, \quad i = 1, 2 \quad (59)$$

or

$$\kappa_{i,h} \geq \left(3C_{i,h} - \frac{\gamma_{ii} L_{f'}^2}{2} \|(-\Delta_h)^{-1}\| \right)^2 \frac{\epsilon}{4}, \quad \beta_{i,h} \geq \frac{L_{f'}^2}{2\tau}, \quad i = 1, 2. \quad (60)$$

The proofs of the above two theorems are similar to the time-discrete analogies in theorem 2.1 and theorem 2.2. The only difference is that $(-\Delta)^{-1}$ is replaced by $(-\Delta_h)^{-1}$. Therefore we omit the details.

3.4. Error analysis of fully-discrete schemes for pACOK. The error estimates for the fully discrete schemes (51) and (52) are similar to the time-discrete case in the section 2.3. For the spatial estimates, we adopt a known result in the error analysis of spectral methods [28]:

$$\|\phi^n - \Phi^n\|_{h,L^2} \leq C(N_x^{-m} + N_y^{-m}), \quad (61)$$

for some generic constant C depending on the regularity of the exact solution.

The following theorem summarizes the combination of the estimate (62) in time and (61) in space for the fully discrete schemes of pACOK. The proof is omitted.

Theorem 3.6. *Given $T > 0$ and an integer $N > 0$ such that $\tau = \frac{T}{N}$ and $t_n = n\tau$ for $n = 0, 1, \dots, N$. Assume that $(W'(\phi))_{tt}, \phi_{ttt} \in L^2(0, T; L^2(\Omega)) \cap L^2(0, T; H^m(\Omega))$, and $(f(\phi))_{tt}, (f'(\phi))_{tt}, \phi_{tt} \in L^2(0, T; L^\infty(\Omega)) \cap L^2(0, T; H^m(\Omega))$. Let $\{\Phi^n\}$ be the numerical solution for the scheme (16) or (17), then for sufficiently small time step τ , we have*

$$\|\phi(t_n) - \Phi^n\|_{h,L^2} \leq C(\tau^2 + N_x^{-m} + N_y^{-m}), \quad n = 1, 2, \dots, N, \quad (62)$$

where C is a generic constant which depends on $\epsilon, \gamma, M, \|(-\Delta)^{-1}\|, |\Omega|, L_{f'}, \tilde{\omega}, \kappa, \beta$, and the regularity of ϕ but is independent of τ, N_x and N_y .

4. Numerical experiments. In this section, we present some numerical solutions to the pACOK (6) and pACON (10) equations with periodic boundary conditions using the suggested BDF schemes. We conduct numerical experiments in two directions. One is to numerically verify the second order rate of convergence, and the other is to observe coarsening dynamics of the binary and ternary systems. The domain for these experiments is $\Omega = [-1, 1]^2 \subset \mathbb{R}^2$. For pACOK, we take $N_x = N_y = 2^8$, and for pACON, we take $N_x = N_y = 2^9$. The grid size is $h = 2/N_x$. The stopping criteria for the time iteration is set to

$$\frac{\|\Phi^{n+1} - \Phi^n\|_{h,L^\infty}}{\tau} \leq 10^{-5}$$

for pACOK, and

$$\frac{\|\Phi_1^{n+1} - \Phi_1^n\|_{h,L^\infty}}{\tau} + \frac{\|\Phi_2^{n+1} - \Phi_2^n\|_{h,L^\infty}}{\tau} \leq 10^{-5}$$

for pACON.

4.1. Rate of convergence. For the pACOK equation (6) of the binary system, we test the rate of convergence using the following initial condition:

$$\phi^0(x, y) = \begin{cases} 1 & \text{if } x^2 + y^2 < r_0^2, \\ 0 & \text{otherwise,} \end{cases}$$

where $r_0 = \sqrt{\omega|\Omega|/\pi} + 0.1$. The test is performed for $\epsilon = 20h, 10h$, and $5h$ up to $T = 0.01$. The parameters are $\omega = 0.1$, $M = 1000$, $\gamma = 100$, $\kappa = 500,000$, and $\beta = 500$. We take the scheme (52) with stabilizer (15) and condition (20) for the numerical simulation.

