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ENERGY STABILITY AND CONVERGENCE OF SAV BLOCK-CENTERED FINITE DIFFERENCE METHOD FOR GRADIENT FLOWS

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Abstract. We present in this paper construction and analysis of a block-centered finite difference method for the spatial discretization of the scalar auxiliary variable Crank-Nicolson scheme (SAV/CN-BCFD) for gradient flows, and show rigorously that the scheme is second-order in both time and space in various discrete norms. When equipped with an adaptive time strategy, the SAV/CN-BCFD scheme is accurate and extremely efficient. Numerical experiments on typical Allen-Cahn and Cahn-Hilliard equations are presented to verify our theoretical results and to show the robustness and accuracy of the SAV/CN-BCFD scheme.

1. Introduction

Gradient flows are widely used in mathematical models for problems in many fields of science and engineering, particularly in materials science and fluid dynamics; cf. [1, 2, 18, 27] and the references therein. Therefore it is important to develop efficient and accurate numerical schemes for their simulation. There exists an extensive literature on the numerical analysis of gradient flows; see for instance [3, 6–8, 11, 12, 20] and the references therein.

In the algorithm design of gradient flows, an important goal is to guarantee the energy stability at the discrete level, in order to capture the correct long-time dynamics of the system and provide enough flexibility for dealing with the stiffness problem induced by the thin interface. Many schemes for gradient flows are based on the traditional fully-implicit or explicit discretization for the nonlinear term, which may suffer from harsh time step constraint due to the thin interfacial width [9, 19]. In order to deal with this problem, the convex splitting approach [13, 15, 21] and linear stabilization approach [14, 19, 24, 29] have been widely used to construct unconditionally energy stable schemes. However, the convex splitting approach usually leads to nonlinear schemes and the linear stabilization approach is usually limited to first-order accuracy.

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Recently, a novel numerical method, the so-called invariant energy quadratization (IEQ), was proposed in [25, 26, 28]. This method is a generalization of the method of Lagrange multipliers or of auxiliary variable. The IEQ approach is remarkable as it permits us to construct linear, unconditionally stable, and second-order unconditionally energy stable schemes for a large class of gradient flows. However, it leads to coupled systems with variable coefficients that may be difficult or expensive to solve. The scalar auxiliary variable (SAV) approach [17, 18] was inspired by the IEQ approach, which inherits its main advantages but overcomes many of its shortcomings. In particular, in a recent paper [16], the authors established the first-order convergence and error estimates for the semidiscrete SAV scheme.

In this paper, we construct a SAV/CN scheme with block-centered finite differences for gradient flows, carry out a rigorous stability and error analysis, and implement an adaptive time stepping strategy so that the time step is only dictated by accuracy rather than by stability. The block-centered finite difference method can be thought of as the lowest order Raviart-Thomas mixed element method with a suitable quadrature. Its main advantage over using a regular finite difference method is that it can approximate both the phase function and chemical potential with Neumann boundary conditions in the mixed formulation to second-order accuracy, and it guarantees local mass conservation. Our approach for error estimates here is very different from that in [16] which is based on deriving H^2 bounds for the numerical solution. However, this approach cannot be used in the fully discrete case with finite-differences in space. The essential tools used in the proof are the summation-by-parts formulae both in space and time to derive energy stability, and an induction process to show that the discrete L^∞ norm of the numerical solution is uniformly bounded, without assuming a uniform Lipschitz condition on the nonlinear potential. To the best of the authors' knowledge, this is the first paper with rigorous proof of second-order convergence both in time and space for a linear scheme to a class of gradient flows without assuming a uniform Lipschitz condition for the nonlinear potential.

The paper is organized as follows. In Section 2, we describe our numerical scheme, including the temporal discretization and spacial discretization. In Section 3, we demonstrate the energy stability for our SAV/CN-BCFD scheme. In Section 4, we carry out error estimates for the SAV/CN-BCFD schemes. In Section 5, we present some numerical experiments to verify the energy stability and accuracy of the proposed schemes.

Throughout the paper we use C, with or without subscript, to denote a positive constant, which could have different values at different places.

2. The SAV/CN-BCFD scheme

Assume given a typical energy functional [16]

$$E(\phi) = \int_\Omega (\frac{\lambda}{2}\phi^2 + \frac{1}{2}|\nabla\phi|^2)d\mathbf{x} + E_1(\phi), \tag{2.1}$$

where Ω is a rectangular domain in $\mathbb{R}^2$, $\lambda \geq 0$, and $E_1(\phi) = \int_\Omega F(\phi)d\mathbf{x} \geq -c_0$ for some $c_0 > 0$, i.e., it is bounded from below. We consider the following gradient flow:

$$\begin{cases} \dfrac{\partial\phi}{\partial t} = M\mathcal{G}\mu, \text{ in } \Omega\times J, \\ \mu = -\Delta\phi + \lambda\phi + F'(\phi), \text{ in } \Omega\times J. \end{cases} \tag{2.2}$$

$J = (0, T]$, and T denotes the final time. M is the mobility constant which is positive. The chemical potential $\mu = \frac{\delta E}{\delta \phi}$. $\mathcal{G} = -1$ for the L^2 gradient flow and $\mathcal{G} = \Delta$ for the H^{-1} gradient flow. $F(\phi)$ is the nonlinear free energy density and we focus on, as an example, when $E_1(\phi) = \int_\Omega \alpha(1-\phi^2)^2 d\mathbf{x}$, the L^2 and H^{-1} gradient flows are the well-known Allen-Cahn and Cahn-Hilliard equations, respectively.

The boundary and initial conditions are

$$\begin{cases} \partial_{\mathbf{n}}\phi|_{\partial\Omega} = 0,\ \partial_{\mathbf{n}}\mu|_{\partial\Omega} = 0, \\ \phi|_{t=0} = \phi_0, \end{cases} \tag{2.3}$$

where $\mathbf{n}$ is the unit outward normal vector of the domain Ω. The equation satisfies the following energy dissipation law:

$$\frac{dE}{dt} = \int_\Omega \frac{\partial \phi}{\partial t}\mu d\mathbf{x} = M\int_\Omega \mu\mathcal{G}\mu d\mathbf{x} \le 0. \tag{2.4}$$

2.1. **The semidiscrete SAV/CN scheme.** We recall the SAV/CN scheme introduced in [18] first.

Let $C_0 > c_0$ so that $E_1(\phi) + C_0 > 0$. Without loss of generality, we substitute E_1 with $E_1 + C_0$ without changing the gradient flow. Then E_1 has a positive lower bound $\hat{C}_0 = C_0 - c_0$, which we still denote as C_0 for simplicity.

In the SAV approach, a scalar variable $r(t) = \sqrt{E_1(\phi)}$ is introduced, and the system (2.2) can be transformed into

$$\begin{cases} \dfrac{\partial \phi}{\partial t} = M\mathcal{G}\mu, & (2.5)\\ \mu = -\Delta\phi + \lambda\phi + \dfrac{r}{\sqrt{E_1(\phi)}}F'(\phi), & (2.6)\\ r_t = \dfrac{1}{2\sqrt{E_1(\phi)}}\displaystyle\int_\Omega F'(\phi)\phi_t d\mathbf{x}. & (2.7) \end{cases}$$

Then, the SAV/CN scheme is given as

$$\begin{cases} \dfrac{\phi^{n+1}-\phi^n}{\Delta t} = M\mathcal{G}\mu^{n+1/2}, & (2.8)\\ \mu^{n+1/2} = -\Delta\phi^{n+1/2} + \lambda\phi^{n+1/2} + \dfrac{r^{n+1/2}}{\sqrt{E_1(\tilde{\phi}^{n+1/2})}}F'(\tilde{\phi}^{n+1/2}), & (2.9)\\ \dfrac{r^{n+1}-r^n}{\Delta t} = \dfrac{1}{2\sqrt{E_1(\tilde{\phi}^{n+1/2})}}\displaystyle\int_\Omega F'(\tilde{\phi}^{n+1/2})\frac{\phi^{n+1}-\phi^n}{\Delta t}d\mathbf{x}, & (2.10) \end{cases}$$

where $\phi^{n+1/2} = \frac{1}{2}(\phi^n + \phi^{n+1})$, $r^{n+1/2} = \frac{1}{2}(r^n + r^{n+1})$, and $\tilde{\phi}^{n+1/2}$ can be any explicit approximation of $\phi(t^{n+1/2})$ with an error of $O(\Delta t^2)$. For instance, we may let $\tilde{\phi}^{n+1/2}$ be the extrapolation by

$$\tilde{\phi}^{n+1/2} = \frac{1}{2}(3\phi^n - \phi^{n-1}). \tag{2.11}$$

2.2. **Spacial discretization.** We apply the BCFD method on the staggered grids for the spacial discretization.

