ERROR ESTIMATES FOR SECOND-ORDER SAV FINITE ELEMENT METHOD TO PHASE FIELD CRYSTAL MODEL

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Abstract. In this paper, the second-order scalar auxiliary variable approach in time and linear finite element method in space are employed for solving the Cahn-Hilliard type equation of the phase field crystal model. The energy stability of the fully discrete scheme and the boundedness of numerical solution are studied. The rigorous error estimates of order $O(\tau^2 + h^2)$ in the sense of L^2-norm is derived. Finally, some numerical results are given to demonstrate the theoretical analysis.

1. **Introduction.** The phase field crystal (PFC) model is proposed by Elder *et al.*[5, 6] to study the microstructural evolution of crystal growth on atomic length and diffusive time scales. The PFC models are applied to describe a broad range of phenomena, including grain boundary dynamics, crystal nucleation, crystal growth, glass formation, crack propagation and many other properties of condensed matter [1].

It is challenging to solve the PFC model numerically due to the high-order derivative and its nonlinearity. Additionally, to obtain physical results of the PFC model, numerical schemes should be constructed to guarantee the energy dissipation. As a well-known approach, the convex splitting approach[8] can guarantee the numerical energy stability. For solving the PFC model, the convex splitting approach combined with different spatial discretization methods is studied, including spectral method[4, 19], finite difference method[13, 16, 29], finite element method[9, 26], and local discontinuous Galerkin method[11, 12]. However, all second-order schemes in the above study are nonlinear, and their implementations are too complex and costly owing to nonlinear equations to be solved at each time step. To obtain linear schemes for this model, the major difficulty is how to discretize the nonlinear and maintain energy stability. As a result, the stabilization method has been presented[22, 30], which adds an extra term with sufficient time accuracy. Yang and Han[31] have constructed linearly unconditionally energy stable schemes by using

the Invariant Energy Quadratization (IEQ) approach. Recently, Shen *et al.*[23] have proposed the scalar auxiliary variable (SAV) approach, which enjoys the advantages and overcomes most of the disadvantages of the IEQ approach. By introducing a scalar auxiliary variable, the SAV approach handles the nonlinear term explicitly and maintains the energy stable. More studies about the PFC problem can be found in recent literature [7, 14, 15, 18, 20, 21, 27].

There are many numerical studies of the PFC model, but few works are about convergence analysis and error estimates. Wise, Wang and Lowengrub[29] have provided the error estimates for the nonlinear first-order finite difference method based on the convex splitting method. Baskaran *et al.*[2] have given the convergence analysis of second-order fully discrete scheme equipped with splitting scheme and cell-centered finite differences method. Grasselli and Pierre[10] have established existence, uniqueness and discrete energy estimate for the semi-discrete and fully discrete finite element scheme for the modified PFC equation. Li and Shen[17] have carried out the analysis of energy stability and convergence for the SAV fourier-spectral method. In [28], we have used the finite element method with first-order SAV approach to solve the Allen-Cahn type equation of the PFC model, and give its energy stability and error analysis. Here, we furthermore give a second-order scheme and its detailed mathematical analysis.

The main contribution of this paper includes two parts. Firstly, we construct a fully discrete scheme for the Cahn-Hilliard type equation of the PFC model by combining linear finite element method and the SAV approach with Crank-Nicolson/Adams-Bashforth scheme. Our numerical scheme has four advantages including, (i) guaranteeing discrete energy stability; (ii) linear equations with constant coefficients is easy to implement at each time step; (iii) high flexibility via C^0 finite elements; (iv) second-order accuracy in time and space. Secondly, we provide rigorous mathematical analysis for the fully discrete scheme. We prove the energy stability and give further the discrete H^2 bound of the numerical solution. Using the discrete Gronwall's inequality, we derive optimal error estimate of the fully discrete scheme in detail.

The rest of this paper is organized as follows. We introduce the Landau-Brazovskii free energy functional, the governing equation and the coupled system in Sec. 2. In Sec. 3, we give the time and space discretization in detail. In Sec. 4, we analyze the mathematical properties of the fully discrete scheme, such as stability, boundedness and convergence. Some numerical experiments are shown to illustrate the accuracy and effectiveness of our scheme in Sec. 5. In Sec. 6, some concluding remarks are given.

2. **Physical model.** The free energy functional of Landau-Brazovskii (LB) model has the dimensionless form

$$\mathcal{E}(\phi(\mathbf{r})) = \int_\Omega \left\{ \frac{\xi^2}{2} [(\Delta + 1)\phi(\mathbf{r})]^2 + \frac{\alpha}{2} [\phi(\mathbf{r})]^2 - \frac{\gamma}{3!} [\phi(\mathbf{r})]^3 + \frac{1}{4!} [\phi(\mathbf{r})]^4 \right\} d\mathbf{r}. \quad (1)$$

The Cahn-Hilliard type dynamical equation of LB model is

$$\phi_t = \Delta \frac{\delta \mathcal{E}}{\delta \phi}. \quad (2)$$

Let $\beta > 0$, and denote that

$$\mathcal{N}(\phi) = \frac{\alpha - \beta}{2} \phi^2 - \frac{\gamma}{3!} \phi^3 + \frac{1}{4!} \phi^4, \quad (3)$$

then

$$\mathcal{N}'(\phi) = (\alpha - \beta)\phi - \frac{\gamma}{2}\phi^2 + \frac{1}{3!}\phi^3, \, \mathcal{N}''(\phi) = (\alpha - \beta) - \gamma\phi + \frac{1}{2}\phi^2, \, \mathcal{N}'''(\phi) = -\gamma + \phi.$$

Therefore, LB model becomes

$$\mathcal{E}(\phi(\mathbf{r})) = \int_\Omega \left\{ \frac{\xi^2}{2}[(\Delta + 1)\phi]^2 + \frac{\beta}{2}\phi^2 + \mathcal{N}(\phi) \right\} d\mathbf{r}. \tag{4}$$

The governing equation can be derived as

$$\phi_t = \Delta\psi, \tag{5a}$$

$$\psi = \xi^2(\Delta + 1)^2\phi + \beta\phi + \mathcal{N}'(\phi), \tag{5b}$$

$$\frac{\partial\phi}{\partial\mathbf{n}} = 0, \quad \frac{\partial(\Delta + 1)\phi}{\partial\mathbf{n}} = 0, \quad \frac{\partial\psi}{\partial\mathbf{n}} = 0 \quad on \, \partial\Omega. \tag{5c}$$

By introducing a new function $\psi = (\Delta + 1)\phi$, we can write Eq. (5) as the coupled system

$$\phi_t = \Delta\psi, \tag{6a}$$

$$\psi = \xi^2(\Delta + 1)\varphi + \beta\phi + \mathcal{N}'(\phi), \tag{6b}$$

$$\varphi = (\Delta + 1)\phi, \tag{6c}$$

$$\frac{\partial\phi}{\partial\mathbf{n}} = 0, \quad \frac{\partial\varphi}{\partial\mathbf{n}} = 0, \quad \frac{\partial\psi}{\partial\mathbf{n}} = 0 \quad on \, \partial\Omega. \tag{6d}$$

Remark 2.1. In Eq. (6), we apply the splitting technique, which is only applicable to convex regions [3].

Remark 2.2. The numerical scheme and analytical techniques in this paper can also be applied to the coupled system (6) with periodic boundary conditions.

3. **The fully discrete numerical scheme.** Here, we shall construct the semi-discrete scheme using the SAV approach, then derive fully discrete scheme by applying linear finite element method.

3.1. **Time discretization, second-order SAV scheme.** Applying the SAV appaorch with Crank-Nicolson/Adams-Bashforth scheme developed by Shen *et al.*[23], we discretize Eq. (6) in time direction.

The inner product and norm of $L^2(\Omega) = H^0(\Omega)$ is denoted as $(w, v) = \int_\Omega wv d\mathbf{r}$ and $\|w\| = (w, w)$, respectively.

