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NUMERICAL ENERGY DISSIPATION FOR TIME-FRACTIONAL PHASE-FIELD EQUATIONS*

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Abstract

The numerical integration of phase-field equations is a delicate task which needs to recover at the discrete level intrinsic properties of the solution such as energy dissipation and maximum principle. Although the theory of energy dissipation for classical phase field models is well established, the corresponding theory for time-fractional phase-field models is still incomplete. In this article, we study certain nonlocal-in-time energies using the first-order stabilized semi-implicit L1 scheme. In particular, we will establish a discrete fractional energy law and a discrete weighted energy law. The extension for a $(2-\alpha)$-order L1 scalar auxiliary variable scheme will be investigated. Moreover, we demonstrate that the energy bound is preserved for the L1 schemes with nonuniform time steps. Several numerical experiments are carried to verify our theoretical analysis.

Mathematics subject classification: 65M06, 65M12, 74A50.
Key words: Time-fractional phased-field equation, Allen-Cahn equations, Cahn-Hilliard equations, Caputo fractional derivative, Energy dissipation.

1. Introduction

A fractional time derivative arises when the characteristic waiting time diverges, which models situations involving memory. In recent years, to model memory effects and subdiffusive regimes in applications such as transport theory, viscoelasticity, rheology and non-Markovian stochastic processes, there has been an increasing interest in the study of time-fractional differential equations, i.e. differential equations where the standard time derivative is replaced by a fractional one, typically a Caputo or a Riemann-Liouville derivative. It has been reported that the presence of nonlocal operators in time in the relevant governing equations may change diffusive dynamics significantly, which can better describe certain fundamental relations between the processes of interest, see, e.g. [1, 4, 6, 18, 26]. It is also noted that an intensive effort

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has been put into investigations on time fractional phase-field models. For instance, phase-field framework has been successfully employed to describe the evolution of structural damage and fatigue [3], in which the damage is described by a variable order time fractional derivative.

Seeking numerical solutions of phase field problems has attracted a lot of recent attentions. The numerical integration of phase-field equations can be a delicate task: it needs to recover at the discrete level intrinsic properties of the solution (energy diminishing, maximum principle) and the presence of small parameter $\varepsilon > 0$ (typically, the interphase length) can generate practical difficulties. Numerical analysis and computation aiming to handle this task for the classical phase field problems have attracted extensive attentions, see, e.g. [8, 12, 35, 39] and the references therein. On the other hand, it is natural to extend the relevant discrete level intrinsic properties, i.e. the maximum principle and energy stability to handle the time-fractional phase-field equations, see, e.g. [9, 21, 23, 24].

This work is concerned with numerical methods for time-fractional phase-field models with the Caputo time-derivative. The time-fractional phase-field equation can be written in the form of

$$\partial_t^\alpha \phi = \gamma\, \mathcal{G} \mu, \tag{1.1a}$$

where $\alpha \in (0,1), \gamma > 0$ is the mobility constant, $\mathcal{G}$ is a nonpositive operator, and ∂_t^α is the Caputo fractional derivative defined by

$$\partial_t^\alpha \phi(t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\phi'(s)}{(t-s)^\alpha}\, \mathrm{d}s, \quad t \in (0,T) \tag{1.1b}$$

with $\Gamma(\cdot)$ the gamma function. Choosing different $\mathcal{G}$ and μ, one derives different phase-field models, such as the Allen-Cahn (AC) model and the Cahn-Hilliard (CH) model. In the AC model and the CH model, $\mathcal{G}$ is taken to be -1 and Δ, respectively, while in both cases μ takes the same form

$$\mu = -\varepsilon^2 \Delta \phi + F'(\phi), \tag{1.2}$$

where $\varepsilon > 0$ is the interface width parameter and F is a double-well potential functional, commonly chosen as $F(\phi) = (1-\phi^2)^2/4$ so that $F'(\phi) = \phi^3 - \phi$. Moreover, the molecular-beam epitaxy (MBE) model has two forms, with or without slope selection [43], where

$$\mathcal{G} = -1, \quad \mu = \varepsilon^2 \Delta^2 \phi + \nabla \cdot \mathbf{f}_{\mathrm{m}}(\nabla \phi) \tag{1.3a}$$

with

$$\mathbf{f}_{\mathrm{m}}(\nabla\phi) = \begin{cases} \nabla\phi - |\nabla\phi|^2 \nabla\phi & \text{with slope selection,} \\ \dfrac{\nabla\phi}{1+|\nabla\phi|^2} & \text{without slope selection.} \end{cases} \tag{1.3b}$$

For sake of simplicity, we consider the periodic boundary condition for above time-fractional phase-field problems.

The classical energy for the standard Allen-Cahn or Cahn-Hilliard equation (i.e. (1.2) with $\alpha = 1$) is

$$E(\phi) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\nabla\phi|^2 + F(\phi) \right) \mathrm{d}x, \tag{1.4}$$

while for the MBE equation (1.3) is given by

$$E(\phi) = \int_\Omega \left(\frac{\varepsilon^2}{2} |\Delta\phi|^2 + F_{\mathrm{m}}(\nabla\phi) \right) \mathrm{d}x \tag{1.5a}$$

with

$$F_{\mathrm{m}}(\nabla\phi) = \begin{cases} \dfrac{1}{4}\left(1-|\nabla\phi|^2\right)^2 & \text{with slope selection,} \\ -\dfrac{1}{2}\ln\left(1+|\nabla\phi|^2\right) & \text{without slope selection.} \end{cases} \tag{1.5b}$$

Applying the definition (1.4) with the time-fractional problem (1.2) gives

$$\frac{\mathrm{d}}{\mathrm{d}t}E(\phi) = \frac{1}{\gamma}\int_\Omega \partial_t\phi\left(\mathcal{G}^{-1}\partial_t^\alpha\phi\right)\mathrm{d}x, \tag{1.6}$$

where $\mathcal{G}^{-1}$ is the inverse of $\mathcal{G}$.

It is well known that when $\alpha = 1$, the Allen-Cahn and Cahn-Hilliard models are gradient flows: The energy associated with these models decays with respect to time, which is the so-called energy dissipation law. This property has been used extensively as a nonlinear numerical stability criterion. However, it is still unknown if such energy dissipation property holds in the general case of $0 < \alpha < 1$. In a recent work [41], it is demonstrated that the classical energy (1.1) is bounded above by the initial energy

$$E(t) \le E(0), \quad \forall\, 0 < t < T, \tag{1.7}$$

which is the first work on the energy stability for time-fractional phase-field equations. Later, Du *et al.* [9] proposed the fractional energy law based on numerical observations and proved for the convex energy (not applicable to nonconvex phase-field models), i.e. the time-fractional derivative of energy is nonpositive

$$\partial_t^\alpha E(t) \le 0, \quad \forall\, 0 < t < T. \tag{1.8}$$

In [27], this fractional energy law was proved for general cases. Still in [27], it is shown that in the continuous case a weighted energy decays with respect to time

$$\partial_t E_\omega(t) \le 0, \quad \forall\, 0 < t < T, \tag{1.9a}$$

where E_ω is defined by

$$E_\omega(t) = \frac{1}{B(\alpha, 1-\alpha)}\int_0^t \frac{E(s)}{s^{1-\alpha}(t-s)^\alpha}\mathrm{d}s. \tag{1.9b}$$

By using the transformation $s = \theta t$, we can obtain

$$E_\omega(t) = \frac{1}{B(\alpha, 1-\alpha)}\int_0^1 \frac{E(\theta t)}{\theta^{1-\alpha}(1-\theta)^\alpha}d\theta.$$

Taking derivative with respect to t and using the transformation $\theta = s/t$ yield

$$E'_\omega(t) = \frac{1}{B(\alpha, 1-\alpha)t}\int_0^t \frac{s^\alpha E'(s)}{(t-s)^\alpha}\mathrm{d}s. \tag{1.10}$$

In other words, the fractional energy law of (1.8) and the weighted energy dissipation law (1.9) are all associated with the Caputo fractional operator, i.e. the dissipation of certain time-fractional form for energy

$$\partial_t^\alpha E(t) \sim \int_0^t \frac{E'(s)}{(t-s)^\alpha}\mathrm{d}s \le 0, \quad E'_\omega(t) \sim \int_0^t \frac{s^\alpha E'(s)}{(t-s)^\alpha}\mathrm{d}s \le 0. \tag{1.11}$$

This paper is concerned with the numerical implementation of the energy stability properties (1.8) and (1.9) by using the first-order stabilized L1 scheme. From a numerical point view, the essential step to study the fractional PDE is to approximate the time-fractional derivative operator. The classical L1 method is naturally derived from the approximation of the fractional integral as a Riemann sum and long known to be consistent (see, e.g. [21]). Moreover, L1 approximation scheme stands out by being able to preserve at the discrete level certain desirable features of the original PDEs, such as maximum principle [11,16,41] and energy stability [9,15]. Our analysis will also be relevant to the convex-splitting schemes [5, 10, 42], the stabilization schemes [36, 43], and the scalar auxiliary variable (SAV) schemes [34]. In particular, we will establish the energy boundedness and the fractional energy law for a $(2-\alpha)$-order L1-SAV scheme with uniform time steps. The energy boundedness under non-uniform time step will be also investigated. All proofs are based on a special Cholesky decomposition proposed recently by us in [27], which seems very useful for studying numerical approximations of time-fractional phase-field equations.

We point out some recent comprehensive and interesting studies for the theory of time-fractional gradient flows. Li *et al.* [20] present the well-posedness and regularity of solutions to a fractional diffusion porous media equation with variable fractional order, and analyze the convergence of a linearly implicit convolution quadrature method. Li and Ma [19] propose an exponential convolution quadrature method for the nonlinear subdiffusion equation with nonsmooth initial data, that has high-order convergence in time. Li and Salgado [21] introduce the notion of energy solutions. The authors provide existence, uniqueness and certain regularizing effects due to the Caputo derivative. The time-fractional phase-field models fit well with the class of the fractional gradient flows. In addition, one can refer to a book by Jin and Zhou [17], that provides a comprehensive survey on the ideas and methods of analysis for solving time-fractional evolution equations.

The paper is organized as follows. Section 2 introduces the L1 approximation of the time-fractional operator and a semi-implicit stabilization technique. We then establish the fractional energy law (1.8) and the weighted energy dissipation law (1.9). In Section 3, we propose a $(2-\alpha)$-order L1-SAV scheme, and establish the corresponding energy boundedness and the fractional energy law. In Section 4, the first-order and $(2-\alpha)$-order L1 schemes are investigated with nonuniform time-steps. Section 5 presents several numerical examples to verify our theoretical results. Some concluding remarks are given in the final section.