The benchmark solution is calculated with the time step $\tau = 1 \times 10^{-6}$. Table 1 shows the errors and the corresponding convergence rates at time $T = 0.01$ using the scheme (52) to solve pACOK equation of the binary system. For each value of $\epsilon = 20h, 10h$ and $5h$, one can see that the numerical rates become very close to the expected value 2 for small τ , which is consistent with the theoretical prediction.

	$\epsilon = 20h$		$\epsilon = 10h$		$\epsilon = 5h$	
τ	Error	Rate	Error	Rate	Error	Rate
6.25000e-4	1.7780e-1	–	2.7611e-1	–	3.0359e-1	–
3.12500e-4	5.7956e-2	1.6173	1.3601e-1	1.0215	2.0887e-1	0.5395
1.56250e-4	1.5596e-2	1.8971	4.3307e-2	1.6510	9.0438e-1	1.2076
7.81250e-5	4.2290e-3	1.8794	1.1944e-2	1.8584	2.7308e-2	1.7276
3.90625e-5	1.2178e-3	1.7960	3.2868e-3	1.8615	7.4445e-3	1.8751
1e-6	–	–	–	–	–	–
(benchmark)						

TABLE 1. Numerical rates of convergence in binary system (pACOK) with parameters $\omega = 0.1$, $M = 1000$, $\gamma = 100$, $\kappa = 500,000$, and $\beta = 500$.

For the pACON equation (10) of the ternary system, we take the initial data as four separated disks, two on each axis.

$$\phi_1^0(x, y) = \begin{cases} 1 & \text{if } (x \pm 0.5)^2 + y^2 < r_1^2/4 + 0.03, \\ 0 & \text{otherwise,} \end{cases}$$

$$\phi_2^0(x, y) = \begin{cases} 1 & \text{if } x^2 + (y \pm 0.5)^2 < r_2^2/4 + 0.03, \\ 0 & \text{otherwise,} \end{cases}$$

where $r_1 = \sqrt{\omega_1|\Omega|/\pi}$ and $r_2 = \sqrt{\omega_2|\Omega|/\pi}$. We choose the parameters as $\omega_1 = \omega_2 = 0.1$, $M_1 = M_2 = 1000$, $\gamma_{11} = \gamma_{22} = 2000$, $\gamma_{12} = \gamma_{21} = 0$, $\kappa_1 = \kappa_2 = 1000$, and $\beta_1 = \beta_2 = 0$. Each test runs up to $T = 0.01$. We take the scheme (53) and condition (59) for the numerical simulation.

Table 2 lists the errors and the numerical convergence rates taken at time $T = 0.01$ using the BDF scheme (53). Our benchmark solution in this example is computed with the time step $\tau = 1 \times 10^{-7}$. Similarly as for the pACOK case, for each value of ϵ , the numerical rates closely match with the theoretical value when τ becomes smaller.

Note that the penalty constant M will potentially increase the stiffness of the model. Two methods are usually adopted to handle the largeness of M while still

maintaining the stability and the numerical accuracy. One is to take a relatively small time step τ , which is what we use in this paper. The other one is to start with a small M so that the initial stiffness is easily controlled, then gradually but slowly increase the value of M . This method has been adopted in some of our earlier work [41, 32].

	$\epsilon = 20h$		$\epsilon = 10h$		$\epsilon = 5h$	
τ	Error	Rate	Error	Rate	Error	Rate
1.9531e-4	6.4752e-2	—	8.6449e-2	—	1.1016e-1	—
9.7656e-5	3.8307e-2	0.7573	5.2877e-2	0.7092	7.4234e-2	0.5694
4.8828e-5	2.0243e-2	0.9202	2.7753e-2	0.9300	4.0591e-2	0.8709
2.4414e-5	9.7032e-3	1.0609	1.3121e-2	1.0807	1.8854e-2	1.1063
1.2207e-5	4.0208e-3	1.2710	5.3810e-3	1.2860	7.6155e-3	1.3078
6.1035e-6	1.0766e-3	1.9010	1.4069e-3	1.9354	1.9639e-3	1.9552
1e-7	—	—	—	—	—	—
(benchmark)						