Let $\mathcal{E}_1(\phi) = (\mathcal{N}(\phi), 1)$, and $u(\phi) = \frac{\mathcal{N}'(\phi)}{\sqrt{\mathcal{E}_1(\phi) + D_0}}$. We introduce the scalar auxiliary variable $s = \sqrt{\mathcal{E}_1(\phi) + D_0}$, where D_0 is a constant which ensures $\mathcal{E}_1(\phi) + D_0 \geq 0$ and write Eq. (6) as

$$\phi_t = \Delta\psi, \tag{7a}$$

$$\psi = \xi^2(\Delta + 1)\varphi + \beta\phi + u(\phi)s, \tag{7b}$$

$$\varphi = (\Delta + 1)\phi, \tag{7c}$$

$$s_t = \frac{1}{2}\big(u(\phi), \phi_t\big). \tag{7d}$$

Denote by f^n the approximation of $f(\mathbf{r}, t^n)$ at time $t^n = n\tau$, where τ is a fixed time step. For any sequence of functions $\{f^n\}_{n=1}^N$, we define

$$D_\tau^1 f^{n+1} = \frac{f^{n+1} - f^n}{\tau}, \quad \bar{f}^{n+1/2} = \frac{f^{n+1} + f^n}{2}, \quad \hat{f}^{n+1/2} = \frac{3f^n - f^{n-1}}{2} \quad (8a)$$

The second-order SAV scheme of Eq. (9) is constructed as follows, for $n \geq 0$, given $(\hat{\phi}^{n+1/2}, \phi^n, \varphi^n, s^n)$, find $(\phi^{n+1}, \psi^{n+1/2}, \varphi^{n+1}, s^{n+1})$ such that

$$D_\tau^1 \phi^{n+1} = \Delta \psi^{n+1/2}, \tag{9a}$$

$$\psi^{n+1/2} = \xi^2(\Delta + 1)\bar{\varphi}^{n+1/2} + \beta\bar{\phi}^{n+1/2} + u(\hat{\phi}^{n+1/2})\bar{s}^{n+1/2}, \tag{9b}$$

$$\varphi^{n+1} = (\Delta + 1)\phi^{n+1}, \tag{9c}$$

$$D_\tau^1 s^{n+1} = \frac{1}{2}\big(u(\hat{\phi}^{n+1/2}), D_\tau^1 \phi^{n+1}\big). \tag{9d}$$

Remark 3.1. There are several semi-discrete schemes based on SAV technique in Ref.[23].

3.2. **Spatial discretization, linear FEM.** We discretize Eq. (9) in space using the linear finite element method. Let $V(\Omega)$ represent the trial and test function spaces

$$V(\Omega) = \{v \in H^1(\Omega), \frac{\partial v}{\partial \mathbf{n}} = 0 \quad on\ \partial\Omega\}. \tag{10}$$

The corresponding Galerkin form of Eq. (9) can be stated as follows, for $n \geq 0$, given $(\hat{\phi}^{n+1/2}, \phi^n, \varphi^n, s^n)$, find $(\phi^{n+1}, \psi^{n+1/2}, \varphi^{n+1}, s^{n+1})$, such that

$$\big(D_\tau^1 \phi^{n+1}, v\big) = -\big(\nabla\psi^{n+1/2}, \nabla v\big) \quad \forall v \in V, \tag{11a}$$

$$\big(\psi^{n+1/2}, \zeta\big) = \xi^2\big(\bar{\varphi}^{n+1/2}, \zeta\big) - \xi^2\big(\nabla\bar{\varphi}^{n+1/2}, \nabla\zeta\big)$$
$$+ \big(\beta\bar{\phi}^{n+1/2}, \zeta\big) + \big(u(\hat{\phi}^{n+1/2})\bar{s}^{n+1/2}, \zeta\big) \quad \forall\zeta \in V, \tag{11b}$$

$$\big(\varphi^{n+1}, \chi\big) = \big(\phi^{n+1}, \chi\big) - \big(\nabla\phi^{n+1}, \nabla\chi\big) \quad \forall\chi \in V, \tag{11c}$$

$$D_\tau^1 s^{n+1/2} = \frac{1}{2}\big(u(\hat{\phi}^{n+1/2}), D_\tau^1 \phi^{n+1}\big), \tag{11d}$$

Let $\mathcal{T}_h = \{K\}$ be a partition of Ω, such as a conforming triangulation in two-dimensional bounded domain, and define the linear finite element space

$$V_h = \{v_h \in C^0(\Omega), v_h|_K \in P_1(K), \forall K \in \mathcal{T}_h\}.$$

Thus, we have the following fully discrete numerical scheme of Eq. (11), for $n \geq 0$, given $(\hat{\phi}_h^{n+1/2}, \phi_h^n, \varphi_h^n, s_h^n)$, find $(\phi_h^{n+1}, \psi_h^{n+1/2}, \varphi_h^{n+1}, s_h^{n+1})$, such that

$$\big(D_\tau^1 \phi_h^{n+1}, v_h\big) = -\big(\nabla\psi_h^{n+1/2}, \nabla v_h\big) \quad \forall v_h \in V_h, \tag{12a}$$

$$\big(\psi_h^{n+1/2}, \zeta_h\big) = \xi^2\big(\bar{\varphi}_h^{n+1/2}, \zeta_h\big) - \xi^2\big(\nabla\bar{\varphi}_h^{n+1/2}, \nabla\zeta_h\big)$$
$$+ \beta\big(\bar{\phi}_h^{n+1/2}, \zeta_h\big) + \big(u(\hat{\phi}_h^{n+1/2})\bar{s}_h^{n+1/2}, \zeta_h\big) \quad \forall\zeta_h \in V_h, \tag{12b}$$

$$\big(\varphi_h^{n+1}, \chi_h\big) = \big(\phi_h^{n+1}, \chi_h\big) - \big(\nabla\phi_h^{n+1}, \nabla\chi_h\big) \quad \forall\chi_h \in V_h, \tag{12c}$$

$$D_\tau^1 s_h^{n+1} = \frac{1}{2}\big(u(\hat{\phi}_h^{n+1/2}), D_\tau^1 \phi_h^{n+1}\big), \tag{12d}$$

where $\hat{\phi}_h^{n+1/2}, \phi_h^n, \phi_h^{n+1}, \varphi_h^n, \varphi_h^{n+1}, \psi_h^{n+1/2} \in V_h$.

Remark 3.2. When $n = 0$, $\hat{\phi}^{1/2}$ in Eq. (12) can be calculated by the following discrete scheme,

$$\big(\frac{\hat{\phi}_h^{1/2} - \phi_h^0}{\tau/2}, v_h\big) = -\big(\nabla\psi_h^{1/2}, \nabla v_h\big) \quad \forall v_h \in V_h, \tag{13a}$$

$$\big(\psi_h^{1/2}, \zeta_h\big) = \xi^2\big(\varphi_h^{1/2}, \zeta_h\big) - \xi^2\big(\nabla\varphi_h^{1/2}, \nabla v_h\big)$$
$$+ \beta\big(\hat{\phi}_h^{1/2}, \zeta_h\big) + \big(u(\phi_h^0)s_h^{1/2}, \zeta_h\big) \quad \forall \zeta_h \in V_h, \tag{13b}$$

$$\big(\varphi_h^{1/2}, \chi_h\big) = \big(\hat{\phi}_h^{1/2}, \chi_h\big) - \big(\nabla\hat{\phi}_h^{1/2}, \nabla\chi_h\big) \quad \forall \chi_h \in V_h, \tag{13c}$$

$$\frac{s_h^{1/2} - s_h^0}{\tau/2} = \frac{1}{2}\big(u(\phi_h^0), \frac{\hat{\phi}_h^{1/2} - \phi_h^0}{\tau/2}\big). \tag{13d}$$

4. **Mathematical analysis of the fully discrete scheme.** In this section, we are devoted to give the detailed mathematical analysis of the fully discrete scheme (9).

4.1. **Stability.** First of all, we shall analyze the energy stability of the scheme (12).

Theorem 4.1. *The scheme* (12) *is unconditionally energy stable with the modified energy* $\tilde{\mathcal{E}}$, *where*

$$\tilde{\mathcal{E}}(\varphi, \phi, s) = \frac{\xi^2}{2}\|\varphi\|^2 + \frac{\beta}{2}\|\phi\|^2 + s^2 - D_0.$$

Proof. We take $v_h = \psi_h^{n+1/2}$ in Eq. (12a) and find

$$\big(D_\tau^1\phi_h^{n+1}, \psi_h^{n+1/2}\big) = -\|\nabla\psi_h^{n+1/2}\|^2. \tag{14}$$

Taking $\zeta_h = D_\tau^1\phi_h^{n+1}$ in Eq. (12b), we have

$$\big(\psi_h^{n+1/2}, D_\tau^1\phi_h^{n+1}\big) = \xi_h^2\big(\bar{\varphi}_h^{n+1/2}, D_\tau^1\phi_h^{n+1}\big) - \xi^2\big(\nabla\bar{\varphi}_h^{n+1/2}, \nabla(D_\tau^1\phi_h^{n+1})\big)$$
$$+ \beta\big(\bar{\phi}_h^{n+1/2}, D_\tau^1\phi^{n+1}\big) + \big(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\phi_h^{n+1}\big)\bar{s}_h^{n+1/2}. \tag{15}$$

According to Eq. (12c), it is easy to obtain

$$\big(D_\tau^1\varphi_h^{n+1}, \chi_h\big) = \big(D_\tau^1\phi_h^{n+1}, \chi_h\big) - \big(\nabla(D_\tau^1\phi_h^{n+1}), \nabla\chi_h\big). \tag{16}$$

Setting $\chi_h = \bar{\varphi}_h^{n+1}$ to Eq. (16), we have

$$\big(D_\tau^1\phi_h^{n+1}, \bar{\varphi}_h^{n+1}\big) - \big(\nabla(D_\tau^1\phi_h^{n+1}), \nabla\bar{\varphi}_h^{n+1}\big)$$
$$= \big(D_\tau^1\varphi_h^{n+1}, \bar{\varphi}_h^{n+1}\big) = \frac{1}{2\tau}(\|\varphi_h^{n+1}\|^2 - \|\varphi_h^n\|^2). \tag{17}$$