2. First Order Stabilized L1 Scheme

We first introduce the discretization of the time fractional derivative. Let $\Delta t = T/N$ be the time step size and $t_n = n\Delta t, 0 \le n \le N$. The L1 approximation of the Caputo time-fractional derivative (1.1b) is given by

$$\bar{\partial}_n^\alpha \phi := \sum_{j=1}^{n} b_{n-j} \overline{\partial}_j \phi, \quad 1 \le n \le N, \tag{2.1a}$$

where $\overline{\partial}_n^\alpha$ denotes the discrete fractional derivative at t_n,

$$b_j = \frac{\Delta t^{1-\alpha}}{\Gamma(2-\alpha)}[(j+1)^{1-\alpha} - j^{1-\alpha}], \quad j \ge 0, \tag{2.1b}$$

and $\overline{\partial}_k$ denotes the discrete first-order derivative at t_k as follows:

$$\overline{\partial}_k \phi := \frac{\phi^k - \phi^{k-1}}{\Delta t}. \tag{2.1c}$$

One can refer to [37] for the analysis of the L1 approximation, where the truncation error of order $2-\alpha$ is derived. A useful reformulation of (2.1a) is

$$\bar{\partial}_n^\alpha \phi = \frac{1}{\Delta t}\left[b_0 \phi^n - \sum_{j=1}^{n-1} (b_{j-1} - b_j)\phi^{n-j} - b_{n-1}\phi^0 \right], \quad 1 \le n \le N, \tag{2.2}$$

where the following relationship holds:

$$b_{j-1} - b_j > 0, \quad b_{n-1} > 0, \quad \sum_{j=1}^{n-1} (b_{j-1} - b_j) + b_{n-1} = b_0. \tag{2.3}$$

We further decompose the energy by the quadratic-nonquadratic splitting as follows:

$$E(\phi) = \frac{1}{2}\langle \phi, \mathcal{L}\phi \rangle + E_1(\phi), \tag{2.4}$$

where $\langle \cdot\,, \cdot \rangle$ denotes the L^2 inner product over Ω, $\mathcal{L}$ is some symmetric nonnegative linear operator ($\mathcal{L} = -\varepsilon^2 \Delta$ for the AC/CH model and $\mathcal{L} = \varepsilon^2 \Delta^2$ for the MBE model), and E_1 is the remaining nonquadratic term. The stabilized L1 scheme for (1.1) is written as

$$\bar{\partial}_{n+1}^\alpha \phi = \gamma\, \mathcal{G}\big(\mathcal{L}\phi^{n+1} + \delta_\phi E_1(\phi^n) + \widetilde{\mathcal{L}}(\phi^{n+1} - \phi^n) \big), \tag{2.5}$$

where $\widetilde{\mathcal{L}}$ is some linear operator in the following form:

$$\widetilde{\mathcal{L}} = \begin{cases} S, & \text{AC or CH model,} \\ -S\Delta, & \text{MBE without slope selection} \end{cases} \tag{2.6}$$

with some positive constant S satisfying

$$S \ge \begin{cases} 2, & \text{AC model,} \\ \dfrac{L}{2}, & \text{CH model,} \\ \dfrac{1}{16}, & \text{MBE without slope selection.} \end{cases} \tag{2.7}$$

Here, $L > 0$ denotes the truncation parameter used for the CH model (see [2, 36]) such that $\max_{\phi \in \mathbb{R}} |E_1''(\phi)| \le L$.

In the classical case of $\alpha = 1$, the following inequality holds for the scheme (2.5):

$$E^{n+1} - E^n \le \frac{1}{\gamma \Delta t} \langle \mathcal{G}^{-1}(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n \rangle \le 0, \tag{2.8}$$

since $\mathcal{G}^{-1}$ is nonpositive definite. Similarly, in the general case of $0 < \alpha < 1$, one can obtain the following inequality characterizing the energy difference between two neighboring time steps.

Lemma 2.1. *Assume that the initial data satisfies $\|\phi^0\|_\infty \le 1$. The energy of the stabilized L1 scheme (2.5) satisfies the following property:*

$$E^{n+1} - E^n \le \frac{1}{\gamma} \big\langle \mathcal{G}^{-1} \overline{\partial}_{n+1}^\alpha \phi, \phi^{n+1} - \phi^n \big\rangle, \quad 0 \le n \le N-1, \tag{2.9}$$

where $E^n = E(\phi^n)$ denotes the classical energy at t_n.

Proof. The proof is quite similar to the classical case of $\alpha = 1$ given by [41]. Here, we only prove the specific case of AC model under the constraint $S \geq 2$. In this case, (2.5) can be rewritten as

$$\left(\frac{b_0}{\Delta t} + \gamma S - \gamma\varepsilon^2\Delta\right)\phi^{n+1} = \gamma(S+1)\phi^n - \gamma(\phi^n)^3 + \sum_{j=0}^{n-1}\frac{(b_j - b_{j+1})}{\Delta t}\phi^{n-j} + \frac{b_n}{\Delta t}\phi^0. \tag{2.10}$$

Since $S \geq 2$, it is not difficult to verify that if $\|\phi^n\|_\infty \leq 1$ then

$$\|(S+1)\phi^n - (\phi^n)^3\|_\infty \leq S.$$

Further, it is known (see, e.g. [40]) that

$$\left\| \left(\frac{b_0}{\Delta t} + \gamma S - \gamma\varepsilon^2\Delta\right)^{-1} \right\|_\infty \leq \left(\frac{b_0}{\Delta t} + \gamma S\right)^{-1}, \tag{2.11}$$

which yields by induction that if $\|\phi^0\|_\infty \leq 1$ then $\|\phi^n\|_\infty \leq 1$, i.e. the maximum bound is preserved. As a consequence, we further obtain

$$\begin{aligned}
&\frac{1}{\gamma}\big\langle \mathcal{G}^{-1}\overline{\partial}_{n+1}^{\alpha}\phi, \phi^{n+1} - \phi^n\big\rangle \\
&= \big\langle -\varepsilon^2\Delta\phi^{n+1} + (\phi^n)^3 - \phi^n + S(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n\big\rangle \\
&= \frac{\varepsilon^2}{2}\big(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2 + \|\nabla\phi^{n+1} - \nabla\phi^n\|^2\big) \\
&\quad + \big\langle (\phi^n)^3 - \phi^n + S(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n\big\rangle \\
&\geq \frac{\varepsilon^2}{2}\big(\|\nabla\phi^{n+1}\|^2 - \|\nabla\phi^n\|^2\big) + \frac{1}{4}\big(\|(\phi^{n+1})^2 - 1\|^2 - \|(\phi^n)^2 - 1\|^2\big) \\
&= E^{n+1} - E^n,
\end{aligned} \tag{2.12}$$

where the following inequality is used:

$$(b^3 - b)(a - b) + (a - b)^2 \geq \frac{1}{4}\left[(a^2-1)^2 - (b^2-1)^2\right], \quad \forall\, a, b \in [-1, 1].$$

This completes the proof of the lemma. □

We point out that when $\alpha = 1$ (2.9) indicates that the discrete energy E^n decays with respect to n. When $0 < \alpha < 1$, (2.9) will be useful in our later analysis for the fractional energy law and the weighted energy dissipation law.

Note that the first-order convex-splitting scheme for (1.1) can be written as

$$\bar{\partial}_{n+1}^{\alpha}\phi = \gamma\,\mathcal{G}\left(\delta_\phi E_{\mathrm{c}}(\phi^{n+1}) - \delta_\phi E_{\mathrm{e}}(\phi^n)\right), \tag{2.13}$$

where $\bar{\partial}_n^{\alpha}$ is given by (2.1a), E_{c} and E_{e} are two convex functionals with respect to ϕ such that $E(\phi) = E_{\mathrm{c}}(\phi) - E_{\mathrm{e}}(\phi)$. The first-order SAV scheme for (1.1) is given by (see, e.g. [35])

$$\bar{\partial}_{n+1}^{\alpha}\phi = \gamma\,\mathcal{G}\mu^{n+1}, \tag{2.14a}$$

$$\mu^{n+1} = \mathcal{L}\phi^{n+1} + \frac{r^{n+1}}{\sqrt{E_1(\phi^n) + C_0}}\delta_\phi E_1(\phi^n), \tag{2.14b}$$

$$r^{n+1} - r^n = \frac{1}{2\sqrt{E_1(\phi^n) + C_0}}\big\langle \delta_\phi E_1(\phi^n), \phi^{n+1} - \phi^n\big\rangle, \tag{2.14c}$$

where $C_0 > 0$ is some positive constant. It can be verified without difficulty that both schemes still satisfy (2.9), implying that the fractional and weighted energy laws in Sections 2.1 and 2.2 also hold.

Before studying the discrete energy laws, we first recall a special Cholesky decomposition result which provides a new way to determine positive definiteness of a symmetric positive matrix.

Lemma 2.2 (A Special Cholesky Decomposition, [27]). *Given an arbitrary symmetric matrix* $\mathbf{S}$ *of size* $N \times N$ *with positive elements, if* $\mathbf{S}$ *satisfies the following properties:*

(P1) $\forall\, 1 \le j < i \le N$, $\mathbf{S}_{i-1,j} \ge \mathbf{S}_{i,j}$,

(P2) $\forall\, 1 < j \le i \le N$, $\mathbf{S}_{i,j-1} < \mathbf{S}_{i,j}$,

(P3) $\forall\, 1 < j < i \le N$, $\mathbf{S}_{i-1,j-1} - \mathbf{S}_{i,j-1} \le \mathbf{S}_{i-1,j} - \mathbf{S}_{i,j}$,

then $\mathbf{S}$ *is a positive definite matrix. Moreover,* $\mathbf{S}$ *has a Cholesky decomposition* $\mathbf{S} = \mathbf{L}\mathbf{L}^{\mathrm{T}}$*, where* $\mathbf{L}$ *is a lower triangular matrix satisfying*

(Q1) $\forall\, 1 \le j \le i \le N$, $[\mathbf{L}]_{ij} > 0$,

(Q2) $\forall\, 1 \le j < i \le N$, $[\mathbf{L}]_{i-1,j} \ge [\mathbf{L}]_{i,j}$.

Note that the property (P1) indicates that the matrix $\mathbf{S}$ is column decreasing, while (P2) means that $\mathbf{S}$ is row increasing. The property (P3) is related to the second-order cross partial derivative from the continuous point of view, see [27] for more details.

