Asymptotically compatible energy of variable-step fractional BDF2 formula for time-fractional Cahn-Hilliard model

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Abstract

A new discrete energy dissipation law of the variable-step fractional BDF2 (second-order backward differentiation formula) scheme is established for time-fractional Cahn-Hilliard model with the Caputo’s fractional derivative of order \( \alpha \in (0, 1) \), under a weak step-ratio constraint \( 0.4753 \leq \frac{\tau_k}{\tau_{k-1}} < r^*(\alpha) \), where \( \tau_k \) is the \( k \)-th time-step size and \( r^*(\alpha) \geq 4.660 \) for \( \alpha \in (0, 1) \).

We propose a novel discrete gradient structure by a local-nonlocal splitting technique, that is, the fractional BDF2 formula is split into a local part analogue to the two-step backward differentiation formula of the first derivative and a nonlocal part analogue to the L1-type formula of the Caputo’s derivative. More interestingly, in the sense of the limit \( \alpha \to 1^- \), the discrete energy and the corresponding energy dissipation law are asymptotically compatible with the associated discrete energy and the energy dissipation law of the variable-step BDF2 method for the classical Cahn-Hilliard equation, respectively. Numerical examples with an adaptive stepping procedure are provided to demonstrate the accuracy and the effectiveness of our proposed method.

Keywords: time-fractional Cahn-Hilliard model, fractional BDF2 formula, discrete gradient structure, asymptotically compatible energy, energy dissipation law

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1 Introduction

Linear and nonlinear diffusion equations with fractional time derivatives have become widely models describing anomalous diffusion processes \[ [8, 12, 33]. \] These models always exhibit multi-scaling time behaviour, which makes them suitable for the description of different diffusive regimes and characteristic crossover dynamics in complex systems. To capture the multi-scale behaviors in time-fractional differential equations, adaptive time-stepping strategies, namely, small time steps are utilized when the solution varies rapidly and large time steps are employed otherwise, would be practically useful especially in the simulations of long-time coarsening dynamics \[ [9, 10, 17, 22, 24]. \] It is natural to require practically and theoretically reliable time-stepping methods on general setting of time step-size variations, or on a wider class of nonuniform time meshes.

This work develops a new discrete energy dissipation law of the second-order fractional backward differentiation formula (FBDF2) for the time-fractional Cahn-Hilliard (TFCH) flow in modelling the coarsening process with a general coarsening rate \[ [2, 6, 10, 25, 30, 31, 33, 34]. \]

\[
\partial_t^\alpha \Phi = \kappa \Delta \mu \quad \text{with} \quad \mu := \frac{\delta E}{\delta \Phi} = f(\Phi) - \epsilon^2 \Delta \Phi, \tag{1.1}
\]

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where \( f(\Phi) := F'(\Phi) \) and \( E[\Phi] \) is the Ginzburg-Landau energy functional
\[
E[\Phi] := \int_\Omega \left( \frac{\epsilon^2}{2} |\nabla \Phi|^2 + F(\Phi) \right) \, dx \quad \text{with the potential } F(\Phi) := \frac{1}{4} (\Phi^2 - 1)^2. \tag{1.2}
\]

The notation \( \partial_t^\alpha := \frac{C}{\Gamma(\alpha)} D_t^\alpha \) represents the Caputo’s derivative of order \( \alpha \in (0, 1) \), defined by
\[
(\partial_t^\alpha v)(t) := \int_0^t \omega_{-\alpha}(t-s)v'(s) \, ds \quad \text{with } \omega_{\beta}(t) := t^{\beta-1}/\Gamma(\beta) \text{ for } \beta > 0. \tag{1.3}
\]

The real valued function \( \Phi \) represents the concentration difference in a binary system on the domain \( \Omega \subseteq \mathbb{R}^2 \), \( \epsilon > 0 \) is an interface width parameter, and \( \kappa > 0 \) is the mobility coefficient.

Let \( \langle \cdot, \cdot \rangle \) and \( \| \cdot \| \) be the \( L^2(\Omega) \) inner product and the associated norm, respectively. Always we use the standard norms of the Sobolev space \( H^m(\Omega) \) and the \( L^p(\Omega) \) space. For \( v \) and \( w \) belonging to the zero-mean space \( \mathbb{V} := \{ v \in L^2(\Omega) \mid \langle v, 1 \rangle = 0 \} \), we use the \( H^{-1} \)-like inner product \( \langle \cdot, \cdot \rangle_{-1} := \langle (-\Delta)^{-1} v, w \rangle \) and the induced norm \( \| v \|_{-1} := \sqrt{\langle v, v \rangle_{-1}} \).

The well-possness of the TFCH model \( (1.1) \) has been established in \( [2,6] \) and the analysis indicated that the solution lacks the smoothness near the initial time while it would be smooth away from \( t = 0 \), also see \( [5,6] \).

As is well known, the CH model \( (1.4) \) conserves the initial volume \( \langle \Phi(t), 1 \rangle = \langle \Phi(0), 1 \rangle \) and has the following energy dissipation law
\[
\frac{dE}{dt} + \kappa \| \nabla \mu \|^2 = 0 \quad \text{for } t > 0. \tag{1.5}
\]

Some efforts have been made to seek the reasonable versions of the energy \( E[\Phi] \) and the energy dissipation law \( (1.5) \) for the TFCH equation \( (1.1) \). Tang, Yu and Zhou \( [33] \) established a global energy dissipation law, \( E[\Phi(t)] \leq E[\Phi(0)] \) for \( t > 0 \), see also \( [9,31] \). In \( [29] \), Quan, Tang and Yang derived a nonlocal energy decaying law, \( \partial_t^\alpha E \leq 0 \), and a weighted energy dissipation law, \( \dot{\partial}_t E_\eta \leq 0 \), for a nonlocal energy \( E_\eta(t) := \int_0^t \eta(\theta) E(\theta t) d\theta \), also cf. the dissipation-preserving augmented energy in \( [6] \). They are quite different from the classical energy law \( (1.5) \). By reformulating the Caputo form \( (1.1) \) into the Riemann-Liouville form and applying the equality in \( [1] \) Lemma 1], one can obtain the following variational energy dissipation law, cf. \( [22] \) Section 1],
\[
\frac{dE_\alpha}{dt} + \frac{\kappa}{2} \omega_\alpha(t) \| \nabla \mu \|^2 - \frac{\kappa}{2} \int_0^t \omega_{\alpha-1}(t-s) \| \nabla \mu(t) - \nabla \mu(s) \|^2 \, ds = 0, \tag{1.6}
\]

where the variational (modified) energy
\[
E_\alpha[\Phi] := E[\Phi] + \frac{\kappa}{2} \int_0^t \| \nabla \mu \|^2 \quad \text{for } t > 0. \tag{1.7}
\]

We remark that the variational energy law \( (1.6) \) is naturally consistent with the energy dissipation law \( (1.5) \) of the CH model. Actually, the discrete energy dissipation laws of the variable-step L1 or L1_1 time-stepping schemes in \( [10,22,24] \) were proven to be asymptotically compatible (in the limit \( \alpha \to 1^- \)) with the associated discrete energy laws of their integer-order counterparts. However, the
variational energy $E_α[Φ]$ is not asymptotically compatible with the Ginzburg-Landau energy $E[Φ]$. Very recently, Quan et al. [30] applied an equivalent definition (obtained from the integration by parts) of the Caputo derivative to find a new energy dissipation law (in our notations)

$$\frac{d\tilde{E}_α}{dt} - \frac{ω_α(t)}{2κ} ||Φ(t) - Φ(0)||^2_1 + \frac{1}{2κ} \int_0^t ω_{α−1}(t−s) ||Φ(t) - Φ(s)||^2_1 ds = 0,$$

(1.8)

where the modified energy $\tilde{E}_α[Φ]$ is defined by

$$\tilde{E}_α[Φ] := E[Φ] + \frac{ω_{1−α}(t)}{2κ} ||Φ(t) - Φ(0)||^2_1 - \frac{1}{2κ} \int_0^t ω_α(t−s) ||Φ(t) - Φ(s)||^2_1 ds.$$

(1.9)

An interesting property is that the new modified energy $\tilde{E}_α[Φ]$ is asymptotically compatible with the Ginzburg-Landau energy [30, Proposition 5.1], that is, $E_α[Φ] → E[Φ]$ as $α → 1^−$. They also derived the modified energy dissipation laws at discrete time levels for the L1 and L2-type implicit-explicit stabilized schemes on the uniform time mesh. Nonetheless, it is noticed that the modified discrete energies of these time-stepping schemes are not asymptotically compatible (except the steady state case) with the associated discrete energies of their integer-order counterparts, see more details in [30, Theorem 5.2] or [30, Theorems 4.1 and 4.2].

The above mentioned variable-step schemes are built by the piecewise linear or piecewise constant interpolating polynomial and only have a low order accuracy of $O(τ^{2−α})$ or $O(τ^{1+α})$ in time, see the related error analysis in [14,18,19,27,28]. In this paper, we shall build a discrete gradient structure (DGS) of fractional BDF2 formula on general nonuniform meshes and establish an asymptotically compatible discrete energy dissipation law at each time level with an asymptotically compatible energy. As far as we know, there are few studies on the high-order energy stable schemes with unequal time-step sizes for time-fractional phase field models, see [9,31,32].

Application of quadratic interpolating polynomial to obtain the high-order approximations of Caputo derivative (1.3) was suggested and investigated in recent years, see [7,20,26]. The so-called L2-type (fractional BDF2) methods in [7,26] were shown to be $(3−α)$-order accurate on the uniform mesh for sufficiently smooth solutions. By using a nonuniform mesh such as the well-known graded meshes [14,15,18,20,32], we will restore the optimal convergence when the solution is not smooth near the initial time. Recently, Kopteva [15] applied the inverse-monotonicity of discrete fractional-derivative operator to obtain sharp pointwise-in-time error bounds on quasi-graded meshes for the linear subdiffusion equation and derived a mild constraint of grading parameter to recover the optimal order convergence at any positive time.