First we give some preliminaries. Let $L^m(\Omega)$ be the standard Banach space with norm

$$\|v\|_{L^m(\Omega)} = \left(\int_\Omega |v|^m d\Omega\right)^{1/m}.$$

For simplicity, let

$$(f,g) = (f,g)_{L^2(\Omega)} = \int_\Omega fg\ d\Omega$$

denote the $L^2(\Omega)$ inner product, $\|v\|_\infty = \|v\|_{L^\infty(\Omega)}$. Let $W^{k,p}(\Omega)$ be the standard Sobolev space

$$W^{k,p}(\Omega) = \{g:\ \|g\|_{W_p^k(\Omega)} < \infty\},$$

where

$$\|g\|_{W^{k,p}(\Omega)} = \left(\sum_{|\alpha|\le k} \|D^\alpha g\|^p_{L^p(\Omega)}\right)^{1/p}. \tag{2.12}$$

The grid points are denoted by

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

and the notation similar to that in [22] is used:

$$\begin{aligned}
&x_i = (x_{i-\frac12} + x_{i+\frac12})/2,\ i = 1, \dots, N_x,\\
&h_x = x_{i+\frac12} - x_{i-\frac12},\ i = 1, \dots, N_x,\\
&y_j = (y_{j-\frac12} + y_{j+\frac12})/2,\ j = 1, \dots, N_y,\\
&h_y = y_{j+\frac12} - y_{j-\frac12},\ j = 1, \dots, N_y,
\end{aligned}$$

where h_x and h_y are grid spacings in x and y directions, and N_x and N_y are the number of grids along the x and y coordinates, respectively.

Let $g_{i,j},\ g_{i+\frac12,j},\ g_{i,j+\frac12}$ denote $g(x_i, y_j),\ g(x_{i+\frac12}, y_j),\ g(x_i, y_{j+\frac12})$. Define the discrete inner products and norms as:

$$\begin{aligned}
(f,g)_m &= \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} h_x h_y f_{i,j} g_{i,j},\\
(f,g)_x &= \sum_{i=1}^{N_x-1}\sum_{j=1}^{N_y} h_x h_y f_{i+\frac12,j} g_{i+\frac12,j},\\
(f,g)_y &= \sum_{i=1}^{N_x}\sum_{j=1}^{N_y-1} h_x h_y f_{i,j+\frac12} g_{i,j+\frac12},\\
(\boldsymbol{v}, \boldsymbol{r})_{TM} &= (v_1, r_1)_x + (v_2, r_2)_y.
\end{aligned}$$

For simplicity, from now on we always omit the superscript n (the time level) if the omission does not cause conflicts. Define

$$\begin{aligned}
&[d_x g]_{i+\frac12,j} = (g_{i+1,j} - g_{i,j})/h_x,\\
&[d_y g]_{i,j+\frac12} = (g_{i,j+1} - g_{i,j})/h_y,\\
&[D_x g]_{i,j} = (g_{i+\frac12,j} - g_{i-\frac12,j})/h_x,\\
&[D_y g]_{i,j} = (g_{i,j+\frac12} - g_{i,j-\frac12})/h_y,\\
&[d_t g]^n_{i,j} = (g^n_{i,j} - g^{n-1}_{i,j})/\Delta t.
\end{aligned}$$

The following discrete-integration-by-part lemma [22] plays an important role in the analysis.

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

$$(q, D_x w_1)_m = -(d_x q, w_1)_x,$$
$$(q, D_y w_2)_m = -(d_y q, w_2)_y.$$

2.2.1. *SAV/CV-BCFD scheme for H^{-1} gradient flow.* Let us denote the BCFD approximations to $\{\phi^n, \mu^n, r^n\}_{n=0}^N$ by $\{Z^n, W^n, R^n\}_{n=0}^N$. The scheme for the H^{-1} gradient flow is as follows: for $1 \le i \le N_x,\ 1 \le j \le N_y$,

$$\begin{cases} [d_t Z]_{i,j}^{n+1} = M[D_x d_x W + D_y d_y W]_{i,j}^{n+1/2}, & (2.13)\\ W_{i,j}^{n+1/2} = -[D_x d_x Z + D_y d_y Z]_{i,j}^{n+1/2} + \lambda Z_{i,j}^{n+1/2} & (2.14)\\ \quad + \dfrac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} F'(\tilde{Z}_{i,j}^{n+1/2}), & \\ d_t R^{n+1} = \dfrac{1}{2\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} (F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m, & (2.15) \end{cases}$$

where $\tilde{Z}^{n+1/2}$ is an approximation of $\tilde{\phi}^{n+1/2}$, and

$$E_1^h(\tilde{Z}^{n+1/2}) = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} h_x h_y F(\tilde{Z}_{i,j}^{n+1/2}).$$

The boundary and initial approximations are

$$(2.16)\qquad \begin{cases} [d_x Z]_{1/2,j}^n = [d_x Z]_{N_x+1/2,j}^n = 0, \quad 1 \le j \le N_y,\\ [d_y Z]_{i,1/2}^n = [d_y Z]_{i,N_y+1/2}^n = 0, \quad 1 \le i \le N_x,\\ [d_x W]_{1/2,j}^n = [d_x W]_{N_x+1/2,j}^n = 0, \quad 1 \le j \le N_y,\\ [d_y W]_{i,1/2}^n = [d_y W]_{i,N_y+1/2}^n = 0, \quad 1 \le i \le N_x,\\ Z_{i,j}^0 = \phi_{0,i,j}, 1 \le i \le N_x, 1 \le j \le N_y. \end{cases}$$

Remark. The solution procedure of the above scheme is described in detail in [17, 18], and hence is omitted here.

2.2.2. *SAV/CV-BCFD scheme for L^2 gradient flow.* Let us denote the BCFD approximations to $\{\phi^n, \mu^n, r^n\}_{n=0}^N$ by $\{Z^n, W^n, R^n\}_{n=0}^N$. The scheme for the L^2 gradient flow is as follows: for $1 \le i \le N_x,\ 1 \le j \le N_y$,

$$\begin{cases} [d_t Z]_{i,j}^{n+1} = -M W_{i,j}^{n+1/2}, & (2.17)\\ W_{i,j}^{n+1/2} = -[D_x d_x Z + D_y d_y Z]_{i,j}^{n+1/2} + \lambda Z_{i,j}^{n+1/2} & (2.18)\\ \quad + \dfrac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} F'(\tilde{Z}_{i,j}^{n+1/2}), & \\ d_t R^{n+1} = \dfrac{1}{2\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} (F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m, & (2.19) \end{cases}$$

where $\tilde{Z}^{n+1/2}$ is an approximation of $\tilde{\phi}^{n+1/2}$. The boundary and initial conditions are given in (2.16).

3. Unconditional energy stability

We demonstrate below that the full discrete SAV/CN-BCFD schemes are unconditionally energy stable with the discrete energy functional

$$E_d(Z^n) = \frac{\lambda}{2}\|Z^n\|_m^2 + \frac{1}{2}\|\mathbf{d}Z^n\|_{TM}^2 + (R^n)^2, \tag{3.1}$$

where $\mathbf{d}Z = (d_x Z, d_y Z)$.