2.1. Fractional energy law

We state and prove the first discrete energy law, called the fractional energy law, proposed by Du *et al.* [9]. Our proof is based on the following lemma.

Lemma 2.3. *For any function* u *defined on* $\Omega \times [0, T]$*, the following inequality holds:*

$$\sum_{k=1}^{n} b_{n-k} \langle \bar{\partial}_k^{\alpha} u, \bar{\partial}_k u \rangle \ge 0, \quad \forall\, n \ge 1. \tag{2.15}$$

Proof. It is sufficient to prove that

$$\mathbf{B} = \begin{bmatrix} b_{n-1} & & & & \\ & b_{n-2} & & & \\ & & \ddots & & \\ & & & b_1 & \\ & & & & b_0 \end{bmatrix} \begin{bmatrix} b_0 & & & & \\ b_1 & b_0 & & & \\ \vdots & \vdots & \ddots & & \\ b_{n-2} & b_{n-3} & \cdots & b_0 & \\ b_{n-1} & b_{n-2} & \cdots & b_1 & b_0 \end{bmatrix} \tag{2.16}$$

is positive definite, which is equivalent to prove that $\mathbf{B} + \mathbf{B}^{\mathrm{T}}$ is positive definite. To do this, we make a congruent transformation of $\mathbf{B} + \mathbf{B}^{\mathrm{T}}$ as follows:

$$\mathbf{S} = P(\mathbf{B} + \mathbf{B}^{\mathrm{T}})P^{\mathrm{T}}, \tag{2.17}$$

where P is an anti-diagonal matrix given by

$$P = \begin{bmatrix} & & & b_0^{-1} \\ & & b_1^{-1} & \\ & \iddots & & \\ b_{n-1}^{-1} & & & \end{bmatrix}. \tag{2.18}$$

It is easy to verify that $\mathbf{S}$ can be written explicitly as

$$\mathbf{S}_{ij} = \begin{cases} 2b_0 b_{i-1}^{-1}, & \text{if} \quad i = j, \\ b_{i-j} b_{i-1}^{-1}, & \text{if} \quad i > j, \\ b_{j-i} b_{j-1}^{-1}, & \text{if} \quad i < j. \end{cases} \tag{2.19}$$

With the above definition, it is not difficult to check that $\mathbf{S}$ satisfies (P1) and (P2) of Lemma 2.2. We now prove that $\mathbf{S}$ also satisfies (P3). In the case of $j = i-1$, it is trivial to see that the property (P3) indeed holds. In the general case of $1 < j < i-1, i \geq 4$, we need to show that

$$\mathbf{S}_{i-1,j-1} - \mathbf{S}_{i,j-1} \leq \mathbf{S}_{i-1,j} - \mathbf{S}_{i,j}, \tag{2.20}$$

that is equivalent to $f(j-1) \leq f(j)$, where

$$f(x) = \frac{(i-x)^{1-\alpha} - (i-x-1)^{1-\alpha}}{(i-1)^{1-\alpha} - (i-2)^{1-\alpha}} - \frac{(i-x+1)^{1-\alpha} - (i-x)^{1-\alpha}}{i^{1-\alpha} - (i-1)^{1-\alpha}}.$$

Note that $f(1) = 0$. Then $f'(x) \geq 0$ for $1 < x \leq i-1$ can ensure the desired inequality. Below we will verify the positivity of $f'(x)$. By direct computation we can that $f'(x) \geq 0$ is equivalent to, for $1 < x \leq i-1$,

$$\frac{1 - (i-x-1)^{\alpha}(i-x)^{-\alpha}}{(i-x-1)^{\alpha}\big((i-1)^{1-\alpha} - (i-2)^{1-\alpha}\big)} \geq \frac{1 - (i-x)^{\alpha}(i-x+1)^{-\alpha}}{(i-x)^{\alpha}\big(i^{1-\alpha} - (i-1)^{1-\alpha}\big)}. \tag{2.21}$$

It is not difficult to see the order of the numerators above

$$1 - (i-x-1)^{\alpha}(i-x)^{-\alpha} \geq 1 - (i-x)^{\alpha}(i-x+1)^{-\alpha}.$$

To prove (2.21), it is now sufficient to show that

$$(i-x-1)^{\alpha}\big((i-1)^{1-\alpha} - (i-2)^{1-\alpha}\big) \leq (i-x)^{\alpha}\big(i^{1-\alpha} - (i-1)^{1-\alpha}\big). \tag{2.22}$$

To show this, we consider the auxiliary function

$$p(y) = y^{\alpha}\big((y+1)^{1-\alpha} - y^{1-\alpha}\big) \quad \text{for} \quad y \in [0, \infty).$$

It is easy to verify that

$$\begin{aligned} p'(y) &= \alpha y^{-(1-\alpha)}(y+1)^{1-\alpha} + (1-\alpha) y^{\alpha}(y+1)^{-\alpha} - 1 \\ &= \alpha z^{1-\alpha} + (1-\alpha) z^{-\alpha} - 1 \geq 0, \end{aligned}$$

where $z = (y+1)/y > 1$. Therefore, we can obtain that $p(i-2) \leq p(i-1)$, i.e.

$$(i-2)^{\alpha}\big((i-1)^{1-\alpha} - (i-2)^{1-\alpha}\big) \leq (i-1)^{\alpha}\big(i^{1-\alpha} - (i-1)^{1-\alpha}\big), \quad i \geq 4. \tag{2.23}$$

By multiplying (2.23) with the following obvious inequality:

$$\Big(1-\frac{x-1}{i-2}\Big)^{\alpha} \le \Big(1-\frac{x-1}{i-1}\Big)^{\alpha},$$

we obtain (2.22) and then (2.21). Therefore, $f(x)$ is monotonically increasing.

In summary, **S** satisfies (P1)-(P3) in Lemma 2.2. We then claim that **S** is positive definite and consequently, **B** is positive definite. □

Theorem 2.1 (Fractional Energy Law). *For the stabilized L1 scheme* (2.5) *to the time-fractional phase-field equations, the following fractional energy law holds:*

$$\overline{\partial}_n^{\alpha} E = \sum_{k=1}^{n} b_{n-k}\overline{\partial}_k E \le 0, \quad \forall\, 1\le n\le N, \tag{2.24}$$

where the discrete fractional derivative $\overline{\partial}_n^{\alpha}$ *is given by* (2.1a), *but now acts on* E^n.

Proof. It follows from Lemma 2.1 and the definition of discrete fractional derivative that

$$\overline{\partial}_n^{\alpha} E \le \frac{1}{\gamma}\sum_{k=1}^{n} b_{n-k}\big\langle \mathcal{G}^{-1}\overline{\partial}_k^{\alpha}\phi, \overline{\partial}_k\phi\big\rangle = -\frac{1}{\gamma}\sum_{k=1}^{n} b_{n-k}\big\langle \overline{\partial}_k^{\alpha}\psi, \overline{\partial}_k\psi\big\rangle, \tag{2.25}$$

where for any $1\le k\le n$,

$$\overline{\partial}_k\psi^k = \begin{cases} \overline{\partial}_k\phi, & \text{Allen-Cahn or MBE model,}\\ \nabla(-\Delta)^{-1}\overline{\partial}_k\phi, & \text{Cahn-Hilliard model.}\end{cases} \tag{2.26}$$

According to Lemma 2.3, we then have $\overline{\partial}_n^{\alpha}E\le 0$. □

We point out that the energy boundedness obtained in [41] is a direct corollary of Theorem 2.1.

Corollary 2.1 (Energy Boundedness). *For the L1 scheme* (2.5) *of the time-fractional phase-field models, the discrete energy at* t_n *is bounded above by the initial energy*

$$E^n \le E^0, \quad \forall\, 1\le n\le N. \tag{2.27}$$

Proof. It follows from (2.24) in Theorem 2.1 that

$$E^n \le \frac{1}{b_0}\sum_{k=1}^{n-1}(b_{n-k-1}-b_{n-k})E^k + \frac{b_{n-1}}{b_0}E^0. \tag{2.28}$$

When $n=1$, this inequality gives $E^1\le E^0$. By induction on n, it is easy to see that $E^n\le E^0$ always holds. □

2.2. Weighted energy dissipation law

In [27], a weighted energy $E_\omega(t)$ is proposed for time-fractional phase-field equations in the form of

$$E_\omega(t) = \frac{1}{B(\alpha,1-\alpha)}\int_0^t \frac{E(s)}{s^{1-\alpha}(t-s)^{\alpha}}\,\mathrm{d}s, \tag{2.29}$$

where $B(\alpha, 1-\alpha)$ is the Beta function. It is proved that this weighted energy decays with time on the continuous level, i.e.

$$E'_\omega(t) \le 0. \tag{2.30}$$

Before stating the discrete weighted energy law, we provide a useful lemma.

Lemma 2.4. *For any function u defined on $\Omega \times [0,T]$, the following inequality holds:*

$$\sum_{k=1}^{n} t_k^\alpha \, b_{n-k} \langle \bar\partial_k^\alpha u, \bar\partial_k u \rangle \ge 0, \quad \forall\, n \ge 1. \tag{2.31}$$

Proof. It is sufficient to prove that

$$\mathbf{B} = \begin{bmatrix} 1^\alpha b_{n-1} & & & & \\ & 2^\alpha b_{n-2} & & & \\ & & \ddots & & \\ & & & (n-1)^\alpha b_1 & \\ & & & & n^\alpha b_0 \end{bmatrix} \begin{bmatrix} b_0 & & & & \\ b_1 & b_0 & & & \\ \vdots & \vdots & \ddots & & \\ b_{n-2} & b_{n-3} & \cdots & b_0 & \\ b_{n-1} & b_{n-2} & \cdots & b_1 & b_0 \end{bmatrix}$$

is positive definite. It is sufficient to show that the symmetric matrix $\mathbf{B} + \mathbf{B}^{\mathrm{T}}$ is positive definite. Similar to the proof of Lemma 2.3, we make the following congruent transformation: $\mathbf{S} = P(\mathbf{B} + \mathbf{B}^{\mathrm{T}})P^{\mathrm{T}}$, where the anti-diagonal matrix P is given by (2.18). Then, $\mathbf{S}$ can be written explicitly as

$$\mathbf{S}_{ij} = \begin{cases} 2(n-i+1)^\alpha b_0 b_{i-1}^{-1}, & \text{if} \quad i = j, \\ (n-j+1)^\alpha b_{i-j} b_{i-1}^{-1}, & \text{if} \quad i > j, \\ (n-i+1)^\alpha b_{j-i} b_{j-1}^{-1}, & \text{if} \quad i < j. \end{cases} \tag{2.32}$$

To prove the positive definiteness of $\mathbf{S}$, we need to show that $\mathbf{S}$ satisfies the three properties (P1)-(P3) in Lemma 2.2.