We study the variable-step fractional BDF2 scheme on a general class of time meshes. Consider the nonuniform time levels $0 = t_0 < t_1 < \cdots < t_{k−1} < t_k < \cdots < t_N = T$ with the time-step sizes $τ_k := t_k - t_{k−1}$ for $1 ≤ k ≤ N$ and the maximum time-step size $τ := \max_{1 ≤ k ≤ N} τ_k$. Also, let $t_{k−1/2} := (t_k + t_{k−1})/2$ for $k ≥ 1$, and the adjacent time-step ratio $r_1 := 0$ and $r_k := τ_k/τ_{k−1}$ for $k ≥ 2$. For any time sequence $v^k = v(t_k)$, define the backward difference $\nabla_τ v^k := v^{k−1} - v^{k−1}$ and the difference quotient $\partial_τ v^k := \nabla_τ v^k/τ_k$. Let $Π_{2,k}v$, $k ≥ 1$, denote the quadratic interpolant with respect to three nodes $t_{k−1}$, $t_k$ and $t_{k+1}$ for $k ≥ 1$. It is easy to find (for instance, by using the Newton forms of the interpolating polynomials) that

$$(Π_{2,k}v)' = \partial_τ v^k + \frac{2(t - t_{k−1/2})}{τ_k + τ_{k+1}} (\partial_τ v^{k−1} - \partial_τ v^k) = \partial_τ v^k + \frac{2(t - t_{k+1/2})}{τ_k + τ_{k+1}} (\partial_τ v^{k+1} - \partial_τ v^k).$$

For any time-level $t_n$ with $n ≥ 2$, applying the quadratic interpolating polynomial $Π_{2,k}v$, we have
the following \((3 - \alpha)\)-order BDF2 type formula \([7, 26]\) of Caputo derivative \((1.3)\)

\[
(\partial^\alpha \tau)^n := \int_{t_{n-1}}^{t_n} \omega_{1-\alpha}(t_n - s) (\Pi_{2,n-1} v)'(s) \, ds + \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_n - s) (\Pi_{2,k} v)'(s) \, ds
\]

\[
= \sum_{k=1}^{n} a_{n-k}^{(n)} \nabla_{\tau} v^k + \frac{\tau_n \eta_0^{(n)}}{1 + \tau_n} (\nabla_{\tau} v^n - r_n \nabla_{\tau} v^{n-1}) + \sum_{k=1}^{n-1} \eta_{n-k}^{(n)} \frac{(\nabla_{\tau} v^{k+1} - r_{k+1} \nabla_{\tau} v^k)}{r_{k+1}(1 + r_{k+1})} \tag{1.10}
\]

for \(n \geq 2\), where the positive coefficients \(a_{n-k}^{(n)}\) and \(\eta_{n-k}^{(n)}\) are defined by

\[
a_{n-k}^{(n)} := \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_n - s) \, ds \quad \text{for} \quad 1 \leq k \leq n, \tag{1.11}
\]

\[
\eta_{n-k}^{(n)} := \frac{2}{\tau_k} \int_{t_{k-1}}^{t_k} \frac{s - t_{k-1/2}}{\tau_k} \omega_{1-\alpha}(t_n - s) \, ds \quad \text{for} \quad 1 \leq k \leq n. \tag{1.12}
\]

To start with the stepping formula \((1.10)\), we use the standard L1 formula at the first time level,

\[
(\partial^\alpha \tau)^1 \triangleq a_0^{(1)} \nabla_{\tau} v^1 \quad \text{with} \quad a_0^{(1)} := \frac{1}{\tau_1} \int_{t_0}^{t_1} \omega_{1-\alpha}(t_1 - s) \, ds. \tag{1.13}
\]

Notice that if the fractional order \(\alpha \to 1^-\), then \(\omega_{3-\alpha}(t) \to t, \omega_{2-\alpha}(t) \to 1\) and \(\omega_{1-\alpha}(t) \to 0\), uniformly for \(t > 0\). Thus, \(a_0^{(n)} = \omega_{2-\alpha}(\tau_n)/\tau_n \to 1/\tau_n\) and \(\eta_0^{(n)} = \alpha \tau_n^{-\alpha}/\Gamma(3 - \alpha) \to 1/\tau_n\), whereas \(a_{n-k}^{(n)} \to 0\) and \(\eta_{n-k}^{(n)} \to 0\) for \(1 \leq k \leq n - 1\). We shall call \((1.10)\) together with \((1.13)\) as the fractional BDF2 (FBDF2) formula for brevity, since the approximation \((1.10)\) degrades into the standard BDF2 formula \([16, 17, 21, 23]\) of the derivative \(\partial_\tau v\), that is,

\[
(\partial^\alpha \tau)^n \to D_2 v^n := \frac{1 + 2 \tau_n}{(1 + \tau_n) \tau_n} \nabla_{\tau} v^n - \frac{r_n^2}{(1 + r_n) \tau_n} \nabla_{\tau} v^{n-1} \quad \text{as} \quad \alpha \to 1^- \tag{1.14}
\]

We can reformulate \((1.10)\) and \((1.13)\) into a compact form,

\[
(\partial^\alpha \tau)^n \triangleq \sum_{k=1}^{n} B_{n-k}^{(n)} \nabla_{\tau} v^k \quad \text{for} \quad n \geq 1, \tag{1.15}
\]

where the kernels \(B_{n-k}^{(n)}\) are determined via \((1.10)\) and \((1.13)\). The above asymptotic property \((1.14)\) arises the main difficulty in the numerical analysis of the FBDF2 formula \((1.10)\). That is, the second kernel \(B_{n-k}^{(n)}\) would be negative when \(\alpha\) is close to 1, and the discrete kernels \(B_{n-k}^{(n)}\) lose the monotonicity. The established stability and convergence theory \([14, 18–20]\) for the variable-step L1 and L2-1_\(\sigma\) formulas can not be applied here directly. Recently, the uniform FBDF2 formula was showed in \([31]\) to be positive semidefinite with the BDF2 multiplier \(D_2 v^n\), that is, \(\sum_{k=1}^{n}(D_2 v^k)(\partial^\alpha \tau)^k \geq 0\). By combining with the recent scalar auxiliary variable technique, the resulting time-stepping scheme was proven to preserve a global energy law \([33]\) of time-fractional phase-field equations. Quan and Wu \([32]\) investigated the \(H^1\) stability of the FBDF2 formula \((1.10)\) on general nonuniform time meshes for a linear subdiffusion equation and established the positive semidefiniteness with the difference multiplier \(\nabla_{\tau} v^n\), that is, \(\sum_{k=1}^{n}(\nabla_{\tau} v^k)(\partial^\alpha \tau)^k \geq 0\), under the following step-ratio condition

\[
0.4573328 \leq r_k \leq 3.5615528 \quad \text{for} \quad k \geq 2. \tag{1.16}
\]

Nonetheless, these results in \([31, 32]\) would be inadequate to build an asymptotically compatible discrete energy law for the TFCH equation \((1.1)\).
The current work is inspired by the following DGS \cite{17} of the BDF2 formula,
\[(\nabla v^n)D_2v^n \geq \frac{3r_{n-1}}{2(1+r_{n-1})\tau_n}(\nabla v^n)^2 - \frac{3r_n}{2(1+r_n)\tau_n}(\nabla v^{n-1})^2 \quad \text{for } n \geq 2. \tag{1.17}\]
This DGS holds if the adjacent step-ratio restriction \(0 < r_k < r^* \approx 4.864\) for \(k \geq 2\), where \(r^*\) is the positive root of \(1 + 2r^* - (r^*)^{3/2} = 0\). This DGS has been proven to be useful to establish the discrete energy dissipation laws at each time level of the BDF2 scheme for the classical gradient flows \cite{17}. It is natural to ask whether the FBDF2 formula \cite{1.10} has a similar gradient structure under some constraint on the step-ratio \(r_k\), and whether the resulting FBDF2 time-stepping for time-fractional gradient flows also has an energy dissipation law at discrete time levels.

In the next section, we update the step-ratio stability constraint \(1.16\) into
\[0.4753 \leq r_k < r^*(\alpha) \quad \text{for } k \geq 2 \quad \text{with } r^*(\alpha) \geq 4.660, \]
and establish a novel DGS for the FBDF2 formula \cite{1.10}. Our main tools include a novel local-nonlocal splitting technique and the step-scaling technique so that the present analysis is quite different and would be more concise than those in \cite{30,32}. As an application, we consider an implicit FBDF2 stepping for the TFCH model \cite{1.1} in Section 3 and prove that it is uniquely solvable and has an asymptotically compatible energy law at each time level. More importantly, our discrete energy is also asymptotically compatible with the associated discrete energy of the BDF2 scheme for the CH equation. Numerical tests show that the proposed method is accurate with an order of \(O(\tau^{3-\alpha})\) in time. An adaptive time-stepping procedure is also provided to speedup the simulations of long-time coarsening dynamics.

\section{Discrete gradient structure of FBDF2 formula}

To derive the DGS of the nonuniform FBDF2 formula \cite{1.10}, we propose a local-nonlocal splitting technique by splitting it into two parts
\[\sum_{k=1}^{n} \tilde{a}_{n-k} \nabla v^n \quad \text{for } n \geq 2, \tag{2.1}\]
where the discrete kernels \(\tilde{a}_{n-k}^{(n)}\) are defined by
\[\tilde{a}_{n-1}^{(n)} := a_{n-1}^{(n)} = a_{n}^{(n)} := \frac{1}{2-\alpha} a_{n}^{(n)} + \frac{n_{n-1}^{(n)}}{r_n(1+r_n)} \quad \text{for } n \geq 2, \tag{2.2}\]
\[\tilde{a}_{n-k}^{(n)} := a_{n-k}^{(n)} - \frac{n_{n-k}^{(n)}}{r_n(1+r_n)} \quad \text{for } 2 \leq k \leq n-1 \quad (n \geq 3), \tag{2.3}\]
\[\tilde{a}_{n-k}^{(n)} := a_{n-k}^{(n)} - \frac{n_{n-k}^{(n)}-1}{r_n(1+r_n)} \quad \text{for } n \geq 2. \tag{2.4}\]

The first part \(j_{B2}^{(n)}\) represents a variable-step BDF2-type formula \cite{16,17,21,23}. The second part \(j_{L1}^{(n)}\) represents the nonuniform L1-type formula \cite{19,24} of Caputo derivative \cite{1.3}. As seen, the discrete kernel \(a_{n}^{(n)}\) is split into two parts with different weights \(\frac{1}{2-\alpha}\) and \(\frac{1}{r_n-\alpha}\). The technical reason of the above local-nonlocal splitting is that the local term \(\tilde{a}_{n}^{(n)} \to D_2v^n\) as \(\alpha \to 1^-\), while the convoluted kernels \(\tilde{a}_{n-k}^{(n)}\) \((n \geq 2)\) of the nonlocal term \(j_{L1}^{(n)}\) will vanish, \(\tilde{a}_{n-k}^{(n)} \to 0\) as \(\alpha \to 1^-\). So we can build a discrete energy that is asymptotically compatible with the discrete energy of the BDF2 scheme for the CH model, see Remark \cite{4}. It significantly updates the previous energy laws in \cite{10,22,24}, in which the discrete energies are always not asymptotically compatible in the fractional order limit \(\alpha \to 1^-\) although the associated energy laws are asymptotically compatible.
2.1 DGS of local part

We shall handle the local term $J_{B2}^n$ by applying the recent step-scaling technique \[17\] for the BDF2 formula. Next lemma presents an upper bound of step-ratio $r_k$ to ensure the DGS of $J_{B2}^n$.

**Lemma 2.1.** For any fractional index $\alpha \in (0, 1)$, it holds that

\[
g(x, y, \alpha) := \frac{2 + 2(1 + \alpha)x - \alpha x^{2 - \frac{2}{\alpha}}}{1 + x} - \frac{\alpha y^{2 - \frac{2}{\alpha}}}{1 + y} > 0 \quad \text{for} \quad 0 \leq x, y < r^*,
\]

where $r^* = r^*(\alpha)$ be the unique root of the equation $1/\alpha + (1 + 1/\alpha)r^* - (r^*)^{2-\frac{2}{\alpha}} = 0$.

**Proof.** At first, we show the well-poseness of $r^*$ for $\alpha \in (0, 1)$. Consider an auxiliary function

\[
g_1(z, \alpha) := 1/\alpha + (1 + 1/\alpha)z - z^{2-\frac{2}{\alpha}} \quad \text{for} \quad z > 0
\]

with $\partial_z g_1(z, \alpha) := 1 + 1/\alpha - (2 - \alpha/2)z^{1-\frac{2}{\alpha}}$. Obviously, the equation $\partial_z g_1(z, \alpha) = 0$ has a unique root $z_1 > 1$ since $\partial_z g_1(1, \alpha) = 1 + 1/\alpha + 2 - 1 > 0$. Thus for any $\alpha \in (0, 1)$, $g_1(z, \alpha)$ is increasing in $(0, z_1)$ and decreasing in $(z_1, +\infty)$ with respect to $z$. We have

\[
g_1(z_1, \alpha) = 1/\alpha + 1 - \alpha/2 \quad (1 + 1/\alpha)z_1 > 0 \quad \text{and} \quad g_1(+\infty, \alpha) < 0.
\]

Thus there exists a unique $r^* \in (z_1, +\infty)$ such that $g_1(r^*, \alpha) = 0$ for any $\alpha \in (0, 1)$.