Multiplying Eq. (12d) with $2\bar{s}_h^{n+1}$ leads to

$$\bar{s}_h^{n+1}\big(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\phi_h^{n+1}\big) = 2\bar{s}_h^{n+1}D_\tau^1 s_h^{n+1} = \frac{1}{\tau}\{(s_h^{n+1})^2 - (s_h^n)^2\}. \tag{18}$$

Combining Eq. (14), Eq. (15), Eq. (17) and Eq. (18), we find

$$\tilde{\mathcal{E}}_1(\varphi_h^{n+1}, \phi_h^{n+1}, s_h^{n+1}) - \tilde{\mathcal{E}}_1(\varphi_h^n, \phi_h^n, s_h^n)$$
$$= \frac{\xi^2}{2}\|\varphi_h^{n+1}\|^2 - \frac{\xi^2}{2}\|\varphi_h^n\|^2 + \frac{\beta}{2}\|\phi_h^{n+1}\|^2 - \frac{\beta}{2}\|\phi_h^n\|^2 + (s_h^{n+1})^2 - (s_h^n)^2 \tag{19}$$
$$= -\tau\|\psi_h^{n+1/2}\|^2 \leq 0.$$

$\square$

4.2. **Boundedness of numerical solution.** Let $L_0^2(\Omega), = \{v \in L^2(\Omega) | (v, 1) = 0\}$ and $\mathring{V} = L_0^2 \cap V$, where $V \subset L^2(\Omega)$.

We define the discrete Laplace operator $\Delta_h, V_h \to \mathring{V}_h$ such that

$$(\Delta_h w_h, v_h) = (-\nabla w_h, \nabla v_h), \quad \forall v_h \in V_h. \tag{20}$$

and the inverse discrete Laplace operator $(-\Delta_h)^{-1}, \mathring{V}_h \to \mathring{V}_h$ such that

$$(\nabla(-\Delta_h)^{-1} w_h, \nabla v_h) = (w_h, v_h), \quad \forall v_h \in V_h. \tag{21}$$

Then the discrete H^2 norm and H^{-1} norm can be defined as follows

$$\|v_h\|_{H^2} = \|v_h\| + \|\nabla v_h\| + \|\Delta_h v_h\|, \forall v_h \in V_h, \tag{22a}$$

$$\|v_h\|_{H^{-1}} = \sqrt{((-\Delta_h)^{-1} v_h, v_h)}, \forall v_h \in \mathring{V}_h. \tag{22b}$$

We shall establish the H^2-boundedness for the numerical solution of the scheme (12), which is of great significance to the derivation of error estimate.

Lemma 4.2. *Let ϕ_h^n be solutions of the scheme* (12). *There exists a positive constant C such that,*

$$\|\phi_h^n\|_{H^2} \leq C. \tag{23}$$

Proof. According to Theorem 4.1, there exists a positive constant C such that ,

$$\frac{\xi^2}{2} \|\varphi_h^k\|^2 + \frac{\beta}{2} \|\phi_h^k\|^2 + (s_h^k)^2 \leq C, \quad \forall k \geq 0, \tag{24}$$

then

$$\|\phi_h^k\| \leq C, \quad \|\varphi_h^k\| \leq C. \tag{25}$$

Thanks to Eq. (12c), we have

$$\begin{aligned} (\nabla \phi_h^k, \nabla \phi_h^k) &= (\phi_h^k, \phi_h^k) - (\varphi_h^k, \phi_h^k), \\ (\nabla \phi_h^k, \nabla \Delta_h \phi_h^k) &= (\phi_h^k, \Delta_h \phi_h^k) - (\varphi_h^k, \Delta_h \phi_h^k), \end{aligned}$$

it follows that

$$\begin{aligned} \|\nabla \phi_h^k\|^2 &\leq \|\phi_h^k\|^2 + \|\phi_h^k\| \|\varphi_h^k\| \leq C, \\ \|\Delta_h \phi_h^k\|^2 &\leq \|\phi_h^k\| \|\Delta_h \phi_h^k\| + \|\varphi_h^k\| \|\Delta_h \phi_h^k\|, \\ \|\Delta_h \phi_h^k\| &\leq \|\phi_h^k\| + \|\varphi_h^k\| \leq C. \end{aligned} \tag{26}$$

Using Eq. (25) and Eq. (26), we can deduce Eq. (23). □

4.3. **Error estimate.** Here, we shall derive error estimates with further assumption of the smoothness of the exact solution.

For simplification, we define

$$\begin{aligned} T_f^{1,n+1/2} &= D_\tau^1 f(t^{n+1}) - f_t(t^{n+1/2}), \\ \bar{T}_f^{n+1/2} &= \bar{f}(t^{n+1/2}) - f(t^{n+1/2}), \\ \tilde{T}_f^n &= 2f^n - f^{n-1} - f^{n+1}. \end{aligned} \tag{27}$$

Lemma 4.3. *For $\nu = -1, 0, 1, 2$, the following estimates hold,*

$$\|T_f^{1,n+1/2}\|_{H^\nu}^2 \leq \tau^3 \int_{t^n}^{t^{n+1}} \|\phi_{ttt}(r)\|_{H^\nu}^2 \mathrm{d}r,$$

$$\|\bar{T}_f^{n+1/2}\|_{H^\nu}^2 \leq \tau^3 \int_{t^n}^{t^{n+1}} \|\phi_{ttt}(r)\|_{H^\nu}^2 \mathrm{d}r, \tag{28}$$

$$\|\tilde{T}_f^n\|_{H^\nu}^2 \leq \tau^3 \int_{t^{n-1}}^{t^{n+1}} \|\phi_{tt}(r)\|_{H^\nu}^2 \mathrm{d}r.$$

Lemma 4.4. *If w is the solution of Eq. (9) or Eq. (12), using Lemma 4.2, we have*

$$|\mathcal{N}(w)|, |\mathcal{N}'(w)|, |\mathcal{N}''(w)| \leq C. \tag{29}$$

Lemma 4.5. *For s in Eq. (9), and assuming that $\|\nabla\phi\|_{L^\infty((0,T)\times\Omega)} \leq C$, it follows that*

$$\int_{t^n}^{t^{n+1}} |s_{tt}(r)|^2 \mathrm{d}r \leq C \int_{t^n}^{t^{n+1}} \|\phi_t(r)\|_{H^1}^4 + \|\phi_{tt}(r)\|^2 \mathrm{d}r, \tag{30}$$

$$\int_{t^n}^{t^{n+1}} |s_{ttt}(r)|^2 \mathrm{d}r \leq C \int_{t^n}^{t^{n+1}} (\|\phi_t(r)\|_{H^1}^4 + \|\phi_t(r)\|_{H^1}^6$$
$$+ \|\phi_{tt}(r)\|^4 + \|\phi_{ttt}(r)\|_{H^{-1}}^2) \mathrm{d}r. \tag{31}$$

Proof. Using Lemma 4.4, we obtain

$$s_{tt} = -\frac{1}{4\sqrt{(\mathcal{E}_1(\phi) + D_0)^3}} \left(\int_\Omega \mathcal{N}'(\phi)\phi_t \mathrm{d}r\right)^2$$
$$+ \frac{1}{2\sqrt{\mathcal{E}_1(\phi) + D_0}} \int_\Omega [\mathcal{N}''(\phi)\phi_t^2 + \mathcal{N}'(\phi)\phi_{tt}] \mathrm{d}r$$
$$\leq C\{\|\mathcal{N}'(\phi)\|^2\|\phi_t\|_{L^6}^2 + \|\mathcal{N}''(\phi)\|\|\phi_t\|_{L^6}^2 + \|\mathcal{N}'(\phi)\|\|\phi_{tt}\|\}$$
$$\leq C\{\|\phi_t\|_{H^1}^2 + \|\phi_{tt}\|\},$$

and

$$s_{ttt} = \frac{3}{8\sqrt{(\mathcal{E}_1(\phi) + D_0)^5}} \left(\int_\Omega \mathcal{N}'(\phi)\phi_t \mathrm{d}r\right)^3$$
$$- \frac{3}{4\sqrt{(\mathcal{E}_1(\phi) + D_0)^3}} \int_\Omega \mathcal{N}'(\phi)\phi_t \mathrm{d}r \int_\Omega (\mathcal{N}''(\phi)\phi_t^2 + \mathcal{N}'(\phi)\phi_{tt}) \mathrm{d}r$$
$$+ \frac{1}{2\sqrt{\mathcal{E}_1(\phi) + D_0}} \int_\Omega (\mathcal{N}'''(\phi)\phi_t^3 + 3\mathcal{N}''(\phi)\phi_t\phi_{tt} + \mathcal{N}'(\phi)\phi_{ttt}) \mathrm{d}r$$
$$\leq C\{\|\mathcal{N}'(\phi)\|^3\|\phi_t\|_{L^6}^3 + \|\mathcal{N}'(\phi)\|\|\phi_t\|_{L^6}(\|\mathcal{N}''(\phi)\|\|\phi_t\|_{L^6}^2 + \|\mathcal{N}'(\phi)\|\|\phi_{tt}\|)$$
$$+ \|\mathcal{N}'''(\phi)\|\|\phi_t\|_{L^6}^3 + \|\phi_t\|_{L^6}\|\mathcal{N}''(\phi)\|\|\phi_{tt}\|$$
$$+ \|\mathcal{N}''(\phi)\|\|\nabla\phi\|_{L^\infty((0,T)\times\Omega)}\|\phi_{ttt}\|_{H^{-1}}\}$$
$$\leq C\{\|\phi_t\|_{H^1}^2 + \|\phi_t\|_{H^1}^3 + \|\phi_{tt}\|^2 + \|\phi_{ttt}\|_{H^{-1}}\}.$$