We first check (P1). In fact, it is sufficient to show that for any fixed j, the following inequality holds for all $i \ge j \ge 1$:

$$\begin{aligned} \frac{b_{i-j}}{b_{i-1}} &= \frac{(i-j+1)^{1-\alpha} - (i-j)^{1-\alpha}}{i^{1-\alpha} - (i-1)^{1-\alpha}} \\ \ge \frac{b_{i-j+1}}{b_i} &= \frac{(i-j+2)^{1-\alpha} - (i-j+1)^{1-\alpha}}{(i+1)^{1-\alpha} - i^{1-\alpha}}, \end{aligned}$$

which is equivalent to

$$\frac{(i+1)^{1-\alpha} - i^{1-\alpha}}{i^{1-\alpha} - (i-1)^{1-\alpha}} \ge \frac{(i-j+2)^{1-\alpha} - (i-j+1)^{1-\alpha}}{(i-j+1)^{1-\alpha} - (i-j)^{1-\alpha}}. \tag{2.33}$$

We consider the following function:

$$f(x) = \frac{(x+1)^{1-\alpha} - x^{1-\alpha}}{x^{1-\alpha} - (x-1)^{1-\alpha}}, \quad x \ge 1.$$

It is easy to verify that

$$f'(x) = \frac{(1-\alpha)\big(2x^\alpha - (x-1)^\alpha - (x+1)^\alpha\big)}{x^\alpha (x-1)^\alpha (x+1)^\alpha \big(x^{1-\alpha} - (x-1)^{1-\alpha}\big)^2} \ge 0.$$

Since $j \geq 1$, we can then claim that $f(i) \geq f(i-j+1)$. Hence (2.33) is true. Consequently, $\mathbf{S}$ satisfies the property (P1).

We then check (P2). We shall prove that for any fixed i, the following inequality holds for $1 \leq j < i \leq n$:

$$(n-j+1)^{\alpha} b_{i-j} \leq (n-j)^{\alpha} b_{i-j-1},$$

which is equivalent to

$$\begin{aligned} &(n-j+1)^{\alpha}\left((i-j+1)^{1-\alpha}-(i-j)^{1-\alpha}\right) \\ \leq\ &(n-j)^{\alpha}\left((i-j)^{1-\alpha}-(i-j-1)^{1-\alpha}\right). \end{aligned}$$

Consider the auxiliary function

$$g(x)=(n-x+1)^{\alpha}\left((i-x+1)^{1-\alpha}-(i-x)^{1-\alpha}\right), \quad 1 \leq x < i.$$

Below we show that $g'(x) \geq 0$. Straightforward computation gives

$$g'(x) = -\frac{(1-\alpha)n+\alpha i-x+1}{(n-x+1)^{1-\alpha}(i-x+1)^{\alpha}}+\frac{(1-\alpha)n+\alpha i-x+1-\alpha}{(n-x+1)^{1-\alpha}(i-x)^{\alpha}}.$$

For any $1 \leq x < i$, $g'(x) \geq 0$ is equivalent to

$$\left(\frac{i-x+1}{i-x}\right)^{\alpha} \geq \frac{(1-\alpha)n+\alpha i-x+1}{(1-\alpha)n+\alpha i-x+1-\alpha}. \tag{2.34}$$

Since $i \leq n$, the right-hand side of (2.34) satisfies for $1 \leq x < i$,

$$\frac{(1-\alpha)n+\alpha i-x+1}{(1-\alpha)n+\alpha i-x+1-\alpha} \leq \frac{i-x+1}{i-x+1-\alpha}.$$

In order to obtain (2.34), it is sufficient to show the following inequality:

$$\left(\frac{i-x+1}{i-x}\right)^{\alpha} \geq \frac{i-x+1}{i-x+1-\alpha},$$

that is,

$$i-x+1-\alpha \geq (i-x+1)\left(1-\frac{1}{i-x+1}\right)^{\alpha}. \tag{2.35}$$

It can be easily verify by using Taylor expansion that

$$\left(1-\frac{1}{i-x+1}\right)^{\alpha} \leq 1-\frac{\alpha}{i-x+1}, \tag{2.36}$$

which yields (2.35). Consequently, (2.34) is true. Therefore, $g'(x) \geq 0$ which verifies (P2).

Thirdly, we check (P3). In the case of $j = i-1$, it is trivial to show that the property (P3) holds according to (P1) and (P2). In the general case of $2 \leq j \leq i-2$ (hence, $4 \leq i \leq n$), we shall prove

$$\mathbf{S}_{i-1,j-1}-\mathbf{S}_{i,j-1} \leq \mathbf{S}_{i-1,j}-\mathbf{S}_{i,j}, \tag{2.37}$$

which is equivalent to $h(j-1) \leq h(j)$, where

$$h(x)=(n-x+1)^{\alpha}\left[\frac{(i-x)^{1-\alpha}-(i-x-1)^{1-\alpha}}{(i-1)^{1-\alpha}-(i-2)^{1-\alpha}}-\frac{(i-x+1)^{1-\alpha}-(i-x)^{1-\alpha}}{i^{1-\alpha}-(i-1)^{1-\alpha}}\right]$$

with $2 \leq x \leq i-2$. Similar to the proof of positivity of $f'(x)$ and $g'(x)$, we can prove that $h'(x) \geq 0$. Therefore, the property (P3) holds for $\mathbf{S}$.

In summary, $\mathbf{S}$ satisfies (P1)-(P3) in Lemma 2.2. Consequently, $\mathbf{S}$ is positive definite and therefore $\mathbf{B}$ is positive definite. □

Theorem 2.2 (Weighted Energy Dissipation). *For any $\alpha \in (0,1)$, the energy of the stabilized L1 scheme* (2.5) *for the time-fractional phase-field equations satisfies*

$$\widetilde{E}^n \leq \widetilde{E}^{n-1}, \quad \forall\, 1 \leq n \leq N, \tag{2.38}$$

where $\widetilde{E}^n$ denotes the following discrete weighted energy:

$$\widetilde{E}^n = E^0 + \Delta t \sum_{m=1}^{n} D^m, \quad D^m = \frac{1}{\Gamma(\alpha) t_m} \sum_{k=1}^{m} t_k^\alpha \, b_{m-k} \, \overline{\partial}_k E. \tag{2.39}$$

Proof. Note that D^n is an approximation to the derivative of weighted energy in (2.30). To derive (2.38), it is sufficient to prove $D^n \leq 0$ for all $1 \leq n \leq N$. According to (2.9), we have the following inequality:

$$\begin{aligned} \Gamma(\alpha) t_n D^n &= \sum_{k=1}^{n} t_k^\alpha b_{n-k} \overline{\partial}_k E \leq \frac{1}{\gamma} \sum_{k=1}^{n} t_k^\alpha b_{n-k} \big\langle \mathcal{G}^{-1} \overline{\partial}_k^\alpha \phi, \overline{\partial}_k \phi \big\rangle \\ &= -\frac{1}{\gamma} \sum_{k=1}^{n} t_k^\alpha b_{n-k} \big\langle \overline{\partial}_k^\alpha \psi, \overline{\partial}_k \psi \big\rangle, \end{aligned} \tag{2.40}$$

where ψ^k is given by (2.26). Combining Lemma 2.4 and (2.40), we conclude that $D^n \leq 0$. □

We point out that Corollary 2.1 can also be deduced from Theorem 2.2. Further, the weighted energy dissipation law is even stronger than the fractional energy law result. In fact, Theorems 2.1 and 2.2 state the following two inequalities respectively:

$$b_0(E^n - E^0) \leq \sum_{k=1}^{n-1} (b_{n-k-1} - b_{n-k})(E^k - E^0), \tag{2.41}$$

$$b_0 n^\alpha (E^n - E^0) \leq \sum_{k=1}^{n-1} \big[(k+1)^\alpha b_{n-k-1} - k^\alpha b_{n-k}\big](E^k - E^0). \tag{2.42}$$

We can show that (2.41) can be deduced from (2.42). This proof is technical and is omitted here.

3. $(2-\alpha)$-order L1-SAV Scheme

We have provided two discrete energy laws for the first-order stabilized L1 scheme, corresponding to the energy property of the governing equation introduced in [9, 27]. We will show in this section that Lemma 2.2 can also be used to analyze the energy stability of high order scheme, i.e. the energy boundedness and the fractional energy law of a $(2-\alpha)$-order L1-SAV scheme.

Inspired by the extended SAV scheme in [14], we consider a semi-discrete implicit scheme using the L1 approximation for the fractional derivative, the Crank-Nicolson discretization of the Laplace term, and the SAV technique [35] for the nonlinear term

$$\bar{\partial}^{\alpha}_{n+\frac{1}{2}}\phi = \gamma\mathcal{G}\mu^{n+\frac{1}{2}}, \tag{3.1a}$$

$$\mu^{n+\frac{1}{2}} = \mathcal{L}\phi^{n+\frac{1}{2}} + \frac{r^{n+\frac{1}{2}}}{\sqrt{E_1(\bar{\phi}^{n+\frac{1}{2}}) + C_0}}\delta_\phi E_1(\bar{\phi}^{n+\frac{1}{2}}), \tag{3.1b}$$

$$r^{n+1} - r^n = \frac{1}{2\sqrt{E_1(\bar{\phi}^{n+\frac{1}{2}}) + C_0}}\langle \delta_\phi E_1(\bar{\phi}^{n+\frac{1}{2}}), \phi^{n+1} - \phi^n \rangle \tag{3.1c}$$

with

$$\phi^{n+\frac{1}{2}} = \frac{1}{2}(\phi^{n+1} + \phi^n), \quad r^{n+\frac{1}{2}} = \frac{1}{2}(r^{n+1} + r^n), \quad \bar{\phi}^{n+\frac{1}{2}} = \frac{3}{2}\phi^n - \frac{1}{2}\phi^{n-1}.$$

The discrete fractional derivative operator $\bar{\partial}^{\alpha}_{n+1/2}$ is given by (see [14])

$$\bar{\partial}^{\alpha}_{n+\frac{1}{2}}\phi = \sum_{j=0}^{n} \tilde{b}_{n-j}\bar{\partial}_{j+1}\phi, \tag{3.2}$$

where $\tilde{b}_0 = \Delta t^{1-\alpha}2^{\alpha-1}/\Gamma(2-\alpha)$ and

$$\tilde{b}_j = \frac{\Delta t^{1-\alpha}}{\Gamma(2-\alpha)}\left[\left(j+\frac{1}{2}\right)^{1-\alpha} - \left(j-\frac{1}{2}\right)^{1-\alpha}\right], \quad j \geq 1.$$

It is shown in [14] that the order of truncation error of $\bar{\partial}^{\alpha}_{n+1/2}\phi$ to $\partial_t^{\alpha}\phi(t_{n+1/2})$ is $2-\alpha$. Hence, the scheme (3.1) is $(2-\alpha)$-order in time.