Differentiating the function $g$ with respect to $x$ gives $\partial_x g = \frac{\alpha}{2(1+x^\gamma)} g_2(x, \alpha)$ with an auxiliary function $g_2(x, \alpha) := 4 - (4 - \alpha)x^{1-\frac{2}{\alpha}} - (2 - \alpha)x^{2-\frac{2}{\alpha}}$. Obviously, the function $g_2$ is decreasing with respect to $x > 0$ and $g_2(0, \alpha)g_2(1, \alpha) < 0$ such that $g_2(x, \alpha)$ has a unique zero point $x_1 \in (0, 1)$ for any $\alpha \in (0, 1)$. Thus, $g$ is increasing in $(0, x_1)$ and decreasing in $(x_1, +\infty)$ for $x > 0$. Furthermore, $g$ is decreasing with respect to $y$ due to the simple fact $\partial_y g < 0$. It holds that

\[
g(x, y, \alpha) > \min\{g(0, r^*, \alpha), g(r^*, r^*, \alpha)\} = g(r^*, r^*, \alpha) = \frac{2\alpha}{1 + r^*} g_1(r^*, \alpha) = 0,
\]

since $r^* > z_1 > 1 > x_1$. This completes the proof. \qed

![Figure 1: Solution curves of $g_1(r^*, \alpha) = 0$ and $g_1(2\gamma_{\text{max}} - 1, \alpha) = 0$.](image)

**Remark 1.** It is easy to check that $r^*(1) = r^* \approx 4.864$ and $r^*(\alpha) \to +\infty$ as $\alpha \to 0^+$; but we are not able to find an explicit solution $r^*(\alpha)$ of $g_1(r^*, \alpha) = 0$. Differentiating this equation with respect to $\alpha$ gives

\[
\frac{dr^*}{d\alpha} = \frac{\frac{1}{2}\alpha^2(r^*)^{2-\frac{2}{\alpha}} \ln r^* - 1 - r^*}{(2 - \frac{2}{\alpha})\alpha^2(r^*)^{1-\frac{2}{\alpha}} - \alpha - \alpha^2} = \frac{(r^*)^{2-\frac{2}{\alpha}} g_3(r^*, \alpha)}{(2 - \frac{2}{\alpha})\alpha(r^*)^{1-\frac{2}{\alpha}} - 1 - \alpha},
\]
where the function \( g_3(z, \alpha) := \frac{1}{2} \alpha \ln z - \frac{1+z}{2(1+z+\alpha z)} \). Since the partial derivative \( \partial_2 g_3 > 0 \) for \( z > 0 \), it is not difficult to check that \( g_3(z, \alpha) = 0 \) has a unique positive root for any \( \alpha \in (0, 1) \). We solve the simultaneous equations of \( g_1(r^*, \alpha) = 0 \) and \( g_2(r^*, \alpha) = 0 \) numerically, and find a pair of approximate solutions \( (r^*, \alpha) \approx (4.660, 0.7881) \). Let \( R^* := 4.660 \). It is checked that the function \( g_1(R^*, \alpha) \) defined by (2.3) has the minimum value, that is, \( g_1(R^*, \alpha) \geq g_1(R^*, 0.7881) \approx 6.67e-4 \) for any \( \alpha \in (0, 1) \). That is to say, the solution of \( g_1(r^*, \alpha) = 0 \) has a low bound \( R^* \) such that \( r^*(\alpha) > R^* \) for any \( \alpha \in (0, 1) \), see Figure 7 (a), and the result of Lemma 2.1 holds for \( 0 \leq x, y \leq R^* = 4.660 \).

**Remark 2.** In resolving the initial singularity of time-fractional problem (1.1), the graded or quasi-graded meshes would be practical to restore the convergence rate of our time-stepping scheme. Due to the nonuniform setting, the FBDF2 method (1.10) is naturally applicable to these graded-like meshes; however, the step-ratio bound \( r^*(\alpha) \) in Lemma 2.1 always restricts the value of graded parameter \( \gamma \), which is adapted to the strength of the singularity. For the standard graded mesh \( t_k = T_0(k/N_0) \) with a grading parameter \( \gamma \geq 1 \), the step-ratios \( r_k = \frac{k^{\gamma}-(k-1)^\gamma}{(k-1)^\gamma-(k-2)^\gamma} \) is decreasing with respect to the level index \( k \) with the maximum one \( r_2 = 2^\gamma - 1 \). According to Remark 7, the maximum permissible parameter \( \gamma_{\text{max}} = \gamma_{\text{max}}(\alpha) \) can be determined by the equation \( g_1(2^{\gamma_{\text{max}}} - 1, \alpha) = 0 \). Figure 7 (b) shows that \( \gamma_{\text{max}}(\alpha) > 3 - \alpha \) for any \( \alpha \in (0, 1) \). Thanks to the theoretical results [13, Theorem 4.1 and Remarks 4.2-4.4], it is adequate to attain the optimal convergence rate at any positive time for the FBDF2 method (1.10). Nonetheless, the step-ratio bound \( r^*(\alpha) \) in Lemma 2.1 is always inadequate to achieve the optimal rate of global convergence since the maximum permissible parameter \( \gamma_{\text{max}}(\alpha) \leq (3 - \alpha)/\alpha \) on the standard graded mesh.

**Lemma 2.2.** Let \( r_k < r^*(\alpha) \) for \( k \geq 2 \). For the local term \( J^n_{B2} \) in (2.1), it holds that

\[
(\nabla_\tau v^n)J^n_{B2} \geq \frac{\alpha r_n^{2-\alpha}}{2(1+r_n)\tau_n^2} \frac{\Gamma(3-\alpha)}{\Gamma(3-\alpha)} - \frac{\alpha r_n^{2-\alpha}}{2(1+r_n)\tau_n^2} \frac{(\nabla_\tau v^n)^2}{\Gamma(3-\alpha)} + g(r_n, r_{n+1}, \alpha)\frac{\alpha r_n^{2-\alpha}}{2(1+r_n)\tau_n^2} \frac{(\nabla_\tau v^n)^2}{\Gamma(3-\alpha)}
\]

for \( n \geq 2 \), where the bound \( r^*(\alpha) \) and \( g(x, y, \alpha) \) are defined by Lemma 2.1.

**Proof.** We introduce the sequence \( w_k \) via \( \nabla_\tau v^n = r_k^{\alpha/2}w_k \) and derive from (2.1) that

\[
(\nabla_\tau v^n)J^n_{B2} = \frac{1}{\Gamma(3-\alpha)} w_n^2 + \frac{r_n}{1+r_n} \frac{\eta_{0}^{(n)}}{\tau_n} w_n^2 - \frac{r_n}{1+r_n} \frac{\eta_{0}^{(n)}}{\tau_n} r_n^{\alpha/2} w_n w_{n-1}- \frac{r_n}{1+r_n} \frac{\eta_{0}^{(n)}}{\tau_n} \frac{\eta_{0}^{(n)}}{\tau_n} r_n^{\alpha/2} w_n w_{n-1} \]

\[
= \frac{w_n^2}{\Gamma(3-\alpha)} + \frac{\alpha r_n}{1+r_n} \frac{w_n^2}{\Gamma(3-\alpha)} - \frac{\alpha r_n}{1+r_n} \frac{\eta_{0}^{(n)}}{\tau_n} \frac{\eta_{0}^{(n)}}{\tau_n} r_n^{\alpha/2} w_n w_{n-1} \]

\[
\geq \frac{1}{1+r_n} \frac{w_n^2}{\Gamma(3-\alpha)} - \frac{\alpha r_n}{1+r_n} \frac{\eta_{0}^{(n)}}{\tau_n} \frac{\eta_{0}^{(n)}}{\tau_n} r_n^{\alpha/2} w_n w_{n-1} \]

\[
= \frac{g(r_n, r_{n+1}, \alpha)}{2\Gamma(3-\alpha)} w_n^2 + \frac{\alpha r_n^{2-\alpha}}{2(1+r_n)\tau_n} w_n^2 - \frac{\alpha r_n^{2-\alpha}}{2(1+r_n)\tau_n} \frac{\eta_{0}^{(n)}}{\tau_n} \frac{\eta_{0}^{(n)}}{\tau_n} r_n^{\alpha/2} w_n w_{n-1}. \]

It leads to the claimed result by using \( w_k = r_k^{\alpha/2}v_k \) for \( k \geq 1 \). \( \square \)

### 2.2 DGS of nonlocal part

To build up a DGS for the nonlocal term \( J^n_{L1} \) in (2.1), we need the following lemma, which is inspired by the proofs of [10, Theorem 2.1] and [30, Lemma 4.1].

**Lemma 2.3.** For any fixed index \( n \geq 2 \) and any positive kernels \( \{\lambda_{n-j})_{j=1}^{n}\} \), define the following auxiliary kernels \( a_{n-j}^{(n)} := (2 - \sigma_{\text{min}})\lambda_{n-j}^{(n)} \) and \( a_{n-j}^{(n)} := \lambda_{n-j}^{(n)} \) for \( 1 \leq j \leq n-1 \). Assume that there exists a constant \( \sigma_{\text{min}} \in [0, 2) \) such that the modified kernels \( a_{n-j}^{(n)} \) satisfy
(Row decrease) \( a_{n-j-1}^{(n)} \geq a_{n-j}^{(n)} > 0 \) for \( 1 \leq j \leq n-1 \);

(Column decrease) \( a_{n-j-1}^{(n-1)} \geq a_{n-j}^{(n)} \) for \( 1 \leq j \leq n-1 \);

(Algebraic convexity) \( a_{n-j-1}^{(n-2)} - a_{n-j-1}^{(n-1)} \geq a_{n-j}^{(n)} - a_{n-j-1}^{(n)} \) for \( 1 \leq j \leq n-2 \).

