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High-Efficiency and Positivity-Preserving Stabilized SAV Methods for Gradient Flows

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Abstract. The scalar auxiliary variable (SAV)-type methods are very popular techniques for solving various nonlinear dissipative systems. Compared to the semi-implicit method, the baseline SAV method can keep a modified energy dissipation law but doubles the computational cost. The general SAV approach does not add additional computation but needs to solve a semi-implicit solution in advance, which may potentially compromise the accuracy and stability. In this paper, we construct a novel first- and second-order unconditional energy stable and positivity-preserving stabilized SAV (PS-SAV) schemes for L^2 and H^{-1} gradient flows. The constructed schemes can reduce nearly half computational cost of the baseline SAV method and preserve its accuracy and stability simultaneously. Meanwhile, the introduced auxiliary variable is always positive while the baseline SAV cannot guarantee this positivity-preserving property. Unconditionally energy dissipation laws are derived for the proposed numerical schemes. In addition we propose an energy optimization technique to optimize the modified energy close to the original energy. Several interesting numerical examples are presented to demonstrate the accuracy and effectiveness of the proposed methods. Finally, we establish a rigorous error analysis of the fully discrete PS-SAV scheme.

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1 Introduction

The gradient flows are very important models in physics, engineering, materials science and mathematics that can accurately and effectively describe the complex interfacial be-

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havior of multi-phase materials. Many modern scientific problems, such as multi-phase industrial alloy casting, metal additive manufacturing, shale oil and gas development, image processing, biomedicine, chip packaging, and many other practical applications can be described by corresponding gradient flow models [4, 22, 31, 32]. In recent years, they have also gained rapid development in many high-precision fields, such as integrated circuits, lithium-ion batteries, 3D printing, etc. [18, 38, 44].

In this paper, we consider the following gradient flow with respect to the following free energy $E(\phi)$:

$$E(\phi)=\frac{\epsilon^2}{2}(A\phi,\phi)+\int_\Omega F\big(\phi(\mathbf{x},t)\big)d\mathbf{x},$$

where $\epsilon>0$ denotes the interfacial width, A is a linear self-adjoint elliptic operator and $F(\phi)$ is a nonlinear potential functional. By introducing a chemical potential $\mu=\delta E/\delta\phi$, we can write the gradient flow as follows:

$$\begin{aligned} &\frac{\partial\phi}{\partial t}=-M\mathcal{G}\mu,\\ &\mu=\epsilon^2A\phi+F'(\phi) \end{aligned} \tag{1.1}$$

with periodic or homogeneous Neumann boundary condition, $M>0$ is a mobility constant and $\mathcal{G}$ is a positive definite operator. For instance, if we let the operator $\mathcal{G}=I$, $A=-\Delta$ and $F(\phi)=(\phi^2-1)^2/4$, the above gradient flow (1.1) will be the known Allen-Cahn model

$$\frac{\partial\phi}{\partial t}=M\epsilon^2\Delta\phi-MF'(\phi). \tag{1.2}$$

The gradient flow is generally a high-order nonlinear partial differential equation, which is a complex system with energy dissipation law. However, it is very difficult to design efficient and energy stable numerical algorithms. In general, the fully explicit discrete scheme for the nonlinear term of the gradient flow (1.1) cannot preserve its physical constraints of the original system. Fully implicit schemes can guarantee the structure of the model, but such methods may require strict time-step restrictions to guarantee the unique solvability and need to solve nonlinear equations at each step, so they are not efficient in practice. The more widely used and effective methods mainly include convex splitting methods [3, 17], stabilization methods [5, 35, 39], exponential time-differencing (ETD) methods [15, 16, 21], invariant energy quadratization (IEQ) methods [40, 41, 43], scalar auxiliary variable methods [1,19,33,34,36], Lagrange multiplier methods [8,10], etc.

In recent years, the SAV-type methods have attracted much attention in numerical solutions for various nonlinear dissipative systems due to their inherent advantage of preserving energy dissipation law. In these SAV-type methods, the baseline SAV method [33] can keep a modified energy dissipation law but doubles the computational cost compared with a semi-implicit approach. It has attracted a lot of attention and has been successfully applied to solve various kinds of complex nonlinear problems, such as various phase field models [9, 11, 20, 25, 26, 29, 30], the Navier-Stokes equation [24, 28], the

Schrödinger equation [2], the magnetohydrodynamic (MHD) equation [27], etc. The recently general SAV (GSAV) approach [19] does not add additional computation but needs to solve a semi-implicit solution in advance which may weaken the accuracy and stability. The main purpose of this paper is to construct a positivity-preserving stabilized SAV approach which enjoys the following advantages:

- The introduced scalar auxiliary variable always keeps a positive property, whereas most SAV-type schemes such as the baseline SAV [33, 34] and the extrapolated RK-SAV [1, 36] fail to do so.
- It only requires solving one linear system with constant coefficients as opposed to the two linear systems by the baseline SAV approach, thus the computational cost of the proposed approach is essentially half that of the SAV approach.
- It provides an enhanced stability and accuracy compared to the GSAV approach, while maintaining nearly identical computational costs.

More specifically, for the E-SAV method [29], the bound of the discrete energy can not be guaranteed due to the uncertainty of the lower bound of $\ln R^{n+1}$ which leads to a lot of difficulties in convergence analysis, whereas our PS-SAV schemes can guarantee the boundedness of R^{n+1}. Besides, compared with the generalised SAV method [19] and its relaxation version [42], the convergence order of the discrete energy is only first-order which will affect the dynamic evolution of energy. However, our second-order PS-SAV scheme can obtain second-order accuracy for the discrete energy.

We prove the unconditional energy dissipation law for the proposed numerical schemes. Furthermore, a rigorous error analysis is derived for the fully-discrete finite difference method with first-order accuracy in time. In particular, it is important to note that the major difficulty in the error estimate is caused by the implicit treatment for R_h and explicit discretization for $\Delta_h \phi_h$ in time. The essential tools used in the proof are unconditional energy dissipation law, the induction process to give a first estimates for the phase function and show that the discrete l^∞ norm of the numerical solution is uniformly bounded. Thus, by establishing several auxiliary lemmas, we finally obtain the optimal convergence rates for the phase function in $l^\infty(0,T;H^1(\Omega))$ norm. We believe that our constructed schemes and optimal error estimate are the first linear, positivity-preserving and unconditionally energy stable method with implicit treatment for the scalar auxiliary variable.

The rest of this paper is organized as follows. In Section 2, we provide a brief review of the SAV-type approaches such as the baseline SAV and GSAV methods for gradient flows. In Section 3, we present the first and second-order semi-discrete positivity-preserving stabilized SAV schemes for L^2 gradient flows together with the energy dissipation law. A semi-discrete numerical scheme based on the PS-SAV approach for H^{-1} gradient flow models is given in Section 4. In Section 5, an energy optimization technique is proposed to optimize the modified energy close to the original energy. In Section 6, we give some comparisons of the proposed PS-SAV approach with the baseline SAV and

GSAV approaches to validate its high efficiency. In the last section, we give a rigorous error analysis for the phase function in $l^\infty(0,T;H^1(\Omega))$ norm.

2 A brief review of the SAV-type approaches

In this section, we give a brief review of the SAV-type methods for the gradient flow (1.1) to better introduce our newly proposed methods.

2.1 The baseline SAV approach

Assume the nonlinear free energy $E_1(\phi)=\int_\Omega F(\phi(\mathbf{x}))d\mathbf{x}$ is bound from below, that is $E_1(\phi)+C>0$ for some constant $C>0$. Let us introduce an auxiliary variable $q(t)=\sqrt{E_1(\phi)+C}$ and reformulate the gradient flow (1.1) to the following equivalent system:

$$\frac{\partial\phi}{\partial t}=-M\mathcal{G}\mu, \tag{2.1a}$$

$$\mu=\epsilon^2A\phi+\frac{q(t)}{\sqrt{E_1(\phi)+C}}F'(\phi), \tag{2.1b}$$

$$\frac{dq}{dt}=\frac{1}{2\sqrt{E_1(\phi)+C}}\left(F'(\phi),\frac{\partial\phi}{\partial t}\right). \tag{2.1c}$$

Before giving a semi-discrete formulation, we let $N>0$ be a positive integer and set

$$\Delta t=\frac{T}{N},\quad t^n=n\Delta t,\quad 0\le n\le N.$$

Then we give the following first-order SAV scheme:

$$\begin{aligned}
&\frac{\phi^{n+1}-\phi^n}{\Delta t}=-M\mathcal{G}\mu^{n+1},\\
&\mu^{n+1}=\epsilon^2A\phi^{n+1}+\frac{q^{n+1}}{\sqrt{E_1(\phi^n)+C}}F'(\phi^n),\\
&\frac{q^{n+1}-q^n}{\Delta t}=\frac{1}{2\sqrt{E_1(\phi^n)+C}}\left(F'(\phi^n),\frac{\phi^{n+1}-\phi^n}{\Delta t}\right).
\end{aligned} \tag{2.2}$$

The scheme (2.2) is unconditionally energy stable in the sense that

$$\left(\frac{\epsilon^2}{2}(A\phi^{n+1},\phi^{n+1})+|q^{n+1}|^2\right)-\left(\frac{\epsilon^2}{2}(A\phi^n,\phi^n)+|q^n|^2\right)\le -M\Delta t(\mathcal{G}\mu^{n+1},\mu^{n+1})\le 0.$$

The above first-order SAV scheme requires the solution of two linear systems with constant coefficients at each time step. The unknown q^{n+1} and ϕ^{n+1} can be calculated decoupled. By setting $\phi^{n+1}=\phi_1^{n+1}+q^{n+1}\phi_2^{n+1}$, we find that ϕ_1^{n+1} and ϕ_2^{n+1} are solutions of the following two linear equations with constant coefficients:

$$(I+M\Delta t\epsilon^2\mathcal{G}A)\phi_1^{n+1}=\phi^n, \quad (I+M\Delta t\epsilon^2\mathcal{G}A)\phi_2^{n+1}=-\frac{M\Delta t}{\sqrt{E_1(\phi^n)+C}}\mathcal{G}F'(\phi^n).$$

Once ϕ_1^{n+1} and ϕ_2^{n+1} are known, we can determine q^{n+1} explicitly by the following equation:

$$\left[1-\frac{1}{2\sqrt{E_1(\phi^n)+C}}\big(F'(\phi^n),\phi_2^{n+1}\big)\right]q^{n+1}=q^n+\frac{1}{2\sqrt{E_1(\phi^n)+C}}\big(F'(\phi^n),\phi_1^{n+1}-\phi^n\big). \tag{2.3}$$

Remark 2.1. The unknown variables q^{n+1} and ϕ^{n+1} in the SAV scheme (2.2) can be calculated decoupled. It requires solving two linear equations with constant coefficients at each time step, so its computational cost is essentially double of the semi-implicit approach.

2.2 The general SAV approach

To reduce the computational cost, Huang *et al.* [19] considered a general SAV approach that is based on a semi-implicit correction. Firstly, assume that the free energy $E(\phi)$ is bounded from below which means $E(\phi)+C>0$ for a positive constant C. Introduce a scalar variable $R(t)=E(\phi)+C$ and rewrite the gradient flow (1.1) as the following equivalent system:

$$\begin{aligned} &\frac{\partial\phi}{\partial t}=-M\mathcal{G}\mu,\\ &\mu=\epsilon^2A\phi+F'(\phi),\\ &\xi=\frac{R(t)}{E(\phi)+C},\\ &\frac{dR}{dt}=-M\xi(\mathcal{G}\mu,\mu). \end{aligned} \tag{2.4}$$

It is not difficult to obtain the following modified energy dissipation law for above equivalent system

$$\frac{dR(t)}{dt}=\frac{d}{dt}\big(E(\phi)+C\big)=-M\xi(\mathcal{G}\mu,\mu)\le 0.$$

We discretisize the state variable ϕ and the introducing variable R implicitly and discretize the energy density function $F'(\phi)$ explicitly to obtain the following k-th order implicit-explicit (IMEX) schemes:

$$\frac{\alpha_k\overline{\phi}^{n+1}-\beta_k(\phi^n)}{\Delta t}=-M\mathcal{G}\overline{\mu}^{n+1}, \tag{2.5a}$$

$$\overline{\mu}^{n+1}=\epsilon^2A\overline{\phi}^{n+1}+F'(\widehat{\phi}^{n+1}), \tag{2.5b}$$

$$\xi^{n+1}=\frac{R^{n+1}}{E(\overline{\phi}^{n+1})+C}, \tag{2.5c}$$

$$\frac{R^{n+1}-R^n}{\Delta t}=-M\xi^{n+1}(\mathcal{G}\overline{\mu}^{n+1},\overline{\mu}^{n+1}), \tag{2.5d}$$

$$\phi^{n+1}=\left[1-(1-\xi^{n+1})^{k+1}\right]\overline{\phi}^{n+1}. \tag{2.5e}$$

Here α_k,β_k and $\widehat{\phi}^{n+1}$ are different for k-th order schemes. For example, they can be defined as follows.

First-order:

$$\alpha_k=1, \quad \beta_k(\phi^n)=\phi^n, \quad \widehat{\phi}^{n+1}=\phi^n,$$

Second-order:

$$\alpha_k=\frac{3}{2}, \quad \beta_k(\phi^n)=2\phi^n-\frac{1}{2}\phi^{n-1}, \quad \widehat{\phi}^{n+1}=2\phi^n-\phi^{n-1}.$$

For more details, please see [42].

The above numerical schemes (2.5) is unconditional energy stable with a modified energy $\mathcal{E}=R^{n+1}-C$ to keep $R^{n+1}\leq R^n$.

Remark 2.2. The k-th order GSAV scheme (2.5) requires solving only one linear equation with constant coefficients at each time step. However, it requires a semi-implicit solution in advance at each time step, which may weaken its stability and accuracy. In practical calculations, it may be necessary to use smaller time steps to achieve long time simulations.

3 A positivity-preserving stabilized SAV method

In this section, we consider a positivity-preserving stabilized SAV method for solving the gradient flow (1.1) effectively. This new proposed method holds the positivity-preserving property of the introduced auxiliary variable. Meanwhile, it reduces the computational cost of the baseline SAV method and preserve its accuracy and stability. We first consider the semi-discrete and fully discrete schemes based on PS-SAV method for the L^2 gradient flow.