3.1. H^{-1} gradient flow.

Theorem 2. *The scheme* (2.13)–(2.15) *is unconditionally stable and the following discrete energy law holds for any* Δt*:*

$$\frac{1}{\Delta t}[E_d(Z^{n+1}) - E_d(Z^n)] = -M\|\mathbf{d}W^{n+1/2}\|_{TM}^2 \quad \forall n \geq 0. \tag{3.2}$$

Proof. Multiplying equation (2.13) by $W_{i,j}^{n+1/2} h_x h_y$, and making summation on i, j for $1 \leq i \leq N_x,\ 1 \leq j \leq N_y$, we have

$$(d_t Z^{n+1}, W^{n+1/2})_m = M(D_x d_x W^{n+1/2} + D_y d_y W^{n+1/2}, W^{n+1/2})_m. \tag{3.3}$$

Using Lemma 1, equation (3.3) can be transformed into the following:

$$\begin{aligned}(d_t Z^{n+1}, W^{n+1/2})_m =& - M(\|d_x W^{n+1/2}\|_x^2 + \|d_y W^{n+1/2}\|_y^2)\\ =& - M\|\mathbf{d}W^{n+1/2}\|_{TM}^2.\end{aligned} \tag{3.4}$$

Multiplying equation (2.14) by $d_t Z_{i,j}^{n+1} h_x h_y$, and making summation on i, j for $1 \leq i \leq N_x,\ 1 \leq j \leq N_y$, we have

$$\begin{aligned}(d_t Z^{n+1}, W^{n+1/2})_m =& - (D_x d_x Z^{n+1/2} + D_y d_y Z^{n+1/2}, d_t Z^{n+1})_m\\ &+ \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m\\ &+ \lambda(Z^{n+1/2}, d_t Z^{n+1})_m.\end{aligned} \tag{3.5}$$

Using Lemma 1 again, the first term on the right-hand side of equation (3.5) can be written as

$$\begin{aligned}&- (D_x d_x Z^{n+1/2} + D_y d_y Z^{n+1/2}, d_t Z^{n+1})_m\\ =&(d_x Z^{n+1/2}, d_t d_x Z^{n+1})_x + (d_y Z^{n+1/2}, d_t d_y Z^{n+1})_y\\ =&\frac{\|\mathbf{d}Z^{n+1}\|_{TM}^2 - \|\mathbf{d}Z^n\|_{TM}^2}{2\Delta t}.\end{aligned} \tag{3.6}$$

Multiplying equation (2.15) by $R^{n+1} + R^n$ leads to

$$\frac{(R^{n+1})^2 - (R^n)^2}{\Delta t} = \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_M. \tag{3.7}$$

Combining equation (3.7) with equations (3.4)–(3.6) gives that

$$\begin{aligned}&\frac{(R^{n+1})^2 - (R^n)^2}{\Delta t} + \lambda\frac{\|Z^{n+1}\|_m^2 - \|Z^n\|_m^2}{2\Delta t}\\ &+ \frac{\|\mathbf{d}Z^{n+1}\|_{TM}^2 - \|\mathbf{d}Z^n\|_{TM}^2}{2\Delta t}\\ =& - M\|\mathbf{d}W^{n+1/2}\|_{TM}^2 \leq 0,\end{aligned} \tag{3.8}$$

which implies the desired results (3.2). ∎

3.2. L^2 **gradient flow.** For the L^2 gradient flow, we shall only state the result, as its proof is essentially the same as for the H^{-1} gradient flow.

Theorem 3. *The scheme* (2.17)–(2.19) *is unconditionally stable and the following discrete energy law holds for any* Δt*:*

$$\frac{1}{\Delta t}[E_d(Z^{n+1}) - E_d(Z^n)] = -M\|W^{n+1/2}\|_m^2 \quad \forall n \geq 0. \tag{3.9}$$

4. Error estimates

In this section, we derive our main results of this paper, i.e., error estimates for the fully discrete SAV/CN-BCFD schemes.

For simplicity, we set

$$e_\phi^n = Z^n - \phi^n, \; e_\mu^n = W^n - \mu^n, \; e_r^n = R^n - r^n.$$

4.1. H^{-1} **gradient flow.** We shall first derive error estimates for the case of the H^{-1} gradient flow.

Theorem 4. *Assume* $F(\phi) \in C^3(\mathbb{R})$, $\phi \in W^{1,\infty}(J; W^{4,\infty}(\Omega)) \cap W^{3,\infty}(J; W^{1,\infty}(\Omega))$, *and* $\mu \in L^\infty(J; W^{4,\infty}(\Omega))$. *Let* $\Delta t \leq C(h_x + h_y)$. *Then for the discrete scheme* (2.13)–(2.15), *there exists a positive constant* C *independent of* h_x, h_y, *and* Δt *such that*

$$\begin{aligned}
&\|Z^{k+1} - \phi^{k+1}\|_m + \|\mathbf{d}Z^{k+1} - \mathbf{d}\phi^{k+1}\|_{TM} + |R^{k+1} - r^{k+1}| \\
&\quad + \left(\sum_{n=0}^{k} \Delta t \|\mathbf{d}W^{n+1/2} - \mathbf{d}\mu^{n+1/2}\|_{TM}^2\right)^{1/2} \\
&\quad + \left(\sum_{n=0}^{k} \Delta t \|W^{n+1/2} - \mu^{n+1/2}\|_m^2\right)^{1/2} \\
&\leq C(\|\phi\|_{W^{1,\infty}(J;W^{4,\infty}(\Omega))} + \|\mu\|_{L^\infty(J;W^{4,\infty}(\Omega))})(h_x^2 + h_y^2) \\
&\quad + C\|\phi\|_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}\Delta t^2.
\end{aligned} \tag{4.1}$$

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

Lemma 5. *Under the conditions of Theorem* 4, *there exists a positive constant* C *independent of* h_x, h_y, *and* Δt *such that*

$$\begin{aligned}
&(e_r^{k+1})^2 + \frac{1}{2}\|\mathbf{d}e_\phi^{k+1}\|_{TM}^2 + \frac{\lambda}{2}\|e_\phi^{k+1}\|_m^2 + \frac{M}{2}\sum_{n=0}^{k} \Delta t \|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2 \\
&\leq C\sum_{n=0}^{k+1} \Delta t \|\mathbf{d}e_\phi^n\|_{TM}^2 + \frac{M}{2}\sum_{n=0}^{k+1} \Delta t \|e_\mu^{n+1/2}\|_m^2 \\
&\quad + C\sum_{n=0}^{k+1} \Delta t \|e_\phi^n\|_m^2 + C\sum_{n=0}^{k+1} \Delta t (e_r^n)^2 \\
&\quad + C(\|\phi\|_{W^{1,\infty}(J;W^{4,\infty}(\Omega))}^2 + \|\mu\|_{L^\infty(J;W^{4,\infty}(\Omega))}^2)(h_x^4 + h_y^4) \\
&\quad + C\|\phi\|_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}^2 \Delta t^4.
\end{aligned} \tag{4.2}$$

Proof. Denote

$$\delta_x(\phi) = d_x\phi - \frac{\partial \phi}{\partial x},\ \delta_y(\phi) = d_y\phi - \frac{\partial \phi}{\partial y},$$
$$\delta_x(\mu) = d_x\mu - \frac{\partial \mu}{\partial x},\ \delta_y(\mu) = d_y\mu - \frac{\partial \mu}{\partial y}.$$

Subtracting equation (2.5) from equation (2.13), we obtain

$$\begin{aligned} [d_t e_\phi]_{i,j}^{n+1} =& M[D_x(d_x e_\mu + \delta_x(\mu)) + D_y(d_y e_\mu + \delta_y(\mu))]_{i,j}^{n+1/2} \\ &+ T_{1,i,j}^{n+1/2} + T_{2,i,j}^{n+1/2}, \end{aligned} \tag{4.3}$$

where

$$T_{1,i,j}^{n+1/2} = \frac{\partial \phi}{\partial t}\Big|_{i,j}^{n+1/2} - [d_t\phi]_{i,j}^{n+1} \leq C\|\phi\|_{W^{3,\infty}(J;L^\infty(\Omega))}\Delta t^2, \tag{4.4}$$

$$\begin{aligned} T_{2,i,j}^{n+1/2} &= M[D_x\frac{\partial \mu}{\partial x} + D_y\frac{\partial \mu}{\partial y}]_{i,j}^{n+1/2} - M\Delta\mu_{i,j}^{n+1/2} \\ &\leq CM(h_x^2 + h_y^2)\|\mu\|_{L^\infty(J;W^{4,\infty}(\Omega))}. \end{aligned} \tag{4.5}$$

Subtracting equation (2.6) from equation (2.14) leads to

$$\begin{aligned} e_{\mu,i,j}^{n+1/2} =& -[D_x(d_x e_\phi + \delta_x(\phi)) + D_y(d_y e_\phi + \delta_y(\phi))]_{i,j}^{n+1/2} \\ &+ \lambda e_{\phi,i,j}^{n+1/2} + \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}F'(\tilde{Z}_{i,j}^{n+1/2}) \\ &- \frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}F'(\phi_{i,j}^{n+1/2}) + T_{3,i,j}^{n+1/2}, \end{aligned} \tag{4.6}$$

where

$$\begin{aligned} T_{3,i,j}^{n+1/2} &= \Delta\phi_{i,j}^{n+1/2} - [D_x\frac{\partial \phi}{\partial x} + D_y\frac{\partial \phi}{\partial y}]_{i,j}^{n+1/2} \\ &\leq C(h_x^2 + h_y^2)\|\phi\|_{L^\infty(J;W^{4,\infty}(\Omega))}. \end{aligned} \tag{4.7}$$