Then for any real sequence \( \{w_k\}_{k=1}^n \), the following discrete gradient structure holds,

\[
2w_n \sum_{j=1}^n \chi_{n-j}^{(n)} w_j = Y[\vec{w}_n] - Y[\vec{w}_{n-1}] + \sigma_{\min} \chi_0^{(n)} w_n^2 + Y_R[\vec{w}_n] \quad \text{for } n \geq 1,
\]

where \( \vec{w}_n = (w_n, w_{n-1}, \ldots, w_1)^T \), and the nonnegative functionals \( Y \) and \( Y_R \) are defined by

\[
Y[\vec{w}_n] := \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) \left( \sum_{\ell=j+1}^n w_\ell \right)^2 + a_{n-1}^{(n)} \left( \sum_{\ell=1}^n w_\ell \right)^2 \quad \text{for } n \geq 1,
\]

\[
Y_R[\vec{w}_n] := \sum_{j=1}^{n-2} (a_{n-j-2}^{(n-1)} - a_{n-j-1}^{(n-1)} - a_{n-j-1}^{(n)} + a_{n-j}^{(n)}) \left( \sum_{\ell=j+1}^{n-1} w_\ell \right)^2 + (a_{n-2}^{(n-1)} - a_{n-1}^{(n)}) \left( \sum_{\ell=1}^{n-1} w_\ell \right)^2
\]

for \( n \geq 2 \). Then the discrete convolution kernels \( \chi_{n-k}^{(n)} \) are positive definite in the sense that

\[
2 \sum_{k=1}^n w_k \sum_{j=1}^k \chi_{k-j}^{(k)} w_j \geq Y[\vec{w}_n] + \sigma_{\min} \sum_{k=1}^n \chi_{k-0}^{(k)} w_k^2 \quad \text{for } n \geq 1.
\]

**Proof.** Fix \( n \) and let \( u_k := \sum_{\ell=1}^k w_\ell \) for \( 0 \leq k \leq n \) such that \( u_0 = 0 \) and \( \nabla_\tau u_k = w_k \) for \( 1 \leq k \leq n \). Recalling the following fact \( \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) = a_0^{(n)} - a_{n-1}^{(n)} \), we derive that

\[
2w_n \sum_{k=1}^n a_{n-k}^{(n)} w_k = 2(\nabla_\tau u_n) \sum_{k=1}^n a_{n-k}^{(n)} \nabla_\tau u_k = 2(\nabla_\tau u_n) \left[ a_0^{(n)} u_n - \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) u_j \right]
\]

\[
= 2(\nabla_\tau u_n) \left[ \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) (u_n - u_j) + a_{n-1}^{(n)} u_n \right].
\]

By using the fact \( 2 \nabla_\tau u_n (u_n - u_j) = (u_n - u_j)^2 - (u_{n-1} - u_j)^2 + (\nabla_\tau u_n)^2 \), it follows that

\[
2w_n \sum_{k=1}^n a_{n-k}^{(n)} w_k = \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) (u_n - u_j)^2 + a_{n-1}^{(n)} u_n^2
\]

\[
= \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) (u_n - u_j)^2 - a_{n-1}^{(n)} u_n^2 + a_{n-1}^{(n)} (\nabla_\tau u_n)^2
\]

\[
= \sum_{j=1}^{n-1} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) (u_n - u_j)^2 + a_{n-1}^{(n)} u_n^2
\]

\[
- \sum_{j=1}^{n-2} (a_{n-j-1}^{(n)} - a_{n-j}^{(n)}) (u_n - u_j)^2 - a_{n-1}^{(n)} u_n^2 + a_0^{(n)} w_n^2.
\]

By replacing the sequence \( \{u_k\} \) with \( \{w_k\} \), it is easy to find that

\[
a_0^{(n)} w_n^2 + 2w_n \sum_{k=1}^{n-1} a_{n-k}^{(n)} w_k = Y[\vec{w}_n] - Y[\vec{w}_{n-1}] + Y_R[\vec{w}_n].
\]

The definition of \( a_{n-j}^{(n)} \) implies the claimed equality and completes the proof. \( \square \)
Now we present the discrete gradient structure of the nonlocal part \( J_{L1}^n \) in (2.1).

**Theorem 2.1.** For the discrete kernels \( \hat{a}_{n-k}^{(n)} \) in [2.2]–[2.4], define the following auxiliary kernels

\[
A_0^{(n)} := 2\hat{a}_0^{(n)} \quad \text{and} \quad A_{n-k}^{(n)} := \hat{a}_{n-k}^{(n)} \quad \text{for} \quad 1 \leq k \leq n-1. \tag{2.6}
\]

If the time-step ratios \( r_k \) fulfill

\[
r_k \geq R_* = \frac{1}{9} \sqrt[3]{\frac{1}{2} (189 - 81\sqrt{5}) + \frac{1}{3} \sqrt[3]{\frac{1}{2} (7 + 3\sqrt{5})}} \approx 0.4753 \quad \text{for} \quad k \geq 2,
\]

then the auxiliary convolution kernels \( A_{n-k}^{(n)} \) satisfy

(a) \( A_{n-k-1}^{(n)} > A_{n-k}^{(n)} > 0 \) for \( 1 \leq k \leq n-1 \) \( (n \geq 2) \);

(b) \( A_{n-1-k}^{(n-1)} > A_{n-k}^{(n)} \) for \( 1 \leq k \leq n-1 \) \( (n \geq 2) \);

(c) \( A_{n-2-k}^{(n-1)} - A_{n-1-k}^{(n-1)} > A_{n-k-1}^{(n)} - A_{n-k}^{(n)} \) for \( 1 \leq k \leq n-2 \) \( (n \geq 3) \).

Then for the nonlocal term \( J_{L1}^n \) in (2.1) with \( n \geq 2 \), it holds that

\[
(\nabla \tau v^n) \sum_{k=1}^n A_{n-k}^{(n)} (\nabla \tau v^k) \geq \frac{1}{2} \left[ \sum_{j=1}^{n-1} (A_{n-j}^{(n)} - A_{n-j}) \left( \sum_{\ell=j+1}^{n} (\nabla \tau v^\ell)^2 \right) + A_{n-1}^{(n)} \left( \sum_{\ell=1}^{n} (\nabla \tau v^\ell)^2 \right) \right] - \frac{1}{2} \left[ \sum_{j=1}^{n-2} (A_{n-j-1}^{(n-1)} - A_{n-j-1}) \left( \sum_{\ell=j+1}^{n-1} (\nabla \tau v^\ell)^2 \right) + A_{n-2}^{(n-1)} \left( \sum_{\ell=1}^{n-1} (\nabla \tau v^\ell)^2 \right) \right].
\]

**Proof.** Consider a function \( g_4(z) := 3 - \frac{1}{z^2(1+z^2)} \), with \( g_4'(z) = -\frac{3z^2+2}{z^4(z^2+1)^2} > 0 \) for \( z > 0 \). It is easy to check that \( R_* \) is the unique positive root of \( g_4(z) = 0 \). If \( r_k \geq R_* \) for \( k \geq 2 \), it holds that

\[
3 - \frac{1}{r_k^2(1+r_k)} \geq g_4(R_*) = 0 \quad \text{for} \quad 2 \leq k \leq n. \tag{2.7}
\]

According to Lemma 2.3 with \( \sigma_{\min} = 0 \), it remains to verify the three properties (a)-(c) of the kernels \( A_{n-k}^{(n)} \). The remainder of this proof is presented separately in Section 4. \( \square \)

By applying Lemma 2.2 and Theorem 2.1 we obtain the DGS of the variable-step FBDF2 formula (1.10) via the splitting equality (2.1) and the definitions (2.2)–(2.4).

**Theorem 2.2.** For \( n \geq 1 \), define a nonnegative functional \( G \) as follows,

\[
G[w_n] := \frac{\alpha r_{n+1}^{2-\alpha}}{2(1+r_{n+1})r_{n}^{\alpha} \Gamma(3-\alpha)} \frac{w_n^2}{n} + \frac{1}{2} \sum_{j=1}^{n-1} (A_{n-j}^{(n)} - A_{n-j}) \left( \sum_{\ell=j+1}^{n} w_\ell \right)^2 + \frac{1}{2} A_{n-1}^{(n)} \left( \sum_{\ell=1}^{n} w_\ell \right)^2.
\]

Assume that the time-step ratios \( r_k \) fulfill

\[
R_* \leq r_k < r^*(\alpha) \quad \text{for} \quad k \geq 2, \tag{2.8}
\]

where the lower bound \( R_* \) and the upper bound \( r^*(\alpha) > R_* \approx 4.660 \) are given in Theorem 2.1 and Lemma 2.1 together with Remark 1 respectively. Then it holds that

\[
(\nabla \tau v^n)(\partial^*_\tau v)^n \geq G[\nabla \tau v^n] - G[\nabla \tau v^{n-1}] + \frac{g(r_n,r_{n+1},\alpha)}{2\Gamma(3-\alpha) r_n^\alpha} (\nabla \tau v^n)^2 \quad \text{for} \quad n \geq 2.
\]
3 The FBDF2 scheme and discrete energy law

Now we apply the FBDF2 formula (1.10) to time integration of TFCH flow (1.1) and construct the following time-discrete scheme

\[(\partial^n_t \phi)^n = \kappa \Delta \mu^n \quad \text{with} \quad \mu^n = f(\phi^n) - \epsilon^2 \Delta \phi^n \quad \text{for} \ n \geq 1. \tag{3.1}\]

Note that, the numerical scheme and the subsequent analysis can be extended in a straightforward way to the fully discrete numerical schemes with some appropriate spatial discretization preserving the discrete integration-by-parts formulas, such as the Fourier pseudo-spectral method [3,4].

Obviously, the FBDF2 scheme (3.1) preserves the volume. Actually, by taking the inner product of (3.1) with 1, one applies the Green’s formula to find that

\[\langle (\partial^n_t \phi)^n, 1 \rangle = \kappa \langle \Delta \mu^n, 1 \rangle = 0.\]

Then the simple induction yields that \(\langle \phi^n, 1 \rangle = \langle \phi^{n-1}, 1 \rangle \) for \(n \geq 1\) with the help of the discrete formulas (1.10) and (1.13). Then we obtain \(\langle \phi^n, 1 \rangle = \langle \phi^0, 1 \rangle \) for \(n \geq 1\).

**Theorem 3.1.** Under the time-step restriction

\[\tau_n \leq \frac{\sqrt{4 \epsilon^2 \frac{2 - \alpha + 2r_n}{\kappa (1 + r_n) \Gamma(3 - \alpha)}}}{\kappa} \quad \text{for} \ n \geq 1, \tag{3.2}\]

the variable-step FBDF2 scheme (3.1) is uniquely solvable.

**Proof.** For any fixed time-level index \(n \geq 1\), we consider the following energy functional \(Q[z]\) on the space \(\mathcal{V}^* := \{z \in L^2(\Omega) \mid \langle z, 1 \rangle = \langle \phi^{n-1}, 1 \rangle\}\),

\[Q[z] := \frac{1}{2} \|z - \phi^{n-1}\|_1^2 + \langle \mathcal{L}^{n-1}, z - \phi^{n-1}\rangle_1 + \frac{\kappa \epsilon^2}{2} \|\nabla z\|^2 + \frac{\kappa}{4} \|z\|^{4}_{L^4} \left(\frac{\kappa}{2}\right) \|z\|^2,\]

where we denote \(\mathcal{L}^{n-1} := \sum_{k=1}^{n-1} B_{n-k}^{(n)} \nabla \phi^k\) from the compact formulation (1.15). With the help of the definitions (1.10) and (1.13) together with (1.11)-(1.12), the restriction (3.2) implies that

\[B_0^{(n)} \geq a_0^{(n)} + \frac{\epsilon^2}{2} \frac{r_n}{1 + \epsilon^2 r_n} \tau_n^2 \geq \frac{2 - \alpha + 2r_n}{(1 + r_n) \Gamma(3 - \alpha) \tau_n^2} \geq \frac{\kappa}{4 \epsilon^2}.\]

By using the generalized Hölder inequality

\[\|v\|^2 \leq \|\nabla v\| \|v\|_{-1} \leq \epsilon^2 \|\nabla v\|^2 + \frac{1}{4 \epsilon^2} \|v\|_{-1}^2 \quad \text{for any} \ v \in \mathcal{V},\]

we see that the energy functional \(Q[z]\) is convex with respect to \(z\), that is,

\[\frac{d^2 Q[z + \epsilon \psi]}{d \epsilon^2} \bigg|_{\epsilon = 0} = B_0^{(n)} \|\psi\|_{-1}^2 + \kappa \epsilon^2 \|\nabla \psi\|^2 + \kappa \|\psi\|^2 + 3\kappa \|z \psi\|^2 \geq \left(B_0^{(n)} - \frac{\kappa}{4 \epsilon^2}\right) \|\psi\|_{-1}^2 + 3 \kappa \|z \psi\|^2 > 0.\]

