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ERROR ESTIMATION OF AN IMPROVED HIGH-ORDER SCHEME FOR HIGH DIMENSIONAL TIME-FRACTIONAL NONLINEAR DIFFUSION EQUATION*

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Abstract In this work, an improved numerical scheme for high dimensional time-fractional nonlinear diffusion equation is proposed. By applying the L2 numerical scheme to the time derivative at every step, we obtain a fully discrete scheme exhibiting locally uniform $3-\theta$ order accuracy with a high-dimensional compact finite difference method for spatial discretization. The core idea of this framework lies in reformulating the high-order uniform temporal convergence scheme into the form to enable to the application of the discrete fractional Grönwall inequality. It is shown that the scheme achieves a temporal convergence order of $3-\theta$ and fourth-order spatial accuracy. Several numerical experiments for nonlinear high-dimensional time-fractional diffusion equations are presented to verify the theoretical results.

Keywords Time-fractional nonlinear diffusion equation, error estimation, compact finite difference scheme, high-order temporal scheme.

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1. Introduction

Fractional-order equations capture the memory, long-range correlations, and non-locality of complex systems, remedying the shortfall of integer-order equations that describe only local, instantaneous interactions, such as complex time-dependent dynamics [9], image super-resolution [6], option price [26,37], fluid flow [5].

In this work, we are concerned with the following class of high-dimensional nonlinear time-

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fractional diffusion equations:

$$ {}_0\partial_t^\theta u(\mathbf{x},t) - \sum_{l=1}^{n} \kappa_l \partial_{x_l}^2 u(\mathbf{x},t) = f(\mathbf{x},t,u(\mathbf{x},t)),\ \ \mathbf{x}\in\Omega,\ \ t\in(0,T], \tag{1.1} $$

where $\kappa_l > 0, l = 1, 2, \cdots, n$, $\mathbf{x} = (x_1, x_2, \cdots, x_n) \in \mathbb{R}^n, \partial_{x_l}^2 = \frac{\partial^2}{\partial x_l^2}$, with the dimension of the space being $n \geq 1$ and $\Omega = [-1, 1]^n$, T is a bounded normal number, and $\partial\Omega$ and $\overline{\Omega}$ represent the boundary and closure of Ω, respectively. The equation (1.1) is subject to the following specified initial and boundary conditions:

$$ \begin{aligned} &u(\mathbf{x},0) = \varphi(\mathbf{x}),\ \ \mathbf{x}\in\Omega,\\ &u(\mathbf{x},t) = 0,\ \ \mathbf{x}\in\partial\Omega,\ \ t\in(0,T]. \end{aligned} \tag{1.2} $$

In addition, the notation ${}_0\partial_t^\theta u(\mathbf{x},t)$ stands for the Caputo fractional-order derivative of order θ with

$$ {}_0\partial_t^\theta u(\mathbf{x},t) = \frac{1}{\Gamma(1-\theta)} \int_0^t (t-s)^{-\theta} \frac{\partial u(\mathbf{x},s)}{\partial s} ds,\ \ 0<\theta<1, \tag{1.3} $$

where $\Gamma(\cdot)$ is the Gamma function.

Assuming that the nonlinear source function $f(\mathbf{x}, t, u(\mathbf{x}, t))$ is a continuous function and satisfies the Lipschitz condition, with a positive Lipschitz constant $L > 0$, it can be expressed as

$$ |f(\mathbf{x},t,u_1(\mathbf{x},t)) - f(\mathbf{x},t,u_2(\mathbf{x},t))| \leq L\ |u_1(\mathbf{x},t) - u_2(\mathbf{x},t)|. \tag{1.4} $$

