Numerical Energy Dissipation for Time-Fractional Phase-Field Equations

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Abstract

The energy dissipation is an important and essential property of classical phase-field equations. However, it is still unknown if the phase-field models with Caputo time-fractional derivative preserve this property, which is challenging due to the existence of both nonlocality and nonlinearity. Our recent work shows that on the continuous level, the time-fractional energy dissipation law and the weighted energy dissipation law can be achieved. Inspired by them, we study in this article the energy dissipation of some numerical schemes for time-fractional phase-field models, including the convex-splitting scheme, the stabilization scheme, and the scalar auxiliary variable scheme. Based on a lemma about a special Cholesky decomposition, it can be proved that the discrete fractional derivative of energy is nonpositive, i.e., the discrete time-fractional energy dissipation law, and that a discrete weighted energy can be constructed to be dissipative, i.e., the discrete weighted energy dissipation law. In addition, some numerical tests are provided to verify our theoretical analysis.

Keywords. time-fractional phased-field equation, Allen–Cahn equations, Cahn–Hilliard equations, Caputo fractional derivative, energy dissipation

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1 Introduction

In recent years, to model memory effects and subdiffusive regimes, there has been an increasing interest in time-fractional differential equations, where the classical time derivative is replaced by a fractional one, typically a Caputo or a Riemann-Liouville derivative. In practice, the Caputo derivative seems more widely used due to its more convenient form. For example, Allen, Caffarelli, and Vasseur \cite{2} studied the regularity of a parabolic problem with a Caputo time-derivative. Luchko
and Yamamoto discussed the maximum principle for a class of time-fractional diffusion equation with the Caputo time-derivative in [2]. Li et al. investigated in [3] some important properties of the solutions, including the nonnegativity preservation, mass conservation and blowup behaviors, for nonlinear time-fractional Keller–Segel equation with the Caputo time-derivative. In [4], Giga and Namba investigated the well-posedness of Hamilton–Jacobi equations with a Caputo derivative, with a main purpose of finding a proper notion of viscosity solutions so that the underlying Hamilton–Jacobi equation is well-posed. A further study along this line is recently provided by Camilli and Goffi [5]. Their study relies on a combination of a gradient bound for the time-fractional Hamilton–Jacobi equation obtained via nonlinear adjoint method and sharp estimates in Sobolev and Hölder spaces for the corresponding linear problem. There are also some numerical works for nonlinear time-fractional problems with real applications, including the time-fractional Schrödinger equations [6], the time-fractional plasma turbulence models [7, 8], the time-fractional porous medium models [9, 10], and the time-fractional ground water equation [11]. Generally speaking, the historic memory described by the time-fractional derivative can play a significant role, although the whole evolution process may be slower due to the memory effect. For governing equations with time-fractional fractional derivative, it is usually expected that the main regularity properties, nonlinear stability and other main features could be preserved.

In this work, we are concerned with the time-fractional phase-field equations. It is well-known that the phase-field models were originally derived for the microstructure evolution and phase transition, but now have been widely-used in many areas, such as material sciences, multiphase flows, biology, and image processing, etc. We aim to study the energy property of numerical schemes for phase-field models with Caputo time-derivative, inspired by our recent theoretical results in [13]. In general, the time-fractional phase-field equation can be written in the form of

$$\partial^\alpha_t \phi = \gamma \mathcal{G} \mu,$$

(1.1)

where \(\alpha \in (0, 1)\), \(\gamma > 0\) is the mobility constant, \(\mathcal{G}\) is a nonpositive operator depending on the phase-field model, and \(\partial^\alpha_t\) is the Caputo fractional derivative [14] defined by

$$\partial^\alpha_t \phi(t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\phi'(s)}{(t-s)^\alpha} \, ds, \quad t \in (0, T)$$

(1.2)

with \(\Gamma(\cdot)\) the gamma function. Taking different functional \(\mu\), one can obtain different phase-field models, for example, the Allen–Cahn (AC) model [15], the Cahn–Hilliard (CH) model [16], and the molecular beam epitaxy (MBE) model [17]. More specifically, in the AC model [15] and the CH model [16], \(\mu\) is taken to be

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

(1.3)

where \(\varepsilon > 0\) is the interface width parameter and \(F\) is a double-well potential functional. We take the common choice \(F(\phi) = \frac{1}{4} (1 - \phi^2)^2\) in this article so that \(F'(\phi) = \phi^3 - \phi\). When \(\mathcal{G} = -1\), (1.1) is the AC equation, while when \(\mathcal{G} = \Delta\), (1.1) is the CH equation. The MBE model has two forms, with or without slope selection [17, 10], where \(\mathcal{G} = -1\) and \(\mu\) is taken to be

$$\mu = \varepsilon^2 \Delta^2 \phi + \nabla \cdot f_m(\nabla \phi)$$

(1.4)

with

$$f_m(\nabla \phi) = \begin{cases} \nabla \phi - |\nabla \phi|^2 \nabla \phi & \text{with slope selection}, \\ \frac{\nabla \phi}{1 + |\nabla \phi|^2} & \text{without slope selection}. \end{cases}$$

(1.5)
For the sake of simplicity, we consider the periodic boundary condition for the time-fractional phase-field equation (1.1). It is known that when $\alpha = 1$, i.e., the classical case, the Allen–Cahn, Cahn–Hilliard, and MBE models are gradient flows. So the energy associated with these models decay with time, which is the so-called energy dissipation law. This dissipation law has been used extensively as a nonlinear numerical stability criteria. However, it is still unknown if such energy dissipation property holds in the general case of $0 < \alpha < 1$.