It is easy to show that the functional \(Q[z]\) is coercive on \(\mathcal{V}^*\), that is,

\[Q[z] \geq \frac{\kappa}{4} \|z\|^{4}_{L^4} - \frac{\kappa}{2} \|z\|^2 - \frac{1}{2B_0^{(n)}} \|\mathcal{L}^{n-1}\|^2 \geq \frac{\kappa}{2} \|z\|^2 - \frac{1}{2B_0^{(n)}} \|\mathcal{L}^{n-1}\|^2 - \kappa |\Omega|,\]

where the inequality \(\|v\|_{L^4}^4 \geq 4 \|v\|^2 - 4 |\Omega|\) has been used in the last step. So the functional \(Q[z]\) has a unique minimizer, which implies that the FBDF2 scheme (3.1) exists a unique solution.
Remark 3. As $\alpha \to 1^-$, the variable-step FBDF scheme (3.1) approaches the BDF2 scheme
\begin{equation}
D_2 \phi^n = \kappa \Delta \mu^n \quad \text{with} \quad \mu^n = (\phi^n)^3 - \phi^n - \epsilon^2 \Delta \phi^n \quad \text{for } n \geq 1,
\end{equation}
which is uniquely solvable if the time-step size $\tau_n \leq \frac{4(1+2\alpha)\kappa^2}{(1+\tau_n)\kappa}$, cf. [17, 21]. As seen, the time-step condition (3.2) is asymptotically compatible in the fractional order limit $\alpha \to 1^-.$

Let $E[\phi^n]$ be the discrete version of the free energy functional (1.2),
\begin{equation}
E[\phi^n] := \frac{\epsilon}{2} \left\| \nabla \phi^n \right\|^2 + \left\langle F(\phi^n), 1 \right\rangle \quad \text{with} \quad F(\phi^n) := \frac{1}{4} \left( (\phi^n)^2 - 1 \right)^2 \quad \text{for } n \geq 0.
\end{equation}
With the nonnegative functional $G$ in Theorem 2.2 we define a modified energy functional
\begin{equation}
E_\alpha[\phi^n] := E[\phi^n] + \frac{1}{\kappa} \left\langle G[\nabla_\tau \phi^n], 1 \right\rangle \quad \text{for } n \geq 1.
\end{equation}

Theorem 3.2. Under the step-ratio constraint (2.8) with the following step-size condition
\begin{equation}
\tau_n \leq \sqrt{\frac{4\epsilon^2 g(r_n, r_{n+1}, \alpha)}{\kappa \Gamma(3-\alpha)}} \quad \text{for } n \geq 2,
\end{equation}
the variable-step FBDF2 scheme (3.1) preserves the following discrete energy dissipation law
\begin{equation}
\partial_\tau E_\alpha[\phi^n] \leq 0 \quad \text{for } 2 \leq n \leq N.
\end{equation}

Proof. Making the inner product of the equation (3.1) by $(-\Delta)^{-1} \nabla_\tau \phi^n / \kappa$, one obtains
\begin{equation}
\frac{1}{\kappa} \left\langle (\partial^2_{\tau} \phi^n), \nabla_\tau \phi^n \right\rangle + \left\langle (\phi^n)^3 - \phi^n, \nabla_\tau \phi^n \right\rangle - \epsilon^2 \left\| \Delta \phi^n, \nabla_\tau \phi^n \right\|^2 = 0.
\end{equation}
Recalling the simple inequality $4(a^3 - a)(a - b) \geq (a^2 - 1)^2 - (b^2 - 1)^2 - 2(a - b)^2$, we can bound the second term of (3.7) by
\begin{equation}
\left\langle f(\phi^n), \nabla_\tau \phi^n \right\rangle \geq \left\langle F(\phi^n), 1 \right\rangle - \left\langle F(\phi^n-1), 1 \right\rangle - \frac{1}{2} \left\| \nabla_\tau \phi^n \right\|^2.
\end{equation}
Applying the identity $2a(a - b) = a^2 - b^2 + (a - b)^2$, we formulate the third term of (3.7) as
\begin{equation}
-\epsilon^2 \left\| \Delta \phi^n, \nabla_\tau \phi^n \right\|^2 = \frac{\epsilon^2}{2} \left\| \nabla \phi^n \right\|^2 - \frac{\epsilon^2}{2} \left\| \nabla \phi^{n-1} \right\|^2 + \frac{\epsilon^2}{2} \left\| \nabla_\tau \nabla \phi^n \right\|^2.
\end{equation}
Substituting the above results into (3.7), one has
\begin{equation}
\frac{1}{\kappa} \left\langle (\partial^2_{\tau} \phi^n), \nabla_\tau \phi^n \right\rangle + \frac{\epsilon^2}{2} \left\| \nabla_\tau \nabla \phi^n \right\|^2 - \frac{1}{2} \left\| \nabla_\tau \phi^n \right\|^2 + E[\phi^n] \leq E[\phi^{n-1}].
\end{equation}
For the first term of (3.8), Theorem 2.2 yields
\begin{equation}
\frac{1}{\kappa} \left\langle (\partial^2_{\tau} \phi^n), \nabla_\tau \phi^n \right\rangle \geq \frac{1}{\kappa} \left\langle G[\nabla_\tau \phi^n], 1 \right\rangle - \frac{1}{\kappa} \left\langle G[\nabla_\tau \phi^{n-1}], 1 \right\rangle - \frac{g(r_n, r_{n+1}, \alpha)}{2\kappa \Gamma(3-\alpha) \tau_n} \left\| \nabla_\tau \phi^n \right\|^2.
\end{equation}
By the generalized Hölder inequality, we have
\begin{equation}
-\frac{1}{2} \left\| \nabla_\tau \phi^n \right\|^2 \geq -\frac{1}{8\epsilon^2} \left\| \nabla_\tau \phi^n \right\|^2 - \frac{\epsilon^2}{2} \left\| \nabla_\tau \nabla \phi^n \right\|^2.
\end{equation}
Inserting the above two estimates into (3.8), one gets
\begin{equation}
\frac{1}{2\kappa} \left( \frac{g(r_n, r_{n+1}, \alpha)}{\Gamma(3-\alpha) \tau_n^\alpha} - \frac{\kappa}{4\epsilon^2} \right) \left\| \nabla_\tau \phi^n \right\|^2 \leq E_\alpha[\phi^n] \leq E_\alpha[\phi^{n-1}].
\end{equation}
Then the claimed result follows from the time-step condition (3.6) immediately.\qed
Remark 4 (asymptotical compatibility). Under the time-step restriction, cf. [17],
\[
\tau_n \leq \frac{4\epsilon^2}{\kappa} \left( \frac{2 + 4r_n - r_n^{3/2}}{1 + r_n} - \frac{3/2}{1 + r_{n+1}} \right) = 4g(r_n, r_{n+1}, 1)\epsilon^2/\kappa \quad \text{for } n \geq 2,
\]
the BDF2 scheme (3.3) for the classical CH model preserves the energy dissipation law,
\[
\partial_t \mathcal{E}[\phi^n] \leq 0 \quad \text{for } 2 \leq n \leq N,
\]
where the modified energy
\[
\mathcal{E}[\phi^n] := E[\phi^n] + \frac{\sqrt{r_{n+1}r_{n+1}}}{2\kappa(1 + r_{n+1})} \left\| \partial_t \phi^n \right\|_{-1}^2 \quad \text{for } 1 \leq n \leq N.
\]
As the fractional index \( \alpha \to 1^− \), the definition (2.6) together with (2.2)-(2.4) shows that the discrete kernels \( A_{n-k}^{(n)} \to 0 \) for \( 1 \leq k \leq n \). According to Theorem 2.2, the discrete energy (3.5) is asymptotically compatible with the modified energy (3.10), that is,
\[
\mathcal{E}_\alpha[\phi^n] \rightarrow \mathcal{E}[\phi^n] \quad \text{as } \alpha \to 1^−.
\]
Also, the energy dissipation law in Theorem 3.2 is asymptotically compatible with the energy dissipation law (3.9) in the sense that
\[
\partial_t \mathcal{E}_\alpha[\phi^n] \leq 0 \rightarrow \partial_t \mathcal{E}[\phi^n] \leq 0 \quad \text{as } \alpha \to 1^−.
\]
Additionally, it is not difficult to check that the modified energy (3.10) of BDF2 scheme and the discrete energy (3.5) of the FBDF2 scheme degrade into the original Ginzburg-Landau energy \( E[\phi^n] \) in approaching the steady state (\( \nabla_\tau \phi^n \to 0 \)), that is,
\[
\mathcal{E}_\alpha[\phi^n] \rightarrow E[\phi^n] \quad \text{and} \quad \mathcal{E}[\phi^n] \rightarrow E[\phi^n] \quad \text{as } t_n \to +\infty.
\]
Remark 5. To make the presentation more clear, the fully implicit time-stepping scheme for the TFCH model is only considered in this paper; however, Theorem 2.2 would be useful to derive the discrete energy dissipation laws of some other FBDF2 approximations, such as convex splitting scheme, stabilized scheme and linearized schemes using the recent SAV techniques, for other time-fractional phase-field models. Since the discrete convolution kernels \( B_k^{(n)} \) in (1.15) lack the monotonicity [15, 26] with respect to the subscript \( k \), another essential difficulty in theory is to establish optimal \( L^2 \)-norm error estimate of the FBDF2 schemes on general nonuniform grids with the step-ratio constraint (2.8). These issues will be studied and presented in separate reports.

4 Proof of Theorem 2.1 (a)-(c)

From the definition (2.6) together with the discrete kernels \( a_{n-k}^{(n)} \) defined in (2.2)-(2.4), we see that the discrete kernels \( A_{n-k}^{(n)} \) are defined by \( a_{n-k}^{(n)} \) and \( \eta_{n-k}^{(n)} \). Some technical lemmas on the positive coefficients \( a_{n-k}^{(n)} \) and \( \eta_{n-k}^{(n)} \) will be established firstly via their definitions (1.11) and (1.12).

Lemma 4.1. For \( n \geq 2 \), define the following “bridging” integrals \( I_{n-k}^{(n)} \) and \( J_{n-k}^{(n)} \) as follows,
\[
I_{n-k}^{(n)} := \int_{t_{k-1}}^{t_k} \frac{t - t_k}{\tau_k} \omega_\alpha(t_n - t) \, dt \quad \text{for } 1 \leq k \leq n,
\]
\[
J_{n-k}^{(n)} := \int_{t_{k-1}}^{t_k} \frac{t_k - t}{\tau_k} \omega_\alpha(t_n - t) \, dt \quad \text{for } 1 \leq k \leq n - 1.
\]
The positive coefficients \( a_{n-k}^{(n)} \) in (1.11) satisfy
(i) \( a_{n-k-1}^{(n)} - a_{n-k}^{(n)} = I_{n-k-1}^{(n)} + J_{n-k}^{(n)} \) for \( 1 \leq k \leq n - 1 \).

(ii) \( \frac{2(1-\alpha)}{2-\alpha} a_0^{(n)} - a_1^{(n)} = \frac{\alpha}{2-\alpha} \omega_1-\alpha(\tau_n) + J_1^{(n)} \).