We now state two properties of the operator $\bar{\partial}^{\alpha}_{n+1/2}$, which ensures the energy boundedness and the fractional energy law.

Lemma 3.1. *For any function u defined on $\Omega \times [0,T]$, the following inequalities hold:*

$$\sum_{k=0}^{n} \langle \bar{\partial}^{\alpha}_{k+\frac{1}{2}}u, \bar{\partial}_{k+1}u \rangle \geq 0, \qquad \forall\, n \geq 0, \tag{3.3}$$

$$\sum_{k=0}^{n} \tilde{b}_{n-k}\langle \bar{\partial}^{\alpha}_{k+\frac{1}{2}}u, \bar{\partial}_{k+1}u \rangle \geq 0, \quad \forall\, n \geq 0. \tag{3.4}$$

Proof. We provide a brief schematic of the proof. Rewriting (3.3) into a quadratic form (omitting details here), it is sufficient to prove that

$$\mathbf{A} = \begin{bmatrix} \tilde{b}_0 & & & & \\ \tilde{b}_1 & \tilde{b}_0 & & & \\ \vdots & \vdots & \ddots & & \\ \tilde{b}_{n-1} & \tilde{b}_{n-2} & \cdots & \tilde{b}_0 & \\ \tilde{b}_n & \tilde{b}_{n-1} & \cdots & \tilde{b}_1 & \tilde{b}_0 \end{bmatrix} \tag{3.5}$$

is positive definite. Using the facts $2\tilde{b}_0 > \tilde{b}_1$ and $2\tilde{b}_0 + \tilde{b}_2 > 2\tilde{b}_1$, it is easy to verify that $\mathbf{A} + \mathbf{A}^{\mathrm{T}}$ satisfies the three conditions in Lemma 2.2 and is therefore positive definite. Thus, $\mathbf{A}$ is positive definite.

Similarly, to prove (3.4) it is sufficient to prove that

$$\mathbf{B} = \begin{bmatrix} \tilde{b}_n & & & & \\ & \tilde{b}_{n-1} & & & \\ & & \ddots & & \\ & & & \tilde{b}_1 & \\ & & & & \tilde{b}_0 \end{bmatrix} \begin{bmatrix} \tilde{b}_0 & & & & \\ \tilde{b}_1 & \tilde{b}_0 & & & \\ \vdots & \vdots & \ddots & & \\ \tilde{b}_{n-1} & \tilde{b}_{n-2} & \cdots & \tilde{b}_0 & \\ \tilde{b}_n & \tilde{b}_{n-1} & \cdots & \tilde{b}_1 & \tilde{b}_0 \end{bmatrix} \tag{3.6}$$

is positive definite. We consider the following congruent transformation of $\mathbf{B}+\mathbf{B}^{\mathrm{T}}$:

$$\mathbf{S} = P\left(\mathbf{B}+\mathbf{B}^{\mathrm{T}}\right)P^{\mathrm{T}}, \tag{3.7}$$

where P is an anti-diagonal matrix

$$P = \begin{bmatrix} & & & \tilde{b}_0^{-1} \\ & & \tilde{b}_1^{-1} & \\ & \iddots & & \\ \tilde{b}_n^{-1} & & & \end{bmatrix}. \tag{3.8}$$

Similar to the proof of Lemma 2.3, one can also verify that $\mathbf{S}$ satisfies the three conditions in Lemma 2.2 and is therefore positive definite. In particular, we used the facts that

$$2\tilde{b}_0\tilde{b}_2 \geq \tilde{b}_1^2, \quad \tilde{b}_{j-1}\tilde{b}_{j+1} \geq \tilde{b}_j^2 \quad \text{for} \quad j \geq 2,$$

which are useful in the verification. The details are omitted here. □

By taking the inner product of (3.1b) with $\Delta t\bar{\partial}_{n+1}\phi$ and multiplying (3.1c) with $2r^{n+1/2}$, we can obtain

$$\bar{\partial}_{n+1}E \leq \langle \mu^{n+\frac{1}{2}}, \bar{\partial}_{n+1}\phi \rangle, \tag{3.9}$$

where

$$E^n = \frac{1}{2}\langle \mathcal{L}\phi^n, \phi^n \rangle + (r^n)^2$$

is the modified energy. Combining (3.1a), (3.3), (3.4), and (3.9), we then derive the energy boundedness for the modified energy as stated below.

Theorem 3.1 (Energy Boundedness and Fractional Energy Law). *For the $(2-\alpha)$-order L1-SAV scheme* (3.1)*, the energy boundedness*

$$E^{n+1} \leq E^0, \quad \forall\, n \geq 0, \tag{3.10}$$

and the fractional energy law

$$\bar{\partial}^{\alpha}_{n+\frac{1}{2}}E = \sum_{k=0}^{n} \tilde{b}_{n-k}\bar{\partial}_{k+1}E \leq 0, \quad \forall\, n \geq 0, \tag{3.11}$$

hold true, where E^n is the modified energy.

We point out that in the case of $\tilde{b}_0 \geq \tilde{b}_1$, i.e. $\alpha \geq \ln_3(3/2) \approx 0.3691$, the fractional energy law (3.11) can lead directly to the energy boundedness (3.10) by induction.

4. L1 Schemes with Nonuniform Time Steps

We will demonstrate in this section that Lemma 2.2 can be extended to handle L1 schemes with nonuniform time steps. To this end, consider the general nonuniform time mesh in the form

$$\tau_j = t_j - t_{j-1}, \quad 1 \le j \le N, \tag{4.1}$$

where τ_j denotes the j-th time step. For the nonuniform time mesh (4.1), the corresponding L1 approximation to $\partial_t^\alpha \phi$ at t_n and $(t_{n+1}+t_n)/2$ becomes

$$D_n^\alpha \phi = \sum_{j=1}^{n} d_{n,j} D_j \phi, \quad D_{n+\frac{1}{2}}^\alpha \phi = \sum_{j=0}^{n} \bar{d}_{n,j} D_{j+1}\phi, \tag{4.2}$$

respectively, where

$$d_{n,j} = \frac{(t_n - t_{j-1})^{1-\alpha} - (t_n - t_j)^{1-\alpha}}{\Gamma(2-\alpha)\tau_j}, \tag{4.3a}$$

$$\bar{d}_{n,j} = \frac{\left(t_{n+1} + t_n - 2t_j\right)^{1-\alpha} - \left(t_{n+1} + t_n - 2t_{j+1}\right)^{1-\alpha}}{\Gamma(2-\alpha)2^{1-\alpha}\tau_{j+1}}, \tag{4.3b}$$

$$\bar{d}_{n,n} = \frac{\left(t_{n+1} - t_n\right)^{1-\alpha}}{\Gamma(2-\alpha)2^{1-\alpha}\tau_{n+1}}, \tag{4.3c}$$

and $D_j\phi := \phi^j - \phi^{j-1}$. Note that the notations $D_n^\alpha\phi, D_{n+1/2}^\alpha\phi, D_j\phi, d_{n,j}, \bar{d}_{n,j}$ correspond respectively to the previous notations $\overline{\partial}_n^\alpha \phi, \bar{\partial}_{n+1/2}^\alpha\phi, \overline{\partial}_j\phi, b_{n-j}, \tilde{b}_{n-j}$, but now for nonuniform time meshes.

Lemma 4.1. *For any function u defined on $[0,T]\times\Omega$, the following properties hold:*

$$\sum_{k=1}^{n} \left\langle D_k^\alpha u, D_k u\right\rangle \ge 0, \qquad \forall\, n \ge 1, \tag{4.4}$$

$$\sum_{k=0}^{n} \left\langle D_{k+\frac{1}{2}}^\alpha u, D_{k+1} u\right\rangle \ge 0, \quad \forall\, n \ge 0, \tag{4.5}$$

where D_k^α and $D_{k+1/2}^\alpha$ are given by (4.2) for nonuniform time steps.

Proof. To derive (4.4), we need to prove that

$$\mathbf{D} = \begin{bmatrix} d_{1,1} & & & & \\ d_{2,1} & d_{2,2} & & & \\ \vdots & \vdots & \ddots & & \\ d_{n-1,1} & d_{n-1,2} & \cdots & d_{n-1,n-1} & \\ d_{n,1} & d_{n,2} & \cdots & d_{n,n-1} & d_{n,n} \end{bmatrix} \tag{4.6}$$

is positive definite. Similarly, to derive (4.5) we need to show that

$$\widetilde{\mathbf{D}} = \begin{bmatrix} \bar{d}_{0,0} & & & & \\ \bar{d}_{1,0} & \bar{d}_{1,1} & & & \\ \vdots & \vdots & \ddots & & \\ \bar{d}_{n-1,0} & \bar{d}_{n-1,1} & \cdots & \bar{d}_{n-1,n-1} & \\ \bar{d}_{n,0} & \bar{d}_{n,1} & \cdots & \bar{d}_{n,n-1} & \bar{d}_{n,n} \end{bmatrix} \tag{4.7}$$

is positive definite. Without much difficulty, one can verify that $\mathbf{D}+\mathbf{D}^{\mathrm{T}}$ and $\widetilde{\mathbf{D}}+\widetilde{\mathbf{D}}^{\mathrm{T}}$ both satisfy the three conditions in Lemma 2.2 and are therefore positive definite. Here, we show details on the positive definiteness of $\mathbf{S}$

$$\begin{aligned}\mathbf{S}_{ij} &= \Gamma(2-\alpha)(\mathbf{D}+\mathbf{D}^{\mathrm{T}})_{ij}\\ &= \begin{cases} 2\tau_i^{-\alpha}, & \text{if} \quad i=j,\\ \tau_j^{-1}\left[(t_i-t_{j-1})^{1-\alpha}-(t_i-t_j)^{1-\alpha}\right], & \text{if} \quad i>j,\\ \mathbf{S}_{ji}, & \text{if} \quad i<j.\end{cases}\end{aligned} \tag{4.8}$$