In a recent work [10], the authors demonstrated that the classical energy of (1.1) is bounded above by the initial energy, i.e., $E(t) \leq E(0)$ for all $t > 0$, which is the first work on the energy stability of time-fractional phase-field equations. Later, we showed in [13] that the time-fractional derivative of energy is nonpositive, i.e., the time-fractional energy law,

$$\partial_t^\alpha E(t) \leq 0, \quad \forall \ 0 < t < T,$$

and that the weighted energy can be constructed to decay with respect to time, i.e., the weighted energy dissipation law,

$$\partial_t E_\omega(t) \leq 0, \quad \forall \ 0 < t < T,$$

where $E_\omega(t) = \int_0^1 \omega(\theta) E(\theta t) \, d\theta$ under the constraint that $\omega(\theta) \theta^{1-\alpha}(1-\theta)^\alpha$ is nonincreasing with respect to $\theta$. It is natural to ask if the above energy analysis also holds on the discrete level for the numerical schemes for time-fractional phase-field equations. We address this issue in this article. To be precise, we will state and prove two discrete energy results for the L1 schemes for time-fractional phase-field equations, including the convex-splitting scheme [18, 19], the stabilization scheme [20, 21], and the scalar auxiliary variable (SAV) scheme [22, 23]. We will show the discrete time-fractional energy law

$$\bar{\partial}_t^\alpha E^n \leq 0, \quad \forall \ 1 \leq n \leq N,$$

and the discrete weighted energy dissipation law

$$\bar{\tilde{E}}^n \leq \bar{\tilde{E}}^{n-1}, \quad \forall \ 1 \leq n \leq N,$$

where $\bar{\partial}_t^\alpha$ is the discrete fractional derivative, $E^n$ is the discrete classical energy, and $\bar{\tilde{E}}^n$ is a newly-defined discrete weighted energy, see Section 3 for details. It should be mentioned that on the discrete level, the weighted energy dissipation law is even stronger than the time-fractional energy law, both of which are stronger than the energy boundedness result in [10]. The proofs are based on a special Cholesky decomposition proposed recently by us in [13], which provides a sufficient condition for judging the positive definiteness of a symmetric positive matrix.

The paper is organized as follows. Section 2 provides three temporal discretizations, namely the L1 approximation of the time-fractional operator combing with convex splitting technique, semi-implicit stabilization technique, and SAV technique respectively. In Section 3 we state and prove two main theorems on the discrete energy, i.e., the time-fractional energy law and the weighted energy dissipation law. Then, in Section 4 we give some numerical results to verify our theoretical analysis. Some concluding remarks are given in the final section.

### 2 Temporal discretizations

We consider the discretization of the time fractional derivative on the left-hand side of (1.1). Let $\Delta t = \frac{T}{N}$ be the time step size and $t_n = n\Delta t$, $0 \leq n \leq N$. The L1 approximation of Caputo
time-fractional derivative (see [24, 25, 10]) is given by:
\[ \partial_t^\alpha \phi^{n+1} := \sum_{j=0}^{n} b_j \left( \phi^{n+1-j} - \phi^{n-j} \right) \Delta t, \quad 0 \leq n \leq N - 1, \] (2.1)

where \( \partial_t^\alpha \) is the discrete fractional derivative and
\[ b_j = \frac{\Delta t^{1-\alpha}}{\Gamma(2-\alpha)} \left[ (j+1)^{1-\alpha} - j^{1-\alpha} \right], \quad j \geq 0. \] (2.2)

One can refer to [24] or [10, Section 3] for the derivation of the above L1 approximation. A useful reformulation of (2.1) is
\[ \partial_t^\alpha \phi^{n+1} = \frac{1}{\Delta t} \left[ b_0 \phi^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1}) \phi^{n-j} - b_n \phi^0 \right], \quad 0 \leq n \leq N - 1, \] (2.3)

where the following relationship holds:
\[ b_j - b_{j+1} > 0, \quad b_n > 0, \quad \sum_{j=0}^{n-1} (b_j - b_{j+1}) + b_n = b_0. \] (2.4)

Before discretizing the right-hand side of (1.1), we recall the energy formulas of phase-field equations, their derivatives, and splittings, that will be helpful to state the numerical schemes. The classical energy functional of the time-fractional Allen–Cahn or Cahn–Hilliard equation (1.3) is
\[ E(\phi) = \int_{\Omega} \left( \frac{\varepsilon^2}{2} |\nabla \phi|^2 + F(\phi) \right) \, dx. \] (2.5)

Straightforward computation of its derivative with respect to time gives
\[ \frac{d}{dt} E(\phi) = \int_{\Omega} \partial_t \phi \left( -\varepsilon^2 \Delta \phi + F'(\phi) \right) \, dx = \frac{1}{\gamma} \int_{\Omega} \partial_t \phi \left( \mathcal{G}^{-1} \partial_t^\alpha \phi \right) \, dx, \] (2.6)

where \( \mathcal{G}^{-1} \) is the inverse of \( \mathcal{G} \). Further, the classical energy functional of the time-fractional MBE equation (1.4) is given by
\[ E_m(\phi) = \int_{\Omega} \left( \frac{\varepsilon^2}{2} |\Delta \phi|^2 + F_m(\nabla \phi) \right) \, dx \] (2.7)

with
\[ F_m(\nabla \phi) = \begin{cases} \frac{1}{4} \left( 1 - |\nabla \phi|^2 \right)^2 & \text{with slope selection,} \\ -\frac{1}{2} \log \left( 1 + |\nabla \phi|^2 \right) & \text{without slope selection,} \end{cases} \] (2.8)

which also yields that
\[ \frac{d}{dt} E_m(\phi) = \frac{1}{\gamma} \int_{\Omega} \partial_t \phi \left( \mathcal{G}^{-1} \partial_t^\alpha \phi \right) \, dx. \] (2.9)
In the following content, we use a consistent notation $E$ to represent $E$ in (2.5) or $E_m$ in (2.7). We mention that the free energy $E$ satisfies $\mu = \delta \phi E$. Usually, one can decompose the energy by two ways: the quadratic-nonquadratic splitting

$$E(\phi) = \frac{1}{2} \langle \phi, L \phi \rangle_\Omega + E_1(\phi),$$  

(2.10)

where $L$ is a symmetric nonnegative linear operator (for example, $L = -\varepsilon^2 \Delta$ for the AC/CH model and $L = \varepsilon^2 \Delta^2$ for the MBE model) and $E_1$ is the remaining nonquadratic term s.t. $\delta \phi E_1 = F$ or $F_m$, and the convex splitting

$$E(\phi) = E_c(\phi) - E_e(\phi),$$  

(2.11)

where $E_c$ and $E_e$ are two convex functionals with respect to $\phi$.