3.1 The L^2 gradient flow

Firstly, we set $\mathcal{G}=I$ to transform the gradient flow (1.1) into the following L^2 gradient flow:

$$\begin{aligned}&\frac{\partial\phi}{\partial t}=-M\mu,\\&\mu=\epsilon^2A\phi+F'(\phi).\end{aligned} \tag{3.1}$$

Similar as the general SAV approach, we also assume $E(\phi)+C>0$ for a positive constant C and introduce a same scalar variable $R(t)=E(\phi)+C$. Then, we change the Eq. (2.1c) in the equivalent system (2.1) by the following formulation:

$$\frac{dR}{dt}=\frac{dE}{dt}=\left(\frac{\delta E}{\delta\phi},\frac{\partial\phi}{\partial t}\right)=\left(\mu,\frac{\partial\phi}{\partial t}\right)=-\frac{1}{M}\left(\frac{\partial\phi}{\partial t},\frac{\partial\phi}{\partial t}\right). \tag{3.2}$$

Combining above equation (3.2) with the L^2 gradient flow (3.1), we can reformulate it to the following equivalent system:

$$\frac{\partial\phi}{\partial t}=-M\mu, \tag{3.3a}$$

$$\mu=\frac{R(t)}{E(\phi)+C}\left(\epsilon^2A\phi+F'(\phi)\right), \tag{3.3b}$$

$$\frac{dR}{dt}=-\frac{1}{M}\left(\frac{\partial\phi}{\partial t},\frac{\partial\phi}{\partial t}\right). \tag{3.3c}$$

Obviously, the Eq. (3.3c) can keep the energy dissipation law.

Based on such an equivalent form (3.3), we next give the first-order semi-discrete PS-SAV scheme.

3.2 First-order semi-discrete PS-SAV scheme

A first-order positivity-preserving stabilized SAV scheme based on backward Euler formulation is given by

$$\frac{\phi^{n+1}-\phi^n}{\Delta t}=-M\mu^{n+1}, \tag{3.4a}$$

$$\mu^{n+1}=s\epsilon^2(A\phi^{n+1}-A\phi^n)+\frac{R^{n+1}}{E(\phi^n)+C}[\epsilon^2A\phi^n+F'(\phi^n)], \tag{3.4b}$$

$$\frac{R^{n+1}-R^n}{\Delta t}=-\frac{1}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right), \tag{3.4c}$$

where $s>0$ is a stabilizing constant. If we choose $s=1$, the above scheme is equivalent to the following formulation:

$$\begin{aligned}
&\frac{\phi^{n+1}-\phi^n}{\Delta t}=-M\mu^{n+1},\\
&\mu^{n+1}=\epsilon^2A\phi^{n+1}+\frac{R^{n+1}}{E(\phi^n)+C}F'(\phi^n)+\left(\frac{R^{n+1}}{E(\phi^n)+C}-1\right)\epsilon^2A\phi^n,\\
&\frac{R^{n+1}-R^n}{\Delta t}=-\frac{1}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right).
\end{aligned}$$

From the Eqs. (3.4a) and (3.4b), we can rewrite (3.4) equivalently as the following formulation:

$$\big(E(\phi^n)+C\big)(I+Ms\epsilon^2\Delta tA)\frac{\phi^{n+1}-\phi^n}{\Delta t}=-MR^{n+1}[\epsilon^2A\phi^n+F'(\phi^n)], \tag{3.5a}$$

$$\frac{M}{\Delta t}(R^{n+1}-R^n)=-\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right). \tag{3.5b}$$

Setting $\phi^{n+1}=\phi^n+\Delta tR^{n+1}\phi_1^{n+1}$, we find that ϕ_1^{n+1} is the solution of the following linear equation with constant coefficients:

$$(I+Ms\epsilon^2\Delta tA)\phi_1^{n+1}=-\frac{M}{E(\phi^n)+C}[\epsilon^2A\phi^n+F'(\phi^n)]. \tag{3.6}$$

Once ϕ_1^{n+1} is known, noting that

$$\phi^{n+1}-\phi^n=\Delta tR^{n+1}\phi_1^{n+1}, \tag{3.7}$$

and combining it with the Eq. (3.5b), we obtain

$$\big(\phi_1^{n+1},\phi_1^{n+1}\big)(R^{n+1})^2+\frac{M}{\Delta t}R^{n+1}-\frac{M}{\Delta t}R^n=0. \tag{3.8}$$

If $\phi_1^{n+1}=0$, we obtain $(\phi_1^{n+1},\phi_1^{n+1})=0$. Then we directly get $\phi^{n+1}=\phi^n$ and $R^{n+1}=R^n$. If $\phi_1^{n+1}\neq 0$, we obtain $(\phi_1^{n+1},\phi_1^{n+1})\neq 0$. The above equation (3.8) is a quadratic equation with one variable for R^{n+1}.

Theorem 3.1. *The quadratic equation with one variable for R^{n+1}* (3.8) *exists and has only one positive solution*

$$R^{n+1}=\frac{-M/\Delta t+\sqrt{M^2/\Delta t^2+4(M/\Delta t)R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)}}{2\big(\phi_1^{n+1},\phi_1^{n+1}\big)}>0. \tag{3.9}$$

Proof. Noting that $R^0=E(\phi^0)+C>0$, then we assume that $R^n>0$. The quadratic equation (3.8) is determined to have a solution because of

$$\Delta=\frac{M^2}{\Delta t^2}+4\frac{M}{\Delta t}R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)>\frac{M^2}{\Delta t^2}>0.$$

One can obviously see that (3.8) has the following two solutions:

$$R_1^{n+1}=\frac{-M/\Delta t-\sqrt{M^2/\Delta t^2+4(M/\Delta t)R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)}}{2\big(\phi_1^{n+1},\phi_1^{n+1}\big)}<0,$$

$$R_2^{n+1}=\frac{-M/\Delta t+\sqrt{M^2/\Delta t^2+4(M/\Delta t)R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)}}{2\big(\phi_1^{n+1},\phi_1^{n+1}\big)}>0.$$

By the positive property of R, we have that $R^{n+1}=R_2^{n+1}$. □

Then we can obtain ϕ^{n+1} directly by the following equation:

$$\phi^{n+1}=\phi^n+\Delta t R^{n+1}\phi_1^{n+1}. \tag{3.10}$$

To summarize, the first-order PS-SAV scheme (3.4) can be implemented as follows:

- solve ϕ_1^{n+1} from (3.6),
- compute R^{n+1} from (3.9),
- update $\phi^{n+1}=\phi^n+\Delta t R^{n+1}\phi_1^{n+1}$ and goto next time step.

We observe that the above procedure only requires solving one linear equation with constant coefficients as in a semi-implicit scheme with stabilization. As for the energy stability, we have the following result.

Theorem 3.2. *Given $R^0>0$, we have $R^n>0$, and the first-order PS-SAV scheme* (3.4) *is unconditionally energy stable in the sense that*

$$R^{n+1}-R^n=-\frac{\Delta t}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)\leq 0.$$

3.3 Second-order PS-SAV scheme

A similar PS-SAV approach can also be extended to construct a second-order Crank-Nicloson formulation for the L^2 gradient flow. We find that a straightforward extension of the first-order PS-SAV scheme to the second-order scheme can not preserve the positive property of R^{n+1}. we add a stabilization term $s^{n+1}\Delta t(R^{n+1}-R^n)$ to overcome this problem.

The second-order PS-SAV scheme based on the Crank-Nicolson formulation is given by

$$\frac{\phi^{n+1}-\phi^n}{\Delta t}=-M\mu^{n+\frac{1}{2}}, \tag{3.11a}$$

$$\begin{aligned}\mu^{n+\frac{1}{2}}=&\frac{1}{2}\epsilon^2 A(\phi^{n+1}+\phi^n)+\left(\frac{R^{n+1}+R^n}{2\big(E(\widehat{\phi}^{n+\frac{1}{2}})+C\big)}-1\right)\epsilon^2 A\phi^n\\&+\frac{R^{n+1}+R^n}{2\big(E(\widehat{\phi}^{n+\frac{1}{2}})+C\big)}F'(\widehat{\phi}^{n+\frac{1}{2}}),\end{aligned} \tag{3.11b}$$

$$\frac{R^{n+1}-R^n}{\Delta t}+s^{n+1}\Delta t(R^{n+1}-R^n)=-\frac{1}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right). \tag{3.11c}$$

The Eq. (3.11b) can be rewritten as the following equivalent system:

$$\mu^{n+\frac{1}{2}}=\frac{1}{2}\epsilon^2 A(\phi^{n+1}-\phi^n)+\frac{R^{n+1}+R^n}{2\big(E(\widehat{\phi}^{n+1/2})+C\big)}\big[\epsilon^2 A\phi^n+F'(\widehat{\phi}^{n+\frac{1}{2}})\big], \tag{3.12}$$

where $\widehat{\phi}^{n+1/2}$ is any explicit $\mathcal{O}((\Delta t)^2)$ approximation for $\phi(t^{n+1/2})$. For example, we can choose $\widehat{\phi}^{n+1/2}=3\phi^n/2-\phi^{n-1}/2$ for $n\geq 1$ or we can use a simple first-order scheme to obtain it, such as the semi-implicit scheme

$$\frac{\widehat{\phi}^{n+1/2}-\phi^n}{\Delta t/2}=-M\epsilon^2 A\widehat{\phi}^{n+\frac{1}{2}}-MF'(\phi^n),$$

which has a local truncation error of $\mathcal{O}((\Delta t)^2)$.

Combining the Eq. (3.11a) with the equivalent equation (3.12) of the second one, we can rewrite (3.11) equivalently as the following formulation:

$$2\big(E\big(\widehat{\phi}^{n+\frac{1}{2}}\big)+C\big)\left(I+\frac{1}{2}M\epsilon^2\Delta tA\right)\frac{\phi^{n+1}-\phi^n}{\Delta t}=-M(R^{n+1}+R^n)\big[\epsilon^2 A\phi^n+F'\big(\widehat{\phi}^{n+\frac{1}{2}}\big)\big], \tag{3.13a}$$

$$\frac{1}{\Delta t}(R^{n+1}-R^n)+s^{n+1}\Delta t(R^{n+1}-R^n)=-\frac{1}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right). \tag{3.13b}$$

Setting $\phi^{n+1}=\phi^n+\Delta t(R^{n+1}+R^n)\phi_1^{n+1}$, we also find that ϕ_1^{n+1} is the solution of the following linear equation with constant coefficients:

$$(I+M\epsilon^2\Delta tA)\phi_1^{n+1}=-\frac{M}{2\big(E\big(\widehat{\phi}^{n+1/2}\big)+C\big)}\big[\epsilon^2 A\phi^n+F'\big(\widehat{\phi}^{n+\frac{1}{2}}\big)\big]. \tag{3.14}$$

Once ϕ_1^{n+1} is known, noting that

$$\phi^{n+1}-\phi^n=\Delta t(R^{n+1}+R^n)\phi_1^{n+1}, \tag{3.15}$$

and combining it with the Eq. (3.13b), we get

$$a(R^{n+1})^2+bR^{n+1}+c=0, \tag{3.16}$$

where the coefficients a,b and c of the above quadratic equation satisfy

$$\begin{aligned}
&a=\big(\phi_1^{n+1},\phi_1^{n+1}\big), \quad b=\frac{M}{\Delta t}+Ms^{n+1}\Delta t+2R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big),\\
&c=(R^n)^2\big(\phi_1^{n+1},\phi_1^{n+1}\big)-\frac{M}{\Delta t}R^n-Ms^{n+1}\Delta tR^n.
\end{aligned}$$

If $\phi_1^{n+1}=0$, we set $s^{n+1}=0$. Then we have $a=0$, $b=M/\Delta t$ and $c=-(M/\Delta t)R^n$, then we immediately obtain $\phi^{n+1}=\phi^n$ and $R^{n+1}=R^n$. If $\phi_1^{n+1}\neq 0$, we obtain $(\phi_1^{n+1},\phi_1^{n+1})>0$. Then the above equation (3.16) is a quadratic equation with one variable for R^{n+1}.

Theorem 3.3. *If we choose the stabilized variable s^{n+1} to satisfy*

$$s^{n+1}=\begin{cases}0, & R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)\leq\dfrac{M}{\Delta t},\\[2mm] \dfrac{1}{M\Delta t}R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)-\dfrac{1}{\Delta t^2}, & R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)>\dfrac{M}{\Delta t},\end{cases} \tag{3.17}$$

then the quadratic equation with one variable for R^{n+1} (3.16) *exists and has only one positive solution*

$$R^{n+1}=\frac{-b+\sqrt{b^2-4ac}}{2a}>0. \tag{3.18}$$

Proof. Noting that $R^0=E(\phi^0)+C>0$, we then assume that $R^n>0$. Noting that $a>0$, if the stabilized variable s^{n+1} is chosen as in (3.17), then we are easy to obtain $c\le 0$. Then the quadratic equation (3.16) is determined to have a solution because of

$$\Delta=b^2-4ac>0.$$

Similarly, one can see that (3.16) has the following two solutions:

$$R_1^{n+1}=\frac{-b-\sqrt{b^2-4ac}}{2a}<0,$$
$$R_2^{n+1}=\frac{-b+\sqrt{b^2-4ac}}{2a}>0.$$

By the positive property of R, we have that $R^{n+1}=R_2^{n+1}$. □

Then we can compute ϕ^{n+1} by the following equation:

$$\phi^{n+1}=\phi^n+\Delta t(R^{n+1}+R^n)\phi_1^{n+1}.$$

To summarize, the second-order PS-SAV scheme (3.13) can be implemented as follows:

- solve ϕ_1^{n+1} from (3.14),
- compute R^{n+1} from (3.18),
- update $\phi^{n+1}=\phi^n+\Delta t(R^{n+1}+R^n)\phi_1^{n+1}$ and goto next time step.

We observe that the above procedure only requires solving one linear equation with constant coefficients as in a semi-implicit scheme with stabilization. As for the energy stability, we have the following result easily.

Theorem 3.4. *Given* $R^0>0$, *we have* $R^n>0$ *for all* $n>0$, *and the second-order PS-SAV scheme* (3.13) *is unconditionally energy stable in the sense that*

$$R^{n+1}-R^n\le -\frac{\Delta t}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)\le 0.$$

Remark 3.1. The stabilized terms are different between the first-order (3.4) and second-order schemes (3.11). The first-order scheme (3.4) employs stabilized term $s\epsilon^2(A\phi^{n+1}-A\phi^n)$ to compute ϕ_1^{n+1}, while the second-order scheme (3.11) utilizes stabilized term $s^{n+1}\Delta t(R^{n+1}-R^n)$ to ensure the existence and uniqueness of solutions for R^{n+1}.