Subtracting equation (2.7) from equation (2.15) gives that

$$\begin{aligned} d_t e_r^{n+1} =& \frac{1}{2\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}), d_t Z^{n+1})_m \\ &- \frac{1}{2\sqrt{E_1(\phi^{n+1/2})}}\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2}d\mathbf{x} + T_4^{n+1/2}, \end{aligned} \tag{4.8}$$

where

$$T_4^{n+1/2} = r_t^{n+1/2} - d_t r^{n+1} \leq C\|r\|_{W^{3,\infty}(J)}\Delta t^2. \tag{4.9}$$

Multiplying equation (4.3) by $e_{\mu,i,j}^{n+1/2}h_xh_y$, and making summation on i,j for $1\leq i\leq N_x,\ 1\leq j\leq N_y$, we have

$$
\begin{aligned}
&(d_te_\phi^{n+1},e_\mu^{n+1/2})_m\\
=&M\left(D_x(d_xe_\mu+\delta_x(\mu))^{n+1/2}+D_y(d_ye_\mu+\delta_y(\mu))^{n+1/2},e_\mu^{n+1/2}\right)_m\\
&+(T_1^{n+1/2},e_\mu^{n+1/2})_m+(T_2^{n+1/2},e_\mu^{n+1/2})_m.
\end{aligned}\tag{4.10}
$$

Using Lemma 1, we can write the first term on the right-hand side of equation (4.10) as

$$
\begin{aligned}
&M\left(D_x(d_xe_\mu+\delta_x(\mu))^{n+1/2}+D_y(d_ye_\mu+\delta_y(\mu))^{n+1/2},e_\mu^{n+1/2}\right)_m\\
=&-M\left((d_xe_\mu+\delta_x(\mu))^{n+1/2},d_xe_\mu^{n+1/2}\right)_x-M\left((d_ye_\mu+\delta_y(\mu))^{n+1/2},d_ye_\mu^{n+1/2}\right)_y\\
=&-M\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2-M(\delta_x(\mu)^{n+1/2},d_xe_\mu^{n+1/2})_x\\
&-M(\delta_y(\mu)^{n+1/2},d_ye_\mu^{n+1/2})_y.
\end{aligned}\tag{4.11}
$$

Thanks to the Cauchy-Schwarz inequality, the last two terms on the right-hand side of equation (4.11) can be transformed into

$$
\begin{aligned}
&-M(\delta_x(\mu)^{n+1/2},d_xe_\mu^{n+1/2})_x-M(\delta_y(\mu)^{n+1/2},d_ye_\mu^{n+1/2})_y\\
\leq&\frac{M}{6}\|\mathbf{d}\mu^{n+1/2}\|_{TM}^2+C\|\mu\|_{L^\infty(J;W^{3,\infty}(\Omega))}^2(h_x^4+h_y^4).
\end{aligned}\tag{4.12}
$$

Multiplying equation (4.6) by $d_te_{\phi,i,j}^{n+1}h_xh_y$, and making summation on i,j for $1\leq i\leq N_x,\ 1\leq j\leq N_y$, we have

$$
\begin{aligned}
&(e_\mu^{n+1/2},d_te_\phi^{n+1})_m=-(D_x(d_xe_\phi+\delta_x(\phi))^{n+1/2}+D_y(d_ye_\phi+\delta_y(\phi))^{n+1/2},d_te_\phi^{n+1})_m\\
&+(\frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}F'(\tilde{Z}^{n+1/2})-\frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}F'(\phi^{n+1/2}),d_te_\phi^{n+1})_m\\
&+\lambda(e_\phi^{n+1/2},d_te_\phi^{n+1})_m+(T_3^{n+1/2},d_te_\phi^{n+1})_m.
\end{aligned}\tag{4.13}
$$

Similar to the estimate of equation (3.6), the first term on the right-hand side of equation (4.13) can be transformed into the following:

$$
\begin{aligned}
&-(D_x(d_xe_\phi+\delta_x(\phi))^{n+1/2}+D_y(d_ye_\phi+\delta_y(\phi))^{n+1/2},d_te_\phi^{n+1})_m\\
=&(d_xe_\phi^{n+1/2},d_td_xe_\phi^{n+1})_x+(d_ye_\phi^{n+1/2},d_td_ye_\phi^{n+1})_y\\
&+(\delta_x(\phi)^{n+1/2},d_td_xe_\phi^{n+1/2})_x+(\delta_y(\phi)^{n+1/2},d_td_ye_\phi^{n+1/2})_y\\
=&\frac{\|\mathbf{d}e_\phi^{n+1}\|_{TM}^2-\|\mathbf{d}e_\phi^{n}\|_{TM}^2}{2\Delta t}+(\delta_x(\phi)^{n+1/2},d_td_xe_\phi^{n+1/2})_x\\
&+(\delta_y(\phi)^{n+1/2},d_td_ye_\phi^{n+1/2})_y.
\end{aligned}\tag{4.14}
$$

The second term on the right-hand side of equation (4.13) can be rewritten as follows:

$$
\begin{aligned}
&\Big(\frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}F'(\tilde{Z}^{n+1/2}) - \frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}F'(\phi^{n+1/2}), d_t e_\phi^{n+1}\Big)_m \\
=& r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, d_t e_\phi^{n+1}\Big)_m \\
&+ r^{n+1/2}\Big(\frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}} - \frac{F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}}, d_t e_\phi^{n+1}\Big)_m \\
&+ e_r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}, d_t e_\phi^{n+1}\Big)_m.
\end{aligned}
\tag{4.15}
$$

Recalling equation (4.3), the first term on the right-hand side of equation (4.15) can be transformed into the following:

$$
\begin{aligned}
& r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, d_t e_\phi^{n+1}\Big)_m \\
=& M r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, D_x(d_x e_\mu + \delta_x(\mu))^{n+1/2}\Big)_m \\
&+ M r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, D_y(d_y e_\mu + \delta_y(\mu))^{n+1/2}\Big)_m \\
&+ r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}, T_1^{n+1/2} + T_2^{n+1/2}\Big)_m.
\end{aligned}
\tag{4.16}
$$

Next, we shall first make the hypothesis that there exists a positive constant C_* such that

$$
\|Z^n\|_\infty \le C_*. \tag{4.17}
$$

This hypothesis will be verified in Lemma 7 using a bootstrap argument.

Since $F(\phi) \in C^3(\mathbb{R})$, we have

$$
\begin{aligned}
& \frac{d_x F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}} - \frac{d_x F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}} \\
=& d_x F'(\tilde{\phi}^{n+1/2}) \frac{E_1^h(\tilde{\phi}^{n+1/2}) - E_1^h(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2}) E_1^h(\tilde{\phi}^{n+1/2})}(E_1^h(\tilde{Z}^{n+1/2}) + E_1^h(\tilde{\phi}^{n+1/2}))} \\
&+ \frac{d_x F'(\tilde{Z}^{n+1/2}) - d_x F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}.
\end{aligned}
\tag{4.18}
$$

Using the above and the Cauchy-Schwartz inequality, we can deduce that

$$\begin{aligned}
&Mr^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}},D_x(d_xe_\mu+\delta_x(\mu))^{n+1/2}\Big)_m\\
=&-Mr^{n+1/2}\Big(\frac{d_xF'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{d_xF'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}},(d_xe_\mu+\delta_x(\mu))^{n+1/2}\Big)_x\\
\leq&\frac{M}{6}\|d_xe_\mu^{n+1/2}\|_x^2+C\|r\|^2_{L^\infty(J)}(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2)\\
&+C\|r\|^2_{L^\infty(J)}(\|d_xe_\phi^n\|_x^2+\|d_xe_\phi^{n-1}\|_x^2)\\
&+C\|\mu\|^2_{L^\infty(J;W^{3,\infty}(\Omega))}(h_x^4+h_y^4).
\end{aligned}\tag{4.19}$$

Similarly we can obtain

$$\begin{aligned}
&Mr^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}},D_y(d_ye_\mu+\delta_y(\mu))^{n+1/2}\Big)_m\\
\leq&\frac{M}{6}\|d_ye_\mu^{n+1/2}\|_y^2+C\|r\|^2_{L^\infty(J)}(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2)\\
&+C\|r\|^2_{L^\infty(J)}(\|d_ye_\phi^n\|_y^2+\|d_ye_\phi^{n-1}\|_y^2)\\
&+C\|\mu\|^2_{L^\infty(J;W^{3,\infty}(\Omega))}(h_x^4+h_y^4).
\end{aligned}\tag{4.20}$$