TABLE 2. Numerical rates of convergence in ternary system (pACON) with parameters $\omega_1 = \omega_2 = 0.1$, $M_1 = M_2 = 1000$, $\gamma_{11} = \gamma_{22} = 2000$, $\gamma_{12} = \gamma_{21} = 0$, $\kappa_1 = \kappa_2 = 1000$, and $\beta_1 = \beta_2 = 0$.

4.2. Coarsening dynamics. In the second experiment, we focus on the dynamics of the pACOK and pACON equations with the suggested schemes (51) and (53), respectively. As we discussed in Remark 1, choosing stabilizer (14) or (25) with mildly large stabilization constants would allow a relatively large step size and not cause too much error in the computation.

When the relative volumes of the constituents in these systems (ω in pACOK, and ω_1, ω_2 in pACON) are small compared to the total volume, and the strengths of long-range interactions (γ in pACOK, and γ_{11}, γ_{22} in pACON) are relatively large, we can observe the equilibria as several types of bubble assemblies.

Our initial data are randomly generated on a uniform mesh of the domain $\Omega = [-1, 1]^2$ with the mesh size $16h$. The MATLAB command for such functions is `repelem(rand(N/ratio, N/ratio), ratio, ratio)`. We use `ratio = 16` in all our experiments and each experiment starts from a random initial state. In the binary system, the fixed parameters are $\tau = 1 \times 10^{-3}$, $\omega = 0.1$, $\kappa = 2000$, $\beta = 5$, and $M = 1000$. In the ternary system, we fix $\tau = 1 \times 10^{-3}$, $\omega_1 = \omega_2 = 0.1$, $\kappa_1 = \kappa_2 = 1000$, $\beta_1 = \beta_2 = 5$, and $M = 1000$. Note that the time step $\tau = 1 \times 10^{-3}$ is taken to be mildly small. This is because on one hand we need a small τ to catch the quick phase separation in detail during the initial short period of time; on the other hand, an extremely small τ will cause numerical inefficiency, therefore, a mildly small value of $\tau = 1 \times 10^{-3}$ is taken.

Equilibria in the binary system are single bubbles captured in Figure 1, where we vary γ as $\gamma = 5000, 8000$. In the top subfigure, the random initial is phase separated quickly within a very short time period, resulting in a group of bubbles with different sizes, then the tiny bubbles disappear, other bubbles evolve into an equal size, and eventually all the equally-sized bubbles become equally distanced, forming a hexagonal pattern in the 2D domain Ω . The insets are snapshots taken

at $t = 1, 10, 50, 150$, each of which has a colored title indicating the corresponding colored marker on the monotone decreasing energy curve.