The intrinsic memory dependence in time render the derivation of analytical solutions for nonlinear time-fractional diffusion equations exceptionally challenging. Consequently, scholarly endeavors have predominantly concentrated on devising robust numerical schemes. In [12], they adopted a nonuniform $L1$ scheme for the time Caputo fractional derivative of order $\theta \in (1, 2)$. In [21], a nonlinear time-fractional diffusion model possessing a generalized memory kernel was analyzed via the $L1$ numerical scheme. In [11], an effective high-accuracy numerical scheme was established for tackling time-space-fractional reaction-diffusion models. In [27], a linearized finite difference spectral Galerkin scheme is proposed for nonlinear variable-order time-fractional diffusion reaction equations with fixed delay. The method combines the $L1$ approximation in time with Legendre spectral discretization in space, and avoids iterative treatment of the nonlinear terms. Stability and convergence are theoretically established, while numerical experiments confirm the effectiveness of the proposed scheme. In [10], a linearized finite difference scheme is constructed for two-dimensional nonlinear time-fractional diffusion problems with weak singular solutions. This method combines the backward discretization of nonlinear terms with the $L1$ approximation on a uniform mesh. Strict theoretical analysis has proved the stability and point-by-point time convergence of this scheme, and numerical experiments have further verified the compactness of the theoretical error bound. In [24], a compact difference method with high efficiency was proposed for two-dimensional nonlinear time fractional diffusion wave equations, where a fast nonuniform mesh-based $L2\text{-}1_\sigma$ formula was employed for temporal discretization and the compact difference method was applied for spatial approximation. In [23], an innovative and practical two-grid algorithm based on the nonuniform $L1$ formula was proposed for nonlinear multi-term time-fractional diffusion equations with variable coefficients. In [29], a finite

difference approach founded on the shifted fractional trapezoidal rule with a particular shift parameter was proposed for nonlinear time-fractional diffusion equations. In [15], an effective numerical scheme for nonlinear time-fractional diffusion equations was designed by transforming the original problem into an equivalent integral equation and coupling the fractional rectangle method with the fractional trapezoidal method.

Alikhanov [3] construct an $L2$-type difference approximation operator for Caputo fractional derivatives, and use it to develop difference schemes for the linear time-fractional diffusion equation with temporally $3-\theta$ order accuracy except the first layer. Additionally, the fractional Grönwall inequality is generalized to the $L2$-type scheme. In [1], for the multi-time fractional-order nonlinear Sobolev type convection-diffusion equations with constant delay, a linearized high-order $L2$-compact difference scheme was developed. An efficient numerical approach for distributed-order TFDEs based on the temporal $L1$ formula was presented in [19]. More recently, a spatial sixth-order finite difference scheme was designed for TFDEs with the Caputo-Fabrizio fractional derivative [31]. A second-order accurate temporal finite difference scheme was presented in [2] for the numerical treatment of nonlinear delayed time-fractional diffusion-wave equations. The work in [20] introduced a combined finite difference-local discontinuous Galerkin scheme tailored for the numerical solution of fourth-order time-fractional diffusion-wave problems. A high-accuracy stable scheme targeting time-fractional convection-diffusion-reaction equations was established in [32]. This study [25] proposed a high-order fully discrete discontinuous Galerkin scheme for 2D unsteady natural convection heat transfer governed by tempered fractional constitutive models. In [36], two implicit Alikhanov $L2$-1_σ-based finite difference schemes are developed for variable-coefficient time-fractional reaction-diffusion equations in one and two dimensions, with unconditional stability and $L2$-convergence rigorously established. In [35], they developed an adaptive time-stepping strategy for Volterra subdiffusion with weakly singular kernels, partitioning the domain to apply graded and uniform $L1$ schemes separately. For further details, we refer the reader to [7, 18], and [34]. A linearized compact difference method combined with Richardson extrapolation was developed in [28] to solve nonlinear Sobolev-type delay differential equations. Further reading is suggested in the references [14, 17] and [8].

Most existing studies mainly focus on low-dimensional problems or linear models, while the theoretical analysis for nonlinear high-dimensional time-fractional problems remains relatively limited. However, in general, the constraint condition A1 in (2.3) does not hold for the coefficients of the $L2$ formula developed in [4]. Therefore, the discrete Grönwall inequality for fractional order presented in [16] cannot be directly applied to this discrete scheme. We find that the existing literature has not presented a systematic and rigorous proof for the high-dimensional temporal fractional nonlinear problems pertaining to the temporal $L2$ scheme and spatial compact finite difference scheme with locally uniform $3-\theta$ order accuracy. The stability and convergence analysis of high-dimensional nonlinear time-fractional problems is generally challenging due to the nonlocal nature of fractional-order derivatives and nonlinear coupling effects. This paper provides a rigorous analysis of the proposed method for solving high-dimensional nonlinear fractional partial differential equations (FPDEs) using discrete fractional Grönwall-type inequalities.