Then equation (4.16) can be estimated by

$$\begin{aligned}
&r^{n+1/2}\Big(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}},d_te_\phi^{n+1}\Big)_m\\
\leq&\frac{M}{6}\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2+C\|r\|_{L^\infty(J)}(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2)\\
&+C\|r\|_{L^\infty(J)}(\|\mathbf{d}e_\phi^n\|_{TM}^2+\|\mathbf{d}e_\phi^{n-1}\|_{TM}^2)\\
&+C\|\mu\|^2_{L^\infty(J;W^{4,\infty}(\Omega))}(h_x^4+h_y^4)+C\|\phi\|^2_{W^{3,\infty}(J;L^\infty(\Omega))}\Delta t^4.
\end{aligned}\tag{4.21}$$

Similar to (4.16), the second term on the right-hand side of equation (4.15) can be controlled by

$$\begin{aligned}
&r^{n+1/2}\Big(\frac{F'(\tilde{\phi}^{n+1/2})}{\sqrt{E_1^h(\tilde{\phi}^{n+1/2})}}-\frac{F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}},d_te_\phi^{n+1}\Big)_m\\
\leq&\frac{M}{6}\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2+C\|\mu\|^2_{L^\infty(J;W^{4,\infty}(\Omega))}(h_x^4+h_y^4)\\
&+C\|\phi\|^2_{L^\infty(J;W^{2,\infty}(\Omega))}(h_x^4+h_y^4)\\
&+C\|\phi\|^2_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}\Delta t^4.
\end{aligned}\tag{4.22}$$

The third term on the right-hand side of equation (4.13) can be estimated by

$$\lambda(e_\phi^{n+1/2},d_te_\phi^{n+1})_m=\lambda\frac{\|e_\phi^{n+1}\|_m^2-\|e_\phi^n\|_m^2}{2\Delta t}.\tag{4.23}$$

Multiplying equation (4.8) by $e_r^{n+1}+e_r^n$ leads to

$$\begin{aligned}\frac{(e_r^{n+1})^2-(e_r^n)^2}{\Delta t}=&\frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}),d_tZ^{n+1})_m\\&-\frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2}d\mathbf{x}\\&+T_4^{n+1/2}\cdot(e_r^{n+1}+e_r^n).\end{aligned}\tag{4.24}$$

The first and second terms on the right-hand side of equation (4.24) can be transformed into

(4.25)

$$\begin{aligned}&\frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}),d_tZ^{n+1})_m-\frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2}d\mathbf{x}\\=&\frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\left((F'(\phi^{n+1/2}),d_t\phi^{n+1})_m-\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2}d\mathbf{x}\right)\\&+\frac{e_r^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}(F'(\tilde{Z}^{n+1/2}),d_te_\phi^{n+1})_m\\&+e_r^{n+1/2}(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}},d_t\phi^{n+1})_m.\end{aligned}$$

Since $F(\phi)\in C^3(\mathbb{R})$, we have that

$$\begin{aligned}&e_r^{n+1/2}(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}},d_t\phi^{n+1})_m\\=&e_r^{n+1/2}(\frac{F'(\tilde{Z}^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\phi^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}},d_t\phi^{n+1})_m\\&+e_r^{n+1/2}(\frac{F'(\phi^{n+1/2})}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}-\frac{F'(\phi^{n+1/2})}{\sqrt{E_1(\phi^{n+1/2})}},d_t\phi^{n+1})_m\\\le&C(e_r^{n+1/2})^2+C\|\phi\|^2_{W^{1,\infty}(J;L^\infty(\Omega))}(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2).\end{aligned}\tag{4.26}$$

Recalling the midpoint approximation property of the rectangle quadrature formula, we can obtain that

$$\begin{aligned}&\frac{e_r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}\left((F'(\phi^{n+1/2}),d_t\phi^{n+1})_m-\int_\Omega F'(\phi^{n+1/2})\phi_t^{n+1/2}d\mathbf{x}\right)\\&\le C(e_r^{n+1/2})^2+C\|\phi\|^2_{W^{1,\infty}(J;W^{2,\infty}(\Omega))}(h_x^4+h_y^4).\end{aligned}\tag{4.27}$$

Combining equation (4.24) with equations (4.10)–(4.27) and using the Cauchy-Schwarz inequality results in

$$
\begin{aligned}
&\frac{(e_r^{n+1})^2-(e_r^n)^2}{\Delta t}+\frac{\|\mathbf{d}e_\phi^{n+1}\|_{TM}^2-\|\mathbf{d}e_\phi^n\|_{TM}^2}{2\Delta t}\\
&+\lambda\frac{\|e_\phi^{n+1}\|_m^2-\|e_\phi^n\|_m^2}{2\Delta t}+M\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2\\
\le\ &\frac{M}{2}\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2+C\|r\|_{L^\infty(J)}^2(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2)\\
&+C\|r\|_{L^\infty(J)}^2(\|\mathbf{d}e_\phi^n\|_{TM}^2+\|\mathbf{d}e_\phi^{n-1}\|_{TM}^2)\\
&-(\delta_x(\phi)^{n+1/2},d_td_xe_\phi^{n+1/2})_x-(\delta_y(\phi)^{n+1/2},d_td_ye_\phi^{n+1/2})_y\\
&+(T_3^{n+1/2},d_te_\phi^{n+1})_m-(T_1^{n+1/2},e_\mu^{n+1/2})_m\\
&-(T_2^{n+1/2},e_\mu^{n+1/2})_m+T_4^{n+1/2}\cdot(e_r^{n+1}+e_r^n)\\
&+C(e_r^{n+1/2})^2+C\|\phi\|_{W^{1,\infty}(J;L^\infty(\Omega))}^2(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2)\\
&+C(\|\phi\|_{W^{1,\infty}(J;W^{2,\infty}(\Omega))}^2+\|\mu\|_{L^\infty(J;W^{4,\infty}(\Omega))}^2)(h_x^4+h_y^4)\\
&+C\|\phi\|_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}^2\Delta t^4.
\end{aligned}
\tag{4.28}
$$

From the discrete-integration-by-parts,

$$
\begin{aligned}
\sum_{n=0}^{k}\Delta t(f^n,d_tg^{n+1})=&-\sum_{n=1}^{k}\Delta t(d_tf^n,g^n)\\
&+(f^k,g^{k+1})+(f^0,g^0),
\end{aligned}
\tag{4.29}
$$

we find

$$
\begin{aligned}
&\sum_{n=0}^{k}\Delta t(T_3^{n+1/2},d_te_\phi^{n+1})\\
=&-\sum_{n=1}^{k}\Delta t(d_tT_3^{n+1/2},e_\phi^n)+(T_3^{k+1/2},e_\phi^{k+1})+(T_3^{1/2},e_\phi^0)\\
\le& C\sum_{n=1}^{k}\Delta t\|e_\phi^n\|_m^2+\frac{\lambda}{4}\|e_\phi^{k+1}\|_m^2+C\|\phi\|_{W^{1,\infty}(J;W^{4,\infty}(\Omega))}^2(h_x^4+h_y^4).
\end{aligned}
\tag{4.30}
$$

Similarly we have

$$
\begin{aligned}
&-\sum_{n=0}^{k}\Delta t(\delta_x(\phi)^{n+1/2},d_td_xe_\phi^{n+1/2})_x-\sum_{n=0}^{k}\Delta t(\delta_y(\phi)^{n+1/2},d_td_ye_\phi^{n+1/2})_y\\
\le& C\sum_{n=1}^{k}\Delta t\|\mathbf{d}e_\phi^n\|_{TM}^2+\frac{\lambda}{4}\|e_\phi^{k+1}\|_m^2+C\|\phi\|_{W^{1,\infty}(J;W^{3,\infty}(\Omega))}^2(h_x^4+h_y^4).
\end{aligned}
\tag{4.31}
$$

Multiplying equation (4.28) by Δt, summing over n, $n=0,1,\dots,k$, and combining with equations (4.30) and (4.31), we can obtain (4.2). □