Then Lemma 4.5 is obtained.   □

Assuming that the solutions ϕ, ψ and φ of Eq. (9) exist and satisfy

$$
\begin{aligned}
&\|\psi\|_{H^2} + \|\psi_t\|_{H^2} + \|\varphi\|_{H^2} + \|\varphi_t\|_{H^2} \\
&\quad + \|\phi\|_{H^2} + \|\phi_t\|_{H^2} + \|\phi_{tt}\|_{H^2} + \|\phi_{ttt}\|_{H^2} \leq C, \\
&\|\phi\|_{L^\infty(0,T;W^{1,\infty})} + \|\phi_t\|_{L^\infty(0,T,L^2)} + \|\phi_t\|_{L^2(0,T;H^1)} + \|\phi_{tt}\|_{L^2(0,T;L^2)} \\
&\quad + \|\phi_{ttt}\|_{L^2(0,T;H^{-1})} + \|\varphi_{tt}\|_{L^2(0,T;H^3)} \leq C.
\end{aligned}
\tag{32}
$$

Let

$$
\theta_w = w_h - R_h w, \quad \rho_w = R_h w - w(t),
\tag{33}
$$

where $R_h w \in V_h$ is the standard elliptic projection operator of w_h, i.e.

$$
(\nabla(R_h w - w(t)), \nabla v_h) = 0, \quad \forall v_h \in V_h.
\tag{34}
$$

It is easy to know

$$
e_w^n = w_h^n - w(t^n) = \theta_w^n + \rho_w^n.
\tag{35}
$$

Lemma 4.6. ([25]) *If* $w, w_t \in C(0,T;H^2)$, *there exists a positive constant* C *indepentent of* $t \in [0,T]$, *such that*

$$
\|\rho_w\| + h\|\nabla\rho_w\| \leq Ch^2,
\tag{36}
$$

$$
\|\rho_{w_t}\| + h\|\nabla\rho_{w_t}\| \leq Ch^2.
\tag{37}
$$

Theorem 4.7. *Let* ϕ *and* ϕ_h^n *be solutions of Eq. (9) and Eq. (12), respectively. Assume* $\phi^0 \in H^2$ *and the assumption* (32) *holds, we have*

$$
\|e_\psi^n\|^2 + \|e_\phi^n\|^2 + (e_s^n)^2 \leq C(\tau^4 + h^4), \quad 0 < n < T/\tau.
\tag{38}
$$

Proof. We shall show the proving process in six steps.

Step 1. we construct the error equaiton (43) by using Eq. (9) and Eq. (12).

Eq. (9) can be reformulated as

$$
\big(\phi_t(t^{n+1/2}), v_h\big) = -\big(\nabla\psi(t^{n+1/2}), \nabla v_h\big),
\tag{39a}
$$

$$
\begin{aligned}
\big(\psi(t^{n+1/2}), \zeta_h\big) = {}& \xi^2\big(\varphi(t^{n+1/2}), \zeta_h\big) - \xi^2\big(\nabla\varphi(t^{n+1/2}), \nabla\zeta_h\big) \\
&+ \beta\big(\phi(t^{n+1/2}), \zeta_h\big) + \big(u(\phi(t^{n+1/2}))s(t^{n+1/2}), \zeta_h\big),
\end{aligned}
\tag{39b}
$$

$$
\big(\varphi(t^{n+1}), \chi_h\big) = \big(\phi(t^{n+1}), \chi_h\big) - \big(\nabla\phi(t^{n+1}), \nabla\chi_h\big),
\tag{39c}
$$

$$
s_t(t^{n+1/2}) = \frac{1}{2}\big(u(\phi(t^{n+1/2})), \phi_t(t^{n+1/2})\big).
\tag{39d}
$$

Subtracting Eq. (39) from Eq. (12) leads to

$$
\big(D_\tau^1 e_\phi^{n+1} + T_\phi^{1,n+1/2}, v_h\big) = -\big(\nabla e_\psi^{n+1/2}, \nabla v_h\big),
\tag{40a}
$$

$$
\begin{aligned}
\big(e_\psi^{n+1/2}, \zeta_h\big) = {}& \xi^2\big(\bar{e}_\varphi^{n+1/2} + \bar{T}_\varphi^{n+1/2}, \zeta_h\big) - \xi^2\big(\nabla(\bar{e}_\varphi^{n+1/2} + \bar{T}_\varphi^{n+1/2}), \nabla\zeta_h\big) \\
&+ \beta\big(\bar{e}_\phi^{n+1/2}, \zeta_h\big) + \big(u(\hat{\phi}_h^{n+1/2})\bar{s}_h^{n+1/2} - u(\phi(t^{n+1/2}))s(t^{n+1/2}), \zeta_h\big),
\end{aligned}
\tag{40b}
$$

$$
\big(e_\varphi^{n+1}, \chi_h\big) = \big(e_\phi^{n+1}, \chi_h\big) - \big(\nabla e_\phi^{n+1}, \nabla\chi_h\big),
\tag{40c}
$$

$$
D_\tau^1 e_s^{n+1} + T_s^{1,n+1/2} = \frac{1}{2}\{\big(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\phi_h^{n+1}\big) - \big(u(\phi(t^{n+1/2})), \phi_t(t^{n+1/2})\big)\}.
\tag{40d}
$$

Let $\hat{e}_u^{n+1/2} = u(\hat{\phi}_h^{n+1/2}) - u(\phi(t^{n+1/2}))$, we obtain

$$u(\hat{\phi}_h^{n+1/2})\bar{s}_h^{n+1/2} - u(\phi(t^{n+1/2}))s(t^{n+1/2})$$
$$= u(\hat{\phi}_h^{n+1/2})(\bar{e}_s^{n+1/2} + \bar{T}_s^{n+1/2}) + \hat{e}_u^{n+1/2}s(t^{n+1/2}), \tag{41a}$$

$$\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\phi_h^{n+1}\right) - \left(u(\phi^{n+1/2}), \phi_t(t^{n+1/2})\right)$$
$$= \left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1 e_\phi^{n+1} + T_\phi^{1,n+1/2}\right) + \left(\hat{e}_u^{n+1/2}, \phi_t(t^{n+1/2})\right). \tag{41b}$$

Then we can write Eq. (40) as

$$\left(D_\tau^1 e_\phi^{n+1}, v_h\right) = -\left(T_\phi^{1,n+1/2}, v_h\right) - \left(\nabla e_\psi^{n+1/2}, \nabla v_h\right), \tag{42a}$$

$$\left(e_\psi^{n+1/2}, \zeta_h\right) = \xi^2\left(\bar{e}_\varphi^{n+1/2} + \bar{T}_\varphi^{n+1/2}, \zeta_h\right) - \xi^2\left(\nabla(\bar{e}_\varphi^{n+1/2} + \bar{T}_\varphi^{n+1/2}), \nabla\zeta_h\right)$$
$$+ \beta\left(\bar{e}_\phi^{n+1/2}, \zeta_h\right)$$
$$+ \left(u(\hat{\phi}_h^{n+1/2})(\bar{e}_s^{n+1/2} + \bar{T}_s^{n+1/2}) + \hat{e}_u^{n+1/2}s(t^{n+1/2}), \zeta_h\right), \tag{42b}$$

$$\left(e_\varphi^{n+1}, \chi_h\right) = \left(e_\phi^{n+1}, \chi_h\right) - \left(\nabla e_\phi^{n+1}, \nabla\chi_h\right), \tag{42c}$$

$$D_\tau^1 e_s^{n+1} = \frac{1}{2}\left\{\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1 e_\phi^{n+1} + T_\phi^{1,n+1/2}\right)\right.$$
$$\left. + \left(\hat{e}_u^{n+1/2}, \phi_t(t^{n+1/2})\right)\right\} - T_s^{1,n+1/2}. \tag{42d}$$