4 The PS-SAV approach for H^{-1} gradient flow

The proposed positivity-preserving technique can also be used to solve H^{-1} gradient flow. By setting $\mathcal{G}=-\Delta$ to transform the gradient flow (1.1) into the following H^{-1} gradient flow:

$$\begin{aligned}&\frac{\partial\phi}{\partial t}=M\Delta\mu,\\&\mu=\epsilon^2A\phi+F'(\phi).\end{aligned}\tag{4.1}$$

The H^{-1} gradient flow model (4.1) is mass preserving since

$$\forall t\geq 0,\quad \frac{d}{dt}\int_\Omega\phi d\mathbf{x}=\int_\Omega\frac{\partial\phi}{\partial t}d\mathbf{x}=0.$$

To construct PS-SAV scheme for the H^{-1} gradient flow (4.1), we need to define the H^{-1}_{per} inner product firstly. Suppose $f\in L^2_0(\Omega)=\{v\in L^2(\Omega)|(v,1)=0\}$, define $\mu_f\in H^2_{per}(\Omega)\cap L^2_0(\Omega)$ to be the unique solution to the following problem with periodic boundary condition:

$$-\Delta\mu_f=f\quad\text{in }\ \Omega.\tag{4.2}$$

We then define $\mu_f:=(-\Delta)^{-1}f$, and for any $f,g\in L^2_0(\Omega)$, the H^{-1}_{per} inner product and norm can be defined as follows:

$$(f,g)_{-1}=(\nabla\mu_f,\nabla\mu_g),\quad \|f\|_{-1}=\sqrt{(f,f)_{-1}}.\tag{4.3}$$

It is easy to obtain the following identity:

$$(f,g)_{-1}=\big((-\Delta)^{-1}f,g\big)=\big(f,(-\Delta)^{-1}g\big)=(g,f)_{-1}.\tag{4.4}$$

Given a same SAV $R(t)$ with (3.3), the corresponding derivative equation for R will take the following formulation:

$$\frac{dR}{dt}=\frac{dE}{dt}=\left(\frac{\delta E}{\delta\phi},\frac{\partial\phi}{\partial t}\right)=\left(\mu,\frac{\partial\phi}{\partial t}\right)=\frac{1}{M}\left(-(-\Delta)^{-1}\frac{\partial\phi}{\partial t},\frac{\partial\phi}{\partial t}\right)=-\frac{1}{M}\left(\frac{\partial\phi}{\partial t},\frac{\partial\phi}{\partial t}\right)_{-1}.\tag{4.5}$$

Combining above equation (4.5) with (4.1), we can reformulate the H^{-1} gradient flow to the following equivalent system:

$$\frac{\partial\phi}{\partial t}=M\Delta\mu,\tag{4.6a}$$

$$\mu=\frac{R(t)}{E(\phi)+C}\big(\epsilon^2A\phi+F'(\phi)\big),\tag{4.6b}$$

$$\frac{dR}{dt}=-\frac{1}{M}\left(\frac{\partial\phi}{\partial t},\frac{\partial\phi}{\partial t}\right)_{-1}.\tag{4.6c}$$

One can see the Eq. (4.6c) can keep the energy dissipation law.

Similar as the PS-SAV schemes for the L^2 gradient flow, the first-order PS-SAV scheme based on the backward Euler formulation for the H^{-1} gradient flow (4.1) can be given by

$$\frac{\phi^{n+1}-\phi^n}{\Delta t}=M\Delta\mu^{n+1}, \tag{4.7a}$$

$$\mu^{n+1}=s\epsilon^2(A\phi^{n+1}-A\phi^n)+\frac{R^{n+1}}{E(\phi^n)+C}[\epsilon^2A\phi^n+F'(\phi^n)], \tag{4.7b}$$

$$\frac{R^{n+1}-R^n}{\Delta t}=-\frac{1}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)_{-1}. \tag{4.7c}$$

From the Eqs. (4.7a) and (4.7b), we can rewrite (4.7) equivalently as the following:

$$\begin{aligned}&\big(E(\phi^n)+C\big)(I-M\epsilon^2s\Delta t\Delta A)\frac{\phi^{n+1}-\phi^n}{\Delta t}=MR^{n+1}[\epsilon^2\Delta A\phi^n+\Delta F'(\phi^n)],\\ &\frac{M}{\Delta t}(R^{n+1}-R^n)=-\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)_{-1}.\end{aligned} \tag{4.8}$$

Setting $\phi^{n+1}=\phi^n+\Delta tR^{n+1}\phi_1^{n+1}$, we also find that ϕ_1^{n+1} is the solution of the following linear equation with constant coefficients:

$$(I-Ms\epsilon^2\Delta t\Delta A)\phi_1^{n+1}=\frac{M}{E(\phi^n)+C}[\epsilon^2\Delta A\phi^n+\Delta F'(\phi^n)]. \tag{4.9}$$

Once ϕ_1^{n+1} is known, to compute R^{n+1}, we need to solve the following quadratic equation:

$$a(R^{n+1})^2+bR^{n+1}+C=0, \tag{4.10}$$

where the coefficients a, b and c satisfy

$$a=\big(\phi_1^{n+1},\phi_1^{n+1}\big)_{-1},\quad b=\frac{M}{\Delta t},\quad c=-\frac{M}{\Delta t}R^n. \tag{4.11}$$

If $\phi_1^{n+1}=0$, we can immediately obtain $\phi^{n+1}=\phi^n$ and $R^{n+1}=R^n$. If $\phi_1^{n+1}\neq 0$, we obtain $(\phi_1^{n+1},\phi_1^{n+1})_{-1}>0$. Then the above equation (4.10) is a quadratic equation with one variable for R^{n+1}.

Theorem 4.1. *The quadratic equation with one variable for* R^{n+1} (4.10) *only has one positive solution*

$$R^{n+1}=\frac{-M/\Delta t+\sqrt{M^2/\Delta t^2+4(M/\Delta t)R^n\big(\phi_1^{n+1},\phi_1^{n+1}\big)_{-1}}}{2\big(\phi_1^{n+1},\phi_1^{n+1}\big)_{-1}}>0. \tag{4.12}$$

As for the energy stability, we have the following result easily.

Theorem 4.2. *Given $R^0>0$, we have $R^n>0$ for all $n>0$, and the first-order PS-SAV scheme* (4.7) *is unconditionally energy stable in the sense that*

$$R^{n+1}-R^n=-\frac{\Delta t}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)_{-1}\leq 0.$$

Remark 4.1. The first-order PS-SAV scheme (4.7) also only requires solving one linear equation with constant coefficients as in a semi-implicit scheme with stabilization. In addition, it may add some additional small computation cost to obtain $(\phi_1^{n+1},\phi_1^{n+1})_{-1}$.

Remark 4.2. Similar to the framework for second-order PS-SAV schemes for the L^2 gradient flow, the second-order Crank-Nicolson scheme for the H^{-1} gradient flow is given by

$$\begin{aligned}
&\frac{\phi^{n+1}-\phi^n}{\Delta t}=M\Delta\mu^{n+\frac{1}{2}},\\
&\mu^{n+\frac{1}{2}}=\frac{1}{2}\epsilon^2A(\phi^{n+1}+\phi^n)+\left(\frac{R^{n+1}+R^n}{2\big(E\big(\widehat{\phi}^{n+\frac{1}{2}}\big)+C\big)}-1\right)\epsilon^2A\phi^n\\
&\qquad+\frac{R^{n+1}+R^n}{2\big(E\big(\widehat{\phi}^{n+\frac{1}{2}}\big)+C\big)}F'\big(\widehat{\phi}^{n+\frac{1}{2}}\big),\\
&\frac{R^{n+1}-R^n}{\Delta t}+s^{n+1}\Delta t(R^{n+1}-R^n)=-\frac{1}{M}\left(\frac{\phi^{n+1}-\phi^n}{\Delta t},\frac{\phi^{n+1}-\phi^n}{\Delta t}\right)_{-1}.
\end{aligned}\tag{4.13}$$

For brevity, we omit the proofs of existence and convergence for the solutions of the above scheme.

Remark 4.3. The positivity-preserving property of the auxiliary variable in our proposed PS-SAV schemes is independent of the type of nonlinear functional F. This approach remains effective and positivity-preserving for both L^2 gradient flows and H^{-1} gradient flows with double-well potentials or Flory-Huggins energy potentials, though additional techniques (e.g. cut-off approach [23], implicit treatment [6, 7, 13, 14]) are required to ensure the positivity for the logarithmic arguments.

5 An energy optimization technique

Noting that the proposed PS-SAV schemes are unconditionally energy stable with a modified energy, we give an energy optimization technique to make the modified energy to be close to the original energy.

At each time step, after obtaining R^{n+1}, we calibrate it by using the following equation:

$$R^{n+1}=\min\{R^n,E(\phi^{n+1})+C\}.\tag{5.1}$$

The above correction technique will not affect the energy dissipation law and the convergence rates.

We take the first-order PS-SAV scheme (3.4) for the L^2 gradient flow as an example.

Theorem 5.1. *The first-order PS-SAV scheme* (3.4) *with a relaxed correction technique* (5.1) *(R-PS-SAV) is unconditionally energy stable in the sense that*

$$\mathcal{E}^{n+1}-\mathcal{E}^n\leq 0, \tag{5.2}$$

where $\mathcal{E}^n=R^n-C$ is the modified energy.

We further have the following original energy dissipation law:

$$E(\phi^{n+1})\leq E(\phi^n)$$

under the condition of $E(\phi^{n+1})+C\leq R^n$. Here

$$E(\phi^n)=\frac{\epsilon^2}{2}(A\phi^n,\phi^n)+\big(F(\phi^n),1\big)$$

is the original energy.

Proof. From the correction equation (5.1), we get $R^{n+1}\leq R^n$, then one can immediately obtain

$$\mathcal{E}^{n+1}-\mathcal{E}^n\leq 0.$$

We can also obtain $R^{n+1}\leq E(\phi^{n+1})+C$ from (5.1), then the following inequality is satisfied:

$$\mathcal{E}^{n+1}=R^{n+1}-C\leq E(\phi^{n+1}),$$

which means

$$\mathcal{E}(\phi^n)\leq E(\phi^n),\quad \forall n\geq 0. \tag{5.3}$$

If $E(\phi^{n+1})+C\leq R^n$, we get $R^{n+1}=\min\{R^n,E(\phi^{n+1})+C\}=E(\phi^{n+1})+C$, then the following equation will hold:

$$\mathcal{E}(\phi^{n+1})=R^{n+1}-C=E(\phi^{n+1}). \tag{5.4}$$

Combining the inequality (5.2) with (5.3) and (5.4), we obtain

$$E(\phi^{n+1})=\mathcal{E}(\phi^{n+1})\leq\mathcal{E}(\phi^n)\leq E(\phi^n), \tag{5.5}$$

which means the first-order PS-SAV scheme (3.4) with correction technique (5.1) is unconditionally energy stable with original energy under the condition of $E(\phi^{n+1})+C\leq R^n$. □

Remark 5.1. The energy optimization technique step (5.1) for R^{n+1} will force the modified energy $R^{n+1}-C$ be closer to the original free energy $E(\phi^{n+1})$. Meanwhile, the updated R^{n+1} will be used to calculate R^{n+2} by the following equation:

$$\big(\phi_1^{n+2},\phi_1^{n+2}\big)(R^{n+2})^2+\frac{M}{\Delta t}R^{n+2}-\frac{M}{\Delta t}R^{n+1}=0,$$

and then ϕ^{n+2} will be computed by R^{n+2}. It means the updated R^{n+1} will affect the value of ϕ^{n+2}.

6 Examples and discussion

In this section, we consider some numerical examples to illustrate the simplicity and efficiency of our proposed method. Unless otherwise specified, we consider the periodic boundary conditions and use a Fourier spectral method in space. We use $\|\cdot\|_{L^2}$ is to denote the norm in $L^2(\Omega)$.

Example 6.1. The following Allen-Cahn equation is under our consideration:

$$\frac{\partial \phi}{\partial t} = M\big(\alpha_0 \Delta \phi + (1-\phi^2)\phi\big) \tag{6.1}$$

subject to periodic boundary conditions.

Case A. We give the exact solution

$$\phi(x,y,t) = \exp\big(\sin(\pi x)\sin(\pi y)\big)\sin(t), \tag{6.2}$$

by introducing an external force f into (6.1) in the domain $\Omega=(0,2)^2$. We set the values of the parameters M and α_0 to 1 and 0.01^2, respectively. To effectively and clearly compare CPU times for different numerical schemes, we use the finite element method for spatial discretization in this study. To ensure that the spatial discretization error is significantly smaller than the time discretization error, we generate a mesh with a resolution of 128^2 for the spatial discretization.

In Tables 1 and 2, we present the L^2-norm error convergence rate for semi-implicit, SAV, GSAV and PS-SAV approaches at $T=1$ obtained using first-order and Crank-Nicolson scheme, respectively. We have observed that the expected convergence rates are achieved for all cases. Fig. 1 illustrates the comparison of CPU times for different approaches. The CPU times are ranked in the following order: semi-implicit $<$ PS-SAV $<$ GSAV $<$ SAV. Among these, the semi-implicit scheme requires the shortest computation time, while the PS-SAV scheme takes slightly longer but is still the fastest among the other SAV-type schemes. In contrast, the SAV scheme demands the longest computation time. These results align with theoretical expectations. Theoretically, the semi-implicit scheme only requires solving a single linear equation at each time step. The SAV

Table 1: Example 6.1 (Case A). Convergence test for Allen-Cahn equation using the first-order scheme by different approaches.

Δt	Semi-implicit		SAV		GSAV		PS-SAV	
	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate
1.00E-1	1.40E-01	–	1.32E-01	–	2.81E-01	–	1.39E-01	–
5.00E-2	6.91E-02	1.01	6.22E-02	1.08	1.07E-01	1.39	6.85E-02	1.02
2.50E-2	3.43E-02	1.01	3.02E-02	1.04	4.94E-02	1.12	3.40E-02	1.01
1.25E-2	1.71E-02	1.01	1.49E-02	1.02	2.38E-02	1.05	1.69E-02	1.01
6.25E-3	8.53E-03	1.00	7.42E-03	1.01	1.17E-02	1.02	8.43E-03	1.00

Table 2: Example 6.1 (Case A). Convergence test for Allen-Cahn equation using the Crank-Nicolson scheme by different approaches.