Lemma 6. *Under the conditions of Theorem 4, there exists a positive constant C independent of h_x, h_y, and Δt such that*

$$\begin{aligned}
&\|e_\phi^{k+1}\|_m^2 + M\sum_{n=0}^{k}\Delta t\|e_\mu^{n+1/2}\|_m^2\\
\le& C\sum_{n=0}^{k}\Delta t(e_r^{n+1})^2 + C\sum_{n=0}^{k}\Delta t\|e_\phi^n\|_m^2\\
&+\frac{M}{4}\sum_{n=0}^{k}\Delta t\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2 + C\sum_{n=0}^{k}\Delta t\|\mathbf{d}e_\phi^{n+1/2}\|_{TM}^2\\
&+C(\|\mu\|^2_{L^\infty(J;W^{4,\infty}(\Omega))} + \|\phi\|^2_{L^\infty(J;W^{4,\infty}(\Omega))})(h_x^4+h_y^4)\\
&+C\|\phi\|^2_{W^{3,\infty}(J;L^\infty(\Omega))}\Delta t^4.
\end{aligned} \tag{4.32}$$

Proof. Multiplying equation (4.3) by $e_{\phi,i,j}^{n+1/2}h_xh_y$, and making summation on i,j for $1\le i\le N_x,\ 1\le j\le N_y$, we have

$$\begin{aligned}
&(d_te_\phi^{n+1}, e_\phi^{n+1/2})_m\\
=&M\left(D_x(d_xe_\mu+\delta_x(\mu))^{n+1/2} + D_y(d_ye_\mu+\delta_y(\mu))^{n+1/2}, e_\phi^{n+1/2}\right)_m\\
&+(T_1^{n+1/2}, e_\phi^{n+1/2})_m + (T_2^{n+1/2}, e_\phi^{n+1/2})_m.
\end{aligned} \tag{4.33}$$

Using Lemma 1, the first term on the right-hand side of equation (4.33) can be transformed into the following:

$$\begin{aligned}
&M\left(D_x(d_xe_\mu+\delta_x(\mu))^{n+1/2} + D_y(d_ye_\mu+\delta_y(\mu))^{n+1/2}, e_\phi^{n+1/2}\right)_m\\
=&-M\left((d_xe_\mu+\delta_x(\mu))^{n+1/2}, d_xe_\phi^{n+1/2}\right)_x\\
&-M\left((d_ye_\mu+\delta_y(\mu))^{n+1/2}, d_ye_\phi^{n+1/2}\right)_y.
\end{aligned} \tag{4.34}$$

The first term on the right-hand side of equation (4.34) can be estimated as

$$\begin{aligned}
&-M\left((d_xe_\mu+\delta_x(\mu))^{n+1/2}, d_xe_\phi^{n+1/2}\right)_x\\
=&-M\left(d_xe_\mu^{n+1/2}, (d_xe_\phi+\delta_x(\phi))^{n+1/2}\right)_x\\
&+M(d_xe_\mu^{n+1/2}, \delta_x(\phi)^{n+1/2})_x - M(\delta_x(\mu)^{n+1/2}, d_xe_\phi^{n+1/2})_x\\
\le& M\left(e_\mu^{n+1/2}, D_x(d_xe_\phi+\delta_x(\phi))^{n+1/2}\right)_m\\
&+\frac{M}{4}\|d_xe_\mu^{n+1/2}\|_x^2 + C\|d_xe_\phi^{n+1/2}\|_x^2\\
&+C(\|\mu\|^2_{L^\infty(J;W^{3,\infty}(\Omega))} + \|\phi\|^2_{L^\infty(J;W^{3,\infty}(\Omega))})(h_x^4+h_y^4).
\end{aligned} \tag{4.35}$$

In the y direction, we have similar estimates. Then the left-hand side in (4.34) can be bounded by

$$\begin{aligned}
&M\left(D_x(d_x e_\mu+\delta_x(\mu))^{n+1/2}+D_y(d_y e_\mu+\delta_y(\mu))^{n+1/2}, e_\phi^{n+1/2}\right)_m\\
\le& M\left(e_\mu^{n+1/2}, D_x(d_x e_\phi+\delta_x(\phi))^{n+1/2}+D_y(d_y e_\phi+\delta_y(\phi))^{n+1/2}\right)_m\\
&+\frac{M}{4}\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2+C\|\mathbf{d}e_\phi^{n+1/2}\|_{TM}^2\\
&+C(\|\mu\|^2_{L^\infty(J;W^{3,\infty}(\Omega))}+\|\phi\|^2_{L^\infty(J;W^{3,\infty}(\Omega))})(h_x^4+h_y^4).
\end{aligned} \tag{4.36}$$

Thanks to (4.6) and (4.15), the first term on the right-hand side of (4.36) can be estimated as follows:

$$\begin{aligned}
&M\left(e_\mu^{n+1/2}, D_x(d_x e_\phi+\delta_x(\phi))^{n+1/2}+D_y(d_y e_\phi+\delta_y(\phi))^{n+1/2}\right)_m\\
=&M\left(e_\mu^{n+1/2}, \frac{R^{n+1/2}}{\sqrt{E_1^h(\tilde{Z}^{n+1/2})}}F'(\tilde{Z}^{n+1/2})-\frac{r^{n+1/2}}{\sqrt{E_1(\phi^{n+1/2})}}F'(\phi^{n+1/2})\right)_m\\
&+M(e_\mu^{n+1/2},\lambda e_\phi^{n+1/2})_m+M(e_\mu^{n+1/2},T_3^{n+1/2})_m-M\|e_\mu^{n+1/2}\|_m^2\\
\le&\frac{M}{2}\|e_\mu^{n+1/2}\|_m^2+C(e_r^{n+1}+e_r^n)^2+C(\|e_\phi^n\|_m^2+\|e_\phi^{n-1}\|_m^2)\\
&-M\|e_\mu^{n+1/2}\|_m^2+C\|\phi\|^2_{L^\infty(J;W^{4,\infty}(\Omega))}(h_x^4+h_y^4).
\end{aligned} \tag{4.37}$$

Combining equation (4.33) with equations (4.36) and (4.37) and multiplying equation (4.28) by $2\Delta t$, summing over n, $n=0,1,\ldots,k$, leads to (4.32). □

Lemma 7. *Under the conditions of Theorem 4, there exists a positive constant C_* independent of h_x, h_y, and Δt such that*

$$\|Z^n\|_\infty\le C_* \ \textit{ for all } \ n.$$

Proof. We proceed in two steps.

Step 1 (Definition of C_*). Using the scheme (2.13)–(2.15) for $n=0$ and applying the inverse assumption, we can get the approximation Z^1 with the following property:

$$\begin{aligned}
\|Z^1\|_\infty\le&\|Z^1-\phi^1\|_\infty+\|\phi^1\|_\infty\le\|Z^1-\Pi_h\phi^1\|_\infty+\|\Pi_h\phi^1-\phi^1\|_\infty+\|\phi^1\|_\infty\\
\le&Ch^{-1}(\|Z^1-\phi^1\|_m+\|\phi^1-\Pi_h\phi^1\|_m)+\|\Pi_h\phi^1-\phi^1\|_\infty+\|\phi^1\|_\infty\\
\le&C(h+h^{-1}\Delta t^2)+\|\phi^1\|_\infty\le C,
\end{aligned}$$

where $h=\max\{h_x,h_y\}$ and Π_h is a bilinear interpolant operator with the following estimate [5]:

$$\|\Pi_h\phi^1-\phi^1\|_\infty\le Ch^2. \tag{4.38}$$

Thus we can choose the positive constant C_* independent of h and Δt such that

$$C_*\ge\max\{\|Z^1\|_\infty, 2\|\phi^n\|_\infty\}.$$

Step 2 (Induction). By the definition of C_*, it is trivial that hypothesis (4.17) holds true for $l=1$. Supposing that $\|Z^{l-1}\|_\infty\le C_*$ holds true for an integer $l=1,\ldots,k+1$, with the aid of the estimate (4.41), we have that

$$\|Z^l-\phi^l\|_m\le C(\Delta t^2+h^2).$$

Next we prove that $\|Z^l\|_\infty \le C_*$ holds true. We have

$$\begin{aligned}\|Z^l\|_\infty \le&\|Z^l-\phi^l\|_\infty+\|\phi^l\|_\infty \le \|Z^l-\Pi_h\phi^l\|_\infty+\|\Pi_h\phi^l-\phi^l\|_\infty+\|\phi^l\|_\infty\\ \le&Ch^{-1}(\|Z^l-\phi^l\|_m+\|\phi^l-\Pi_h\phi^l\|_m)+\|\Pi_h\phi^l-\phi^l\|_\infty+\|\phi^l\|_\infty\\ \le&C_1(h+h^{-1}\Delta t^2)+\|\phi^1\|_\infty.\end{aligned} \tag{4.39}$$

Let $\Delta t \le C_2 h$ and let a positive constant h_1 be small enough to satisfy

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

Then for $h\in(0,h_1]$, we derive from (4.39) that

$$\begin{aligned}\|Z^l\|_\infty \le&C_1(h+h^{-1}\Delta t^2)+\|\phi^l\|_\infty\\ \le&C_1(h_1+C_2^2h_1)+\frac{C_*}{2}\le C_*.\end{aligned}$$

This completes the induction. □

We are now in position to prove our main results.