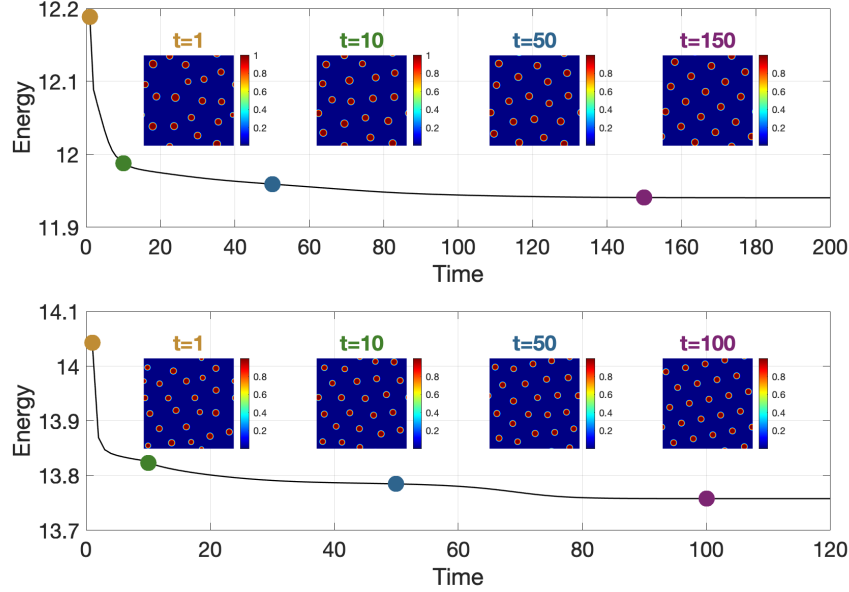


FIGURE 1. (Color online) Coarsening dynamics in binary system with $\gamma = 5000$ (top) and $\gamma = 8000$ (bottom). The larger the repulsive force γ is, the more bubbles are generated from random initial.

When the value of γ becomes larger, say $\gamma = 8000$, but other parameters are fixed, the stronger long-range repulsive interaction between bubbles lead to more bubbles of equal size and equal distance. The result is depicted in bottom subfigure.

The ternary system has more equilibrium types as shown in Figure 2. For the top subfigure in Figure 2, we take $\gamma_{11} = \gamma_{22} = 2000, \gamma_{12} = \gamma_{21} = 0$. Starting from a random initial generated by `repelem`, the system quickly goes through the phase separation within a very short time period ($t = 1$), with some being double-bubbles, and others single bubbles in either red or yellow. Then the tiny single bubbles disappear ($t = 10$), and other single bubbles with different colors merge to form double-bubbles, reaching to all double bubbles with equal size and equal distance in hexagonal pattern ($t = 100$). Most importantly in the coarsening dynamics for the pACON system, it takes very long time ($t = 300$) for all the double-bubbles to be polarized along the same direction. Here we define the polarity direction as the direction pointing from the center of the mass of the red component from that of the yellow component.

For the middle subfigure in Figure 2, we take $\gamma_{11} = \gamma_{22} = 2000$ unchanged but increase the value of $\gamma_{12} = \gamma_{21} = 1350$. While γ_{11} (γ_{22} , respectively) can be understood as the splitting strength for the red component (yellow component, respectively), $\gamma_{12} = \gamma_{21}$ accounts for the splitting strength between red and yellow components. When $\gamma_{12} = \gamma_{21}$ is small (for instance, the top subfigure case), the splitting strength between red and yellow components is weak, therefore red and yellow components are adhered together (weak splitting leads to strong adhesion);