**Proof.** The original idea comes from [20, Lemma 4.6] but we include the proof for completeness. Applying the definition (1.11), we exchange the order of integration to find

\[
a_{n-k-1}^{(n)} - \omega_1-\alpha(t_n - t_k) = \int_{t_k}^{t_{k+1}} \omega_1-\alpha(t_n - s) - \omega_1-\alpha(t_n - t_k) \, ds
\]

\[
= - \frac{1}{\tau_{k+1}} \int_{t_k}^{t_{k+1}} \int_{t_k}^{s} \omega_\alpha(t_n - t) \, dt \, ds = \int_{t_k}^{t_{k+1}} \frac{t - t_{k+1}}{\tau_{k+1}} \omega_\alpha(t_n - t) \, dt = I_{n-k-1}^{(n)}
\]

for \( 0 \leq k \leq n - 1 \), and similarly,

\[
\omega_1-\alpha(t_n - t_k) - a_{n-k}^{(n)} = \int_{t_{k-1}}^{t_k} \frac{\omega_1-\alpha(t_n - t_k) - \omega_1-\alpha(t_n - s)}{\tau_k} \, ds = J_{n-k}^{(n)}
\]

for \( 1 \leq k \leq n - 1 \). Hence the claimed equality (i) is obtained by summing up the above two equalities (4.3) and (4.4) for \( 1 \leq k \leq n - 1 \). Now taking the index \( k = n - 1 \) in (4.4) yields \( \omega_1-\alpha(\tau_n) = a_1^{(n)} + J_{1}^{(n)} \). By using the simple fact \( a_0^{(n)} = \omega_1-\alpha(\tau_n)/(1-\alpha) \), we have

\[
\frac{2(1-\alpha)}{2-\alpha} a_0^{(n)} - a_1^{(n)} = \frac{\alpha}{2-\alpha} a_1^{(n)} + \frac{2}{2-\alpha} J_{1}^{(n)} = \frac{\alpha}{2-\alpha} \omega_1-\alpha(\tau_n) + J_{1}^{(n)}.
\]

This confirms the result (ii) and completes the proof. \( \square \)

**Lemma 4.2.** The positive coefficients \( \eta_{n-k}^{(n)} \) in (1.12) satisfy

(i) \( \eta_{n-k}^{(n)} < \eta_{n-k-1}^{(n-1)} \) for \( 1 \leq k \leq n - 1 \).

(ii) \( \eta_{n-k-1}^{(n)} > \tau_{k+1} \eta_{n-k}^{(n)} \) for \( 1 \leq k \leq n - 1 \) and

\[
\eta_{n-k-1}^{(n)} - \tau_{k+1} \eta_{n-k}^{(n)} < \eta_{n-k-2}^{(n-1)} - \tau_{k+1} \eta_{n-k-2}^{(n-1)} \) for \( 1 \leq k \leq n - 2 \).

**Proof.** The integration by parts yields, also see [20, Lemma 2.1],

\[
\eta_{n-k}^{(n)} = - \frac{1}{\tau_k^2} \int_{t_{k-1}}^{t_k} (s - t_{k-1})(t_k - s) \omega_\alpha(t_n - s) \, ds > 0 \quad \text{for} \quad 1 \leq k \leq n.
\]

Then it is easy to check that

\[
\eta_{n-k}^{(n)} < - \frac{1}{\tau_k^2} \int_{t_{k-1}}^{t_k} (s - t_{k-1})(t_k - s) \omega_\alpha(t_n - s) \, ds = \eta_{n-k-1}^{(n-1)} \quad \text{for} \quad 1 \leq k \leq n - 1.
\]

The result (i) is verified. Now consider an auxiliary function

\[
\eta_{n,k}(z) := \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k+2\tau_k} \frac{2s - 2t_{k-1} - z\tau_k}{\tau_k} \omega_1-\alpha(t_n - s) \, ds \quad \text{for} \quad 1 \leq k \leq n
\]

with the first and second derivatives

\[
\eta_{n,k}'(z) = z \omega_1-\alpha(t_n - t_{k-1} - z\tau_k) - \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k+2\tau_k} \omega_1-\alpha(t_n - s) \, ds \quad \text{for} \quad 1 \leq k \leq n,
\]

\[
\eta_{n,k}''(z) = - z \tau_k \omega_\alpha(t_n - t_{k-1} - z\tau_k) \quad \text{for} \quad 1 \leq k \leq n.
\]
Notice that $\eta_{n,k}(1) = \eta_{n-k}^{(n)}$, $\eta_{n,k}(0) = 0$ and $\eta_{n,k}'(0) = 0$ for $1 \leq k \leq n$. The Cauchy differential mean-value theorem says that there exist $z_{1k}, z_{2k} \in (0, 1)$ such that

$$\frac{\eta_{n,k-1}^{(n)}}{\eta_{n-k}^{(n)}} = \frac{\eta_{n,k+1}(1)}{\eta_{n,k}(1)} = \frac{\eta_{n,k+1}'(z_{1k})}{\eta_{n,k}'(z_{1k})} = \frac{\eta_{n,k+1}''(z_{2k})}{\eta_{n,k}''(z_{2k})} = \frac{\tau_{k+1}}{\tau_k}\left(\frac{t_n - t_{k+1} - z_{2k}\tau_{k+1}}{t_n - t_k - z_{2k}\tau_k}\right)^{1+\alpha} > r_{k+1} \quad \text{for } 1 \leq k \leq n - 1.$$

To process the proof, we introduce another auxiliary function $\Pi_{n,k}(z) := \eta_{n,k+1}(z) - r_{k+1}\eta_{n,k}(z)$ for $1 \leq k \leq n - 1$

such that $\Pi_{n,k}(1) = \eta_{n-k}^{(n)} - r_{k+1}\eta_{n-k}^{(n)}$. Thanks to the Cauchy differential mean-value theorem, there exist $z_{3n}, z_{4n} \in (0, 1)$ such that

$$\frac{\Pi_{n,k}(1)}{\Pi_{n-1,k}(1)} = \frac{\Pi_{n,k}'(z_{3n})}{\Pi_{n-1,k}'(z_{3n})} = \frac{\Pi_{n,k}''(z_{4n})}{\Pi_{n-1,k}''(z_{4n})} = \frac{-\omega\omega(t_n - t_k - z_{4n}\tau_k) + \omega(t_n - t_{k-1} - z_{4n}\tau_k)}{-\omega\omega(t_n - t_k - z_{4n}\tau_k) + \omega(t_n - t_{k-1} - z_{4n}\tau_k)} < 1$$

for $1 \leq k \leq n - 2$, where the last inequality comes from the convexity of function $t^{-1-\alpha}$. Thus the two inequalities of (ii) are valid and the proof is completed. \hfill \Box

**Lemma 4.3.** For $n \geq 2$, the positive coefficients $\eta_{n-k}^{(n)}$ in (1.12) satisfy

(i) $I_{n-k}^{(n)} > \eta_{n-k}^{(n)}$ for $1 \leq k \leq n$, and

$$I_{n-k}^{(n)} - \eta_{n-k}^{(n)} < I_{n-k-1}^{(n)} - \eta_{n-k-1}^{(n)} \quad \text{for } 1 \leq k \leq n - 1.$$

(ii) $J_{n-k}^{(n)} > 3\eta_{n-k}^{(n)}$ for $1 \leq k \leq n - 1$, and

$$J_{n-k}^{(n)} - 3\eta_{n-k}^{(n)} < J_{n-k-1}^{(n)} - 3\eta_{n-k-1}^{(n)} \quad \text{for } 1 \leq k \leq n - 2.$$

**Proof.** By using the definition (4.1) of $I_{n-k}^{(n)}$ and the formula (4.5), one gets

$$I_{n-k}^{(n)} - \eta_{n-k}^{(n)} = \frac{1}{\tau_k^2} \int_{t_{k-1}}^{t_k} (t_k - t)^2 \omega\omega(t_n - t) \, dt > 0 \quad \text{for } 1 \leq k \leq n,$$

and

$$I_{n-k}^{(n)} - \eta_{n-k}^{(n)} = \frac{1}{\tau_k^2} \int_{t_{k-1}}^{t_k} (t_k - t)^2 \omega\omega(t_n - t) \, dt = I_{n-k-1}^{(n)} - \eta_{n-k-1}^{(n)} \quad \text{for } 1 \leq k \leq n - 1.$$

Thus the result (i) is verified. Moreover, the definition (4.2) gives

$$J_{n-k}^{(n)} - 3\eta_{n-k}^{(n)} = -\frac{3}{\tau_k^2} \int_{t_{k-1}}^{t_k} (t_k - t_{k-1})(t_k - t_{k-1} - 2\tau_k/3) \omega\omega(t_n - t) \, dt > 0$$

for $1 \leq k \leq n - 1$ because $(t_n - t)^{-1-\alpha}$ is increasing with respect to $t$ and

$$\int_{t_{k-1}}^{t_k} (t_k - t_{k-1})(t_k - t_{k-1} - 2\tau_k/3) \omega\omega(t_n - t) \, dt = \tau_k^3 \int_{0}^{1} s(s - 2/3) \, ds = 0.$$

In the similar way,

$$J_{n-k}^{(n)} - 3\eta_{n-k}^{(n)} = -\frac{3}{\tau_k^2} \int_{t_{k-1}}^{t_k} (t_k - t_{k-1})(t_k - t_{k-1} - 2\tau_k/3) \omega\omega(t_n - t) \, dt = J_{n-k-1}^{(n)} - 3\eta_{n-k-1}^{(n)} \quad \text{for } 1 \leq k \leq n - 2.$$

They verify the result (ii). It completes the proof. \hfill \Box
4.1 Proof of Theorem 2.1 (a)

It is in the position to show that the discrete kernels $A_j^{(n)}$ in (2.6) are positive and monotonically decreasing with respect to $j$.

Proof of Theorem 2.1 (a). The definitions (2.2)-(2.4) of discrete convolution kernels $a_n^{(n)}$ will be used frequently. With the definitions (1.11)-(1.12), one has $A_0^{(n)} > 0$ and

$$A_{n-k}^{(n)} \geq a_{n-k}^{(n)} - \frac{1}{1 + r_{k+1}} \eta_{n-k}^{(n)} = \int_{t_{k-1}}^{t_k} \frac{t_{k+1} + t_k - 2s}{1 + r_{k+1}} \omega_{1-\alpha}(t_n - s) \, ds > 0 \quad (4.8)$$

for $1 \leq k \leq n - 1$ due to the simple fact $\int_{t_{k-1}}^{t_k} (t_{k+1} + t_k - 2s) \, ds > 0$. It remains to prove the decreasing property $A_{n-k-1}^{(n)} \geq A_{n-k}^{(n)}$ ($n \geq k + 1 \geq 2$) by the four separate cases: (a.1) $k = 1$ for $n = 2$, (a.2) $k = 1$ for $n \geq 3$, (a.3) $2 \leq k \leq n - 2$ for $n \geq 4$, and (a.4) $k = n - 1$ for $n \geq 3$.