Combining Eq.(42) with Eq.(34)-(35), we arrive at

$$\left(D_\tau^1\theta_\phi^{n+1}, v_h\right) + \left(\nabla\theta_\psi^{n+1/2}, \nabla v_h\right) = -\left(T_\phi^{1,n+1/2}, v_h\right) - \left(D_\tau^1\rho_\phi^{n+1}, v_h\right), \tag{43a}$$

$$\left(\theta_\psi^{n+1/2}, \zeta_h\right) - \xi^2\left(\bar{\theta}_\varphi^{n+1/2}, \zeta_h\right) + \xi^2\left(\nabla\bar{\theta}_\varphi^{n+1/2}, \nabla\zeta_h\right) - \beta\left(\bar{\theta}_\phi^{n+1/2}, \zeta_h\right)$$
$$= \xi^2\left(\bar{T}_\varphi^{n+1/2}, \zeta_h\right) - \xi^2\left(\nabla\bar{T}_\varphi^{n+1/2}, \nabla\zeta_h\right) + \left(\xi^2\bar{\rho}_\varphi^{n+1/2} - \rho_\psi^{n+1/2}, \zeta_h\right)$$
$$+ \beta\left(\bar{\rho}_\phi^{n+1/2}, \zeta_h\right) + \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), \zeta_h\right)$$
$$+ \bar{T}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), \zeta_h\right) + s(t^{n+1/2})\left(\hat{e}_u^{n+1/2}, \zeta_h\right), \tag{43b}$$

$$\left(\theta_\varphi^{n+1}, \chi_h\right) - \left(\theta_\phi^{n+1}, \chi_h\right) + \left(\nabla\theta_\phi^{n+1}, \nabla\chi_h\right) = \left(\rho_\phi^{n+1} - \rho_\varphi^{n+1}, \chi_h\right), \tag{43c}$$

$$2D_\tau^1 e_s^{n+1} = \left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\theta_\phi^{n+1}\right) + \left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\rho_\phi^{n+1}\right)$$
$$+ \left(u(\hat{\phi}_h^{n+1/2}), T_\phi^{1,n+1/2}\right) + \left(\hat{e}_u^{n+1/2}, \phi_t(t^{n+1/2})\right) - 2T_s^{1,n+1/2}. \tag{43d}$$

Step 2. we derive the error estimate formulas (48) on the basis of Eqs. (43).
Setting $v_h = \theta_\psi^{n+1/2}$ in Eq. (43a) gives

$$\left(D_\tau^1\theta_\phi^{n+1}, \theta_\psi^{n+1/2}\right) + \|\nabla\theta_\psi^{n+1/2}\|^2 = -\left(T_\phi^{1,n+1/2}, \theta_\psi^{n+1/2}\right) - \left(D_\tau^1\rho_\phi^{n+1}, \theta_\psi^{n+1/2}\right). \tag{44}$$

Taking $\zeta_h = D_\tau^1\theta_\phi^{n+1}$ in Eq. (43b) leads to

$$\left(\theta_\psi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) - \xi^2\left(\bar{\theta}_\varphi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) + \xi^2\left(\nabla\bar{\theta}_\varphi^{n+1/2}, \nabla D_\tau^1\theta_\phi^{n+1}\right) - \frac{\beta}{2}D_\tau^1\|\theta_\phi^{n+1}\|^2$$
$$= \xi^2\left(\bar{T}_\varphi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) - \xi^2\left(\nabla\bar{T}_\varphi^{n+1/2}, \nabla D_\tau^1\theta_\phi^{n+1}\right) + \left(\xi^2\bar{\rho}_\varphi^{n+1/2} - \rho_\psi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right)$$
$$+ \beta\left(\bar{\rho}_\phi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) + \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\theta_\phi^{n+1}\right)$$
$$+ \bar{T}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\theta_\phi^{n+1}\right) + s(t^{n+1/2})\left(\hat{e}_u^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right). \tag{45}$$

Using Eq. (43c) and writing $\chi_h = \bar{\theta}_\varphi^{n+1/2}$, we have

$$\frac{1}{2}D_\tau^1\|\theta_\varphi^{n+1}\|^2 - \left(D_\tau^1\theta_\phi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\right) + \left(\nabla(D_\tau^1\theta_\phi^{n+1}), \nabla\bar{\theta}_\varphi^{n+1/2}\right)$$
$$= \left(D_\tau^1\rho_\phi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\right) - \left(D_\tau^1\rho_\varphi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\right). \tag{46}$$

Multiplying Eq. (43d) by $\bar{e}_s^{n+1/2}$ gives rise to

$$D_\tau^1(e_s^{n+1})^2 = \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\theta_\phi^{n+1}\right) + \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\rho_\phi^{n+1}\right)$$
$$+ \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), T_\phi^{1,n+1/2}\right) + \bar{e}_s^{n+1/2}\left(\hat{e}_u^{n+1/2}, \phi_t(t^{n+1/2})\right)$$
$$- 2\bar{e}_s^{n+1/2}T_s^{1,n+1/2}. \tag{47}$$

Together with Eq. (44)-Eq. (47), we can derive

$$\frac{\xi^2}{2}D_\tau^1\|\theta_\varphi^{n+1}\|^2 + \frac{\beta}{2}D_\tau^1\|\theta_\phi^{n+1}\|^2 + D_\tau^1(e_s^{n+1})^2 + \|\nabla\theta_\psi^{n+1/2}\|^2$$
$$= -\left(T_\phi^{1,n+1/2}, \theta_\psi^{n+1/2}\right) - \left(D_\tau^1\rho_\phi^{n+1}, \theta_\psi^{n+1/2}\right)$$
$$- \xi^2\left(\bar{T}_\varphi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) + \xi^2\left(\nabla\bar{T}_\varphi^{n+1/2}, \nabla D_\tau^1\theta_\phi^{n+1}\right)$$
$$- \left(\xi^2\bar{\rho}_\varphi^{n+1/2} - \rho_\psi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) - \beta\left(\bar{\rho}_\phi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right)$$
$$- \bar{T}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\theta_\phi^{n+1}\right) - s(t^{n+1/2})\left(\hat{e}_u^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right)$$
$$+ \xi^2\left(D_\tau^1\rho_\phi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\right) - \xi^2\left(D_\tau^1\rho_\varphi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\right)$$
$$+ \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\rho_\phi^{n+1}\right) + \bar{e}_s^{n+1/2}\left(u(\hat{\phi}_h^{n+1/2}), T_\phi^{1,n+1/2}\right)$$
$$+ \bar{e}_s^{n+1/2}\left(\hat{e}_u^{n+1/2}, \phi_t(t^{n+1/2})\right) - 2\bar{e}_s^{n+1/2}T_s^{1,n+1/2}. \tag{48}$$

Step 3. we estimate each term at the right of Eq. (48) and obtain Eq. (63).

Using Lemma 4.3 and Lemma 4.6, we find

$$-\left(T_\phi^{1,n+1/2}, \theta_\psi^{n+1/2}\right) \leq 4\|T_\phi^{1,n+1/2}\|_{H^{-1}}^2 + \frac{1}{16}\|\nabla\theta_\psi^{n+1/2}\|^2$$
$$\leq C\tau^4 + \frac{1}{16}\|\nabla\theta_\psi^{n+1/2}\|^2, \tag{49}$$

$$-\left(D_\tau^1\rho_\phi^{n+1}, \theta_\psi^{n+1/2}\right) \leq 4\|D_\tau^1\rho_\phi^{n+1}\|_{H^{-1}}^2 + \frac{1}{16}\|\nabla\theta_\psi^{n+1/2}\|^2$$
$$\leq Ch^6 + \frac{1}{16}\|\nabla\theta_\psi^{n+1/2}\|^2, \tag{50}$$

$$-\xi^2\left(\bar{T}_\varphi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) \leq 4\xi^4\|\bar{T}_\varphi^{n+1/2}\|^2 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2$$
$$\leq C\tau^4 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2, \tag{51}$$

$$-\xi^2\left(\nabla\bar{T}_\varphi^{n+1/2}, \nabla D_\tau^1\theta_\phi^{n+1}\right) \leq 4\xi^4\|\Delta\bar{T}_\varphi^{n+1/2}\|^2 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2$$
$$\leq C\tau^4 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2, \tag{52}$$

and

$$-\left(\xi^2\bar{\rho}_\varphi^{n+1/2} - \rho_\psi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\right) \leq \|\xi^2\bar{\rho}_\varphi^{n+1/2} - \rho_\psi^{n+1/2}\|^2 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2$$
$$\leq Ch^4 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2, \tag{53}$$

$$-\beta\big(\bar{\rho}_\phi^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\big) \le \beta\|\bar{\rho}_\phi^{n+1/2}\|^2 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2$$

$$\le Ch^4 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2, \tag{54}$$

$$\xi^2\big(D_\tau^1\rho_\phi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\big) \le \frac{\xi^2}{4}\|D_\tau^1\rho_\phi^{n+1}\|^2 + \xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2,$$

$$\le Ch^4 + \xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2, \tag{55}$$

$$-\xi^2\big(D_\tau^1\rho_\varphi^{n+1}, \bar{\theta}_\varphi^{n+1/2}\big) \le \frac{\xi^2}{4}\|D_\tau^1\rho_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2,$$

$$\le Ch^4 + \xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2. \tag{56}$$