There are different methods for discretizing the right-hand side of (1.1), for example, the convex-splitting technique [18, 19], the stabilization technique [20, 21], and the scalar auxiliary variable (SAV) technique [22, 23], etc. For the sake of completeness, we show the corresponding L1 schemes as follows:

(1) The convex-splitting scheme for (1.1) is written as

$$\overline{\partial}_t^\alpha \phi^{n+1} = \gamma G \left( \delta \phi E_c(\phi^{n+1}) - \delta \phi E_e(\phi^n) \right),$$  

(2.12)

where $\overline{\partial}_t$ is given by (2.1), $E_c$ and $E_e$ are given by (2.11).

(2) The stabilization scheme for (1.1) is written as

$$\overline{\partial}_t^\alpha \phi^{n+1} = \gamma G \left( L \phi^{n+1} + \delta \phi E_1(\phi^n) + \bar{L} \left( \phi^{n+1} - \phi^n \right) \right),$$  

(2.13)

where $\bar{L}$ is some linear operator. Specifically speaking, for the AC model, one can choose $\bar{L}$ as a positive constant $S \geq 2$, see [26]. For the CH model, one can truncate the functional $\delta \phi E_1$ s.t. $\max \left| (\delta \phi E_1)'' \right| \leq L$ and then choose $\bar{L}$ to be a positive constant $S \geq \frac{L}{2}$, see [10] for details. For the MBE model without slope selection, one can take $\bar{L} = -S \Delta$ with $S \geq \frac{1}{16}$, see [10].

(3) The SAV scheme for (1.1) is written generally as

$$\overline{\partial}_t^\alpha \phi^{n+1} = \gamma G \mu^{n+1},$$  

$$\mu^{n+1} = L \phi^{n+1} + \frac{x^{n+1}}{\sqrt{E_1(\phi^n)}} \delta \phi E_1(\phi^n),$$  

$$\frac{x^{n+1} - x^n}{\Delta t} = \frac{1}{2 \sqrt{E_1(\phi^n)}} \left\langle \delta \phi E_1(\phi^n), \frac{\phi^{n+1} - \phi^n}{\Delta t} \right\rangle_\Omega,$$

(2.14)

where $L$ is a symmetric nonnegative linear operator and $E_1(\phi) > 0$ is given by (2.10) corresponding to the nonlinear term in $\mu$. 
3 Discrete energy laws

It is well-known that in the classical case of $\alpha = 1$, the following inequality holds for the schemes (2.12)–(2.14):

$$E^{n+1} - E^n \leq \frac{1}{\gamma \Delta t} \left( G^{-1}(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n \right)_\Omega \leq 0,$$

(3.1)

since $G^{-1}$ is nonpositive definite. Similarly, in the general case of $0 < \alpha < 1$, we can obtain the following inequality on the energy difference between two neighboring time steps for the schemes (2.12)–(2.14).

Lemma 3.1. The $L^1$ schemes for time-fractional phase-field equations, (2.12)–(2.14), satisfy the following inequality:

$$E^{n+1} - E^n \leq \frac{1}{\gamma} \left( G^{-1}(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n \right)_\Omega, \quad 0 \leq n \leq N - 1,$$

(3.2)

where $E^n = E(\phi^n)$ denotes the classical energy at $t_n$ for the convex-splitting scheme (2.12) and the stabilization scheme (2.13), while $E^n = \frac{1}{2} (\mathcal{L}\phi^n, \phi^n)_\Omega + (r^n)^2$ for the SAV scheme (2.14).

Proof. (1) We first prove (3.2) for the convex-splitting scheme (2.11). Since $E_c$ and $E_e$ are convex functionals, we have

$$E_c(\phi^n) - E_c(\phi^{n+1}) \geq \left( \delta_\phi E_c(\phi^{n+1}), \phi^n - \phi^{n+1} \right)_\Omega,$$

$$E_e(\phi^{n+1}) - E_e(\phi^n) \geq \left( \delta_\phi E_e(\phi^n), \phi^{n+1} - \phi^n \right)_\Omega.$$

(3.3)

Combining these two inequality with (2.11), we can obtain

$$E^{n+1} - E^n = (E_c(\phi^{n+1}) - E_c(\phi^n)) - (E_c(\phi^n) - E_e(\phi^n))$$

$$\leq \left( \delta_\phi E_c(\phi^{n+1}) - \delta_\phi E_e(\phi^n), \phi^{n+1} - \phi^n \right)_\Omega$$

$$= \frac{1}{\gamma} \left( G^{-1}(\phi^{n+1} - \phi^n), \phi^{n+1} - \phi^n \right)_\Omega.$$

(3.4)

(2) Now we want to prove that the stabilization scheme (2.13) also satisfies the inequality (3.2). Here, we prove the specific case of AC model under the constraint $S \geq 2$. In this case, (2.13) can be rewritten as

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

(3.5)

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 well-known (see for example [27]) that

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

(3.6)
Lemma 3.2 results in [13] on continuous level. We first recall a special Cholesky decomposition in [13], which is established.

\[ \text{(3.2)} \]

Remark 3.1.

When \( \alpha = 1 \), the inequality \[ \text{(3.2)} \] indicates that the discrete energy \( E^n \) decays with respect to \( n \). When \( 0 < \alpha < 1 \), \[ \text{(3.2)} \] will be useful in our later analysis. In fact, as long as the inequality \[ \text{(3.2)} \] holds, the time-fractional energy law and the weighted energy dissipation law will be established.