(a.1) The case $k = 1$ ($n = 2$). Lemma 4.1 (ii) gives

$$A_0^{(2)} - A_1^{(2)} = \frac{2 - 2\alpha}{2 - \alpha} a_0^{(2)} - a_1^{(2)} + \frac{(2 + r_2)\eta_1^{(2)}}{r_2(1 + r_2)} = \frac{\alpha \omega_{1-\alpha}(\tau_2)}{2 - \alpha} + J_1^{(2)} + \frac{(2 + r_2)\eta_1^{(2)}}{r_2(1 + r_2)} > 0.$$

(a.2) The case $k = 1$ ($n \geq 3$). Applying Lemma 4.1 (i), we reformulate the difference term $A_{n-2}^{(n)} - A_{n-1}^{(n)}$ into a linear combination with nonnegative coefficients,

$$A_{n-2}^{(n)} - A_{n-1}^{(n)} = a_{n-2}^{(n)} - a_{n-1}^{(n)} + \frac{\eta_{n-2}^{(n)}}{r_2} - \frac{\eta_{n-2}^{(n)}}{1 + r_3} = J_{n-2}^{(n)} + J_{n-1}^{(n)} + \frac{\eta_{n-2}^{(n)}}{r_2} - \frac{\eta_{n-2}^{(n)}}{1 + r_3}$$

$$= (I_{n-2}^{(n)} - \eta_{n-2}^{(n)}) + \frac{r_3 \eta_{n-2}^{(n)}}{1 + r_3} + (J_{n-1}^{(n)} - 3\eta_{n-1}^{(n)}) + \frac{(1 + 3r_2)\eta_{n-1}^{(n)}}{r_2}. \quad (4.9)$$

Then Lemma 4.3 (i)-(ii) yields $A_{n-2}^{(n)} > A_{n-1}^{(n)}$ directly.

(a.3) The general cases $k = 2, 3, \ldots, n - 2$ ($n \geq 4$). Lemma 4.1 (i) gives

$$A_{n-k-1}^{(n)} - A_{n-k}^{(n)} = a_{n-k-1}^{(n)} - a_{n-k}^{(n)} + \frac{\eta_{n-k-1}^{(n)}}{r_{k+1}} - \frac{\eta_{n-k}^{(n)}}{1 + r_{k+2}} - \frac{\eta_{n-k+1}^{(n)}}{r_k(1 + r_k)}$$

$$= (I_{n-k-1}^{(n)} - \eta_{n-k-1}^{(n)}) + \frac{r_{k+2} \eta_{n-k-1}^{(n)}}{1 + r_{k+2}} + \frac{\eta_{n-k}^{(n)} - r_k \eta_{n-k+1}^{(n)}}{r_k^2(1 + r_k)}$$

$$+ (J_{n-k}^{(n)} - 3\eta_{n-k}^{(n)}) + \left(\frac{1}{r_{k+1}} + 3 - \frac{1}{r_k(1 + r_k)}\right) \eta_{n-k}^{(n)}. \quad (4.10)$$

With Lemma 4.2 (ii) and Lemma 4.3 (i)-(ii) together with the step-ratio constraint (2.7), the linear combination (4.10) with nonnegative coefficients lead to the desired inequality.

(a.4) The case $k = n - 1$ ($n \geq 3$). By using Lemma 4.1 (ii), we have

$$A_0^{(n)} - A_1^{(n)} = \frac{2 - 2\alpha}{2 - \alpha} a_0^{(n)} - a_1^{(n)} + \frac{(2 + r_n)\eta_1^{(n)}}{r_n(1 + r_n)} - \frac{\eta_2^{(n)}}{r_{n-1}(1 + r_{n-1})}$$

$$= \frac{\alpha \omega_{1-\alpha}(\tau_n)}{2 - \alpha} + (J_1^{(n)} - 3\eta_1^{(n)}) + \frac{\eta_1^{(n)} - r_n \eta_2^{(n)}}{r_{n-1}^2(1 + r_{n-1})}$$

$$+ \left(\frac{2 + r_n}{r_n(1 + r_n)} + 3 - \frac{1}{r_{n-1}^2(1 + r_{n-1})}\right) \eta_1^{(n)}. \quad (4.11)$$

Thus Lemma 4.2 (ii) and Lemma 4.3 (ii) together with the step-ratio constraint (2.7) arrive at the desired inequality, $A_0^{(n)} > A_1^{(n)}$.

In summary, $A_{n-k-1}^{(n)} > A_{n-k}^{(n)} > 0$ for $1 \leq k \leq n - 1$ such that Theorem 2.1 (a) is verified. □
4.2 Proof of Theorem 2.1 (b)-(c)

It is easy to check that the inequalities of Theorem 2.1 (b)-(c) are equivalent to
\[ A_0^{(n-1)} - A_1^{(n-1)} > A_1^{(n-1)} - A_2^{(n-1)} > \cdots > A_{n-3}^{(n-1)} - A_{n-2}^{(n-1)} > A_{n-2}^{(n-1)} - A_{n-1}^{(n)} > 0 \quad \text{for } n \geq 2. \] (4.12)

Thus we shall prove Theorem 2.1 (b)-(c) by the following two technical steps:

**Step 1.** Check the last inequality, \( A_n^{(n)} < A_{n-2}^{(n-1)} \) for \( n \geq 2 \).

**Step 2.** Verify the general cases of (4.12) via the equivalent inequalities,
\[ A_{n-k-1}^{(n)} - A_{n-k}^{(n)} < A_{n-2-k}^{(n-1)} - A_{n-1-k}^{(n-1)} \quad \text{for } 1 \leq k \leq n-2 \quad (n \geq 3). \] (4.13)

**Proof of Theorem 2.1 (b)-(c).** By the formula (4.8), one has
\[ A_n^{(n)} = a_n^{(n)} - \frac{1}{1 + r_2} \eta_n^{(n)} < \int_{t_0}^{t_1} \frac{t_2 + t_1 - 2s}{(1 + r_2) \tau_1} \omega_{1-a}(t_n - s) \, ds = a_{n-2}^{(n-1)} - \frac{1}{1 + r_2} \eta_{n-2}^{(n-2)} \quad \text{for } n \geq 2. \]

According to the definitions (2.6) and (2.4), it leads to \( A_{n-1}^{(n)} < A_{n-2}^{(n-1)} \) for \( n \geq 3 \). For \( n = 2 \), the definitions (2.2) and (2.4) yield that \( A_1^{(2)} < a_0^{(1)} = \frac{1}{1 + r_2} \eta_0^{(1)} < a_0^{(1)} < A_0^{(1)} \). Thus we obtain that
\[ A_{n-2}^{(n-1)} < A_{n-2}^{(n-1)} \quad \text{for } n \geq 2. \]

To complete this proof, it remains to verify (4.13). Recalling the three different expressions (4.9)-(4.11) of the difference term \( A_{n-k-1}^{(n)} - A_{n-k}^{(n)} \), we will consider the three separate cases: (c.1) \( k = 1 \) for \( n \geq 3 \), (c.2) \( 2 \leq k \leq n-3 \) for \( n \geq 5 \), and (c.3) \( k = n-2 \) for \( n \geq 4 \).

**(c.1) The case \( k = 1 \) (\( n \geq 3 \)).** Applying the linear combination form (4.9), Lemma 4.2 (i) and Lemma 4.3 (i)-(ii), we have
\[ A_{n-2}^{(n)} - A_{n-1}^{(n)} < \left( I_{n-3}^{(n-1)} - \eta_{n-3}^{(n-1)} \right) + \frac{r_3 \eta_{n-3}^{(n-1)}}{1 + r_3} \]
\[ + \left( J_{n-2}^{(n-1)} - 3 \eta_{n-2}^{(n-1)} \right) + \frac{(1 + 3r_2) \eta_{n-2}^{(n-1)}}{r_2} = A_{n-3}^{(n-1)} - A_{n-2}^{(n-1)}. \]

**(c.2) The general cases \( k = 2, 3, \cdots, n-3 \) (\( n \geq 5 \)).** By using the equality (4.10), Lemma 4.2 and Lemma 4.3 (i)-(ii) together with the step-ratio constraint (2.7), we derive that
\[ A_{n-k-1}^{(n)} - A_{n-k}^{(n)} < \left( I_{n-k-2}^{(n-1)} - \eta_{n-k-2}^{(n-1)} \right) + \frac{r_{k+2} \eta_{n-k-2}^{(n-1)}}{1 + r_{k+2}} \]
\[ + \left( J_{n-k-1}^{(n-1)} - 3 \eta_{n-k-1}^{(n-1)} \right) + \frac{1}{r_k (1 + r_k)} \left( \eta_{n-k-1}^{(n-1)} - r_k \eta_{n-k}^{(n-1)} \right) \]
\[ + \left( 1 + \frac{1}{r_{k+1}} + 3 - \frac{1}{r_{k+1} (1 + r_{k+1})} \right) \eta_{n-k-1}^{(n-1)} \quad \text{for } 2 \leq k \leq n-2. \] (4.14)

According to the formula (4.11), the case \( k = n-2 \) in the right hand side of the above inequality does not equal to the difference term \( A_{n-1}^{(n-1)} - A_1^{(n)} \) and will be handled in the next step (c.3). At this moment, the equality (4.10) implies that
\[ A_{n-k-1}^{(n)} - A_{n-k}^{(n)} < A_{n-k-2}^{(n-1)} - A_{n-k-1}^{(n-1)} \quad \text{for } 2 \leq k \leq n-3. \]
The case $k = n - 2$ ($n \geq 4$). By considering the equality (4.10) with $k = n - 2$, we apply Lemma 4.2, Lemma 4.3 (ii) and the condition (2.7) to the last three terms and obtain that

$$A_1^{(n)} - A_2^{(n)} < (I_1^{(n)} - q_1^{(n)}) + \frac{r_n}{1 + r_n} n_1^{(n)} + (J_1^{(n-1)} - 3n_1^{(n-1)})$$

$$+ \frac{n_1^{(n-1)}}{r_{n-2}(1 + r_{n-2})} + \left(\frac{1}{r_{n-1}} + 3 - \frac{1}{r_{n-2}(1 + r_{n-2})}\right)n_1^{(n-1)}.$$

Replacing the index $n$ with $n - 1$ in the formulation (4.11), one has

$$A_0^{(n-1)} - A_1^{(n-1)} = \frac{\alpha \omega_{1-\alpha}(\tau_{n-1})}{2 - \alpha} + (J_1^{(n-1)} - 3n_1^{(n-1)}) + \frac{n_1^{(n-1)}}{r_{n-2}(1 + r_{n-2})}$$

$$+ \left(\frac{1}{r_{n-1}(1 + r_{n-1})} + \frac{1}{r_{n-1}} + 3 - \frac{1}{r_{n-2}(1 + r_{n-2})}\right)n_1^{(n-1)}.$$

Thus, by the equality (4.3) with $k = n - 2$, a simple subtraction yields

$$A_1^{(n)} - A_2^{(n)} - (A_0^{(n-1)} - A_1^{(n-1)}) < I_1^{(n)} - n_1^{(n)} - \frac{\alpha \omega_{1-\alpha}(\tau_{n-1})}{2 - \alpha}$$

$$= a_1^{(n)} - \omega_{1-\alpha}(\tau_n + \tau_{n-1}) - n_1^{(n)} - \frac{\alpha \omega_{1-\alpha}(\tau_{n-1})}{2 - \alpha}$$

$$= -\frac{1}{\tau_{n-1}^\alpha \Gamma(2 - \alpha)} \frac{g_5(r_n, \alpha)}{1 + r_n},$$

(4.15)

where $g_5$ is an auxiliary function defined for $0 < \alpha < 1$ and $z \geq 0$.

$$g_5(z, \alpha) := \frac{\alpha}{2 - \alpha} \left[ (z + 1)^{2-\alpha} - z^{2-\alpha} \right] - \alpha (z + 1)^{1-\alpha} + \frac{\alpha (1 - \alpha)}{2 - \alpha} (z + 1).$$

Note that, the first derivative of $g_5$ with respect to $z$ reads

$$\partial_z g_5 = \alpha (1 - \alpha) \int_0^1 [(z + s)^{-\alpha} - (z + 1)^{-\alpha}] \, ds + \frac{\alpha (1 - \alpha)}{2 - \alpha} > 0 \quad \text{for } z > 0$$

such that $g_5(z, \alpha) > g_5(0, \alpha) = 0$. Then the desired inequality follows from (4.15).