We focus on the lower triangular part of $\mathbf{S}$, i.e. $i\geq j$. Firstly, it is easy to see that $\mathbf{S}_{ij}$ decreases with respect to i, i.e. the property (P1) in Lemma 2.2. Secondly, we have

$$\begin{aligned}\mathbf{S}_{ij} &= \tau_j^{-1}\left[(t_i-t_{j-1})^{1-\alpha}-(t_i-t_j)^{1-\alpha}\right]\\ &= \frac{1-\alpha}{t_j-t_{j-1}}\int_{t_{j-1}}^{t_j}(t_i-s)^{-\alpha}\,\mathrm{d}s\\ &= (1-\alpha)(t_i-\xi_j)^{-\alpha}, \quad \xi_j\in(t_{j-1},t_j), \quad 1\leq j\leq i-1,\end{aligned} \tag{4.9}$$

implying that $\mathbf{S}_{ij}$ increases with respect to $j\in[1,i-1]$. Due to the convexity of $(t_i-s)^{-\alpha}$, we know $\xi_j\in(t_{j-1},t_{j-1}+\tau_j/2)$. Moreover,

$$\mathbf{S}_{i,i-1}=(1-\alpha)(t_i-\xi_{i-1})^{-\alpha}<\mathbf{S}_{ii}=2\tau_i^{-\alpha}. \tag{4.10}$$

Therefore, the property (P2) in Lemma 2.2. Thirdly, from (4.9), we have

$$\begin{aligned}\mathbf{S}_{i-1,j}-\mathbf{S}_{i,j} &= \frac{1-\alpha}{t_j-t_{j-1}}\int_{t_{j-1}}^{t_j}\left[(t_{i-1}-s)^{-\alpha}-(t_i-s)^{-\alpha}\right]\,\mathrm{d}s\\ &= (1-\alpha)\left[(t_{i-1}-\eta_j)^{-\alpha}-(t_i-\eta_j)^{-\alpha}\right], \quad \eta_j\in(t_{j-1},t_j), \quad 1\leq j\leq i-2,\end{aligned} \tag{4.11}$$

implying that $\mathbf{S}_{i-1,j}-\mathbf{S}_{i,j}$ increases with respect to $j\in[1,i-2]$, due to the monotonicity of function $(t_{i-1}-\eta)^{-\alpha}-(t_i-\eta)^{-\alpha}$. Using the fact

$$\mathbf{S}_{i-1,i-1}=2\tau_{i-1}^{-\alpha}=\frac{2(1-\alpha)}{t_{i-1}-t_{i-2}}\int_{t_{i-2}}^{t_{i-1}}(t_{i-1}-s)^{-\alpha}\,\mathrm{d}s, \tag{4.12}$$

we then have

$$\begin{aligned}\mathbf{S}_{i-1,i-1}-\mathbf{S}_{i,i-1} &\geq \frac{1-\alpha}{t_{i-1}-t_{i-2}}\int_{t_{i-2}}^{t_{i-1}}\left[(t_{i-1}-s)^{-\alpha}-(t_i-s)^{-\alpha}\right]\,\mathrm{d}s\\ &= (1-\alpha)\left[(t_{i-1}-\eta_{i-1})^{-\alpha}-(t_i-\eta_{i-1})^{-\alpha}\right]\\ &\geq (1-\alpha)\left[(t_{i-1}-\eta_{i-2})^{-\alpha}-(t_i-\eta_{i-2})^{-\alpha}\right]\\ &= \mathbf{S}_{i-1,i-2}-\mathbf{S}_{i,i-2},\end{aligned} \tag{4.13}$$

where $\eta_{i-1}\in(t_{i-2},t_{i-1})$. Therefore, the property (P3) in Lemma 2.2 holds. In summary, $\mathbf{S}$ is positive definite and consequently, $\mathbf{D}$ is positive definite.

Similar proof can be done for $\widetilde{\mathbf{D}}$. We shall verify that $\widetilde{\mathbf{S}}=2^{1-\alpha}\Gamma(2-\alpha)(\widetilde{\mathbf{D}}+\widetilde{\mathbf{D}}^{\mathrm{T}})$ satisfies the three conditions in Lemma 2.2. The proof is almost the same as before, except the verification of

$$\widetilde{\mathbf{S}}_{j,j}-\widetilde{\mathbf{S}}_{j+1,j}\geq\widetilde{\mathbf{S}}_{j,j-1}-\widetilde{\mathbf{S}}_{j+1,j-1}, \quad \forall\, j\geq 2. \tag{4.14}$$

It can be verified that (4.14) is equivalent to

$$\begin{aligned} &2\tau_{j+1}^{-\alpha} - \tau_{j+1}^{-1}\left[(\tau_{j+2} + 2\tau_{j+1})^{1-\alpha} - \tau_{j+2}^{1-\alpha}\right] \\ \geq\; &\tau_j^{-1}\left[(\tau_{j+1} + 2\tau_j)^{1-\alpha} - \tau_{j+1}^{1-\alpha}\right] \\ &- \tau_j^{-1}\left[(\tau_{j+2} + 2\tau_{j+1} + 2\tau_j)^{1-\alpha} - (\tau_{j+2} + 2\tau_{j+1})^{1-\alpha}\right]. \end{aligned} \tag{4.15}$$

Let

$$\begin{aligned} Q(a,b) = &2a^{1-\alpha} - (b+2a)^{1-\alpha} + b^{1-\alpha} \\ &- a\left[(a+2)^{1-\alpha} - a^{1-\alpha} - (b+2a+2)^{1-\alpha} + (b+2a)^{1-\alpha}\right]. \end{aligned}$$

For any $a, b > 0$, straightforward computation gives

$$\partial_b Q(a,b) = (1-\alpha)(a+1)\left[\frac{1}{a+1}b^{-\alpha} + \frac{a}{a+1}(b+2a+2)^{-\alpha} - (b+2a)^{-\alpha}\right] \geq 0,$$

where the Jensen's inequality is used. Further, when $b = 0$, we have $Q(a,0) = a^{2-\alpha}p(1/a)$, where

$$p(x) = (1+2x) - (1+2x)^{1-\alpha} + 2^{1-\alpha}(1+x)^{1-\alpha} - 2^{1-\alpha}(1+x).$$

It is easy to find that $p(0) = 0$, $p'(0) \geq 0$, and $p''(x) \geq 0$, so that $p(x) \geq 0$. Since $Q(a,0) \geq 0$ and $\partial_b Q(a,b) \geq 0$, we have $Q(a,b) \geq 0$ for any $a, b > 0$. In particular, we have

$$\tau_{j+1}^{-1}\tau_j^{1-\alpha}Q\big(\tau_{j+1}\tau_j^{-1}, \tau_{j+2}\tau_j^{-1}\big) \geq 0.$$

It can be verified that the above inequality is equivalent to (4.15). This completes the proof of the lemma. □

With nonuniform time mesh, we rewrite the first-order stabilized L1 scheme (2.5) as

$$D_{n+1}^{\alpha}\phi = \gamma\,\mathcal{G}\big(\mathcal{L}\phi^{n+1} + \delta_\phi E_1(\phi^n) + \widetilde{\mathcal{L}}(\phi^{n+1} - \phi^n)\big), \tag{4.16}$$

and the $(2-\alpha)$-order L1-SAV scheme (3.1) as

$$D_{n+\frac{1}{2}}^{\alpha}\phi = \gamma\mathcal{G}\mu^{n+\frac{1}{2}}, \tag{4.17a}$$

$$\mu^{n+\frac{1}{2}} = \mathcal{L}\phi^{n+\frac{1}{2}} + \frac{r^{n+\frac{1}{2}}}{\sqrt{E_1\big(\tilde{\phi}^{n+\frac{1}{2}}\big) + C_0}}\delta_\phi E_1\big(\tilde{\phi}^{n+\frac{1}{2}}\big), \tag{4.17b}$$

$$r^{n+1} - r^n = \frac{1}{2\sqrt{E_1\big(\tilde{\phi}^{n+\frac{1}{2}}\big) + C_0}}\big\langle \delta_\phi E_1\big(\tilde{\phi}^{n+\frac{1}{2}}\big), \phi^{n+1} - \phi^n\big\rangle, \tag{4.17c}$$

where $\mathcal{L}, \widetilde{\mathcal{L}}, E_1$, and C_0 are the same as before, while

$$\tilde{\phi}^{n+\frac{1}{2}} = \phi^n + \frac{\tau_{n+1}}{2\tau_n}(\phi^n - \phi^{n-1}).$$

Using Lemma 4.1 we can derive the energy bound preserving property of the L1 schemes (4.16) and (4.17) with nonuniform time meshes. The details will be omitted here.

Theorem 4.1 (Energy Boundedness). *The energy boundedness holds for the L1 schemes* (4.16) *and* (4.17) *with arbitrary nonuniform time mesh*

$$E^n \leq E^0, \quad \forall\, n \geq 1, \tag{4.18}$$

where E^n denotes the classical discrete energy for (4.16) *and the modified SAV energy for* (4.17).

Remark 4.1. The energy stability of $L2$ schemes for time-fractional phase-field equations have been studied recently in [22,28,29]. Furthermore, a series of works on global-in-time H^1 stability of standard and fast L2 schemes on general nonuniform time meshes for subdiffusion equations have been done in [30–32].

5. Numerical Tests

In this section, we test the proposed schemes for time-fractional phase-field equations to verify our energy stability results. In particular, we test the first order stabilized L1 scheme (2.5) for the time-fractional AC and CH models, and then the $(2-\alpha)$-order L1-SAV scheme (3.1) for the time-fractional MBE model with slope selection. The implementations of these schemes are linearly implicit without using nonlinear iterations.

5.1. Time-fractional Allen-Cahn model

We first test the stabilized L1 scheme (2.5) for the time fractional AC model defined in a two-dimensional domain $\Omega = [0, L_x] \times [0, L_y]$ with periodic boundary conditions. We take $L_x = L_y = 2, \varepsilon = 0.1$, and $\gamma = 1$ in (1.1). The stabilization constant S in scheme (2.5) is set to be $S = 2$ and the time step is set to be $\Delta t = 0.01$. The peuso-spectral method with 128×128 Fourier modes is used for space discretization. The initial phase-field state is taken as

$$\phi_0(x) = \tanh\left[\frac{1}{2\varepsilon}\left(\frac{2r}{3} - \frac{1}{4} - \frac{1+\cos(6\theta)}{16}\right)\right] \tag{5.1}$$

with the polar coordinates $r = \sqrt{x^2+y^2}$ and $\theta = \arctan(y/x)$.