Next, we present two theorems on the discrete energy, which corresponds respectively to the results in [13] on continuous level. We first recall a special Cholesky decomposition in [13], which provides a new tool on determining the positive definiteness of a symmetric positive matrix.

Lemma 3.2 (A special Cholesky decomposition). Given an arbitrary symmetric matrix \( S \) of size \( N \times N \) with positive elements, if \( S \) satisfies the following three properties:
(P1) $1 \leq j < i \leq N$, $[S]_{i-1,j} \geq [S]_{i,j}$;
(P2) $1 < j \leq i \leq N$, $[S]_{i,j-1} < [S]_{i,j}$;
(P3) $1 < j < i \leq N$, $[S]_{i-1,j-1} - [S]_{i,j-1} \leq [S]_{i-1,j} - [S]_{i,j}$,
then $S$ is a positive definite matrix. In particular, $S$ has the following Cholesky decomposition:

$$S = LL^T,$$

where $L$ is a lower triangular matrix, satisfying two properties:

(Q1) $1 \leq j \leq i \leq N$, $[L]_{ij} > 0$;
(Q2) $1 \leq j < i \leq N$, $[L]_{i-1,j} \geq [L]_{i,j}$.

**Remark 3.2.** In the above lemma, the property (P1) means that the matrix $S$ is column decreasing, while (P2) means that $S$ is row increasing. The property (P3) seems complicated and artificial, but is actually related to the second-order cross partial derivative from the continuous point of view.

### 3.1 Time-fractional energy law

We state and prove our first discrete energy law result based on Lemma 3.2 which is called the time-fractional energy law in this article.

**Theorem 3.1.** For the $L_1$ schemes (2.12)–(2.14) of time-fractional phase-field equations, the following time-fractional energy law holds:

$$\partial_t^\alpha E^n := \sum_{j=0}^{n-1} b_j \frac{E^{n-j} - E^{n-j-1}}{\Delta t} \leq 0 \quad \forall 1 \leq n \leq N,$$

where the discrete fractional derivative $\partial_t^\alpha$ is given by (2.1), but now acts on $E^n$.

**Proof.** According to Lemma 3.1 and the definition of discrete fractional derivative, we have

$$\partial_t^\alpha E^n \leq \frac{1}{\gamma \Delta t} \sum_{i=0}^{n-1} b_i \left< G^{-1} \partial_t^\alpha \phi^{n-i}, \phi^{n-i} - \phi^{n-i-1} \right> \Omega$$

$$= \frac{1}{\gamma \Delta t^2} \sum_{i=0}^{n-1} b_i \sum_{j=0}^{n-i-1} b_j \left< G^{-1} (\phi^{n-i-j} - \phi^{n-i-j-1}), \phi^{n-i} - \phi^{n-i-1} \right> \Omega$$

$$= -\frac{1}{\gamma \Delta t^2} \sum_{i=1}^{n} \sum_{j=1}^{i} b_{n-i} b_{i-j} \left< \psi^i, \psi^j \right> \Omega$$

$$= -\frac{1}{\gamma \Delta t^2} \int_{\Omega} [\psi^1, \ldots, \psi^n] B [\psi^1, \ldots, \psi^n]^T$$

$$= -\frac{1}{2\gamma \Delta t^2} \int_{\Omega} [\psi^1, \ldots, \psi^n] (B + B^T) [\psi^1, \ldots, \psi^n]^T,$$

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where \( \forall 1 \leq k \leq n \),
\[
\psi^k = \begin{cases} \phi^k - \phi^k \varepsilon & \text{Allen–Cahn or MBE}, \\
\nabla(-\Delta)^{-1}(\phi^k - \phi^k \varepsilon) & \text{Cahn–Hilliard},
\end{cases}
\]
and
\[
B = \begin{bmatrix}
b_{n-1} & b_{n-2} & \cdots & b_1 & b_0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
b_1 & b_{n-2} & b_{n-3} & \cdots & b_0 \\
b_0 & b_{n-1} & b_{n-2} & \cdots & b_1 \\
\end{bmatrix}.
\]

To prove (3.13), it is only necessary to show that the symmetric matrix \( B + B^T \) is positive definite. To do this, we make a conjugate transformation of \( B + B^T \) as follows:
\[
M = P(B + B^T)P^T,
\]
where \( P \) is an anti-diagonal matrix given by
\[
P = \begin{bmatrix}
b_0^{-1} & b_1^{-1} & \cdots & b_{n-1}^{-1} \\
\vdots & \vdots & \ddots & \vdots \\
b_1^{-1} & b_0^{-1} \\
b_{n-1}^{-1} & \vdots & \vdots & \vdots \\
\end{bmatrix}
\]

As a consequence, we have
\[
[M]_{ij} = \begin{cases} 2b_0b_{i-1}^{-1} & \text{if } i = j, \\
b_{i-j}b_{i-1}^{-1} & \text{if } i > j, \\
b_{j-i}b_{j-1}^{-1} & \text{if } i < j.
\end{cases}
\]

It is sufficient to show that \( M \) is positive definite. It is easy to check that \( M \) satisfies the first two properties (P1) and (P2) in Lemma 3.2. Now we check the property (P3) in Lemma 3.2 for \( M \). 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 should prove
\[
[M]_{i-1,j-1} - [M]_{i,j-1} \leq [M]_{i-1,j} - [M]_{i,j},
\]
that is equivalent to prove
\[
f(j - 1) \leq f(j),
\]
where
\[
f(x) = \frac{(i - x)^{1-\alpha} - (i - x - 1)^{1-\alpha}}{(i - 1)^{1-\alpha} - (i - 2)^{1-\alpha}} - \frac{(i - x + 1)^{1-\alpha} - (i - x)^{1-\alpha}}{i^{1-\alpha} - (i - 1)^{1-\alpha}}, \quad 1 \leq x < i - 1.
\]