Δt	Semi-implicit		SAV		GSAV		PS-SAV	
	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate
1.00E-1	5.00E-03	–	5.23E-03	–	4.96E-03	–	5.09E-03	–
5.00E-2	1.30E-03	1.95	1.34E-03	1.97	1.28E-03	1.95	1.30E-03	1.97
2.50E-2	3.33E-04	1.96	3.39E-04	1.98	3.26E-04	1.98	3.24E-04	2.01
1.25E-2	8.56E-05	1.96	8.55E-05	1.99	8.23E-05	1.99	7.89E-05	2.04
6.25E-3	2.27E-05	1.91	2.17E-05	1.98	2.09E-05	1.98	1.98E-05	1.99

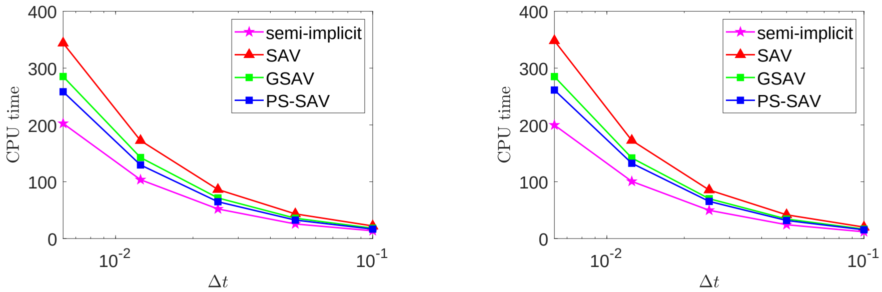


Figure 1: Example 6.1 (Case A). Comparison of CPU time for solving the Allen-Cahn equation using different approaches. First: first-order scheme; Second: Crank-Nicolson scheme.

scheme, however, necessitates solving two linear equations as well as an algebraic equation (2.3) related to q^{n+1} at each time step. The GSAV scheme requires solving one linear equation and an algebraic equation for R^{n+1} (scheme (2.5), Eq. (2.5e)) at each time step. Similarly, the PS-SAV scheme only requires solving one linear equation and an algebraic equation (3.8) for R^{n+1}, whose root is given by Eq. (3.9). The reason the GSAV scheme takes slightly longer than the PS-SAV scheme is that the GSAV scheme involves additional computations when solving the algebraic equation for R^{n+1}. Specifically, it requires the evaluation of $\overline{\mu}^{n+1}$ and $E(\widehat{\phi}^{n+1})$, which entails solving for $\Delta\overline{\phi}^{n+1},\nabla\widehat{\phi}^{n+1}$, and performing an integration.

Case B. We choose the initial condition as

$$\begin{aligned} &\phi(x,y)=\tanh\frac{1.5+1.2\cos(6\theta)-2\pi r}{\sqrt{2\alpha_0}}, \\ &\theta=\arctan\frac{y-0.5L_y}{x-0.5L_x}, \quad r=\sqrt{\left(x-\frac{L_x}{2}\right)^2+\left(y-\frac{L_y}{2}\right)^2}, \end{aligned} \tag{6.3}$$

where (θ,r) are the polar coordinates of (x,y). We set $\Omega=[0,L_x]\times[0,L_y]$ with $L_x=L_y=1$ and the other parameters are $\alpha_0=0.01^2, M=0.1$ and 128^2 Fourier modes. We use the results of the semi-implicit/first-order scheme with $\Delta t=1E\text{-}5$ as the reference solution.

The L^2-norm error of four schemes at $T=200$ with different time steps are shown in Table 3. In this particular case, we observe that the errors of the semi-implicit, SAV, GSAV, and PS-SAV approaches follow the order: PS-SAV $<$ SAV $\approx$ semi-implicit $<$ GSAV. However, upon applying the energy optimization technique, the error of R-PS-SAV approach is slightly larger than that of PS-SAV approach, but still smaller than the errors of semi-implicit, SAV and GSAV approaches. In Fig. 2, we present a comparative analysis of the SAV, GSAV, PS-SAV, and R-PS-SAV approaches, focusing on three aspects: first, the comparison between modified and reference energies; second, the energy error between the modified and reference energies; and third, the error in ξ^{n+1}. What needs illustration is that $\xi=q(t)/\sqrt{E_1(\phi)+C}$ in SAV scheme (2.1) and $\xi=R(t)/(E(\phi)+C)$ in PS-SAV and R-PS-SAV schemes. These results are obtained using the first-order scheme with a time step size of $\Delta t=1E$-3. We can observe that for the majority of the time, the error in modified energy and the error in ξ^{n+1} follow the following order: R-PS-SAV$<$SAV$<$PS-SAV$<$ GSAV. Table 4 presents a comparison of the L^2-errors obtained using different stabilization parameters based on the first-order scheme at $T=200$ for various time steps. It can be observed that the lowest error results can be achieved when $s=0.6$.

Table 3: Example 6.1 (Case B). A comparison of L^2-error obtained by five approaches based on first-order scheme for Allen-Cahn equation at $T=200$ with various time steps.

Δt	Semi-implicit	SAV	GSAV	PS-SAV	R-PS-SAV
1.00E-1	1.75E-03	1.75E-03	3.31E-03	4.88E-04	9.31E-04
5.00E-2	8.79E-04	8.77E-04	1.83E-03	2.48E-04	4.66E-04
1.00E-2	1.76E-04	1.76E-04	4.07E-04	5.03E-05	9.32E-05
5.00E-3	8.79E-05	8.77E-05	2.07E-04	2.51E-05	4.65E-05
1.00E-3	1.74E-05	1.74E-05	4.18E-05	5.04E-06	9.16E-06

Table 4: Example 6.1 (Case B). A comparison of L^2-error obtained by different stabilizations based on first-order scheme for Allen-Cahn equation at $T=200$ with various time steps.

Δt	$s=0$	$s=0.2$	$s=0.5$	$s=0.6$	$s=0.7$	$s=1$	$s=2$
1.00E-1	2.84E-03	1.84E-03	4.88E-04	7.92E-05	3.32E-04	1.44E-03	4.36E-03
1.00E-2	2.73E-04	1.83E-04	5.03E-05	7.19E-06	3.78E-05	1.68E-04	5.91E-04
1.00E-3	2.72E-05	1.83E-05	5.04E-06	7.17E-07	3.85E-06	1.71E-05	6.11E-05

Example 6.2. We consider Cahn-Hilliard equation

$$\frac{\partial\phi}{\partial t}=-M\Delta\left(\alpha_0\Delta\phi+\frac{1}{\epsilon^2}(1-\phi^2)\phi\right). \tag{6.4}$$

Case A. We give the exact solution

$$\phi(x,y,t)=\cos(\pi x)\cos(\pi y)\sin(t) \tag{6.5}$$

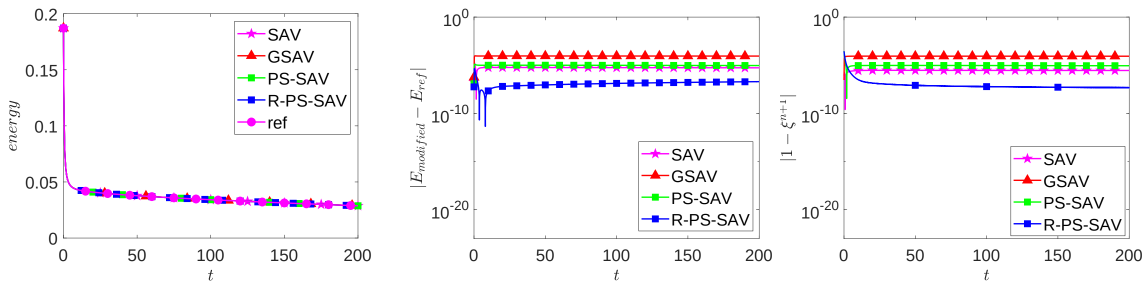


Figure 2: Example 6.1 (Case B). Allen-Cahn equation: comparison of modified and reference energies (first), errors between modified and reference energies (second) and errors of ξ^{n+1} (third) obtained by four approaches with $\Delta t = 1E\text{-}3$ based on first-order scheme.

by introducing an external force f into (6.4) in the domain $\Omega=(0,2)^2$. We set the values of the parameters $\alpha_0=0.04, M=0.005$, and $\epsilon=1$. To ensure that the spatial discretization error is much smaller than the time discretization error, we adopt 128^2 Fourier modes for space discretization.

In Tables 5 and 6, we present the L^2-norm error convergence rate for semi-implicit, SAV, GSAV and PS-SAV approaches at $T=1$ obtained using first-order and Crank-Nicolson scheme, respectively. We can observe that the expected convergence rates are obtained for all cases.

Table 5: Example 6.2 (Case A). Convergence test for Cahn-Hilliard equation using the first-order scheme by different approaches.

Δt	Semi-implicit		SAV		GSAV		PS-SAV	
	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate
1.00E-1	2.87E-02	–	2.89E-02	–	2.87E-02	–	2.30E-02	–
5.00E-2	1.42E-02	1.01	1.43E-02	1.01	1.42E-02	1.01	1.13E-02	1.02
2.50E-2	7.08E-03	1.01	7.14E-03	1.00	7.08E-03	1.01	5.62E-03	1.01
1.25E-2	3.53E-03	1.00	3.56E-03	1.00	3.53E-03	1.00	2.80E-03	1.01
6.25E-3	1.76E-03	1.00	1.78E-03	1.00	1.77E-03	1.00	1.40E-03	1.00

Table 6: Example 6.2 (Case A). Convergence test for Cahn-Hilliard equation using the Crank-Nicolson scheme by different approaches.

Δt	Semi-implicit		SAV		GSAV		PS-SAV	
	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate	$\|e_\phi\|_{L^2}$	Rate
1.00E-1	4.39E-04	–	4.47E-04	–	4.39E-04	–	3.58E-04	–
5.00E-2	1.17E-04	1.91	1.19E-04	1.92	1.17E-04	1.91	9.45E-05	1.92
2.50E-2	3.00E-05	1.96	3.05E-05	1.96	3.00E-05	1.96	2.43E-05	1.96
1.25E-2	7.61E-06	1.98	7.72E-06	1.98	7.61E-06	1.98	6.15E-06	1.98
6.25E-3	1.92E-06	1.99	1.94E-06	1.99	1.92E-06	1.99	1.55E-06	1.99

Case B. As the initial condition, we consider a rectangular arrangement of 19×19 circles

$$\phi^0(x)=360-\sum_{m=1}^{19}\sum_{n=1}^{19}\tanh\left(\frac{\sqrt{(x-x_m)^2+(y-y_n)^2}-r_0}{\sqrt{2}\epsilon}\right), \tag{6.6}$$

where $r_0=0.085, x_m=0.2\times m, y_n=0.2\times n$ for $m,n=1,2,\ldots,19$. For our simulations, we use a computational domain of $[0,4]^2$. The parameters M, α_0, and ϵ are set to $1E$-6, 1.6032, and 0.0079, respectively. We adopt a spatial discretization scheme using 512^2 Fourier modes. The first subfigure of Fig. 3 displays the energy history computed using the semi-implicit/Crank-Nicolson scheme. It is evident that the energy increases rapidly, leading to a blow-up. The PS-SAV approach proposed in this study guarantees the unconditional positivity of the computed $R(t)$ values, regardless of the time step size. Second and third subfigures in Fig. 3 illustrate the time history of the auxiliary variable $r(t)$ computed using the SAV and the auxiliary variable $R(t)$ obtained by the PS-SAV approach, both with a time step size of $\Delta t=0.5$. In the PS-SAV approach, $R(t)$ is computed using a dynamic equation derived from the relation $R(t)=E(\phi)+C>0$, ensuring the positivity of $R(t)$. On the other hand, in the SAV method, the auxiliary variable $r(t)$ is computed using a dynamic equation based on the relation $r(t)=\sqrt{E_1(\phi)+C}$. However, SAV lacks the property of guaranteeing the positivity of the auxiliary variable, and as shown in second subfigure of Fig. 3, the computed $r(t)$ values can take negative values. The fourth subfigure in Fig. 3 gives the history of ξ^{n+1} for SAV, PS-SAV and R-PS-SAV schemes with $\Delta t=1E$-3. In all schemes, ξ^{n+1} is an approximation of 1. Meanwhile, a relaxed correction technique (5.1) for the R-PS-SAV scheme forces ξ^{n+1} closer to 1, which brings the modified energy closer to the original energy. The first two subfigures of Fig. 4 show the snapshots of field function at $T=100$ using SAV and PS-SAV approaches with Euler scheme and a time step size $\Delta t=0.1$. The discrepancy between the two results suggests that the PS-SAV approach yields more accurate results compared to the SAV approach. The last two subfigures of Fig. 4 show the snapshots of field function at $T=100$ using SAV and PS-SAV approaches with Euler scheme and a time step size $\Delta t=1E$-3. The results obtained from both figures are consistent with each other.

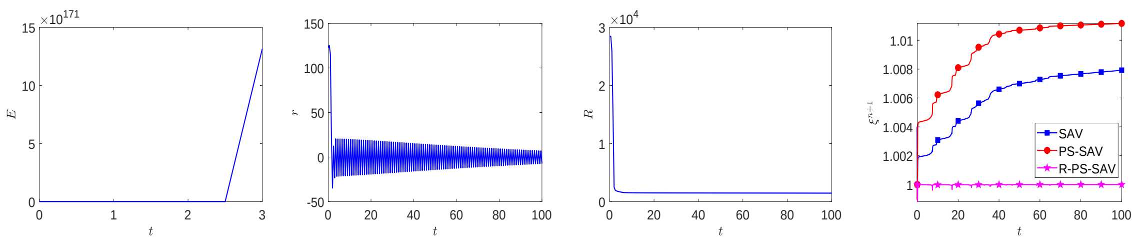


Figure 3: Example 6.2 (Case B). The history of energy obtained by semi-implicit/Crank-Nicolson scheme (first), the history of r obtained by SAV/Crank-Nicolson scheme (second) and the history of R obtained by PS-SAV/Crank-Nicolson scheme (third) with $\Delta t=0.5$. Fourth subfigure is the history of ξ for three schemes with $\Delta t=1E$-3.

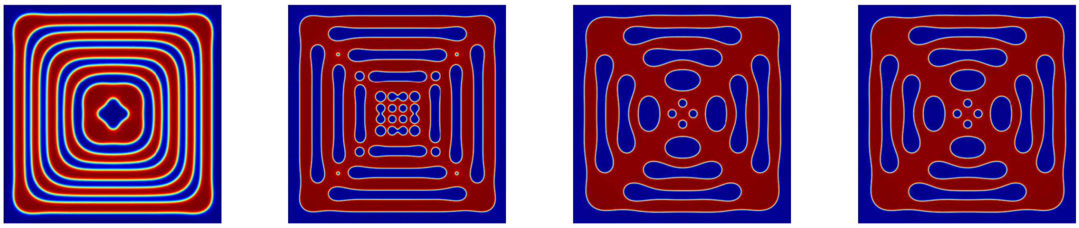


Figure 4: Example 6.2 (Case B). The snapshots of the field function at $T=100$ computed using different schemes and time step sizes: SAV/first-order scheme with $\Delta t=0.1$ (first); PS-SAV/first-order scheme with $\Delta t=0.1$ (second); SAV/first-order scheme with $\Delta t=0.001$ (third); PS-SAV/first-order scheme with $\Delta t=0.001$ (fourth).

Example 6.3. We consider the thin film epitaxy growth model. Let $\phi(\mathbf{x}):\Omega\to\mathbf{R}$ represents the height of the thin film. The total free energy can be expressed as

$$E(\phi)=\int_\Omega\left(F(\nabla\phi)+\frac{\epsilon^2}{2}(\Delta\phi)^2\right)d\mathbf{x}. \tag{6.7}$$

Here, $F(\mathbf{y})$ is a smooth function, and ϵ is the gradient energy coefficient. The first term $\int_\Omega F(\nabla\phi)d\mathbf{x}$ represents a continuum description of the Ehrlich-Schwoedel effect, while the second term $\int_\Omega(\epsilon^2/2)(\Delta\phi)^2d\mathbf{x}$ represents the surface diffusion effect.