Fig. 5.1 illustrates the solution ϕ to the time-fractional AC equation with different orders of derivative $\alpha = 1, 0.8, 0.5, 0.3$. On the left-hand side of Fig. 5.2, one can see that the energy decreases with respect to time. In the middle of Fig. 5.2, it can be observed that the fractional derivative of energy is always nonpositive for different values of α, which is in good agreement with the discrete fractional energy law in Theorem 2.1. On the right-hand side of Fig. 5.2, we plot the derivative of weighted energy with respect to time, which is found to be nonpositive as stated in Theorem 2.2.

5.2. Time-fractional Cahn-Hilliard model

For the time-fractional CH model defined on $[0, L_x] \times [0, L_y]$, we again solve the governing equation using the stabilization scheme (2.5). The following parameters are used: $L_x = L_y = 2$, $\varepsilon = 0.1, \gamma = 0.1, L = 8, S = 4$, and $\Delta t = 0.01$. Still, 128×128 Fourier modes are used in the peuso-spectral method. The initial phase-field state ϕ_0 is taken as the uniformly distributed random field in $[-1, 1]$.

Fig. 5.3 illustrates the phase-field function ϕ with $\alpha = 1, 0.8, 0.5, 0.3$. We observed an interesting phenomena that the steady state with $\alpha = 0.5$ and 0.3 is very different with that of $\alpha = 1$ and 0.8. In addition, it is observed from the left-hand side of Fig. 5.4 the energy decreases with respect to time although its theoretical justification is still unavailable. Furthermore, in the middle of Fig. 5.4, it can be observed that the fractional derivative of energy is always nonpositive as stated in Theorem 2.1. On the right-hand side of Fig. 5.4, the derivative of weighted energy is nonpositive as stated in Theorem 2.2.

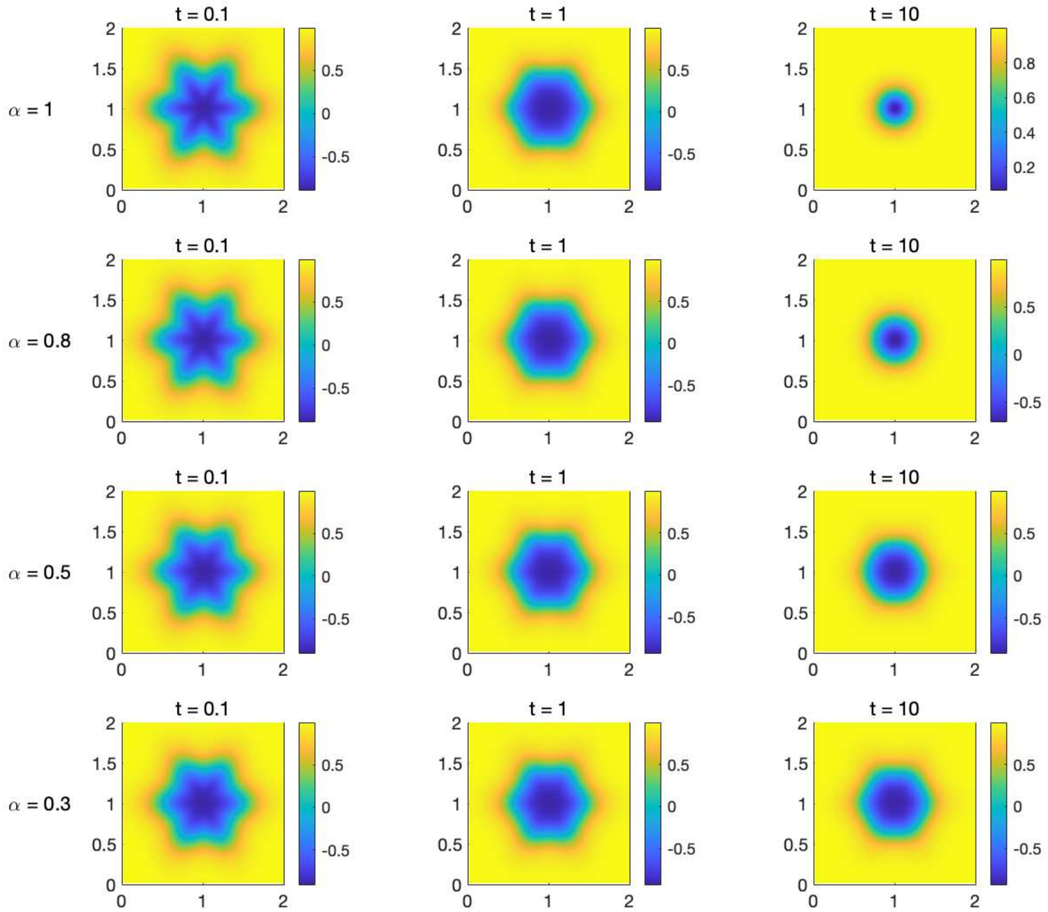

Fig. 5.1. Snapshots of the time-fractional Allen-Cahn solution with $\alpha = 1, 0.8, 0.5, 0.3$.

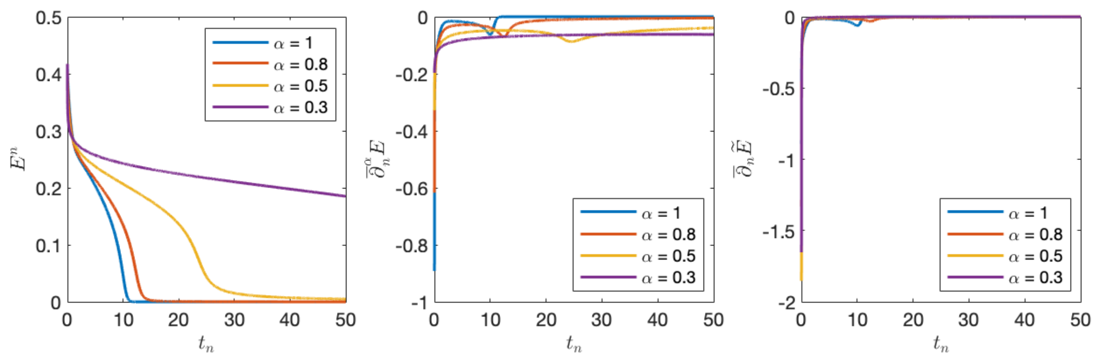

Fig. 5.2. Energy (left), time-fractional derivative of energy (middle), and time derivative of weighted energy (right) with respect to time, for the time-fractional Allen-Cahn model with $\alpha = 1, 0.8, 0.5, 0.3$.

5.3. Time-fractional MBE model with slope selection

We test the $(2-\alpha)$-order L1-SAV schemes (3.1) and (4.17) for solving the time-fractional MBE equation (1.3) with slope selection defined in the domain $[0, 2\pi] \times [0, 2\pi]$. The following

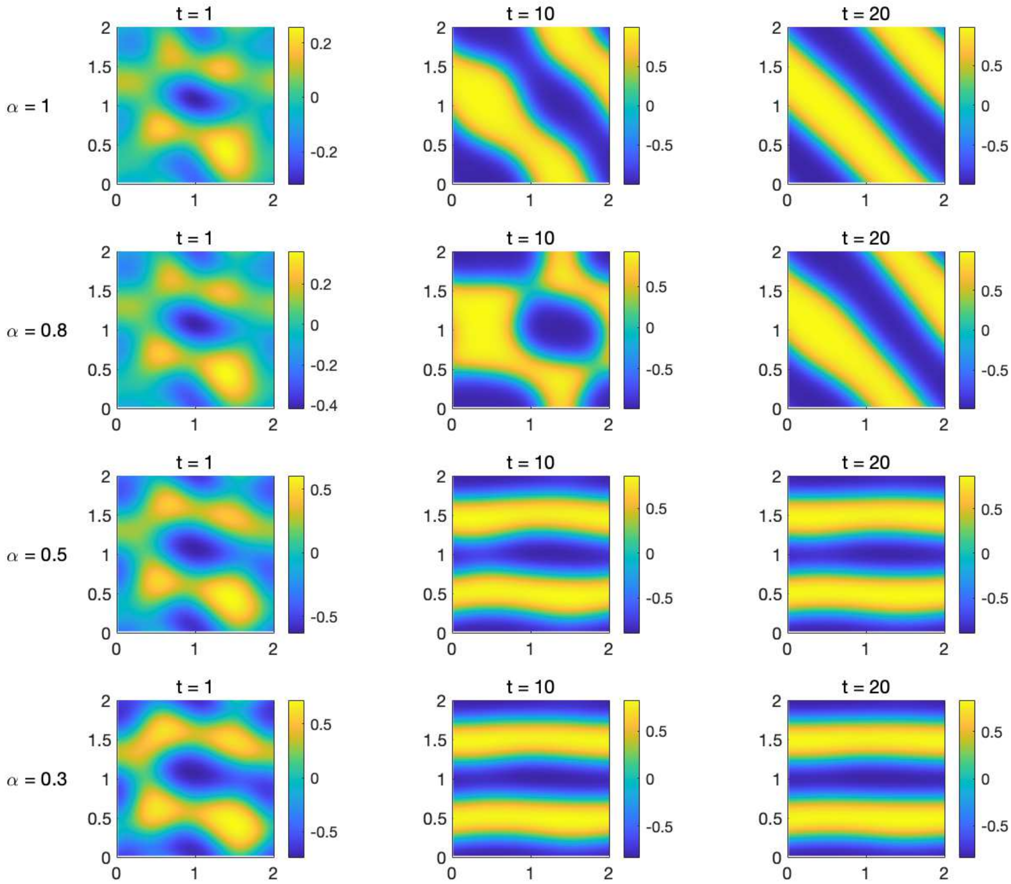

Fig. 5.3. Snapshots of the time-fractional Cahn-Hilliard solution with $\alpha = 1, 0.8, 0.5, 0.3$.