We can find that (3.21) will hold as soon as \( f'(x) \geq 0 \), i.e.,
\[
(i - x)^{-\alpha} + (i - x - 1)^{-\alpha} - (i - x + 1)^{-\alpha} - (i - x)^{-\alpha} \geq 0,
\]
\[
(1 - \alpha)(i - x)^{-\alpha} + (i - x - 1)^{-\alpha} - (i - x + 1)^{-\alpha} - (i - x)^{-\alpha} \geq 0,
\]
that is,
\[
1 - (i - x - 1)^\alpha(i - x)^{-\alpha} \leq \frac{1 - (i - x)^\alpha(i - x + 1)^{-\alpha}}{(i - x - 1)^\alpha((i - 1)^{1-\alpha} - (i - 2)^{1-\alpha})}. \tag{3.24}
\]
It is not difficulty to see that
\[
1 - (i - x - 1)^\alpha(i - x)^{-\alpha} \geq 1 - (i - x)^\alpha(i - x + 1)^{-\alpha}. \tag{3.25}
\]
To prove (3.24), we only need to show
\[
(i - x - 1)^\alpha((i - 1)^{1-\alpha} - (i - 2)^{1-\alpha}) \leq (i - x)^\alpha(i^{1-\alpha} - (i - 1)^{1-\alpha}). \tag{3.26}
\]
We consider an auxiliary function
\[
g(y) = y^\alpha((y + 1)^{1-\alpha} - y^{1-\alpha}), \quad \forall y \geq 0 \tag{3.27}
\]
and its derivative
\[
g'(y) = \alpha y^{-(1-\alpha)}(y + 1)^{1-\alpha} + (1 - \alpha)y^\alpha(y + 1)^{-\alpha} - 1. \tag{3.28}
\]
Letting \( z = \frac{y+1}{y} > 1 \), we can rewrite
\[
h(z) = g'(y) = \alpha z^{1-\alpha} + (1 - \alpha)z^{-\alpha} - 1. \tag{3.29}
\]
Since \( h(1) = 0 \) and \( h'(z) = \alpha(1 - \alpha)z^{-\alpha}(1 - z^{-1}) \geq 0 \), we have \( h(z) \geq 0 \), i.e., \( g'(y) \geq 0 \). Therefore, we can obtain that \( g(i - 2) \leq g(i - 1) \) with \( i \geq 4 \), i.e.,
\[
(i - 2)^\alpha((i - 1)^{1-\alpha} - (i - 2)^{1-\alpha}) \leq (i - 1)^\alpha(i^{1-\alpha} - (i - 1)^{1-\alpha}). \tag{3.30}
\]
By multiplying (3.30) and the following obvious inequality
\[
\left(1 - \frac{x - 1}{i - 2}\right)^\alpha \leq \left(1 - \frac{x - 1}{i - 1}\right)^\alpha, \tag{3.31}
\]
we obtain (3.26) and then (3.24). Therefore, \( f(x) \) is monotonically increasing. As a consequence, (3.24) is true and the property (P3) holds.

In summary, \( \mathbf{M} \) satisfies (P1)–(P3) in Lemma 3.2. Then, we claim that \( \mathbf{M} \) is positive definite and \( \mathbf{B} + \mathbf{B}^T \) is also positive definite. According to (3.14), we then have \( \partial_t E^n \leq 0 \). The proof is done. \( \square \)

Theorem 3.1 can yield directly to the following corollary on the energy boundedness that was proposed in [10]. In other words, Theorem 3.1 is a stronger result.

**Corollary 3.1.** For the L1 schemes (2.12)–(2.14) of the time-fractional phase-field models, the discrete energy is bounded by initial energy:
\[
E^n \leq E^0, \quad \forall 1 \leq n \leq N. \tag{3.32}
\]

**Proof.** The inequality (3.14) in Theorem 3.1 says
\[
E^n \leq \frac{1}{b_0} \sum_{j=0}^{n-2} (b_j - b_{j+1})E^{n-j-1} + \frac{b_{n-1}}{b_0}E^0. \tag{3.33}
\]
When \( n = 1 \), this inequality gives \( E^1 \leq E^0 \). By induction on \( n \), it is easy to see that \( E^n \leq E^0 \) always holds. \( \square \)
3.2 Weighted energy dissipation law

In [13], we proposed a weighted energy $E_\omega(t)$ for time-fractional phase-field models in the form of

$$E_\omega(t) = \int_0^1 \omega(\theta)E(\theta t) d\theta, \quad (3.34)$$

where $\omega(\cdot) \geq 0$ is some weight function satisfying $\int_0^1 \omega(\theta) d\theta = 1$. It has been shown that if $\omega(\theta)\theta^{1-\alpha}(1-\theta)^\alpha$ is nonincreasing with respect to $\theta$, the weighted energy decays with time, i.e.,

$$E'_\omega(t) = \int_0^1 \omega(\theta)\theta E'(\theta t) d\theta \leq 0. \quad (3.35)$$

In the particular case of $\omega(\theta) = \frac{1}{B_\alpha \theta^{1-\alpha}(1-\theta)^\alpha}$, $\quad (3.36)$

where $B_\alpha = B(\alpha, 1 - \alpha)$ is the Beta function, (3.35) becomes

$$E'_\omega(t) = \frac{1}{B_\alpha t} \int_0^t \frac{s^\alpha}{(t-s)^\alpha} E'(s) ds \leq 0. \quad (3.37)$$

**Theorem 3.2.** For any $\alpha \in (0, 1)$, the energy of the L1 schemes (2.12)–(2.14) of time-fractional phase-field equations satisfy

$$\tilde{E}^n \leq \tilde{E}^{n-1}, \quad \forall 1 \leq n \leq N, \quad (3.38)$$

where $\tilde{E}^n$ is a weighted energy given by

$$\tilde{E}^n := E^0 + \sum_{j=1}^n c_j (E^j - E^{j-1}), \quad c_j = \frac{t_j^\alpha}{\Gamma(\alpha)} \sum_{m=j}^n b_{m-j}. \quad (3.39)$$