Proof of Theorem 4. Thanks to the above three lemmas, we can obtain

$$\begin{aligned}&(e_r^{k+1})^2+\frac{1}{2}\|\mathbf{d}e_\phi^{k+1}\|_{TM}^2+\|e_\phi^{k+1}\|_m^2\\ &+\frac{M}{4}\sum_{n=0}^{k}\Delta t\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2+\frac{M}{2}\sum_{n=0}^{k}\Delta t\|e_\mu^{n+1/2}\|_m^2\\ \le&C\sum_{n=0}^{k+1}\Delta t\|\mathbf{d}e_\phi^{n}\|_{TM}^2+C\sum_{n=0}^{k+1}\Delta t\|e_\phi^{n}\|_m^2+C\sum_{n=0}^{k+1}\Delta t(e_r^n)^2\\ &+C(\|\phi\|^2_{W^{1,\infty}(J;W^{4,\infty}(\Omega))}+\|\mu\|^2_{L^{\infty}(J;W^{4,\infty}(\Omega))})(h_x^4+h_y^4)\\ &+C\|\phi\|^2_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}\Delta t^4.\end{aligned} \tag{4.40}$$

Finally applying the discrete Gronwall's inequality, we arrive at the desired result:

$$\begin{aligned}&(e_r^{k+1})^2+\|\mathbf{d}e_\phi^{k+1}\|_{TM}^2+\|e_\phi^{k+1}\|_m^2\\ &+\sum_{n=0}^{k}\Delta t\|\mathbf{d}e_\mu^{n+1/2}\|_{TM}^2+\sum_{n=0}^{k}\Delta t\|e_\mu^{n+1/2}\|_m^2\\ \le&C(\|\phi\|^2_{W^{1,\infty}(J;W^{4,\infty}(\Omega))}+\|\mu\|^2_{L^{\infty}(J;W^{4,\infty}(\Omega))})(h_x^4+h_y^4)\\ &+C\|\phi\|^2_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}\Delta t^4.\end{aligned} \tag{4.41}$$

Thus, the proof of Theorem 4 is complete. □

4.2. L^2 **gradient flow.** For the L^2 gradient flow, we shall only state the error estimates below, as their proofs are essentially the same as for the H^{-1} gradient flow.

Theorem 8. *Assume* $F(\phi)\in C^3(\mathbb{R})$, $\phi\in W^{1,\infty}(J;W^{4,\infty}(\Omega))\cap W^{3,\infty}(J;W^{1,\infty}(\Omega))$, *and* $\Delta t\le C(h_x+h_y)$. *Then for the discrete scheme* (2.17)–(2.19), *there exists a positive constant* C *independent of* h_x, h_y, *and* Δt *such that*

$$\begin{aligned}&\|Z^{k+1}-\phi^{k+1}\|_m+\|\mathbf{d}Z^{k+1}-\mathbf{d}\phi^{k+1}\|_{TM}+|R^{k+1}-r^{k+1}|\\ \le&C\|\phi\|_{W^{3,\infty}(J;W^{1,\infty}(\Omega))}\Delta t^2+C\|\phi\|_{W^{1,\infty}(J;W^{4,\infty}(\Omega))}(h_x^2+h_y^2).\end{aligned} \tag{4.42}$$

5. Numerical simulations

We present in this section various numerical experiments to verify the energy stability and accuracy of the proposed numerical schemes.

5.1. **Accuracy test for Allen-Cahn and Cahn-Hilliard equations.**

We consider the free energy

$$E(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla \phi|^2 + \frac{1}{4\epsilon^2}(\phi^2-1)^2 \right) d\mathbf{x}, \tag{5.1}$$

and for better accuracy rewrite it as

$$E(\phi) = \int_\Omega \left(\frac{1}{2}|\nabla \phi|^2 + \frac{\beta}{2\epsilon^2}\phi^2 + \frac{1}{4\epsilon^2}(\phi^2-1-\beta)^2 - \frac{\beta^2+2\beta}{4\epsilon^2} \right) d\mathbf{x}, \tag{5.2}$$

where β is a positive number to be chosen. To apply our schemes (2.13)–(2.15) or (2.17)–(2.19) to the system (2.2), we drop the constant in the free energy and specify the operator $\mathcal{G}$, the energy $E_1(\phi)$, and λ as follows:

$$\mathcal{G} = -(-\Delta)^s,\ E_1(\phi) = \frac{1}{4\epsilon^2}\int_\Omega (\phi^2-1-\beta)^2 d\mathbf{x},\ \lambda = \frac{\beta}{\epsilon^2}. \tag{5.3}$$

The system (2.2) becomes the standard Allen-Cahn equation with $s=0$, and the standard Cahn-Hilliard equation with $s=1$.

We denote

$$\begin{cases} \|f-g\|_{\infty,2} = \max\limits_{0\le n\le k} \left\{ \|f^{n+q}-g^{n+q}\|_X \right\}, \\ \|f-g\|_{2,2} = \left(\sum\limits_{n=0}^{k} \Delta t \,\|f^{n+q}-g^{n+q}\|_X^2 \right)^{1/2}, \\ \|R-r\|_\infty = \max\limits_{0\le n\le k} \{R^{n+1}-r^{n+1}\}, \end{cases}$$

where $q=\frac{1}{2}$, 1 and $X = m,\ TM$.

In the following simulations, we choose $\Omega=(0,1)\times(0,1)$ and $C_0 = 0$.

5.1.1. *Convergence rates of the SAV/CN-BCFD scheme for the Allen-Cahn equation.*

Example 1. We take $T=0.5,\ \mathcal{G}=-1,\ \beta=0,\ M=0.01,\ \epsilon=0.08,\ \Delta t = 5E-4$, and the initial solution $\phi_0 = \cos(\pi x)\cos(\pi y)$. To get around the fact that we do not have possession of an exact solution, we measure Cauchy error, which is similar to [4, 6, 23]. Specifically, the error between two different grid spacings h and $\frac{h}{2}$ is calculated by $\|e_\zeta\| = \|\zeta_h - \zeta_{h/2}\|$.

The numerical results are listed in Table 1. We observe the second-order convergence predicted by the error estimates in Theorem 8.

TABLE 1. Errors and convergence rates of Example 1.

h	$\|e_Z\|_{\infty,2}$	Rate	$\|e_{\mathbf{d}Z}\|_{\infty,2}$	Rate	$\|e_W\|_{\infty}$	Rate
1/10	6.36E-3	—	5.96E-2	—	5.93E-3	—
1/20	1.59E-3	2.00	1.57E-2	1.93	1.47E-3	2.01
1/40	3.98E-4	2.00	3.98E-3	1.98	3.69E-4	2.00
1/80	9.96E-5	2.00	9.98E-4	1.99	9.23E-5	2.00

5.1.2. *Convergence rates of SAV/CN-BCFD scheme for the Cahn-Hilliard equation.*

Example 2. We take $T = 0.5,\ \mathcal{G} = \Delta,\ \beta = 0,\ M = 0.01,\ \epsilon = 0.2,\ \Delta t = 5E-4$, with the same initial solution as in Example 1. The numerical results are listed in Tables 2 and 3. Again, we observe the expected second-order convergence rate in various discrete norms.

TABLE 2. Errors and convergence rates of Example 2.

h	$\|e_Z\|_{\infty,2}$	Rate	$\|e_{\mathbf{d}Z}\|_{\infty,2}$	Rate	$\|e_R\|_{\infty}$	Rate
1/10	5.49E-3	—	2.78E-2	—	4.88E-3	—
1/20	1.36E-3	2.01	6.91E-3	2.01	1.20E-3	2.02
1/40	3.41E-4	2.00	1.73E-3	2.00	3.00E-4	2.00
1/80	8.51E-5	2.00	4.31E-4	2.00	7.49E-5	2.00

TABLE 3. Errors and convergence rates of Example 2.

h	$\|e_W\|_{2,2}$	Rate	$\|e_{\mathbf{d}W}\|_{2,2}$	Rate
1/10	2.50E-2	—	2.18E-1	—
1/20	6.11E-3	2.03	5.46E-2	2.00
1/40	1.52E-3	2.01	1.37E-2	2.00
1/80	3.79E-4	2.00	3.42E-3	2.00

5.2. **Coarsening dynamics and adaptive time stepping.**

Example 3. In this example, we simulate the coarsening dynamics of the Cahn-Hilliard equation.