Using Lemma 4.2, we can obtain $\|u(\hat{\phi}_h^{n+1/2})\| \le C$. With the assumption (32), we get

$$-\bar{T}_s^{n+1/2}\big(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\theta_\phi^{n+1}\big) \le \|u(\hat{\phi}_h^{n+1/2})\|(\bar{T}_s^{n+1/2})^2 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2$$

$$\le C\tau^4 + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2, \tag{57}$$

$$-s(t^{n+1/2})\big(\hat{e}_u^{n+1/2}, D_\tau^1\theta_\phi^{n+1}\big) \le C\|\hat{e}_u^{n+1/2}\| + \frac{1}{16}\|D_\tau^1\theta_\phi^{n+1}\|^2, \tag{58}$$

$$\bar{e}_s^{n+1/2}\big(u(\hat{\phi}_h^{n+1/2}), D_\tau^1\rho_\phi^{n+1}\big) \le \frac{1}{2}\|u(\hat{\phi}_h^{n+1/2})\|^2\{\|D_\tau^1\rho_\phi^{n+1}\|^2 + (e_s^{n+1})^2 + (e_s^n)^2\}$$

$$\le C\{h^4 + (e_s^{n+1})^2 + (e_s^n)^2\}, \tag{59}$$

$$\bar{e}_s^{n+1/2}\big(u(\hat{\phi}_h^{n+1/2}), T_\phi^{1,n+1/2}\big) \le \frac{1}{2}\|u(\hat{\phi}_h^{n+1/2})\|^2\{\|T_\phi^{1,n+1/2}\|^2 + (e_s^{n+1})^2 + (e_s^n)^2\}$$

$$\le C\{\tau^4 + (e_s^{n+1})^2 + (e_s^n)^2\}, \tag{60}$$

$$\bar{e}_s^{n+1/2}\big(\hat{e}_u^{n+1/2}, \phi_t(t^{n+1/2})\big) \le \frac{1}{2}\|\phi_t(t^{n+1/2})\|^2\{\|\hat{e}_u^{n+1/2}\|^2 + (e_s^{n+1})^2 + (e_s^n)^2\},$$

$$\le C\{\|\hat{e}_u^{n+1/2}\|^2 + (e_s^{n+1})^2 + (e_s^n)^2\}, \tag{61}$$

$$2\bar{e}_s^{n+1/2}T_s^{1,n+1/2} \le \|T_s^{1,n+1/2}\|^2 + (e_s^{n+1})^2 + (e_s^n)^2,$$

$$\le C\tau^4 + (e_s^{n+1})^2 + (e_s^n)^2. \tag{62}$$

Using Eq. (49)-(62), Eq. (48) can be rewritten as

$$\frac{\xi^2}{2}D_\tau^1\|\theta_\varphi^{n+1}\|^2 + \frac{\beta}{2}D_\tau^1\|\theta_\phi^{n+1}\|^2 + D_\tau^1(e_s^{n+1})^2 + \frac{7}{8}\|\nabla\theta_\psi^{n+1/2}\|^2$$

$$\le C(\xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2 + \|\theta_\phi^{n+1}\|^2 + \|\theta_\phi^n\|^2 + (e_s^{n+1})^2$$

$$+ (e_s^n)^2) + C\|\hat{e}_u^{n+1/2}\|^2 + \frac{3}{8}\|D_\tau^1\theta_\phi^{n+1}\|^2 + C(\tau^4 + h^4). \tag{63}$$

Step 4. we eliminate $\|D_\tau^1\theta_\phi^{n+1}\|^2$ at the right hand side of Eq. (63).

Taking $v_h = \theta_\phi^{n+1}$ in Eq. (43a), and we have

$$\big(D_\tau^1\theta_\phi^{n+1}, \theta_\phi^{n+1}\big) + \big(\nabla\theta_\psi^{n+1/2}, \nabla\theta_\phi^{n+1}\big)$$

$$= -\big(T_\phi^{1,n+1/2}, \theta_\phi^{n+1}\big) - \big(D_\tau^1\rho_\phi^{n+1}, \theta_\phi^{n+1}\big),$$

it follows that

$$\frac{1}{2}D_\tau^1\|\theta_\phi^{n+1}\|^2 + \frac{1}{2}\|D_\tau^1\theta_\phi^{n+1}\|^2$$

$$\leq \|\nabla\theta_\phi^{n+1}\|^2 + \|\theta_\phi^{n+1}\|^2 + \frac{1}{4}\|\nabla\theta_\psi^{n+1/2}\|^2 + C(\tau^4 + h^4). \tag{64}$$

Setting $\chi_h = \theta_\phi^{n+1}$ in Eq. (43c) gives that

$$\left(\theta_\varphi^{n+1}, \theta_\phi^{n+1}\right) - \left(\theta_\phi^{n+1}, \theta_\phi^{n+1}\right) + \left(\nabla\theta_\phi^{n+1}, \nabla\theta_\phi^{n+1}\right)$$
$$= \left(\rho_\phi^{n+1} - \rho_\varphi^{n+1}, \theta_\phi^{n+1}\right),$$

then

$$\|\nabla\theta_\phi^{n+1}\|^2 \leq C(\|\theta_\varphi^{n+1}\|^2 + \|\theta_\phi^{n+1}\|^2) + C(\tau^4 + h^4). \tag{65}$$

Using Eq. (64) and Eq. (65), Eq. (63) can be transformed into

$$\frac{\xi^2}{2}D_\tau^1\|\theta_\varphi^{n+1}\|^2 + \frac{\beta+1}{2}D_\tau^1\|\theta_\phi^{n+1}\|^2 + D_\tau^1(e_s^{n+1})^2 + \frac{1}{8}\|D_\tau^1\theta_\phi^{n+1}\|^2 + \frac{5}{8}\|\nabla\theta_\psi^{n+1/2}\|^2$$
$$\leq C(\xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2 + \|\theta_\phi^{n+1}\|^2 + \|\theta_\phi^n\|^2 + (e_s^{n+1})^2 + (e_s^n)^2)$$
$$+ C\|\hat{e}_u^{n+1/2}\|^2 + C(\tau^4 + h^4). \tag{66}$$

Step 5. we estimate $\|\hat{e}_u^{n+1/2}\|^2$ in different situation.

Let $G(w) = \sqrt{\mathcal{E}_1(w) + D_0}$, we can deduce that

$$\hat{e}_u^{n+1/2} = u(\hat{\phi}_h^{n+1/2}) - u(\phi(t^{n+1/2}))$$
$$= \frac{\mathcal{N}'(\hat{\phi}_h^{n+1/2})}{G(\hat{\phi}_h^{n+1/2})} - \frac{\mathcal{N}'(\phi(t^{n+1/2})}{G(\phi(t^{n+1/2}))}$$
$$= \frac{\mathcal{N}'(\hat{\phi}_h^{n+1/2})}{G(\hat{\phi}_h^{n+1/2})} - \frac{\mathcal{N}'(\hat{\phi}_h^{n+1/2})}{G(\phi(t^{n+1/2}))} + \frac{\mathcal{N}'(\hat{\phi}_h^{n+1/2})}{G(\phi(t^{n+1/2}))} - \frac{\mathcal{N}'(\phi(t^{n+1/2}))}{G(\phi(t^{n+1/2}))}$$
$$= \frac{\mathcal{N}'(\hat{\phi}_h^{n+1/2})(\mathcal{E}_1(\phi(t^{n+1/2})) - \mathcal{E}_1(\hat{\phi}_h^{n+1/2}))}{G(\hat{\phi}_h^{n+1/2})G(\phi(t^{n+1/2}))[G(\hat{\phi}_h^{n+1/2}) + G(\phi(t^{n+1/2}))]}$$
$$+ \frac{\mathcal{N}'(\hat{\phi}_h^{n+1/2}) - \mathcal{N}'(\phi(t^{n+1/2}))}{G(\phi(t^{n+1/2}))}. \tag{67}$$

Combining with the assumption of (32) and Lemma 4.4, we get

$$\|\hat{e}_u^{n+1/2}\| \leq C\|\hat{\phi}_h^{n+1/2} - \phi(t^{n+1/2})\|. \tag{68}$$

when $n = 0$, we have

$$\|\hat{e}_u^{1/2}\| = \|\hat{\phi}_h^{1/2} - \phi(t^{1/2})\| \leq \|\hat{\theta}_\phi^{1/2}\| + Ch^2.$$

Starting from Eq. (13), and using a similar process described as step 1-4, we can obtain

$$\frac{\xi^2}{2}D_\tau^1\|\theta_\varphi^{1/2}\|^2 + \frac{\beta+1}{2}D_\tau^1\|\hat{\theta}_\phi^{1/2}\|^2 + D_\tau^1(e_s^{1/2})^2 + \frac{1}{8}\|D_\tau^1\hat{\theta}_\phi^{1/2}\|^2 + \frac{5}{8}\|\nabla\theta_\psi^{1/2}\|^2$$
$$\leq C(\xi^2\|\theta_\varphi^{1/2}\|^2 + \xi^2\|\theta_\varphi^0\|^2 + \|\hat{\theta}_\phi^{1/2}\|^2 + \|\theta_\phi^0\|^2 + (e_s^{1/2})^2 + (e_s^0)^2)$$
$$+ C\|u(\phi_h^0) - u(\phi(t^{1/2}))\|^2 + C(\tau^4 + h^4)$$

$$\leq C(\xi^2 \|\theta_\varphi^{1/2}\|^2 + \xi^2 \|\theta_\varphi^0\|^2 + \|\hat{\theta}_\phi^{1/2}\|^2 + \|\theta_\phi^0\|^2 + (e_s^{1/2})^2 + (e_s^0)^2)$$
$$+ C\|\phi(t^0) - \phi(t^{1/2})\|^2 + C(\tau^4 + h^4)$$
$$\leq C(\xi^2 \|\theta_\varphi^{1/2}\|^2 + \xi^2 \|\theta_\varphi^0\|^2 + \|\hat{\theta}_\phi^{1/2}\|^2 + \|\theta_\phi^0\|^2 + (e_s^{1/2})^2 + (e_s^0)^2)$$
$$+ C(\tau^2 + h^4). \tag{69}$$