**Proof.** We define the following numerical approximation $D^n$ to the left-hand side of (3.37) at $t_n$:

$$D^n = \frac{1}{\Gamma(\alpha)t_n} \sum_{j=0}^{n-1} t_{n-j}^\alpha \frac{E^n - E^{n-1}}{\Delta t}, \quad \forall 1 \leq n \leq N. \quad (3.40)$$

As a consequence, we can rewrite the weighted energy to be

$$\tilde{E}^n = E^0 + \Delta t \sum_{m=1}^n D^m. \quad (3.41)$$

To prove (3.38), it is sufficient to prove $D^n \leq 0$ for all $1 \leq n \leq N$. According to (3.2), we have the
following inequality:

\[
\Gamma(\alpha) t_n D^n = \sum_{i=0}^{n-1} \frac{e_{n-i}^\alpha b_n}{\Delta t} E_{n-i} - E_{n-i-1}
\]

\[
\leq \frac{1}{\gamma \Delta t} \sum_{i=0}^{n-1} e_{n-i}^\alpha b_n \left\langle G^{-1} T^\alpha, \phi_{n-i}, \phi_{n-i} - \phi_{n-i-1} \right\rangle \Omega
\]

\[
= - \frac{1}{\gamma \Delta t^2} \sum_{i=1}^{n} \sum_{j=1}^{i} t_i^\alpha b_{n-i} b_{i-j} \left\langle \psi^i, \psi^j \right\rangle \Omega
\]

\[
= - \frac{1}{2 \gamma \Delta t^{2-\alpha}} \int_{\Omega} \left[ \psi^1, \ldots, \psi^n \right] (B + B^T) \left[ \psi^1, \ldots, \psi^n \right]^T,
\]

where \( \psi^k \) is given by (3.15) and

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

(3.43)

To prove the weighted energy dissipation law, it is only necessary to show that the symmetric matrix \( B + B^T \) is positive definite. To do this, we still make a conjugate transformation as in the proof of Theorem 3.1

\[
M = P (B + B^T) P^T,
\]

(3.44)

where the anti-diagonal matrix \( P \) is given by (3.18). Then, \( M \) can be written explicitly as

\[
[M]_{ij} = \begin{cases}
2(n-i+1)^\alpha b_0 b_{i-1}^{-1} & \text{if } i = j, \\
(n-j+1)^\alpha b_{i-j} b_{i-1}^{-1} & \text{if } i > j, \\
(n-i+1)^\alpha b_{i-j} b_{j-i}^{-1} & \text{if } i < j.
\end{cases}
\]

(3.45)

To prove that \( M \) is positive definite, we check that \( M \) satisfies the three properties (P1)–(P3) in Lemma 3.2.

Firstly, we check the property (P1) in Lemma 3.2 for \( M \). In fact, it is sufficient to show that for any fixed \( j \), the following inequality holds for all \( i \geq j \geq 1 \):

\[
\frac{b_{i-j}}{b_{i-1}} = \frac{(i-j+1)^{1-\alpha} - (i-j)^{1-\alpha}}{i^{1-\alpha} - (i-1)^{1-\alpha}} \geq \frac{b_{i-j+1}}{b_i} = \frac{(i-j+2)^{1-\alpha} - (i-j+1)^{1-\alpha}}{(i+1)^{1-\alpha} - i^{1-\alpha}},
\]

(3.46)

that is equivalent to

\[
\frac{(i+1)^{1-\alpha} - i^{1-\alpha}}{i^{1-\alpha} - (i-1)^{1-\alpha}} \geq \frac{(i-j+2)^{1-\alpha} - (i-j+1)^{1-\alpha}}{(i-j+1)^{1-\alpha} - (i-j)^{1-\alpha}}. 
\]

(3.47)

We consider the following function

\[
f(x) = \frac{(x+1)^{1-\alpha} - x^{1-\alpha}}{x^{1-\alpha} - (x-1)^{1-\alpha}}, \quad x \geq 1,
\]

(3.48)
whose derivative is
\[
 f'(x) = \frac{(1 - \alpha) (2x^\alpha - (x - 1)^\alpha - (x + 1)^\alpha)}{x^\alpha(x - 1)^\alpha (x + 1)^\alpha (x^\alpha - (x - 1)^\alpha - (x + 1)^\alpha)^2} \geq 0. 
\] (3.49)

Since \( j \geq 1 \), we can then claim that \( f(i) \geq f(i - j + 1) \), i.e., the inequality (3.47) is true. Therefore, \( M \) satisfies the property (P1).

Secondly, we check the property (P2) in Lemma 3.2 for \( M \). We shall prove that for any fixed \( i \), the following inequality holds for \( 1 \leq j < i \leq n \):
\[
 (n - j + 1)^\alpha b_{i-j} \leq (n - j)^\alpha b_{i-j+1}, 
\] (3.50)
that is equivalent to
\[
 (n - j + 1)^\alpha \left((i - j + 1)^{1-\alpha} - (i - j)^{1-\alpha}\right) \leq (n - j)^\alpha \left((i - j)^{1-\alpha} - (i - j - 1)^{1-\alpha}\right). 
\] (3.51)

Consider the following function
\[
 g(x) = (n - x + 1)^\alpha \left((i - x + 1)^{1-\alpha} - (i - x)^{1-\alpha}\right) 
\] (3.52)
whose derivative is
\[
 g'(x) = -\alpha(n - x + 1)^{\alpha-1} \left((i - x + 1)^{1-\alpha} - (i - x)^{1-\alpha}\right) 
+ (1 - \alpha)(n - x + 1)^\alpha \left(-(i - x + 1)^{-\alpha} + (i - x)^{-\alpha}\right) 
\]
\[
= -\frac{(1 - \alpha)n + \alpha i - x + 1}{(n - x + 1)^{1-\alpha}(i - x + 1)^\alpha} + \frac{(1 - \alpha)n + \alpha i - x + 1 - \alpha}{(n - x + 1)^{1-\alpha}(i - x)^\alpha}. 
\] (3.53)