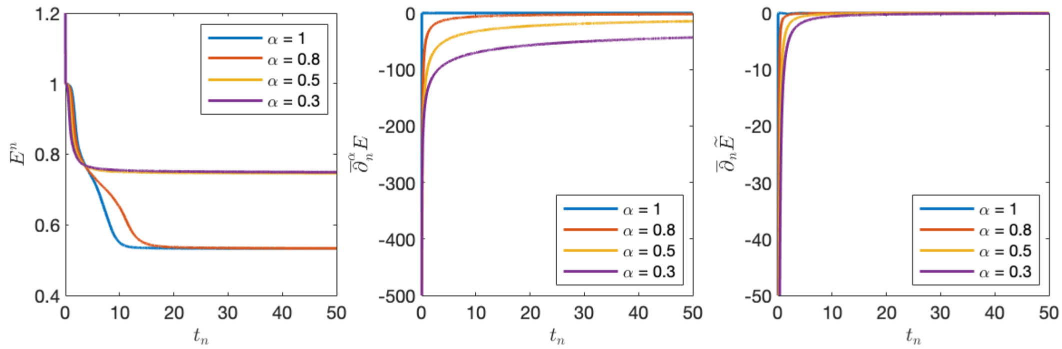

Fig. 5.4. Energy (left), time-fractional derivative of energy (middle), and time derivative of weighted energy (right) with respect to time t, for the time-fractional Cahn-Hilliard equation with $\alpha = 1, 0.8, 0.5, 0.3$.

parameters are used: $\varepsilon^2 = 0.1, \gamma = 1$, and $C_0 = 1$. For the peuso-spectral method, 128×128 Fourier modes are used. The initial phase-field state ϕ_0 is taken to be

$$\phi_0(x, y) = 0.1 \left[\sin(3x)\sin(2y) + \sin(5x)\sin(5y)\right], \quad (x, y) \in [0, 2\pi]^2. \tag{5.2}$$

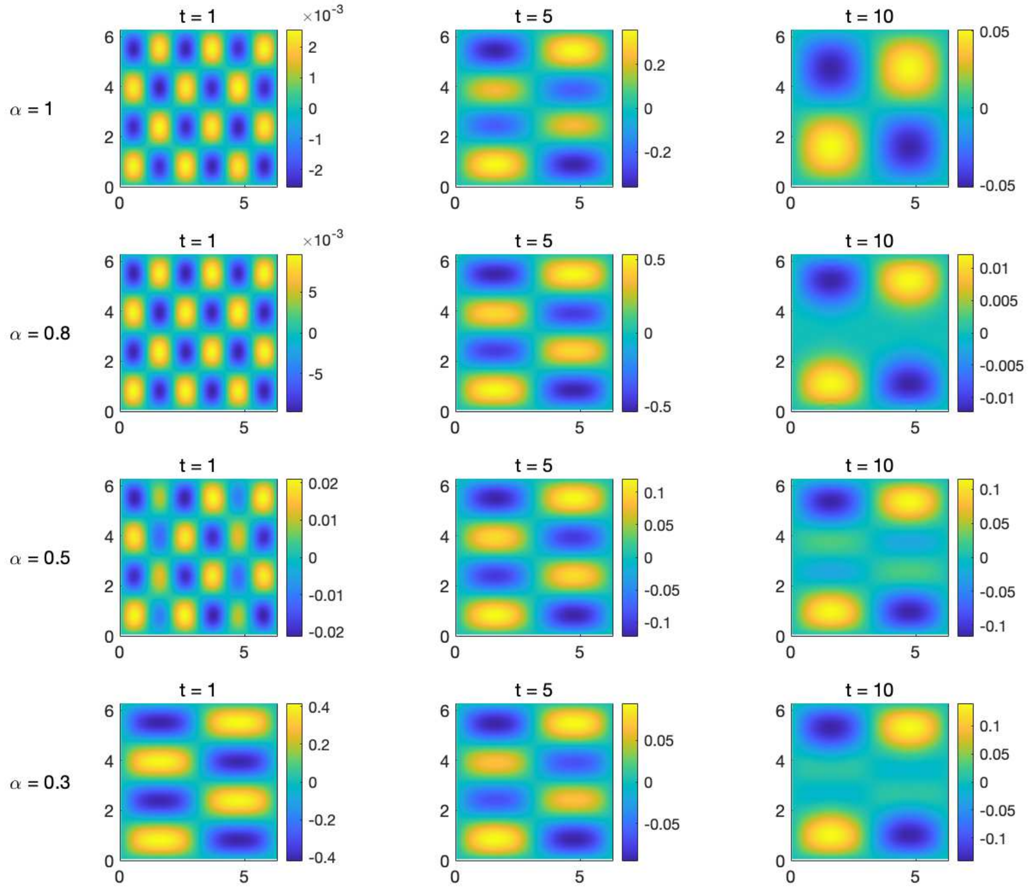

Fig. 5.5. Snapshots of the solution to the time-fractional MBE equation with slope selection with $\alpha = 1, 0.8, 0.5, 0.3$.

First, we test the scheme (3.1) with uniform time step $\Delta t = 0.01$. Fig. 5.5 illustrates the phase solution ϕ to the time-fractional MBE equation with $\alpha = 1, 0.8, 0.5$ and 0.3. It can be observed that when α becomes smaller, the phase changes faster at the beginning but later changes quite slowly. On the left-hand side of Fig. 5.6, the modified energy decreases with respect to time in the case of $\alpha = 1, 0.8$ and 0.5. However, the energy dissipation is violated at $t_n \approx 1.44$ in the case of $\alpha = 0.3$, as observed in [13]. The violation occurs for small α, which requires much smaller mesh sized to obtain satisfactory resolution. Even in this case it is observed that the energy stability (boundedness) is preserved. In the middle of Fig. 5.6, the fractional energy law in Theorem 3.1 is verified. On the right-hand side of the figure, it is found that the derivative of weighted (modified) energy is nonpositive.

Next, we test the scheme (4.17) with graded time mesh (see, e.g. [38])

$$t_j = (j/N)^r \, T, \quad j = 0, 1, \ldots, N, \tag{5.3}$$

where $r \geq 1$ is some constant and N is the total number of time steps. In our test, we set $r = 1.2$ and $T = 10$. Fig. 5.7 illustrate the modified energy for $N = 100, 500$ and 1000 respectively, which corresponds roughly to $\Delta t \approx 0.1, 0.02, 0.01$ away from $t = 0$. It is observed that the computed energy is bounded above by the initial energy, as stated in Theorem 4.1. One can

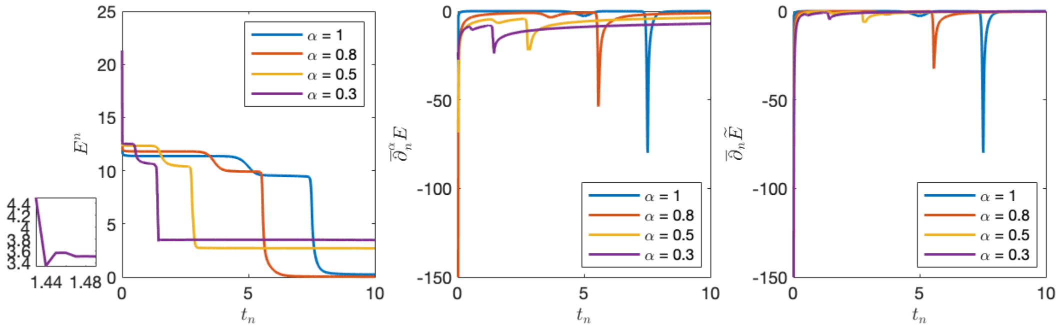

Fig. 5.6. Energy (left), time-fractional derivative of energy (middle), and time derivative of weighted energy (right) with respect to time t, for the time-fractional MBE equation with slope selection with $\alpha = 1, 0.8, 0.5, 0.3$. Here, in the middle and the right-hand side figures, the y-axis is cut for a better illustration.

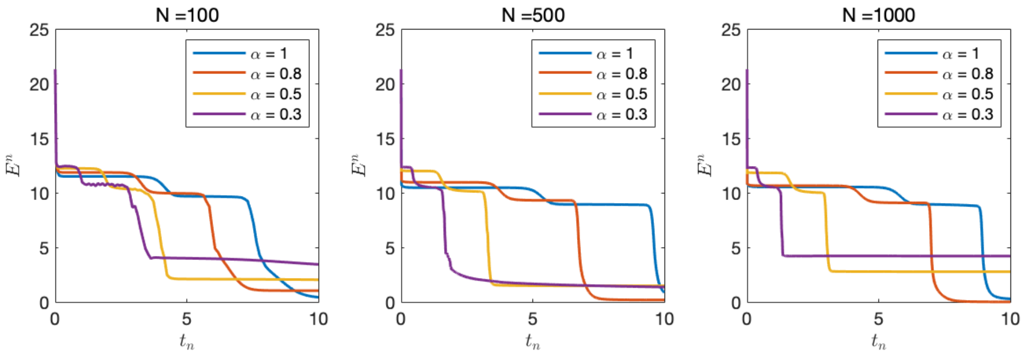

Fig. 5.7. Discrete energy of the L1-SAV scheme on graded time meshes for the time-fractional MBE equation with slope selection, where the number of steps and the fractional order are set to $N = 100, 500, 1000$ and $\alpha = 1, 0.8, 0.5, 0.3$ respectively.

find that in the case of $N = 100$ and $\alpha = 0.3$, the computed energy oscillates despite that the stability can be ensured. We also mention that when $\alpha = 0.3$ and the computed energy at $T = 10$ varies with different values of N.

6. Conclusion

In this work, we applied a special Cholesky decomposition technique to analyze the energy stability of the first-order L1 approximation for time-fractional phase-field equations. From a numerical point view, the essential step to study the fractional PDE is to approximate the time-fractional derivative operator. We use a classical scheme called L1 approximation, which is naturally derived from the approximation of the fractional integral appropriately. In particular, we investigated the discrete versions of the fractional energy law of Du *et al.* [9] and the weighted energy lay of [27], and obtained the dissipation of the fractional/weighted energy associated with numerical schemes. A higher order numerical scheme, i.e. a $(2-\alpha)$-order L1-SAV scheme, is also investigated, while the relevant energy boundedness and the fractional energy law are established. Moreover, we prove that the L1 schemes with nonuniform time steps still preserve the energy boundness.

We point out that the Cholesky decomposition technique is useful for the numerical schemes for time-fractional problems. It is expected that the framework developed in this work can also be employed to study second-order schemes for time-fractional phase-field equations. In fact, there have been extensive works of second-order accurate energy stable numerical schemes for the Cahn-Hilliard and MBE equation, using the convex splitting approach, in the standard temporal derivative case. Both the Crank-Nicolson and the modified BDF2 approaches, with the standard finite difference, mixed finite element and Fourier pseudo-spectral spatial approximations have been reported, see, e.g. [7,25,33]. It is certainly of some theoretical and numerical interests to extend these results to the time-fractional equations. The corresponding analysis for the stability issues seems a challenging issue.

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