Two common choices for the nonlinear potential $F(\nabla\phi)$ are frequently employed:

(i) Double well potential for the model with slope selection

$$F(\nabla\phi)=\frac{1}{4}(|\nabla\phi|^2-1)^2.$$

(ii) Logarithmic potential for the model without slope selection

$$F(\nabla\phi)=-\frac{1}{2}\ln(1+|\nabla\phi|^2).$$

The evolution equation for the height function ϕ is governed by the gradient flow, given by

$$\phi_t=-M\big(\epsilon^2\Delta^2\phi+f(\nabla\phi)\big), \tag{6.8}$$

where M is the mobility constant, and

$$f(\nabla\phi)=-\nabla\cdot F'(\nabla\phi)=\begin{cases}\nabla\cdot\big((1-|\nabla\phi|^2)\nabla\phi\big), & \text{model with slope selection,}\\ \nabla\cdot\left(\dfrac{\nabla\phi}{1+|\nabla\phi|^2}\right), & \text{model without slope selection.}\end{cases}$$

The energy dissipation property for the aforementioned two models can be obtained by taking the L^2 inner product of (6.8) with ϕ_t and applying integration by parts

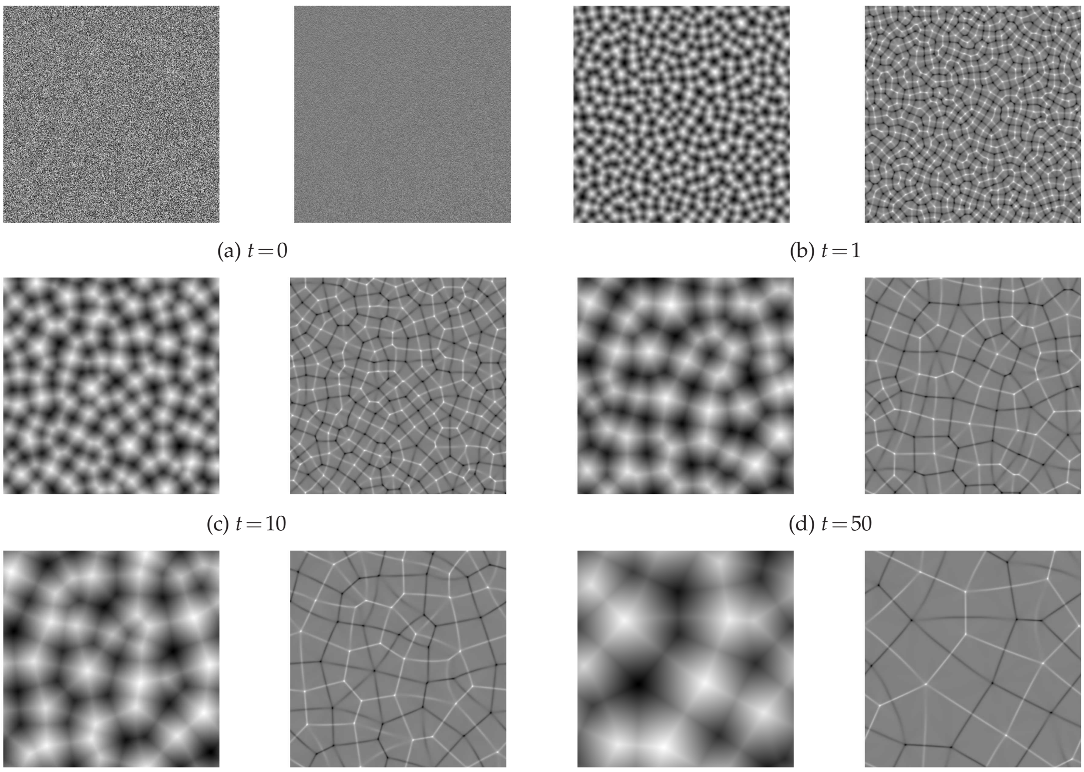
$$\frac{d}{dt}E(\phi) = -\frac{1}{M}\|\phi_t\|^2 \leq 0.$$

To simulate the coarsening dynamics, we select a random initial condition ranging from -0.001 to 0.001. The parameters are as follows:

$$\epsilon = 0.03, \quad M = 1.$$

The computational domain is $\Omega = [0,12.8)^2$, and we utilize 512^2 Fourier modes for spatial discretization. In Figs. 5 and 6, snapshots of the numerical solutions for the height function ϕ and its Laplacian $\Delta\phi$ at different times are presented for both models, respectively.

In the left subplot of Fig. 7, the evolution of energy for the model with slope selection is plotted. It can be observed that the energy decays following a $t^{-1/3}$ trend. In the right subplot of Fig. 7, the evolution of energy for the model without slope selection is depicted. It is notable that the energy decays logarithmically with respect to $-\log_{10}(t)$. These results are consistent with the findings reported in [11].

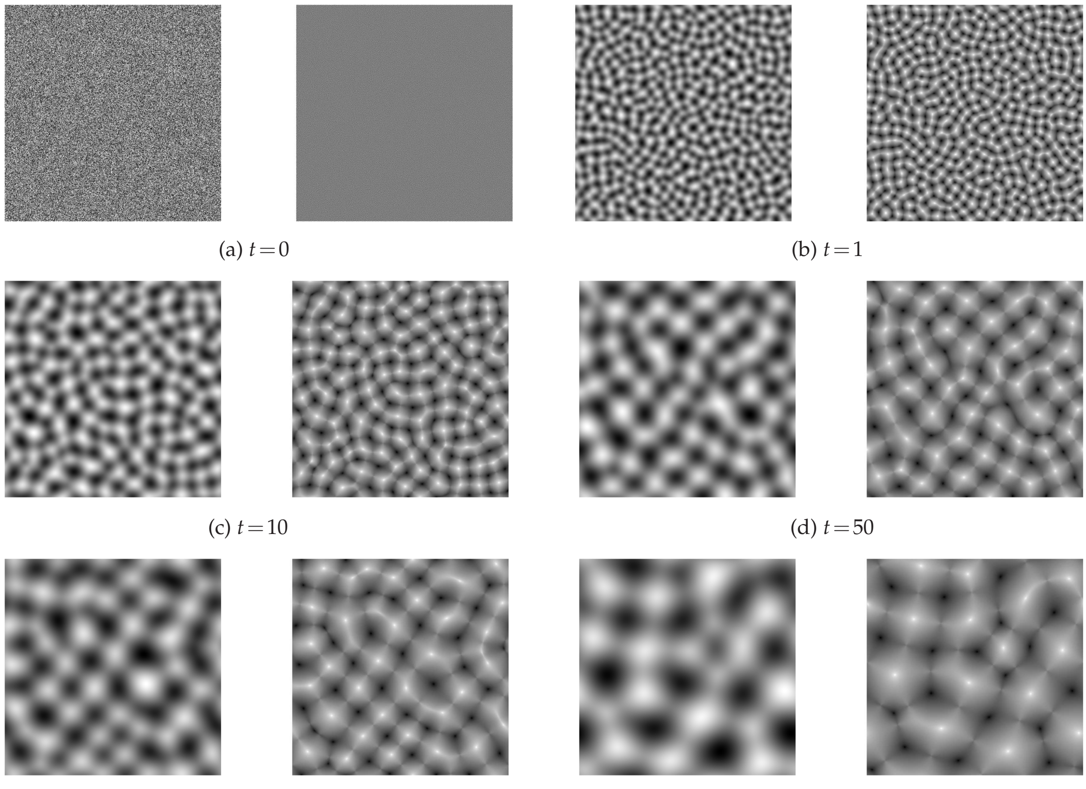


(a) $t=0$ (b) $t=1$

(c) $t=10$ (d) $t=50$

(e) $t=100$ $t=500$

Figure 5: Example 6.3. The isolines of the numerical solutions for the height function ϕ and its $\Delta\phi$ for the thin film epitaxy growth model with slope selection, using a random initial condition. In each subfigure, the left side represents ϕ, while the right side represents $\Delta\phi$.



(a) $t=0$ (b) $t=1$

(c) $t=10$ (d) $t=50$

(e) $t=100$ $t=500$

Figure 6: Example 6.3. The isolines of the numerical solutions for the height function ϕ and its $\Delta\phi$ for the thin film epitaxy growth model without slope selection, using a random initial condition. In each subfigure, the left side represents ϕ, while the right side represents $\Delta\phi$.

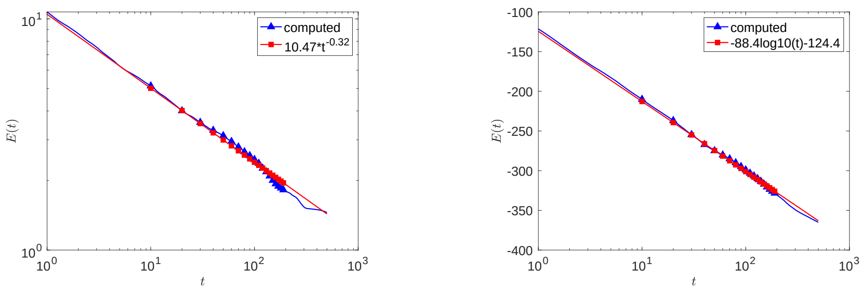


Figure 7: Example 6.3. First: the log-log plots of the free energy for the thin film epitaxy growth model with slope selection. Second: the semi-log plots of the free energy for the thin film epitaxy growth model without slope selection.

7 Error estimates

In this section, we will derive error estimates for the proposed PS-SAV schemes to show the reliability of the constructed schemes. For simplicity, only the first-order PS-SAV scheme based the finite difference method for Allen-Cahn type equation is considered. Note that other spatial discretization methods such as finite element, spectral, etc., can be combined with the schemes constructed above.

We set $h=L/N_{xy}$ to be size of the uniform mesh where N_{xy} is a positive integer. The grid points are denoted by $(x_i,y_j)=(ih,jh)$ for $0\le i,j\le N_{xy}$. The discrete Laplace operator Δ_h is defined by

$$\Delta_h u_{i,j}=\frac{1}{h^2}(u_{i+1,j}+u_{i,j+1}+u_{i-1,j}+u_{i,j-1}-4u_{i,j}),$$

and the discrete gradient operator ∇_h is defined by

$$\begin{aligned}\nabla_h u_{i,j}&=\left(\frac{u_{i+1,j}-u_{i,j}}{h},\frac{u_{i,j+1}-u_{i,j}}{h}\right)\\&=:\left(\nabla_h^1 u_{i+1/2,j},\nabla_h^2 u_{i,j+1/2}\right).\end{aligned}$$

Define the discrete inner products and norms are

$$\begin{aligned}&(u,v)_m=h^2\sum_{i,j=0}^{N_{xy}}u_{i,j}v_{i,j},\quad \|u\|_m^2=(u,u)_m,\\&(u,v)_x=h^2\sum_{i=0}^{N_{xy}-1}\sum_{j=0}^{N_{xy}}u_{i+1/2,j}v_{i+1/2,j},\\&(u,v)_y=h^2\sum_{i=0}^{N_{xy}}\sum_{j=0}^{N_{xy}-1}u_{i,j+1/2}v_{i,j+1/2},\\&\|\nabla_h u\|_{TM}^2=\left(\nabla_h^1 u,\nabla_h^1 u\right)_x+\left(\nabla_h^2 u,\nabla_h^2 u\right)_y.\end{aligned}$$

The following discrete-integration-by-part formula plays an important role in the analysis:

$$(u,\Delta_h v)_m=-\left[\left(\nabla_h^1 u,\nabla_h^1 v\right)_x+\left(\nabla_h^2 u,\nabla_h^2 v\right)_y\right]=(\Delta_h u,v)_m. \tag{7.1}$$

A first-order fully discrete PS-SAV scheme for the Allen-Cahn type model is given by

$$\begin{aligned}&\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}=-M\mu_h^{n+1},\\&\mu_h^{n+1}=-s\epsilon^2\left(\Delta_h\phi_h^{n+1}-\Delta_h\phi_h^n\right)+\frac{R_h^{n+1}}{E_h\left(\phi_h^n\right)+C}\left[-\epsilon^2\Delta_h\phi_h^n+F'\left(\phi_h^n\right)\right],\\&\frac{R_h^{n+1}-R_h^n}{\Delta t}=-\frac{1}{M}\left(\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t},\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}\right)_m,\end{aligned} \tag{7.2}$$

where $s>0$ is a stabilizing constant and the full discretization $E_h(\phi_h^n)$ of $E(\phi(\mathbf{x},t^n))$ is

$$E_h(\phi_h^n)=-\frac{\epsilon^2}{2}\left(\Delta_h\phi_h^n,\phi_h^n\right)_m+\left(F\left(\phi_h^n\right),1\right)_m$$

$$
\begin{aligned}
&=\frac{\epsilon^2}{2}\Big(\big(\nabla_h^1\phi_h^n,\nabla_h^1\phi_h^n\big)_x+\big(\nabla_h^2\phi_h^n,\nabla_h^2\phi_h^n\big)_y\Big)+\frac{1}{4}\Big(\big(\phi_h^n\big)^2-1,\big(\phi_h^n\big)^2-1\Big)_m \\
&=\frac{\epsilon^2}{2}\|\nabla_h\phi_h^n\|_{TM}^2+\frac{1}{4}\|\big(\phi_h^n\big)^2-1\|_m^2.
\end{aligned}
$$

Similar as semi-discrete scheme (3.4), we are easy to obtain the following energy dissipation law.

Theorem 7.1. *Given $R_h^0=R^0>0$, we have $R_h^n>0$, and the first-order fully discrete PS-SAV scheme* (7.2) *is unconditionally energy stable in the sense that*

$$
R_h^{n+1}-R_h^n=-\frac{\Delta t}{M}\left(\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t},\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}\right)_m\le 0.
$$

For simplicity, we set

$$
\begin{aligned}
&e_\phi^{n+1}=\phi_h^{n+1}-\phi(t^{n+1}), \quad && e_\mu^{n+1}=\mu_h^{n+1}-\mu(t^{n+1}),\\
&d_te_\phi^{n+1}=\frac{e_\phi^{n+1}-e_\phi^n}{\Delta t}, && e_R^{n+1}=R_h^{n+1}-R(t^{n+1}).
\end{aligned}
$$

Theorem 7.2. *Assume*

$$
\phi\in W^{2,\infty}\big(0,T;L^2(\Omega)\big)\bigcap W^{1,\infty}\big(0,T;W^{2,2}(\Omega)\big)\bigcap L^\infty\big(0,T;W^{4,\infty}(\Omega)\big),
$$

and $F(\phi)\in C^2(\mathbb{R})$, then for the fully discrete scheme (7.2) *with stabilizing constant $s\ge R^0/K_1$ and $\Delta t\le Ch^{1+\beta}$ with $\beta>0$, there exists a positive constant C independent of h and Δt such that*

$$
\sum_{n=1}^k\Delta t\|d_te_\phi^{n+1}\|_m^2+\|\nabla_he_\phi^{k+1}\|_{TM}^2+\|e_\phi^{k+1}\|_m^2+|e_R^{k+1}|^2\le C\big(h^4+(\Delta t)^2\big),
$$

where the positive constant K_1 is the lower bound of $E_h(\phi_h^n)+C$.