All of the inequalities in (4.13) are verified and the proof of Theorem 2.1 (b)-(c) is completed.

5 Numerical experiments

Some numerical examples are presented to support the theoretical results. Always, we use the Fourier pseudo-spectral method on the domain $\Omega = (0, 2\pi)^2$ with $128 \times 128$ uniform grids. In solving the nonlinear system at each time level, a simple fixed-point iteration is adopted with the tolerance of $10^{-12}$. The so-called SOE technique [11] is applied to speedup the FBDF2 formula (1.10) with the absolute tolerance error $\varepsilon := 10^{-12}$ and the cut-off time $\Delta t := \tau_1$.

Example 1. We consider the forced model $\partial_t^\alpha \Phi = \kappa \Delta \mu - g$ by adding a forcing term $g = g(x, t)$ to the time-fractional Cahn-Hilliard model (1.1) on the domain $x \in (0, 2\pi)^2$. Choose the model data $\kappa = 1$, $\epsilon = 0.5$ and $T = 1$ such that the exact solution $\Phi = \omega_{1+\alpha}(t) \sin x \sin y$.

We examine the temporal accuracy by considering the graded mesh $t_k = (k/N)^{\gamma}$ for six different total number $N = 20 \times 2^{m-1}$ ($1 \leq m \leq 6$) such that the temporal errors dominate the numerical error. In each run of the variable-step FBDF2 scheme (3.1), the error $e(N) := \|\Phi^N - \phi^N\|$ at the
Figure 2: Log-log plots of time accuracy for two different fractional orders.

Finally, time $T = 1$ is recorded. Figure 2 depicts the log-log plots of the numerical errors for two different fractional orders $\alpha = 0.4$ and $0.7$ with three grading parameters. As observed, the FBDF2 scheme (3.1) is accurate with the temporal order about $O(\tau_{\min}^{\gamma(3-\alpha)})$, which is in accordance with the previous results in [15,32].

**Example 2.** Setting the mobility $\kappa = 0.01$ and the interfacial thickness $\epsilon = 0.05$, the coarsening dynamics of the time-fractional Cahn-Hilliard model (1.1) is simulated with a random initial field $\phi_0(x) = \text{rand}(x)$, where $\text{rand}(x)$ generates uniform random numbers between $-0.001$ to $0.001$.

To resolve the initial singularity, the graded time mesh $t_k = T_0(k/N_0)^{\gamma}$ with $T_0 = 0.01$, $\gamma = 2$ and $N_0 = 30$ is applied inside the initial period $[0, T_0]$. Taking the predetermined maximum time-
(a) The fractional order $\alpha = 0.2$, at time $t = 10, 30, 50, 100$

(b) The fractional order $\alpha = 0.5$, at time $t = 10, 30, 50, 100$

(c) The fractional order $\alpha = 0.8$, at time $t = 10, 30, 50, 100$

Figure 5: Snapshots of dynamic coarsening processes for different fractional orders $\alpha$.

Figure 3 shows the numerical results by using the adaptive time-stepping strategy (5.1) for the fractional order $\alpha = 0.5$ with three parameters $\eta = 10, 10^2$ and $10^3$, respectively. In Figure 3, the uniform time step $\tau = 5 \times 10^{-3}$ is used as a the reference solution. Figure 3 plots the original energy curves and the associated time-steps. We choose the parameter $\eta = 10^3$ for further simulations since it admits smaller time-steps in the fast varying region.

Figure 4 depicts the numerical results by using the adaptive time-stepping strategy (5.1) with the parameter $\eta = 10^3$ until time $T = 500$. The curves of original energy $E[\phi^n]$ in (1.2) and the associated adaptive time steps are depicted in Figure 4. The adaptive time-stepping approach seems to be efficient for our numerical simulations since the moment at which the energy decays rapidly can be captured with small time steps. As expected, the value of fractional order $\alpha$ significantly affects the coarsening dynamics process and the energy curves always approach the integer-order one as the fractional order $\alpha \to 1$. The phase profiles at four different times are listed in Figure 5 for three different fractional orders $\alpha = 0.2, 0.5, 0.8$, respectively. They are in accordance with the coarsening dynamics processes reported in [10,25].

References

[1] A. Alsaedi, B. Ahmad and M. Kirane, Maximum principle for certain generalized time and space-fractional diffusion equations, Quart. Appl. Math., 73 (2015), pp. 163-175.
[2] M. Al-Maskari and S. Karaa, The time-fractional Cahn-Hilliard equation: analysis and approximation, IMA J. Numer. Anal., 42 (2022), pp. 1831-1865.

[3] K. Cheng, C. Wang and S. Wise, An energy stable BDF2 Fourier pseudo-spectral numerical scheme for the square phase field crystal equation, Comm. Comput. Phys., 26 (2019), pp. 1335-1364.

[4] K. Cheng, C. Wang, S. Wise and X. Yue, A second-order, weakly energy-stable pseudospectral scheme for the Cahn-Hilliard equation and its solution by the homogeneous linear iteration method, J. Sci. Comput., 69 (2016), pp. 1083-1114.

[5] Q. Du, J. Yang and Z. Zhou, Time-fractional Allen-Cahn equations: analysis and numerical methods, J. Sci. Comput., 85 (2020), num. 42.

[6] M. Fritz, M.L. Rajendran and B. Wohlmuth, Time-fractional Cahn-Hilliard equation: well-posedness, degeneracy and numerical solutions, Comp. Math. Appl., 108 (2022), pp. 66-87.

[7] G. Gao, Z. Sun and H. Zhang, A new fractional numerical differentiation formula to approximate the Caputo derivative and its applications, J. Comput. Phys., 259 (2014), pp. 33-50.

[8] R. Hilfer, Applications of Fractional Calculus in Physics, World Scientific, Singapore, 2000.

[9] B. Ji, H.-L. Liao, Y. Gong and L. Zhang, Adaptive second-order Crank-Nicolson time-stepping schemes for time fractional molecular beam epitaxial growth models, SIAM J. Sci. Comput., 42 (2020), pp. B738-B760.

[10] B. Ji, X. Zhu and H.-L. Liao, Energy stability of variable-step L1-type schemes for time-fractional Cahn-Hilliard model, 2022, arXiv:2201.00920v1.

[11] S. Jiang, J. Zhang, Z. Qian and Z. Zhang, Fast evaluation of the Caputo fractional derivative and its applications to fractional diffusion equations, Comm. Comput. Phys., 21 (2017), pp. 650-678.

[12] A.A. Kilbas, H.M. Srivastava and J.J. Trujillo, Theory and Applications of Fractional Differential Equations, Elsevier Science Limited, Amsterdam, 2006.

[13] S. Karaa, Positivity of discrete time-fractional operators with applications to phase-field equations, SIAM J. Numer. Anal., 59 (2021), pp. 2040-2053.

[14] N. Kopteva, Error analysis of the L1 method on graded and uniform meshes for a fractional derivative problem in two and three dimensions, Math. Comp., 88 (2019), pp. 2135-2155.

[15] N. Kopteva, Error analysis of an L2-type method on graded meshes for a fractional-order parabolic problem, Math. Comp., 90 (2021), pp. 19-40.

[16] Z. Li and H.-L. Liao, Stability of variable-step BDF2 and BDF3 methods, SIAM J. Numer. Anal., 60 (2022), pp. 2253-2272.

[17] H.-L. Liao, B. Ji, L. Wang and Z. Zhang, Mesh-robustness of an energy stable BDF2 scheme with variable steps for the Cahn-Hilliard model, J. Sci. Comput., 92 (2022), num. 52, doi: 10.1007/s10915-022-01861-4, see the fully implicit scheme in arXiv: 2102.03731v1.

[18] H.-L. Liao, D. Li and J. Zhang, Sharp error estimate of nonuniform L1 formula for linear reaction-subdiffusion equations, SIAM J. Numer. Anal., 56 (2018), pp. 1112-1133.

[19] H.-L. Liao, W. McLean and J. Zhang, A discrete Grönwall inequality with application to numerical schemes for subdiffusion problems, SIAM J. Numer. Anal., 57 (2019), pp. 218-237.
[20] H.-L. Liao, W. McLean and J. Zhang, A second-order scheme with nonuniform time steps for a linear reaction-subdiffusion equation, Commu. Comput. Phys., 30 (2021), pp. 567-601.

[21] H.-L. Liao, T. Tang and T. Zhou, On energy stable, maximum-bound preserving, second-order BDF scheme with variable steps for the Allen-Cahn equation, SIAM J. Numer. Anal., 58 (2020), pp. 2294-2314.

[22] H.-L. Liao, T. Tang and T. Zhou, An energy stable and maximum bound preserving scheme with variable time steps for time fractional Allen-Cahn equation, SIAM J. Sci. Comput., 43 (2021), pp. A3503-A3526.

[23] H.-L. Liao and Z. Zhang, Analysis of adaptive BDF2 scheme for diffusion equations, Math. Comp., 90 (2021), pp. 1207-1226.

[24] H.-L. Liao, X. Zhu and J. Wang, The variable-step L1 time-stepping scheme preserving a compatible energy law for the time-fractional Allen-Cahn equation, Numer. Math. Theory Method Appl., 2021, to appear.

[25] H. Liu, A. Cheng, H. Wang and J. Zhao, Time-fractional Allen-Cahn and Cahn-Hilliard phase-field models and their numerical investigation, Comp. Math. Appl., 76 (2018), pp. 1876-1892.

[26] C. Lv and C. Xu, Error analysis of a high order method for time-fractional diffusion equations, SIAM J. Sci. Comput., 38 (2016), pp. A2699-A2724.

[27] K. Mustapha, An implicit finite difference time-stepping method for a subdiffusion equation with spatial discretization by finite elements, IMA J. Numer. Anal., 31 (2011), pp. 719-739.

[28] K. Mustapha and J. AlMutawa, A finite difference method for an anomalous subdiffusion equation: theory and applications, Numer. Algor., 61 (2012), pp. 525-543.

[29] C. Quan, T. Tang and J. Yang, How to define dissipation-preserving energy for time-fractional phase-field equations, CSIAM-AM, 1 (2020), pp. 478-490.

[30] C. Quan, T. Tang, B. Wang and J. Yang, A decreasing upper bound of energy for time-fractional phase-field equations, arXiv:2202.12192v1, 2022.

[31] C. Quan and B. Wang, Energy stable L2 schemes for time-fractional phase-field equations, J. Comput. Phys., 458 (2022), num. 111085.

[32] C. Quan and X. Wu, H1-stability of an L2 method on general nonuniform meshes for subdiffusion equation, arXiv:2205.06060v1, 2022.

[33] T. Tang, H. Yu and T. Zhou, On energy dissipation theory and numerical stability for time-fractional phase-field equations, SIAM J. Sci. Comput., 41 (2019), pp. A3757-A3778.

[34] T. Tang, B. Wang and J. Yang, Asymptotic analysis on the sharp interface limit of the time-fractional Cahn-Hilliard equation, SIAM J. Appl. Math., 82 (2022), pp. 773-792.