We want to prove that \( g'(x) \geq 0 \) for any \( 1 \leq x < i \), which is equivalent to prove
\[
 \left(\frac{i - x + 1}{i - x}\right)^{\alpha} \geq \frac{(1 - \alpha)n + \alpha i - x + 1}{(1 - \alpha)n + \alpha i - x + 1 - \alpha}. 
\] (3.54)

Since \( i \leq n \), the right-hand side of the above inequality satisfies
\[
 \frac{(1 - \alpha)n + \alpha i - x + 1}{(1 - \alpha)n + \alpha i - x + 1 - \alpha} \leq \frac{i - x + 1}{i - x + 1 - \alpha}. 
\] (3.55)

In order to obtain (3.54), it is sufficient to show the following inequality:
\[
 \left(\frac{i - x + 1}{i - x}\right)^{\alpha} \geq \frac{i - x + 1}{i - x + 1 - \alpha}, 
\] (3.56)
that is,
\[
 i - x + 1 - \alpha \geq (i - x + 1) \left(1 - \frac{1}{i - x + 1}\right)^\alpha. 
\] (3.57)

According to the Taylor expansion, it is easy to verify that
\[
 \left(1 - \frac{1}{i - x + 1}\right)^\alpha \leq 1 - \frac{\alpha}{i - x + 1}. 
\] (3.58)
implying that \( (3.57) \) is true and then \( (3.54) \) is true. As a consequence, we know that \( g(x) \) is monotonically increasing and the property (P2) is proved.

Thirdly, we check the property (P3) in Lemma 3.2 for \( M \). 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 \( 2 \leq j \leq i - 2 \) (here, \( 4 \leq i \leq n \)), we shall prove

\[
[M]_{i-1,j-1} - [M]_{i,j} \leq [M]_{i-1,j} - [M]_{i,j},
\]

that 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 \( 2 \leq x \leq i - 2 \). It is sufficient to show that

\[
h'(x)
= -\alpha(n - x + 1)^{\alpha-1} \left[ \frac{(i - x)^{1-\alpha} - (i - x - 1)^{1-\alpha}}{(i - 1)^{1-\alpha} - (i - 2)^{1-\alpha}} - \frac{(i - x + 1)^{1-\alpha} - (i - x)^{1-\alpha}}{i^{1-\alpha} - (i - 1)^{1-\alpha}} \right]
+ (1 - \alpha)(n - x + 1)^{\alpha} \left[ \frac{-(i - x)^{-\alpha} + (i - x - 1)^{-\alpha}}{(i - 1)^{-\alpha} - (i - 2)^{-\alpha}} - \frac{-(i - x + 1)^{-\alpha} + (i - x)^{-\alpha}}{i^{-\alpha} - (i - 1)^{-\alpha}} \right]
\geq 0.
\]

In fact, it is easy to find that

\[
(i - x)^{1-\alpha} - (i - x - 1)^{1-\alpha} = (i - x - 1)^{1-\alpha} \left[ \left( 1 + \frac{1}{i - x - 1} \right)^{1-\alpha} - 1 \right]
\leq (i - x - 1)^{1-\alpha} \frac{1 - \alpha}{i - x - 1} = \frac{1 - \alpha}{(i - x - 1)^{\alpha}}
\]

and similarly,

\[
-(i - x + 1)^{1-\alpha} + (i - x)^{1-\alpha} \leq \frac{1 - \alpha}{(i - x + 1)^{\alpha}}.
\]

Moreover, we have

\[
-(i - x)^{-\alpha} + (i - x - 1)^{-\alpha} = (i - x - 1)^{-\alpha} \left[ -\left( 1 - \frac{1}{i - x} \right)^{\alpha} + 1 \right]
\geq \frac{\alpha}{(i - x)(i - x - 1)^{\alpha}}
\]

and

\[
(i - x + 1)^{-\alpha} - (i - x)^{-\alpha} \geq -\frac{\alpha}{(i - x)(i - x + 1)^{\alpha}}.
\]

Substituting \( (3.63) \)–\( (3.66) \) into \( (3.62) \), we then have

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

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The remaining work it to show that
\[
(i - x - 1)^\alpha((i - 1)^{1-\alpha} - (i - 2)^{1-\alpha}) \leq (i - x + 1)^\alpha(i^{1-\alpha} - (i - 1)^{1-\alpha}).
\] (3.68)

We consider an auxiliary function
\[
p(y) = y^\alpha((y + 1)^{1-\alpha} - y^{1-\alpha}), \quad \forall \ y > 0,
\] (3.69)
whose derivative is
\[
p'(y) = \alpha\left(\frac{y + 1}{y}\right)^{1-\alpha} + (1 - \alpha)\left(\frac{y}{y + 1}\right)^\alpha - 1.
\] (3.70)

Letting \( z = \frac{y + 1}{y} > 1 \), we can rewrite
\[
p'(y) = h(z) = \alpha z^{1-\alpha} + (1 - \alpha)z^{-\alpha} - 1.
\] (3.71)

Since \( h(1) = 0 \) and
\[
h'(z) = \alpha(1 - \alpha)z^{-\alpha}(1 - z^{-1}) \geq 0, \quad \forall \ z \geq 1,
\] (3.72)
we then have
\[
p'(y) \geq 0, \quad \forall \ y > 0.
\] (3.73)

This results in \( p(i - 2) \leq p(i - 1) \) for any \( i \geq 4 \), i.e.,
\[
(i - 2)^\alpha((i - 1)^{1-\alpha} - (i - 2)^{1-\alpha}) \leq (i - 1)^\alpha(i^{1-\alpha} - (i - 1)^{1-\alpha}).
\] (3.74)

Multiplying (3.74) with the following inequality
\[
\left(1 - \frac{x - 1}{i - 2}\right)^\alpha \leq \left(1 - \frac{x - 2}{i - 1}\right)^\alpha,
\] (3.75)
we then obtain (3.68). Therefore, we have \( h'(x) \geq 0 \), implying that the property (P3) holds for \( M \).