We shall split the proof of the above results into three lemmas below.

Lemma 7.1. *Under the conditions of Theorem* 7.2, *there exists positive constants C and K_1 independent of h and Δt such that*

$$
\begin{aligned}
&\frac{K_1}{2}\|d_te_\phi^{n+1}\|_m^2+\left(s-\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}\right)K_1\epsilon^2M\frac{\|\nabla_he_\phi^{n+1}-\nabla_he_\phi^n\|_{TM}^2}{\Delta t}+R_h^{n+1}\epsilon^2M\frac{\|\nabla_he_\phi^{n+1}\|_{TM}^2}{2\Delta t}\\
\le{}& C|e_R^{n+1}|^2+C\|\nabla_he_\phi^n\|_{TM}^2+C\|e_\phi^n\|_m^2+R_h^n\epsilon^2M\frac{\|\nabla_he_\phi^n\|_{TM}^2}{2\Delta t}+C\big(h^4+(\Delta t)^2\big).
\end{aligned} \tag{7.3}
$$

Proof. Subtracting equations in (3.3) from equations in (7.2) respectively, we obtain the following three error equations:

$$\frac{e_\phi^{n+1}-e_\phi^n}{\Delta t}=-Me_\mu^{n+1}+\left.\frac{\partial\phi}{\partial t}\right|_{t^{n+1}}-\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}, \tag{7.4}$$

$$\begin{aligned} e_\mu^{n+1}=&-s\epsilon^2\left(\Delta_h e_\phi^{n+1}-\Delta_h e_\phi^n\right)+\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\left[-\epsilon^2\Delta_h\phi_h^n+F'(\phi_h^n)\right]\\ &-\frac{R(t^{n+1})}{E(\phi(t^{n+1}))+C}\left[-\epsilon^2\Delta\phi(t^{n+1})+F'(\phi(t^{n+1}))\right]\\ &-s\epsilon^2\left(\Delta_h\phi(t^{n+1})-\Delta\phi(t^{n+1})\right)+s\epsilon^2\left(\Delta_h\phi(t^n)-\Delta\phi(t^{n+1})\right), \end{aligned} \tag{7.5}$$

$$\begin{aligned} \frac{e_R^{n+1}-e_R^n}{\Delta t}=&-\frac{1}{M}\left(\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t},\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}\right)_m+\frac{1}{M}\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)\\ &+\left.\frac{dR}{dt}\right|_{t^{n+1}}-\frac{R(t^{n+1})-R(t^n)}{\Delta t},\\ \le&-\frac{1}{M}\left(\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}+\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\phi_h^{n+1}-\phi_h^n}{\Delta t}-\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\\ &+\frac{1}{M}\left[\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)-\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\right]+C|R|_{W^{2,\infty}(0,T)}\Delta t. \end{aligned} \tag{7.6}$$

Next we shall first make the hypotheses that there exist two positive constant C^* and C_* such that

$$\|\phi_h^n\|_\infty\le C^*, \tag{7.7a}$$

$$\|e_\phi^n\|_m+\|\nabla_h e_\phi^n\|_{TM}+|e_R^n|\le C_*(\Delta t+h^2)^{\frac{1}{2}}. \tag{7.7b}$$

These two hypotheses will be verified in Lemma 7.4.

Multiplying (7.4) by $((e_\phi^{n+1}-e_\phi^n)/\Delta t)h^2$ making summation on i,j for $0\le i\le N_{xy}$, $0\le j\le N_{xy}$, we have

$$\|d_te_\phi^{n+1}\|_m^2=-M\left(e_\mu^{n+1},d_te_\phi^{n+1}\right)_m+\left(\left.\frac{\partial\phi}{\partial t}\right|_{t^{n+1}}-\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t},d_te_\phi^{n+1}\right)_m. \tag{7.8}$$

Multiplying (7.5) by $d_te_\phi^{n+1}h^2$ and making summation on i,j for $0\le i\le N_{xy}$, $0\le j\le N_{xy}$, we have

$$\begin{aligned} \left(e_\mu^{n+1},d_te_\phi^{n+1}\right)_m=&-s\epsilon^2\left(\Delta_he_\phi^{n+1}-\Delta_he_\phi^n,d_te_\phi^{n+1}\right)_m\\ &-\epsilon^2\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\Delta_h\phi_h^n-\frac{R(t^{n+1})}{E(\phi(t^{n+1}))+C}\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m \end{aligned}$$

$$
\begin{aligned}
&+\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}F'-\frac{R(t^{n+1})}{E(\phi(t^{n+1}))+C}F'(\phi(t^{n+1})),d_te_\phi^{n+1}\right)_m\\
&-s\epsilon^2\left(\Delta_h\phi(t^{n+1})-\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m\\
&+s\epsilon^2\left(\Delta_h\phi(t^{n})-\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m.
\end{aligned}\tag{7.9}
$$

For the first term in the right-hand side of the Eq. (7.9), we have

$$
-s\epsilon^2\left(\Delta_he_\phi^{n+1}-\Delta_he_\phi^n,d_te_\phi^{n+1}\right)_m=s\epsilon^2\frac{\|\nabla_he_\phi^{n+1}-\nabla_he_\phi^n\|_{TM}^2}{\Delta t},\tag{7.10}
$$

where $\nabla_hf=d_xf+d_yf$.

For the second term in the right-hand side of the Eq. (7.9), we have

$$
\begin{aligned}
&-\epsilon^2\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\Delta_h\phi_h^n-\frac{R(t^{n+1})}{E(\phi(t^{n+1}))+C}\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m\\
=&-\epsilon^2\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\Delta_he_\phi^n,d_te_\phi^{n+1}\right)_m-\epsilon^2\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\left(\Delta_h\phi(t^n)-\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m\\
&-\epsilon^2\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}-\frac{R(t^{n+1})}{E(\phi(t^{n+1}))+C}\right)\left(\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m.
\end{aligned}\tag{7.11}
$$

For the first term in the right-hand side of (7.11), we have

$$
\begin{aligned}
&-\epsilon^2\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\Delta_he_\phi^n,d_te_\phi^{n+1}\right)_m\\
=&\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\epsilon^2\left(\nabla_he_\phi^n,\frac{\nabla_he_\phi^{n+1}-\nabla_he_\phi^n}{\Delta t}\right)_{TM}\\
=&-\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\epsilon^2\left(\frac{\|\nabla_he_\phi^n\|_{TM}^2-\|\nabla_he_\phi^{n+1}\|_{TM}^2}{2\Delta t}+\frac{\|\nabla_he_\phi^n-\nabla_he_\phi^{n+1}\|_{TM}^2}{2\Delta t}\right)\\
=&\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\epsilon^2\left(\frac{\|\nabla_he_\phi^{n+1}\|_{TM}^2-\|\nabla_he_\phi^n\|_{TM}^2}{2\Delta t}-\frac{\|\nabla_he_\phi^n-\nabla_he_\phi^{n+1}\|_{TM}^2}{2\Delta t}\right).
\end{aligned}\tag{7.12}
$$

Noting that $R_h^{n+1}\le R^0\le C_1$ and $E_h(\phi_h^n)+C>K_1>0$, then for the second term in the right-hand side of (7.11), by using Cauchy-Schwartz inequality, we have

$$
\begin{aligned}
&-\epsilon^2\frac{R_h^{n+1}}{E_h(\phi_h^n)+C}\left(\Delta_h\phi(t^n)-\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\right)_m\\
\le&\frac{1}{10M}\|d_te_\phi^{n+1}\|_m^2+C\|\Delta_h\phi(t^n)-\Delta\phi(t^{n+1})\|_m^2
\end{aligned}
$$

$$\leq \frac{1}{10M}\|d_t e_\phi^{n+1}\|_m^2 + C\|\phi\|^2_{L^\infty(0,T;W^{4,\infty}(\Omega))}h^4 + C\|\phi\|^2_{W^{1,\infty}(0,T;W^{2,\infty}(\Omega))}(\Delta t)^2. \tag{7.13}$$

Using inequality (7.7a) and supposing $F(\phi)\in C^2(\mathbb{R})$, then we have the following inequality for the last term in the right-hand side of (7.11):

$$\begin{aligned}
&-\epsilon^2\left(\frac{R_h^{n+1}}{E_h(\phi_h^n)+C} - \frac{R(t^{n+1})}{E(\phi(t^{n+1}))+C}\right)(\Delta\phi(t^{n+1}), d_t e_\phi^{n+1})_m \\
=& -\epsilon^2 \frac{e_R^{n+1}}{E_h(\phi_h^n)+C}(\Delta\phi(t^{n+1}), d_t e_\phi^{n+1})_m \\
&+\epsilon^2 \frac{R(t^{n+1})\big(E(\phi(t^{n+1}))-E_h(\phi_h^n)\big)}{\big[E_h(\phi_h^n)+C\big]\big[E(\phi(t^{n+1}))+C+C\big]}(\Delta\phi(t^{n+1}), d_t e_\phi^{n+1})_m.
\end{aligned} \tag{7.14}$$

Here, for $E(\phi(t^{n+1}))-E_h(\phi_h^n)$, we have

$$\begin{aligned}
&E(\phi(t^{n+1}))-E_h(\phi_h^n) \\
=&\frac{\epsilon^2}{2}\|\nabla\phi(t^{n+1})\|^2 + \big(F(\phi(t^{n+1})),1\big) - \frac{\epsilon^2}{2}\|\nabla_h\phi_h^n\|^2_{TM} + \big(F(\phi_h^n),1\big)_m.
\end{aligned} \tag{7.15}$$

Using the approximation property of the quadrature formula, we obtain

$$\begin{aligned}
&\frac{\epsilon^2}{2}\|\nabla\phi(t^{n+1})\|^2 - \frac{\epsilon^2}{2}\|\nabla_h\phi_h^n\|^2_{TM} \\
=&\frac{\epsilon^2}{2}\Big(\|\nabla\phi(t^{n+1})\|^2 - \|\nabla\phi(t^{n+1})\|^2_{TM}\Big) + \frac{\epsilon^2}{2}\Big(\|\nabla\phi(t^{n+1})\|^2_{TM} - \|\nabla_h\phi_h^n\|^2_{TM}\Big) \\
\leq& Ch^2 + \frac{\epsilon^2}{2}\Big(\|\nabla\phi(t^{n+1})\|_{TM} + \|\nabla_h\phi_h^n\|_{TM}\Big)\Big(\|\nabla\phi(t^{n+1})\|_{TM} - \|\nabla_h\phi_h^n\|_{TM}\Big) \\
\leq& \frac{\epsilon^2}{2}\Big(\|\nabla\phi(t^{n+1})\|_{TM} + \|\nabla_h\phi_h^n\|_{TM}\Big)\|\nabla\phi(t^{n+1}) - \nabla_h\phi_h^n\|_{TM} + Ch^2.
\end{aligned}$$

Taking advantage of the bounded property of $\phi(t^n)$ and the inequality (7.7b), we have $\|\nabla_h\phi_h^n\|_{TM}\leq C$. Then the above inequality will be transformed as

$$\begin{aligned}
&\frac{\epsilon^2}{2}\|\nabla\phi(t^{n+1})\|^2 - \frac{\epsilon^2}{2}\|\nabla_h\phi_h^n\|^2_{TM} \\
\leq& C\|\nabla\phi(t^{n+1}) - \nabla_h\phi_h^n\|_{TM} + Ch^2 \\
\leq& C\Big(\|\nabla\phi(t^{n+1}) - \nabla_h\phi(t^n)\|_{TM} + \|\nabla_h\phi(t^n) - \nabla_h\phi_h^n\|_{TM}\Big) + Ch^2 \\
\leq& C\Big(\|\nabla(\phi(t^{n+1}) - \phi(t^n))\|_{TM} + \|(\nabla-\nabla_h)\phi(t^n)\|_{TM} + \|\nabla_h e_\phi^n\|_{TM}\Big) + Ch^2 \\
\leq& C\|\nabla_h e_\phi^n\|_{TM} + C(\Delta t + h^2).
\end{aligned} \tag{7.16}$$

For the other two terms on the right side of Eq. (7.15), using the midpoint approximation property of the rectangle quadrature formula and inequality (7.7a), we have

$$
\begin{aligned}
&\big(F\big(\phi(t^{n+1})\big),1\big)-\big(F\big(\phi_h^n\big),1\big)_m \\
=&\frac{1}{4}\big\|\big(\phi(t^{n+1})\big)^2-1\big\|^2-\frac{1}{4}\big\|\big(\phi_h^n\big)^2-1\big\|_m^2 \\
=&\frac{1}{4}\big\|\big(\phi(t^{n+1})\big)^2-1\big\|^2-\frac{1}{4}\big\|\big(\phi(t^{n+1})\big)^2-1\big\|_m^2+\frac{1}{4}\big\|\big(\phi(t^{n+1})\big)^2-1\big\|_m^2-\frac{1}{4}\big\|\big(\phi_h^n\big)^2-1\big\|_m^2 \\
\le& Ch^2+\frac{1}{4}\Big(\big\|\big(\phi(t^{n+1})\big)^2-1\big\|_m+\big\|\big(\phi_h^n\big)^2-1\big\|_m\Big)\Big(\big\|\big(\phi(t^{n+1})\big)^2-1\big\|_m-\big\|\big(\phi_h^n\big)^2-1\big\|_m\Big) \\
\le& Ch^2+C\big\|\big(\phi(t^{n+1})\big)^2-\big(\phi_h^n\big)^2\big\|_m \\
\le& Ch^2+C\big\|\phi(t^{n+1})+\phi_h^n\big\|_m\big\|\phi(t^{n+1})-\phi_h^n\big\|_m \\
\le& Ch^2+C\Big(\big\|e_\phi^n\big\|_m+\|\phi(t^n)-\phi(t^{n+1})\|_m\Big) \\
\le& C\|e_\phi^n\|_m+C(\Delta t+h^2).
\end{aligned}
\tag{7.17}
$$

Bringing the inequalities (7.16) and (7.17) into Eq. (7.14), we have

$$
\begin{aligned}
&-\epsilon^2\left(\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}-\frac{R(t^{n+1})}{E\big(\phi(t^{n+1})\big)+C}\right)\big(\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\big)_m \\
\le&\frac{1}{10M}\big\|d_te_\phi^{n+1}\big\|_m^2+C\big|e_R^{n+1}\big|^2+C\big\|\nabla_he_\phi^n\big\|_{TM}^2+C\big\|e_\phi^n\big\|_m^2+C\big(h^4+(\Delta t)^2\big).
\end{aligned}
\tag{7.18}
$$