Owing to $\|\theta_w^0\| \leq Ch^2$ $(w = \phi, \psi, \varphi)$, $e_s^0 = 0$, and ignoring some nonnegative terms, we have

$$\frac{\xi^2}{2}(1 - 2C\tau)\|\theta_\varphi^{1/2}\|^2 + (\frac{\beta+1}{2} - C\tau)\|\hat{\theta}_\phi^{1/2}\|^2 + (1 - C\tau)(e_s^{1/2})^2 \leq C(\tau^3 + h^4),$$

then

$$\|\theta_\varphi^{1/2}\|^2 + \|\hat{\theta}_\phi^{1/2}\|^2 + (e_s^{1/2})^2 \leq C(\tau^3 + h^4). \tag{70}$$

Therefore

$$\|\hat{e}_u^{1/2}\| \leq C(\tau^{3/2} + h^2). \tag{71}$$

When $n \geq 1$, using Lemma 4.3, we can obtain

$$\|\hat{\phi}_h^{n+1/2} - \phi(t^{n+1/2})\| = \|\frac{3\phi_h^n - \phi_h^{n-1}}{2} - \phi(t^{n+1/2})\|$$
$$\leq \|\frac{3\phi_h^n - \phi_h^{n-1}}{2} - \bar{\phi}(t^{n+1/2}) + \bar{\phi}(t^{n+1/2}) - \phi(t^{n+1/2})\|$$
$$\leq \|\frac{3e_\phi^n - e_\phi^{n-1}}{2} + \frac{2\phi(t^n) - \phi(t^{n-1}) - \phi(t^{n+1})}{2} + \bar{T}_\phi(t^{n+1/2})\|$$
$$\leq \|\frac{3e_\phi^n - e_\phi^{n-1}}{2} + \frac{1}{2}\tilde{T}_\phi(t^n) + \bar{T}_\phi(t^{n+1/2})\|$$
$$\leq C(\|e_\phi^n\| + \|e_\phi^{n-1}\|) + C\tau^2$$
$$\leq C(\|\theta_\phi^n\| + \|\theta_\phi^{n-1}\|) + C(\tau^2 + h^2).$$

Then

$$\|\hat{e}_u^{n+1/2}\| \leq C(\|\theta_\phi^n\| + \|\theta_\phi^{n-1}\|) + C(\tau^2 + h^2). \tag{72}$$

Step 6. with the help of the discrete Gronwall's inequality, we obtain the final result, i.e. Eq. (38).

For $n = 0$, Eq. (66) can be written as

$$\frac{\xi^2}{2}D_\tau^1\|\theta_\varphi^1\|^2 + \frac{\beta+1}{2}D_\tau^1\|\theta_\phi^1\|^2 + D_\tau^1(e_s^1)^2 + \frac{1}{8}\|D_\tau^1\theta_\phi^{n+1}\|^2 + \frac{5}{8}\|\nabla\theta_\psi^{n+1/2}\|^2$$
$$\leq C(\xi^2 \|\theta_\varphi^1\|^2 + \xi^2 \|\theta_\varphi^0\|^2 + \|\theta_\phi^1\|^2 + \|\theta_\phi^0\|^2 + (e_s^1)^2 + (e_s^0)^2)$$
$$+ C\|\hat{e}_u^{1/2}\|^2 + C(\tau^4 + h^4)$$
$$\leq C(\xi^2 \|\theta_\varphi^1\|^2 + \|\theta_\phi^1\|^2 + (e_s^1)^2) + C(\tau^3 + h^4). \tag{73}$$

It is easy to obtain

$$\|\theta_\varphi^1\|^2 + \|\hat{\theta}_\phi^1\|^2 + (e_s^1)^2 \leq C(\tau^4 + h^4). \tag{74}$$

For $n \geq 1$, Eq. (66) can be transformed into the following inequality,

$$\frac{\xi^2}{2}D_\tau^1\|\theta_\varphi^{n+1}\|^2 + \frac{\beta+1}{2}D_\tau^1\|\theta_\phi^{n+1}\|^2 + D_\tau^1(e_s^{n+1})^2 + \frac{1}{8}\|D_\tau^1\theta_\phi^{n+1}\|^2 + \frac{5}{8}\|\nabla\theta_\psi^{n+1/2}\|^2$$
$$\leq C(\xi^2\|\theta_\varphi^{n+1}\|^2 + \xi^2\|\theta_\varphi^n\|^2 + \|\theta_\phi^{n+1}\|^2 + \|\theta_\phi^n\|^2 + \|\theta_\phi^{n-1}\|^2$$
$$+ (e_s^{n+1})^2 + (e_s^n)^2) + C(\tau^4 + h^4). \tag{75}$$

Multiplying Eq. (63) by τ and ignoring some nonnegative terms, summing over n, $n = 0, 1, \cdots, m \, (m \geq 1)$, we have

$$\frac{\xi^2}{2}\|\theta_\varphi^{m+1}\|^2 + \frac{\beta+1}{2}\|\theta_\phi^{m+1}\|^2 + (e_s^{m+1})^2$$
$$\leq C\sum_{n=0}^m \tau\xi^2\|\theta_\varphi^n\|^2 + C\sum_{n=0}^m \tau\|\theta_\phi^n\|^2 + C\sum_{n=0}^m \tau(e_s^n)^2 + C(\tau^4 + h^4). \tag{76}$$

Applying the discrete Gronwall's inequality[24], it follows that

$$\|\theta_\varphi^{m+1}\|^2 + \|\theta_\phi^{m+1}\|^2 + (e_s^{m+1})^2 \leq C(\tau^4 + h^4). \tag{77}$$

Thus it is easy to get Eq. (38) by Eq. (74)-(77) and Lemma 4.4. □

5. **Numerical results.** In this section, several numerical examples are given to verify the effectiveness and practicability of our method. Firstly, mesh refinement tests are designed to validate the convergence rate of L^2-norm error of our proposed method in time and space direction. Next, phase transition experiments are used to demonstrate the energy dissipation and numerical effectiveness of the method.

5.1. **Accuracy tests.** In all simulations, we choose $\xi = 1.0, \alpha = -1.0, \gamma = 0.2, \beta = 0.1$ and $D_0 = 50$.

5.1.1. *One dimension.* We consider one-dimensional problem in domain $[0, L_1](L_1 = 4\pi)$ using the uniform mesh of size h and starting with an initial condition $u_0 = cos(x)$.

In Tab 1, the space step size is fixed at $h = 2^{-6}L_1$ and the numerical errors are calculated on $t = 2^{-4}$, then it is easy to observe that the second-order accuracy in the time direction in our simulations. By fixing a small time step as $\tau = 2^{-18}$, we compute every numerical error at $t = 2^{-8}$ for different mesh size. The second-order accuracy in the space direction is shown in Tab. 2.

TABLE 1. Time errors and convergence rates

Coarse τ	Fine τ	$\|e_\psi\|$	rate	$\|e_\phi\|$	rate	$|e_s|$	rate
2^{-10}	2^{-11}	1.13E-6	——	3.72E-7	——	1.86E-8	——
2^{-11}	2^{-12}	2.82E-7	2.01	9.26E-8	2.00	5.74E-9	1.70
2^{-12}	2^{-13}	7.02E-8	2.00	2.31E-6	2.00	1.62E-9	1.83
2^{-13}	2^{-14}	1.75E-8	2.00	5.78E-9	2.00	4.30E-10	1.91
2^{-14}	2^{-15}	4.38E-9	2.00	1.44E-9	2.00	1.11E-10	1.95

TABLE 2. Space errors and convergence rates

Coarse h	Fine h	$\|e_\psi\|$	rate	$\|e_\phi\|$	rate	$|e_s|$	rate
$2^{-4}L_1$	$2^{-5}L_1$	9.42E-2	––	2.87E-4	––	1.63E-2	––
$2^{-5}L_1$	$2^{-6}L_1$	2.41E-2	1.97	7.19E-5	2.06	4.26E-3	1.94
$2^{-6}L_1$	$2^{-7}L_1$	6.05E-3	1.99	1.84E-5	1.97	1.08E-3	1.98
$2^{-7}L_1$	$2^{-8}L_1$	1.51E-3	2.00	4.67E-6	1.98	2.70E-4	2.00
$2^{-8}L_1$	$2^{-9}L_1$	3.78E-4	2.00	1.17E-6	2.00	6.75E-7	2.00

5.1.2. *Two dimension.* Two-dimensional problem with initial value $u_0 = cos(x)$ and domain $\Omega = [0, L_2] \times [0, L_2](L_2 = 2\pi)$ is considered. First, we use $h \times h(h = 2^{-5}L_2)$ as the space step size and choose different time step size to calculate numerical errors at $t = 2^{-4}$. The second-order accuracy in the time direction is shown in Tab 3. Afterward, the second-order accuracy in the space direction is found in Tab. 4, and numerical errors at $t = 2^{-10}$ is computed by fixing the time step $\tau = 2^{-18}$.