In summary, \( M \) satisfies (P1)–(P3) in Lemma 3.2. Then, we can claim that \( M \) is positive definite and therefore, \( B + B^T \) is positive definite. According to (3.42), we then claim that \( D^a \leq 0 \) is true. The proof is completed.

**Remark 3.3.** We mention that Corollary 3.1 can also be deduced directly from Theorem 3.2 as Theorem 3.7. Further, the weighted energy dissipation law result is even stronger than the time-fractional energy law result. In fact, Theorem 3.7 and Theorem 3.2 state the following two inequalities respectively
\[
b_0(E^n - E^0) \leq \sum_{j=1}^{n-1} (b_j - b_{j-1}) \left(E^{n-j} - E^0\right)
\] (3.76)
and
\[
b_0n^\alpha(E^n - E^0) \leq \sum_{j=1}^{n-1} [b_{j-1}(n - j + 1)^\alpha - b_j(n - j)^\alpha] \left(E^{n-j} - E^0\right).
\] (3.77)

It can be shown that (3.76) can be deduced from (3.77). This proof is technical and we leave it to readers.
4 Numerical tests

In this section, we will test the numerical schemes for time-fractional phase-field models, to verify the above energy analysis. For the sake of simplicity, we just test the stabilization scheme (2.13).

4.1 Time-fractional Allen–Cahn model

We first consider the time fractional AC model defined in a two-dimensional domain \(\Omega = [0, L_x] \times [0, L_y]\) with periodic boundary conditions. The pseudo-spectral method is used for space discretization. We use the L1 stabilization scheme (2.13). We mention that the fast sum-of-exponential algorithm [28] could be used for evaluating the time-fractional derivatives. We take \(L_x = L_y = 2\), \(\varepsilon = 0.02\), and \(\gamma = 1\) in (1.1). The stabilization constant \(S\) in scheme (2.13) is set to \(S = 2\gamma\). The 128 \(\times\) 128 Fourier modes are used in the physical domain and the time step size is set to \(\Delta t = 0.1\). The initial phase-field state is taken as

\[
\phi_0(x) = \tanh \left[ \frac{1}{20\varepsilon} \left( \frac{2r}{3} - \frac{1}{4} - \frac{1 + \cos(6\theta)}{16} \right) \right]
\]

with the polar coordinates

\[
r = \sqrt{x^2 + y^2} \quad \text{and} \quad \theta = \arctan \frac{y}{x}.
\]

Figure 1 illustrates the solution \(\phi\) with different \(\alpha = 1, 0.8, 0.5, 0.3\). It is observed that when \(\alpha\) becomes smaller, it takes more time to reach the equilibrium. On the left-hand side of Figure 2, we can see that the energy decreases with respect to \(t\) in this numerical test. In the middle of Figure 2, it can be observed that the fractional derivative of energy is always nonpositive for different \(\alpha\), which is just the time-fractional energy law result in Theorem 3.1. On the right-hand side of Figure 2, we plot the derivative of weighted energy with respect to time, to find it always nonpositive as claimed in Theorem 3.2.

4.2 Time-fractional Cahn–Hilliard model

For the time-fractional CH model defined on \([0, L_x] \times [0, L_y]\), we still solve the governing equation using the stabilization scheme (2.13) with truncation. The following parameters are used: \(L_x = L_y = 2\), \(\varepsilon = 0.05\), \(\gamma = 0.1\), \(S = 20\gamma\), and \(\Delta t = 0.1\). Still, 128 \(\times\) 128 Fourier modes are used in the physical domain. The initial phase-field state \(\phi_0\) is taken as the uniformly distributed field in \([-1, 1]\).

Figure 3 illustrates the phase-field function \(\phi\) with \(\alpha = 1, 0.8, 0.5, 0.3\). It is still observed that when \(\alpha\) decreases, it takes more time to reach the equilibrium. From the left-hand side of Figure 4, we can find that the energy decreases with respect to the time \(t\). However, the theoretical proof is an open question. Furthermore, in the middle of Figure 4, it can be observed that the fractional derivative of energy is always nonpositive with respect to time as stated in Theorem 3.1. That is to say, the time-fractional energy law is preserved in this numerical test on the CH model. On the right-hand side of Figure 4, the derivative of weighted energy is nonpositive as stated in Theorem 3.2.
Figure 1: Snapshots of the solution to the time-fractional Allen–Cahn equation with different values $\alpha = 1, 0.8, 0.5, 0.3$. 
Figure 2: Energy (left), time-fractional derivative of energy (middle), and time derivative of weighted energy (right) with respect to time $t$, for the time-fractional Allen–Cahn equation with different $\alpha = 1, 0.8, 0.5, 0.3$.

5 Conclusion

We have proposed two new discrete energy laws, the time-fractional energy law (Theorem 3.1) and the weighted energy dissipation law (Theorem 3.2), of the L1 schemes for time-fractional phase-field equations. Both results are stronger than the energy boundedness result proposed in [10], since they can yield the boundedness directly by induction. The weighted energy dissipation law is even stronger than the time-fractional energy law. However, it is still an interesting open question whether pointwise energy law is true or not, which is challenging due to existence of both nonlocality and nonlinearity in the governing equations. In addition, it should be further investigated how to generalize the time-fractional energy law and weighted energy dissipation law for high-order schemes for time-fractional phase-field equations.

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Figure 3: Snapshots of the solution to the time-fractional Cahn–Hilliard equation with different $\alpha = 1, 0.8, 0.5, 0.3$. 
Figure 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 different values $\alpha = 1, 0.8, 0.5, 0.3$.

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