Using similar technique and Cauchy-Schwartz inequality, we can obtain the following inequality for the third term in the right-hand side of (7.9):

$$
\begin{aligned}
&\left(\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}F'\big(\phi_h^n\big)-\frac{R(t^{n+1})}{E\big(\phi(t^{n+1})\big)+C}F'\big(\phi(t^{n+1})\big),d_te_\phi^{n+1}\right)_m \\
=&\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}\big(F'\big(\phi_h^n\big)-F'\big(\phi(t^{n+1})\big),d_te_\phi^{n+1}\big)_m \\
&\quad+\left(\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}-\frac{R(t^{n+1})}{E_h\big(\phi(t^{n+1})\big)+C}\right)\big(F'\big(\phi(t^{n+1})\big),d_te_\phi^{n+1}\big)_m \\
\le&\frac{1}{10M}\big\|d_te_\phi^{n+1}\big\|_m^2+C\big\|e_\phi^n\big\|_m^2+C(\Delta t)^2 \\
&\quad+\frac{1}{10M}\big\|d_te_\phi^{n+1}\big\|_m^2+C\big|e_R^{n+1}\big|^2+C\big\|\nabla_he_\phi^n\big\|_{TM}^2+C\big\|e_\phi^n\big\|_m^2+C\big(h^4+(\Delta t)^2\big) \\
\le&\frac{1}{5M}\big\|d_te_\phi^{n+1}\big\|_m^2+C\big\|e_\phi^n\big\|_m^2+C\big|e_R^{n+1}\big|^2+C\big\|\nabla_he_\phi^n\big\|_{TM}^2+C\big(h^4+(\Delta t)^2\big).
\end{aligned}
\tag{7.19}
$$

For the last two terms in the right-hand side of (7.9), using Cauchy-Schwartz inequality, we have

$$
\begin{aligned}
&-s\epsilon^2\big(\Delta_h\phi(t^{n+1})-\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\big)_m+s\epsilon^2\big(\Delta_h\phi(t^n)-\Delta\phi(t^{n+1}),d_te_\phi^{n+1}\big)_m\\
\le&\frac{1}{10M}\|d_te_\phi^{n+1}\|_m^2+C\big(h^4+(\Delta t)^2\big)\Big(\|\phi\|^2_{L^\infty(0,T;W^{4,\infty}(\Omega))}+\|\phi\|^2_{W^{1,\infty}(0,T;W^{2,2}(\Omega))}\Big). \qquad (7.20)
\end{aligned}
$$

Using (7.7a), we obtain that there exists a positive constant K_1 to satisfy

$$
0<K_1<E_h\big(\phi_h^n\big)+C<2\big(E\big(\phi(t^n)\big)+C\big).
$$

We choose $s\ge R^0/K_1$ to satisfy that $s-R_h^{n+1}/(E_h(\phi_h^n)+C)>0$. Combining (7.8) with (7.9)-(7.20), we get

$$
\begin{aligned}
&\frac{K_1}{2}\|d_te_\phi^{n+1}\|_m^2+\left(s-\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}\right)K_1\epsilon^2M\frac{\|\nabla_he_\phi^{n+1}-\nabla_he_\phi^n\|_{TM}^2}{\Delta t}+R_h^{n+1}\epsilon^2M\frac{\|\nabla_he_\phi^{n+1}\|^2_{TM}}{2\Delta t}\\
\le&C|e_R^{n+1}|^2+C\|\nabla_he_\phi^n\|^2_{TM}+C\|e_\phi^n\|_m^2+R_h^n\epsilon^2M\frac{\|\nabla_he_\phi^n\|^2_{TM}}{2\Delta t}+C\big(h^4+(\Delta t)^2\big).
\end{aligned}
$$

The proof is complete. ◻

Lemma 7.2. *Under the conditions of Theorem* 7.2*, there exists a positive constant C independent of h and* Δt *such that*

$$
\begin{aligned}
&\frac{\|e_\phi^{n+1}\|_m^2-\|e_\phi^n\|_m^2}{2\Delta t}+\frac{\|e_\phi^{n+1}-e_\phi^n\|_m^2}{2\Delta t}\\
&\quad+Ms\epsilon^2\left(\frac{\|\nabla_he_\phi^{n+1}\|^2_{TM}-\|\nabla_he_\phi^n\|^2_{TM}}{2}+\frac{\|\nabla_he_\phi^{n+1}-\nabla_he_\phi^n\|^2_{TM}}{2}\right)\\
\le&C\|e_\phi^{n+1}\|_m^2+C\|\nabla_he_\phi^{n+1}\|^2_{TM}+C|e_R^{n+1}|^2+C\big(h^4+(\Delta t)^2\big). \qquad (7.21)
\end{aligned}
$$

Proof. Combining (7.8)-(7.9) with above inequalities (7.10)-(7.20), we can obtain that

$$
\begin{aligned}
&\frac{1}{2}\|d_te_\phi^{n+1}\|_m^2+\left(s-\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}\right)\epsilon^2M\frac{\|\nabla_he_\phi^{n+1}-\nabla_he_\phi^n\|_{TM}^2}{\Delta t}\\
&\quad+\frac{R_h^{n+1}}{E_h\big(\phi_h^n\big)+C}\epsilon^2M\frac{\|\nabla_he_\phi^{n+1}\|^2_{TM}}{2\Delta t}\\
\le&C|e_R^{n+1}|^2+C\|\nabla_he_\phi^n\|^2_{TM}+C\|e_\phi^n\|_m^2+\frac{R_h^n}{E_h\big(\phi_h^n\big)+C}\epsilon^2M\frac{\|\nabla_he_\phi^n\|^2_{TM}}{2\Delta t}+C\big(h^4+(\Delta t)^2\big). \qquad (7.22)
\end{aligned}
$$

Next we multiply (7.4) by $e_\phi^{n+1}h^2$, make summation on i,j for $1\le i\le N_{xy}$, $1\le j\le N_{xy}$, and combine it with (7.5) to obtain

$$\begin{aligned}
&\left(\frac{e_\phi^{n+1}-e_\phi^n}{\Delta t},e_\phi^{n+1}\right)_m - Ms\epsilon^2\left(\Delta_h e_\phi^{n+1}-\Delta_h e_\phi^n,e_\phi^{n+1}\right)_m\\
=&-\Bigg(\frac{MR_h^{n+1}}{E_h(\phi_h^n)+C}\left[-\epsilon^2\Delta_h\phi_h^n+F'(\phi_h^n)\right]\\
&\quad-\frac{MR(t^{n+1})}{E_h(\phi(t^{n+1}))+C}\left[-\epsilon^2\Delta\phi(t^{n+1})+F'(\phi(t^{n+1}))\right],e_\phi^{n+1}\Bigg)_m\\
&\quad+s\epsilon^2M\left(\Delta_h\phi(t^{n+1})-\Delta\phi(t^{n+1}),e_\phi^{n+1}\right)_m - s\epsilon^2M\left(\Delta_h\phi(t^n)-\Delta\phi(t^{n+1}),e_\phi^{n+1}\right)_m\\
&\quad+\left(\frac{\partial\phi}{\partial t}\bigg|_{t^{n+1}}-\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t},e_\phi^{n+1}\right)_m = RHD.
\end{aligned}\tag{7.23}$$

For all terms on the left-hand side of (7.23), we have

$$\begin{aligned}
&\left(\frac{e_\phi^{n+1}-e_\phi^n}{\Delta t},e_\phi^{n+1}\right)_m - Ms\epsilon^2\left(\Delta_h e_\phi^{n+1}-\Delta_h e_\phi^n,e_\phi^{n+1}\right)_m\\
=&\frac{\|e_\phi^{n+1}\|_m^2-\|e_\phi^n\|_m^2}{2\Delta t}+\frac{\|e_\phi^{n+1}-e_\phi^n\|_m^2}{2\Delta t}\\
&\quad+MS\epsilon^2\left(\frac{\|\nabla_h e_\phi^{n+1}\|_{TM}^2-\|\nabla_h e_\phi^n\|_{TM}^2}{2}+\frac{\|\nabla_h e_\phi^{n+1}-\nabla_h e_\phi^n\|_{TM}^2}{2}\right).
\end{aligned}\tag{7.24}$$

Using similar technique for the right-hand side of (7.9), we can obtain the following inequality for the right-hand side of (7.23):

$$RHD\le C\|e_\phi^{n+1}\|_m^2+C\|\nabla_h e_\phi^{n+1}\|_{TM}^2+C|e_R^{n+1}|^2+C\left(h^4+(\Delta t)^2\right).\tag{7.25}$$

Combining (7.23) with above inequalities (7.24)-(7.25), we can obtain that

$$\begin{aligned}
&\frac{\|e_\phi^{n+1}\|_m^2-\|e_\phi^n\|_m^2}{2\Delta t}+\frac{\|e_\phi^{n+1}-e_\phi^n\|_m^2}{2\Delta t}\\
&\quad+MS\epsilon^2\left(\frac{\|\nabla_h e_\phi^{n+1}\|_{TM}^2-\|\nabla_h e_\phi^n\|_{TM}^2}{2}+\frac{\|\nabla_h e_\phi^{n+1}-\nabla_h e_\phi^n\|_{TM}^2}{2}\right)\\
\le& C\|e_\phi^{n+1}\|_m^2+C\|\nabla_h e_\phi^{n+1}\|_{TM}^2+C|e_R^{n+1}|^2+C\left(h^4+(\Delta t)^2\right).
\end{aligned}$$

The proof is complete. □

We next give the estimate analysis for $|e_R^{n+1}|$.

Lemma 7.3. *Under the conditions of Theorem* 7.2, *there exists a positive constant C independent of h and* Δt *such that*

$$\begin{aligned}&\frac{|e_R^{n+1}|^2-|e_R^n|^2}{2\Delta t}+\frac{|e_R^{n+1}-e_R^n|^2}{2\Delta t}\\ \le&\frac{1}{4}\|d_te_\phi^{n+1}\|_m^2+C\|d_te_\phi^{n+1}\|_m^2|e_R^{n+1}|^2+C|e_R^{n+1}|^2+C\big(h^4+(\Delta t)^2\big).\end{aligned}\tag{7.26}$$

Proof. Multiplying (7.6) with e_R^{n+1} results in

$$\begin{aligned}&\frac{|e_R^{n+1}|^2-|e_R^n|^2}{2\Delta t}+\frac{|e_R^{n+1}-e_R^n|^2}{2\Delta t}\\ =&-\frac{e_R^{n+1}}{M}\left(\frac{e_\phi^{n+1}-e_\phi^n}{\Delta t}+\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}+\frac{\partial\phi(t^{n+1})}{\partial t},\frac{e_\phi^{n+1}-e_\phi^n}{\Delta t}+\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}-\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\\ &+\frac{e_R^{n+1}}{M}\left(\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)-\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\right)+C|R|_{W^{2,\infty}(0,T)}\Delta t e_R^{n+1}\\ \le&-\frac{e_R^{n+1}}{M}\|d_te_\phi^{n+1}\|_m^2\\ &-\frac{e_R^{n+1}}{M}\left(\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}+\frac{\partial\phi(t^{n+1})}{\partial t},d_te_\phi^{n+1}+\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}-\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\\ &+C\Delta t\|d_te_\phi^{n+1}\|_m|e_R^{n+1}|+\frac{e_R^{n+1}}{M}\left(\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)-\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\right)\\ &+C|R|_{W^{2,\infty}(0,T)}\Delta t e_R^{n+1}.\end{aligned}\tag{7.27}$$

For the first term in the right-hand side of above equation (7.27), by using Cauchy-Schwartz inequality, we have

$$-\frac{e_R^{n+1}}{M}\|d_te_\phi^{n+1}\|_m^2\le\frac{1}{8}\|d_te_\phi^{n+1}\|_m^2+C\|d_te_\phi^{n+1}\|_m^2|e_R^{n+1}|^2.\tag{7.28}$$

For the second and third terms in the right-hand side of above equation (7.27), we have

$$\begin{aligned}&-\frac{e_R^{n+1}}{M}\left(\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}+\frac{\partial\phi(t^{n+1})}{\partial t},d_te_\phi^{n+1}+\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}-\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\\ &\quad+C\Delta t\|d_te_\phi^{n+1}\|_m|e_R^{n+1}|\\ \le&\frac{|e_R^{n+1}|}{M}\left\|\frac{\phi(t^{n+1})-\phi(t^n)}{\Delta t}+\frac{\partial\phi(t^{n+1})}{\partial t}\right\|_m\|d_te_\phi^{n+1}\|_m+C\Delta t|e_R^{n+1}|+C\Delta t\|d_te_\phi^{n+1}\|_m|e_R^{n+1}|\\ \le&\frac{1}{8}\|d_te_\phi^{n+1}\|_m^2+C|e_R^{n+1}|^2+C(\Delta t)^2.\end{aligned}\tag{7.29}$$

The last two terms in the right-hand side of Eq. (7.27) can be bounded by using the midpoint approximation property of the rectangle quadrature formula

$$\begin{aligned}&\frac{e_R^{n+1}}{M}\left(\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)-\left(\frac{\partial\phi(t^{n+1})}{\partial t},\frac{\partial\phi(t^{n+1})}{\partial t}\right)_m\right)+C|R|_{W^{2,\infty}(0,T)}\Delta t e_R^{n+1}\\&\le C\left|e_R^{n+1}\right|^2+C(\Delta t)^2+Ch^4.\end{aligned}\tag{7.30}$$

Combining (7.27) with above inequalities (7.28)-(7.30), we can obtain that

$$\begin{aligned}&\frac{\left|e_R^{n+1}\right|^2-\left|e_R^n\right|^2}{2\Delta t}+\frac{\left|e_R^{n+1}-e_R^n\right|^2}{2\Delta t}\\&\le\frac{1}{4}\left\|d_te_\phi^{n+1}\right\|_m^2+C\left\|d_te_\phi^{n+1}\right\|_m^2\left|e_R^{n+1}\right|^2+C\left|e_R^{n+1}\right|^2+C\left(h^4+(\Delta t)^2\right).\end{aligned}$$

The proof is complete. □

Lemma 7.4. *Under the conditions of Theorem* 7.2*, there exists two positive constants C^* and C_* independent of h and Δt such that*

$$\begin{aligned}&\left\|\phi_h^n\right\|_\infty\le C^*,\\&\left\|e_\phi^n\right\|_m+\left\|\nabla_he_\phi^n\right\|_{TM}+\left|e_R^n\right|\le C_*(\Delta t+h^2)^{\frac{1}{2}}.\end{aligned}$$