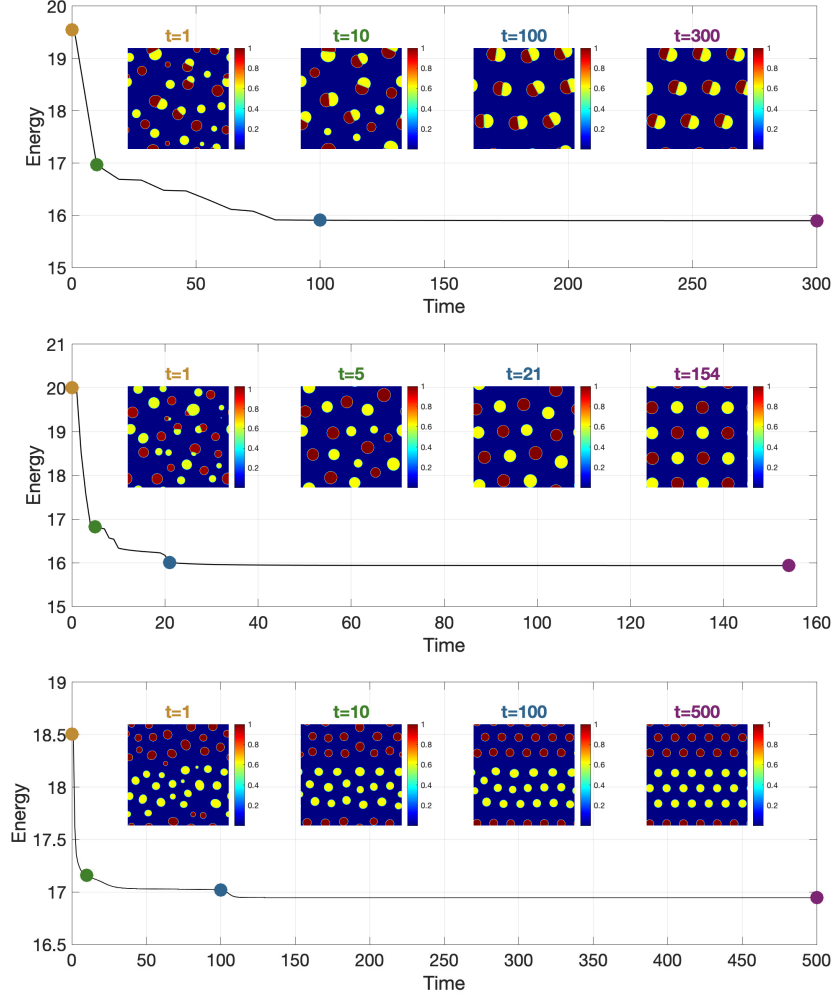


FIGURE 2. (Color online) Coarsening dynamics in ternary system with various $\gamma_{11} = \gamma_{22}$ and $\gamma_{12} = \gamma_{21}$: $\gamma_{11} = \gamma_{22} = 2000$ and $\gamma_{12} = \gamma_{21} = 0$ (top), $\gamma_{11} = \gamma_{22} = 2000$, and $\gamma_{12} = \gamma_{21} = 1350$ (middle), $\gamma_{11} = \gamma_{22} = 10000$, and $\gamma_{12} = \gamma_{21} = 12000$ (bottom). When $\gamma_{12} = \gamma_{21}$ is small, a double-bubble hexagonal pattern is formed, with the same polarity direction. As $\gamma_{12} = \gamma_{21}$ becomes large, double-bubbles are broken, and a perfectly mixed red/yellow single-bubble square pattern is formed. Even larger $\gamma_{12} = \gamma_{21}$ will further push away the two colors, leading to a complete separation between red and yellow, each of which has its own hexagonal pattern.

if $\gamma_{12} = \gamma_{21}$ is large as presented in the middle subfigure, the splitting strength between red and yellow components forces them to break (strong splitting leads to weak adhesion), forming all single bubbles of equal size and equal distance in the pattern of square lattice.

The bottom subfigure in Figure 2 is also interesting. In this case, the $\gamma_{12} = \gamma_{21}$ becomes much larger (even larger than $\gamma_{11} = \gamma_{22}$). Starting from a random initial, we still observe the quick phase separation. Different from the other two cases in which the red and yellow components are well mixed, the large $\gamma_{12} = \gamma_{21}$ separates the two colors. In each colored region, single bubbles of equal size and equal distance are assembled and form hexagonal pattern, similar as the binary case in Figure 1.

5. Concluding remarks. In this paper, we construct second-order stabilized linear semi-implicit schemes for the pACOK and pACON equations. For both binary and ternary systems, we consider two types of stabilizers and prove conditional energy stability in the semi-discrete and fully discrete schemes for the type $[\phi^{n+1} - 2\phi^n + \phi^{n-1}]$, and an unconditional energy stability in the other type $[\tau(\phi^{n+1} - \phi^n)]$.

In the numerical simulations, we observe some hexagonal and square patterns in bubble assemblies by the second-order scheme for pACOK dynamics when one species has much smaller volume than the other species in the binary system. With the second-order scheme for pACON dynamics, the repulsion between different species leads us to various equilibrium types in double bubble assemblies for the ternary system.

Our future research interests include extending the application of the second order scheme proposed in this paper to a disk domain with Neumann boundary condition. This will lead us to the pattern of bubbles, some of which interact with the domain boundary. Some higher-order schemes such as exponential time differencing based Runge-Kutta methods are also within our consideration. Another ongoing work is to consider a general long-range interaction term (not necessarily the term of $(-\Delta)^{-1}$), which might result in more interesting patterns.

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