TABLE 3. Time errors and convergence rates

Coarse τ	Fine τ	$\|e_\psi\|$	rate	$\|e_\phi\|$	rate	$|e_s|$	rate
2^{-7}	2^{-8}	8.06E-5	––	4.84E-5	––	3.79E-6	––
2^{-8}	2^{-9}	2.19E-5	1.88	1.25E-5	1.95	1.03E-6	1.97
2^{-9}	2^{-10}	5.72E-6	1.93	3.21E-6	1.97	2.62E-7	1.97
2^{-10}	2^{-11}	1.47E-6	1.96	8.19E-7	1.89	6.68E-8	1.97
2^{-11}	2^{-12}	3.75E-7	1.97	2.06E-7	1.99	1.69E-8	1.98

TABLE 4. Space errors and convergence rates

Coarse h	Fine h	$\|e_\psi\|$	rate	$\|e_\phi\|$	rate	$|e_s|$	rate
$2^{-2}L_2$	$2^{-3}L_2$	4.93E-1	––	2.72E-2	––	1.34E-2	––
$2^{-3}L_2$	$2^{-4}L_2$	1.57E-2	1.65	9.93E-3	1.45	3.94E-3	1.77
$2^{-4}L_2$	$2^{-5}L_2$	3.84E-2	2.03	3.29E-3	1.59	1.03E-3	1.94
$2^{-5}L_2$	$2^{-6}L_2$	9.43E-3	2.02	9.10E-4	1.85	2.60E-4	1.99
$2^{-6}L_2$	$2^{-7}L_2$	2.35E-2	2.00	2.35E-4	1.96	6.50E-5	2.00

5.2. **Phase transition and energy dissipation.** In these experiments, the processes of phase transition are simulated on a hexagon domain with the radius $r = 2\pi$. The parameters $\xi = 1.0, \alpha = -1.0, \gamma = 0.8, \beta = 0.1, h = 2^{-4}r$. We choose the tetragonal cylinder structure as the initial phase through a given $\phi_0 = 0.5 + 0.5cos(x)cos(y)$.

Firstly, we set $\tau = 0.01$ and select different D_0 as 150, 500 and 1000. The lower energy value of hexagonal cylinder structure compared with tetragonal cylinder structure, and the latter is metastable structure, thus the phase transition from the latter to the former occurs. For different D_0, there are the same dynamical processes of phase evolution in Fig. 1. The modified free energy and the original free energy with different D_0 are given in Fig. 2. We observe that the energy dissipative property is maintained and is independent of the value of D_0.
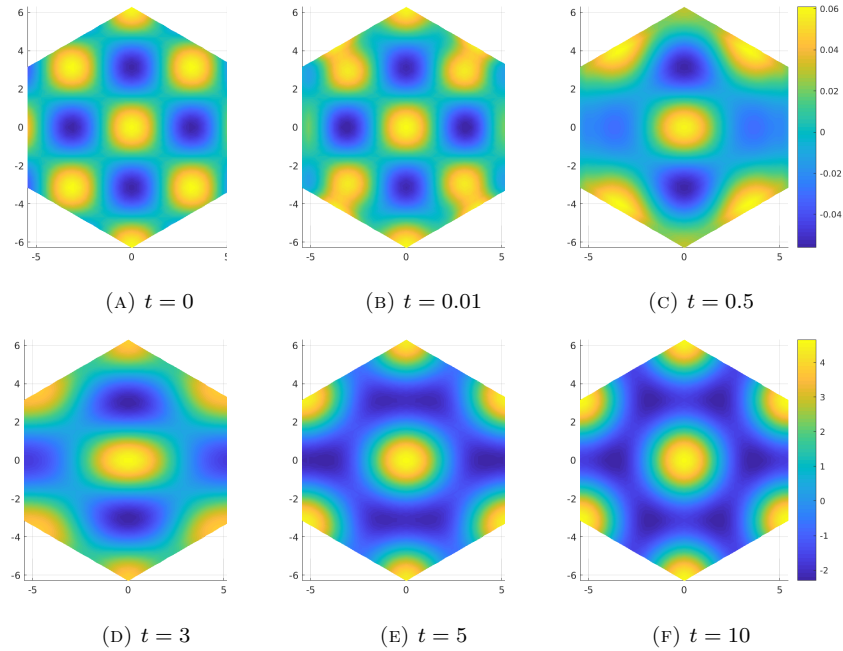
(A) $t = 0$ (B) $t = 0.01$ (C) $t = 0.5$

(D) $t = 3$ (E) $t = 5$ (F) $t = 10$

FIGURE 1. The phase evolution occurs.

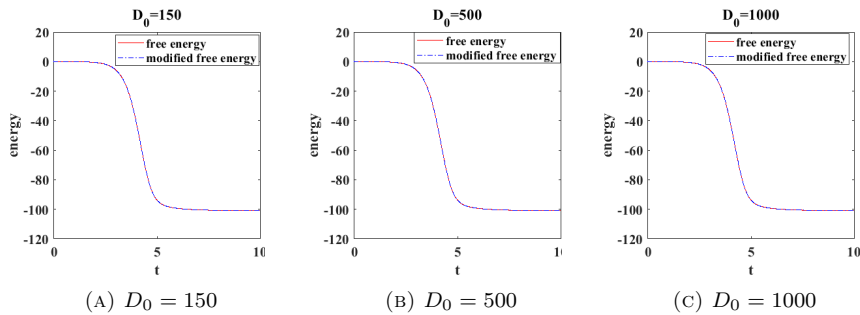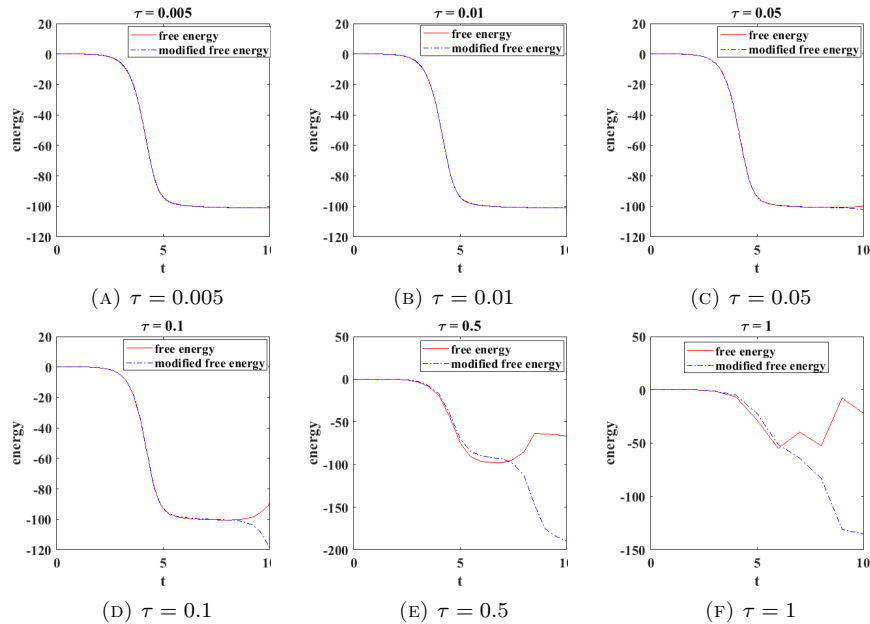(A) $D_0 = 150$ (B) $D_0 = 500$ (C) $D_0 = 1000$

FIGURE 2. The energy dissipative occurs.

Secondly, we choose different τ as 0.005, 0.01, 0.05 0.1, 0.5 1 and fix $D_0 = 250$. We give the processes of energy evolution with time in Fig. 3. As we have seen, for difference values of τ, the modified free energies go down over time. However, with the increase of the value of τ, the original free energy becomes inconsistent with the modified free energy, and the original free energy cannot keep dissipating. It should be pointed out that the modified free energy is different from the original free energy, especially in the case of large time step. In theory, our method only guarantees the unconditional stability of the modified free energy. How to keep the original free energy consistent with the modified free energy for our method needs further study.

6. **Conclusions.** A second-order SAV finite element method equipped with Crank-Nicolson/Adams-Bashforth scheme is present to solve phase field crystal model in

FIGURE 3. The energy energy changing processes with difference τ.

this paper. The stability and convergence of the fully discrete scheme are analyzed in detail. The validity of the proposed method is shown theoretically and numerically. It can be seen from numerical experiments that the energy dissipation of the original free energy for our method cannot be guaranteed when the time step is large. In recent studies, such as [15, 17], the allowable time step can be effectively improved by combining the SAV approach with the stabilization method for time discretization. Therefore, the second-order SAV finite element method can be further developed in the future by incorporating with the stabilization method.

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