Since the scheme (2.13)–(2.15) is unconditionally energy stable, we can choose time steps according to accuracy only with an adaptive time stepping. Actually in many situations, the energy and solution of gradient flows can vary drastically in certain time intervals, but only slightly elsewhere. In order to maintain the desired accuracy, we adjust the time sizes based on an adaptive time-stepping strategy below ([10, 17]). We update the time step size by using the formula

$$A_{dp}(e, \Delta t) = \rho \left(\frac{tol}{e}\right)^{1/2} \Delta t, \tag{5.4}$$

Algorithm 1 Adaptive time stepping procedure

Given: $\mathbf{Z}^n$ and Δt^n.

1: Computer $\mathbf{Z}_{Ref}^{n+1}$ using a first order SAV-BCFD scheme and Δt^n.
2: Computer $\mathbf{Z}^{n+1}$ using the SAV/CN-BCFD scheme (2.13)-(2.15) and Δt^n.
3: Calculate $e^{n+1} = \|\mathbf{Z}_{Ref}^{n+1} - \mathbf{Z}^{n+1}\| / \|\mathbf{Z}^{n+1}\|$.
4: **If** $e^{n+1} > tol$ **then**
    Recalculate time step $\Delta t^n \leftarrow \max\{\Delta t_{min}, \min\{A_{dp}(e^{n+1}, \Delta t^n), \Delta t_{max}\}\}$.
5:     **goto** 1
6: **else**
    Update time step $\Delta t^{n+1} \leftarrow \max\{\Delta t_{min}, \min\{A_{dp}(e^{n+1}, \Delta t^n), \Delta t_{max}\}\}$.
7: **endif**

where ρ is a default safety coefficient, tol is a reference tolerance, and e is the relative error at each time level. In this simulation, we take

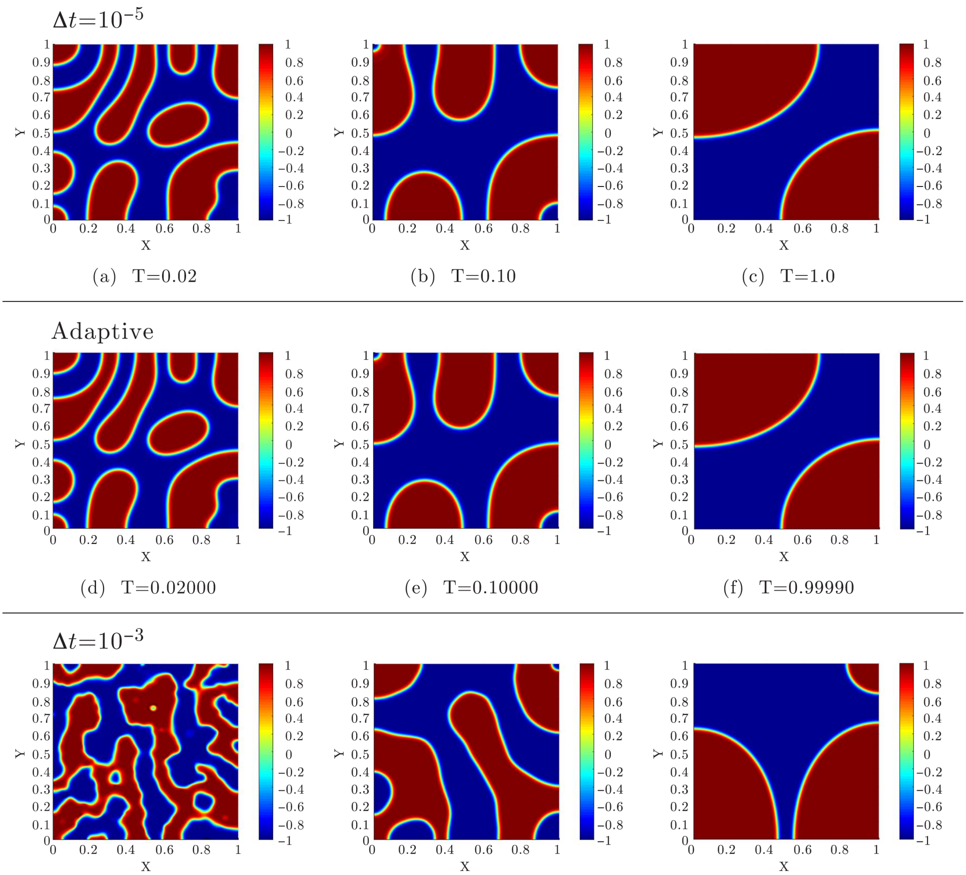
$$\begin{cases} \mathcal{G} = \Delta,\ \Delta t_{max} = 10^{-2},\ \Delta t_{min} = 10^{-5},\ tol = 10^{-3}, \\ M = 0.002,\ \epsilon = 0.01,\ \beta = 6,\ \rho = 0.9, \end{cases}$$

with a random initial condition with values in $[-0.05, 0.05]$, and the initial time step is taken as Δt_{min}.

To demonstrate the effectivity of the SAC/CN-BCFD scheme with adaptive time stepping, we compute the reference solutions with a small uniform time step $\Delta t = 10^{-5}$ and a large uniform time step $\Delta t = 10^{-3}$, respectively. Characteristic evolutions of the phase functions are presented in Figure 1. We also present in Figure 2 the energy evolutions and the roughness of interface, where the roughness measure function $R(t)$ is defined as follows:

$$R(t) = \sqrt{\frac{1}{|\Omega|} \int_\Omega (\phi - \bar{\phi})^2 d\Omega}, \tag{5.5}$$

with $\bar{\phi} = \frac{1}{|\Omega|} \int_\Omega \phi d\Omega$. One observes that the solution obtained with adaptive time steps is consistent with the reference solution obtained with a small time step, while the solution with large time step deviates from the reference solution. This is also verified by both the energy evolutions and roughness measure function $R(t)$. We present in Figure 3 the adaptive time steps for different $\epsilon = 0.02,\ 0.01,\ 0.005$. We observe that there are about two orders of magnitude variation in the time steps with the adaptive time stepping, which indicates that the adaptive time stepping for the SAV/CN-BCFD scheme is very efficient.



(a) T=0.02 (b) T=0.10 (c) T=1.0

(d) T=0.02000 (e) T=0.10000 (f) T=0.99990

(g) T=0.02 (h) T=0.1 (i) T=1.0

FIGURE 1. Snapshots of the phase function among small time steps, adaptive time steps and large time steps in Example 3.

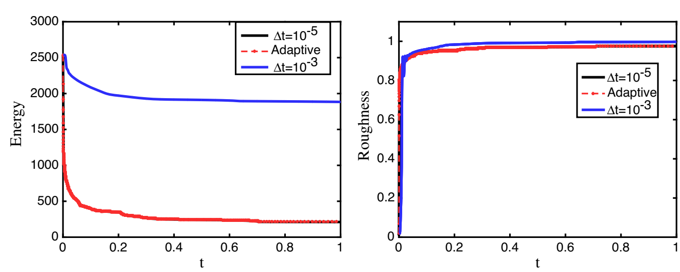


FIGURE 2. Numerical comparisons of discrete scaled surface energy and roughness for the simulation of spinodal decomposition in Example 3.

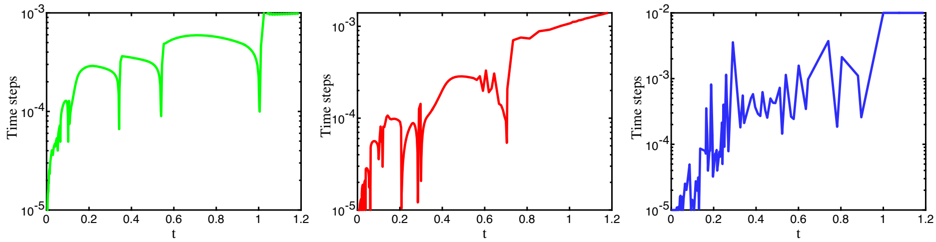


FIGURE 3. Adaptive time steps for different ϵ: (a) $\epsilon = 0.02$, (b) $\epsilon = 0.01$, (c) $\epsilon = 0.005$

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