Proof. Using the scheme (7.2) for $n=0$ and applying the inverse assumption, we can get the approximation ϕ_h^1 with the following property:

$$\begin{aligned}\left\|\phi_h^1\right\|_\infty&\le\left\|\phi_h^1-\phi(t^1)\right\|_\infty+\|\phi(t^1)\|_\infty\\&\le\left\|\phi_h^1-\Pi_h\phi(t^1)\right\|_\infty+\left\|\Pi_h\phi(t^1)-\phi(t^1)\right\|_\infty+\|\phi(t^1)\|_\infty\\&\le Ch^{-1}\left(\left\|\phi_h^1-\phi(t^1)\right\|_m+\left\|\phi(t^1)-\Pi_h\phi(t^1)\right\|_m\right)+\left\|\Pi_h\phi(t^1)-\phi(t^1)\right\|_\infty+\|\phi(t^1)\|_\infty\\&\le C(h+h^{-1}\Delta t)+\|\phi(t^1)\|_\infty\le C.\end{aligned}$$

Here Π_h is an bilinear interpolant operator with the following estimate:

$$\left\|\Pi_h\phi^1-\phi^1\right\|_\infty\le Ch^2.\tag{7.31}$$

Thus, we can choose the positive constant C^* independent of h and Δt such that

$$C^*\ge\max\left\{\left\|\phi_h^1\right\|_\infty,2\|\phi(t^n)\|_\infty\right\}.$$

By the definition of C^*, it is trivial that hypothesis (7.7a) holds true for $n=1$. Supposing that $\|\phi_h^k\|_\infty\le C^*$ holds true for an integer $k=1,\ldots,n$, with the aid of Lemmas 7.1-7.3, we have that

$$\left\|\phi_h^k-\phi(t^k)\right\|_m\le C(\Delta t+h^2).$$

Next, we prove that $\|\phi_h^{n+1}\|_\infty \le C^*$ holds true. Since

$$\begin{aligned}
\|\phi_h^{n+1}\|_\infty &\le \|\phi_h^{n+1}-\phi(t^{n+1})\|_\infty + \|\phi(t^{n+1})\|_\infty \\
&\le \|\phi_h^{n+1}-\Pi_h\phi(t^{n+1})\|_\infty + \|\Pi_h\phi(t^{n+1})-\phi(t^{n+1})\|_\infty + \|\phi(t^{n+1})\|_\infty \\
&\le Ch^{-1}\Big(\|\phi_h^{n+1}-\phi(t^{n+1})\|_m + \|\phi(t^{n+1})-\Pi_h\phi(t^{n+1})\|_m\Big) \\
&\quad + \|\Pi_h\phi(t^{n+1})-\phi(t^{n+1})\|_\infty + \|\phi(t^{n+1})\|_\infty \\
&\le C_1(h+h^{-1}\Delta t) + \|\phi(t^{n+1})\|_\infty.
\end{aligned} \tag{7.32}$$

Let $\Delta t \le C_2 h^{1+\beta}$ with $\beta > 0$ and a positive constant h_1 be small enough to satisfy $h_1 \le 1$ and

$$C_1(1+C_2)h_1^\beta \le \frac{C^*}{2}.$$

Then for $h \in (0,h_1]$, we derive from (7.32) that

$$\begin{aligned}
\|\phi_h^{n+1}\|_\infty &\le C_1(h+h^{-1}\Delta t) + \|\phi(t^{n+1})\|_\infty \\
&\le C_1(h_1+C_2h_1) + \frac{C^*}{2} \le C^*.
\end{aligned}$$

This completes the induction (7.7a).

We next give a proof of the second inequality (7.7b). It is obvious that

$$\|e_\phi^0\|_m + \|\nabla_h e_\phi^0\|_{TM} + |e_R^0| = 0 \le C_*(\Delta t + h^2)^{\frac{1}{2}}.$$

Assume that

$$\|e_\phi^k\|_m + \|\nabla_h e_\phi^k\|_{TM} + |e_R^k| \le C_*(\Delta t + h^2)^{\frac{1}{2}}, \quad \forall n = 1,2,\ldots,k,$$

then for $n = k+1$, as we have stated later in (7.46), we have

$$\|e_\phi^{k+1}\|_m + \|\nabla_h e_\phi^{k+1}\|_{TM} + |e_R^{k+1}| \le C(\Delta t + h^2). \tag{7.33}$$

We choose sufficiently small Δt and h such that $C(\Delta t+h^2)^{1/2} \le C_*$, then above equality (7.33) can be transformed as

$$\|e_\phi^{k+1}\|_m + \|\nabla_h e_\phi^{k+1}\|_{TM} + |e_R^{k+1}| \le C_*(\Delta t + h^2)^{\frac{1}{2}}, \tag{7.34}$$

which completes the proof. □

We are now in position to prove our main results of Theorem 7.2. Combining Lemmas 7.1-7.3, we have

$$\frac{K_1}{4}\|d_t e_\phi^{n+1}\|_m^2 + R_h^{n+1}\epsilon^2 M \frac{\|\nabla_h e_\phi^{n+1}\|_{TM}^2}{2\Delta t} + K_1\frac{\|e_\phi^{n+1}\|_m^2 - \|e_\phi^n\|_m^2}{2\Delta t} + K_1\frac{\|e_\phi^{n+1}-e_\phi^n\|_m^2}{2\Delta t}$$

$$
\begin{aligned}
&+Ms\epsilon^2K_1\frac{\|\nabla_h e_\phi^{n+1}\|_{TM}^2-\|\nabla_h e_\phi^n\|_{TM}^2}{2}+Ms\epsilon^2K_1\frac{\|\nabla_h e_\phi^{n+1}-\nabla_h e_\phi^n\|_{TM}^2}{2}\\
&+K_1\frac{|e_R^{n+1}|^2-|e_R^n|^2}{2\Delta t}+K_1\frac{|e_R^{n+1}-e_R^n|^2}{2\Delta t}\\
&+\left(s-\frac{R^{n+1}}{2\big(E_h(\phi^n)+C\big)}\right)\epsilon^2MK_1\frac{\|\nabla_h e_\phi^{n+1}-\nabla_h e_\phi^n\|_{TM}^2}{\Delta t}\\
\le\, & C|e_R^{n+1}|^2+C\|\nabla_h e_\phi^n\|_{TM}^2+C\|e_\phi^n\|_m^2+C\|d_t e_\phi^{n+1}\|_m^2|e_R^{n+1}|^2\\
&+R_h^n\epsilon^2M\frac{\|\nabla_h e_\phi^n\|_{TM}^2}{2\Delta t}+C\big(h^4+(\Delta t)^2\big). \qquad (7.35)
\end{aligned}
$$

Multiplying both sides of above inequality (7.35) by Δt and making summation on n from 0 to k yields

$$
\begin{aligned}
&\frac{K_1}{4}\sum_{n=0}^k\Delta t\|d_t e_\phi^{n+1}\|_m^2+\frac{\epsilon^2M}{2}\sum_{n=0}^k R_h^{n+1}\|\nabla_h e_\phi^{n+1}\|_{TM}^2+\frac{K_1}{2}\|e_\phi^{k+1}\|_m^2+\frac{K_1}{2}\sum_{n=0}^k\|e_\phi^{n+1}-e_\phi^n\|_m^2\\
&+\frac{Ms\epsilon^2K_1}{2}\Delta t\|\nabla_h e_\phi^{k+1}\|_{TM}^2+\frac{Ms\epsilon^2K_1}{2}\sum_{n=0}^k\Delta t\|\nabla_h e_\phi^{n+1}-\nabla_h e_\phi^n\|_{TM}^2+\frac{K_1}{2}|e_R^{k+1}|^2\\
&+\frac{K_1}{2}\sum_{n=0}^k|e_R^{n+1}-e_R^n|^2+\left(s-\frac{R^{n+1}}{2\big(E_h(\phi^n)+C\big)}\right)\epsilon^2MK_1\sum_{n=0}^k\|\nabla_h e_\phi^{n+1}-\nabla_h e_\phi^n\|_{TM}^2\\
\le\, & C\sum_{n=0}^k\Delta t|e_R^{n+1}|^2+C\sum_{n=0}^k\Delta t\|\nabla_h e_\phi^n\|_{TM}^2+C\sum_{n=0}^k\Delta t\|e_\phi^n\|_m^2+C\sum_{n=0}^k\Delta t\|d_t e_\phi^{n+1}\|_m^2|e_R^{n+1}|^2\\
&+\frac{\epsilon^2M}{2}\sum_{n=0}^k R_h^n\|\nabla_h e_\phi^n\|_{TM}^2+C\big(h^4+(\Delta t)^2\big). \qquad (7.36)
\end{aligned}
$$

Noting that $0<R_h^{n+1}<R_h^0$, we have $|e_R^{n+1}|^2\le C$ for a constant C. Then for the fourth term in the right-hand side of above inequality (7.36), using Lemma 7.1, we have

$$
\begin{aligned}
&C\sum_{n=0}^k\Delta t\|d_t e_\phi^{n+1}\|_m^2|e_R^{n+1}|^2\\
\le\, & C\sum_{n=0}^k\Delta t\|d_t e_\phi^{n+1}\|_m^2\\
\le\, & C\sum_{n=0}^k\Delta t|e_R^{n+1}|^2+C\sum_{n=0}^k\Delta t\|\nabla_h e_\phi^n\|_{TM}^2+C\sum_{n=0}^k\Delta t\|e_\phi^n\|_m^2+C\big(h^4+(\Delta t)^2\big). \qquad (7.37)
\end{aligned}
$$

Substituting above inequality (7.37) into (7.36), we have

$$
\frac{K_1}{4}\sum_{n=0}^k\Delta t\|d_t e_\phi^{n+1}\|_m^2+\frac{\epsilon^2M}{2}R_h^{k+1}\|\nabla_h e_\phi^{k+1}\|_{TM}^2+\frac{K_1}{2}\|e_\phi^{k+1}\|_m^2+\frac{K_1}{2}|e_R^{k+1}|^2
$$

$$\leq C\sum_{n=1}^{k}\Delta t\left|e_R^{n+1}\right|^2+C\sum_{n=1}^{k}\Delta t\left\|\nabla_h e_\phi^n\right\|_{TM}^2+C\sum_{n=1}^{k}\Delta t\left\|e_\phi^n\right\|_m^2+C\left(h^4+(\Delta t)^2\right). \tag{7.38}$$

From energy dissipation law in Theorem 3.2, we know that

$$R_h^{k+1}=R_h^k-\frac{\Delta t}{M}\left\|d_t\phi^{n+1}\right\|_m^2=R_h^k-\frac{\Delta t}{M}\left\|d_te_\phi^{n+1}+d_t\phi(t^{n+1})\right\|_m^2. \tag{7.39}$$

Substituting above equation (7.39) into the second term of the left-hand side of (7.38), we have

$$\begin{aligned}&\frac{\epsilon^2M}{2}R_h^{k+1}\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2\\ =&\frac{\epsilon^2M}{2}R_h^k\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2-\frac{\epsilon^2\Delta t}{2}\left\|d_te_\phi^{k+1}+d_t\phi(t^{k+1})\right\|_m^2\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2.\end{aligned} \tag{7.40}$$

For the first term in the right-hand side of above equation (7.40), noting that $R(t^k)=E(\phi(t^k))+C>K_1$, we have

$$\frac{\epsilon^2M}{2}R_h^k\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2=\frac{\epsilon^2M}{2}\left(e_R^k+R(t^k)\right)\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2\geq\frac{\epsilon^2MK_1}{4}\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2. \tag{7.41}$$

For the second term in the right-hand side of above equation (7.40), using Cauchy-Schwartz inequality, we have

$$\begin{aligned}&\frac{\epsilon^2\Delta t}{2}\left\|d_te_\phi^{k+1}+d_t\phi(t^{n+1})\right\|_m^2\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2\\ \leq&\epsilon^2\Delta t\left(\left\|d_te_\phi^{k+1}\right\|_m^2+\left\|d_t\phi(t^{k+1})\right\|_m^2\right)\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2\\ \leq&\epsilon^2\Delta t\left\|d_te_\phi^{k+1}\right\|_m^2\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2+C\Delta t\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2.\end{aligned} \tag{7.42}$$

Multiplying both sides of above inequality (7.3) by $2\epsilon^2\Delta t$ and using (7.7b) yield

$$\begin{aligned}\epsilon^2\Delta t\left\|d_te_\phi^{k+1}\right\|_m^2\leq&C\Delta t\left|e_R^{k+1}\right|^2+C\Delta t\left\|\nabla_he_\phi^k\right\|_{TM}^2+C\Delta t\left\|e_\phi^k\right\|_m^2\\ &+R_h^k\epsilon^4M\left\|\nabla_he_\phi^k\right\|_{TM}^2+C\left(h^4+(\Delta t)^2\right)\\ \leq&C\Delta t\left|e_R^{k+1}\right|^2+C(\Delta t+h^2).\end{aligned} \tag{7.43}$$

Noting that $0<R_h^{k+1}<R_h^0$ and $K_1<R(t^{k+1})<K_2$, we have $|e_R^{k+1}|<C$. Combining inequality (7.43) with (7.42) and supposing that $\Delta t\geq Ch^2$, we obtain

$$\frac{\epsilon^2\Delta t}{2}\left\|d_te_\phi^{k+1}+d_t\phi(t^{n+1})\right\|_m^2\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2\leq C\Delta t\left\|\nabla_he_\phi^{k+1}\right\|_{TM}^2. \tag{7.44}$$

Substituting (7.39)-(7.44) into (7.38) and supposing that Δt is sufficiently small, we have

$$\begin{aligned}&\frac{K_1}{4}\sum_{n=0}^{k}\Delta t\|d_t e_\phi^{n+1}\|_m^2+\frac{\epsilon^2 MK_1}{4}\|\nabla_h e_\phi^{k+1}\|_{TM}^2+\frac{K_1}{2}\|e_\phi^{k+1}\|_m^2+\frac{K_1}{2}|e_R^{k+1}|^2\\ \leq& C\sum_{n=1}^{k}\Delta t|e_R^{n+1}|^2+C\sum_{n=1}^{k}\Delta t\|\nabla_h e_\phi^n\|_{TM}^2+C\sum_{n=1}^{k}\Delta t\|e_\phi^n\|_m^2+C\big(h^4+(\Delta t)^2\big).\end{aligned} \tag{7.45}$$

Using Gronwall inequality for above inequality, we obtain

$$\begin{aligned}&\frac{K_1}{4}\sum_{n=1}^{k}\Delta t\|d_t e_\phi^{n+1}\|_m^2+\frac{\epsilon^2 MK_1}{4}\|\nabla_h e_\phi^{k+1}\|_{TM}^2+\frac{K_1}{2}\|e_\phi^{k+1}\|_m^2+\frac{K_1}{2}|e_R^{k+1}|^2\\ \leq& C\big(h^4+(\Delta t)^2\big).\end{aligned} \tag{7.46}$$

Remark 7.1. The convergence analysis of the second-order PS-SAV scheme will be deferred to a subsequent study. For details on the proof of convergence of several existing second-order SAV-type schemes, we refer to [12, 34, 37]. Besides, the proposed PS-SAV technique is also extensible to some other gradient flows like the phase field crystal model, with this extension reserved for future research.

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