The framework of the paper is as follows. Section 2 is devoted to introducing a high-order numerical scheme based on the $L2$ formulation, and elaborates on the validity conditions for the discrete fractional Grönwall-type inequalities. Section 3 applies the discrete fractional Grönwall-type inequality to rigorously establish the convergence and stability of the improved fully discrete scheme, which achieves high-order accuracy in both space and time. Section 4

presents numerical results obtained with the proposed scheme for FPDEs featuring smooth solution. Section 5 concludes with a brief summary.

2. Numerical method for the temporal discretization

We introduce a linearized fully discrete numerical method for the time-fractional nonlinear diffusion problem governed by the Caputo-type derivative For the temporal discretization of equations (1.1)-(1.2), we adopt an $L2$-type discretization scheme to approximate the Caputo time-fractional derivative, employing a third-order extrapolation technique to approximate the nonlinear term. Meanwhile, for the spatial discretization, we construct and implement an improved compact difference operator to approximate the spatial derivatives.

Considering the time grid of this problem as $0 = t_0 < t_1 < \cdots < t_K = T$, where an equidistant temporal mesh $t_k = k\Delta t$, $k = 0, 1, \cdots, K$, and the step size $\Delta t = \frac{T}{K}$. The $L1$ formula is derived by directly applying the piecewise linear polynomial approximation of $\frac{\partial u(\mathbf{x},s)}{\partial s}$ in (1.3), its expression is given as

$$ {}_0\partial_t^\theta u(\mathbf{x}, t_k) = {}_0^{L1}\partial_{\Delta t}^\theta u(\mathbf{x}, t_k) + R^k = \sum_{j=1}^{k} \bar{a}_{k-j}^{(\theta)} \left[u(\mathbf{x}, t_j) - u(\mathbf{x}, t_{j-1})\right] + R^k, \tag{2.1} $$

where

$$ \bar{a}_j^{(\theta)} = \frac{\Delta t^{-\theta}}{\Gamma(2-\theta)}\left[(j+1)^{1-\theta} - j^{1-\theta}\right]. $$

The detailed derivation process of (2.1) can be found in reference [17]. The proposed theory requires that $\bar{a}_j^{(\theta)}$ satisfy the following two conditions:

A1: The discrete kernel demonstrates positive definiteness and monotonicity, which satisfies

$$ \bar{a}_0^{(\theta)} \geq \bar{a}_1^{(\theta)} \geq \bar{a}_2^{(\theta)} \geq \cdots \geq \bar{a}_{k-1}^{(\theta)} > 0, \quad \text{for } 1 \leq k \leq K. \tag{2.2} $$

A2: The discrete kernels satisfy a uniform lower bound condition with some positive constant $\pi_{\bar{a}} > 0$, and the kernel

$$ \bar{a}_{k-j}^{(\theta)} \geq \frac{1}{\pi_{\bar{a}}\Delta t}\int_{t_{j-1}}^{t_j} \frac{(t_k - \eta)^{-\theta}}{\Gamma(1-\theta)} d\eta, \quad \text{for } 1 \leq j \leq k \leq K. \tag{2.3} $$

To proceed with the numerical approximation, we construct a uniform grid to discretize the problem. The spatial step size in the kth direction is given separately as $\Delta h_l = 2/M_l$. Each spatial domain is discretized such that M_l for $l = 1, 2, \cdots, n$ and K are positive integers defining the grid. The notation used throughout this paper mainly follows [33].

For $1 \leq l \leq n$, we define $\Theta_l = \{j \in \mathbf{N}^+ | 1 \leq j \leq M_l - 1\}$ and $\ddot{\Theta}_l = \{j \in \mathbf{N}^+ | 0 \leq j \leq M_l\}$, $\psi = \prod_{l=1}^{n} \Theta_l$, $\ddot{\psi} = \prod_{l=1}^{n} \ddot{\Theta}_l$ and $\partial\ddot{\psi} = \ddot{\psi}\backslash\psi$. For simplicity, we set a multi-index $J = (j_1, j_2, \cdots, j_n)$ and denote $\mathbf{x}_J = (x_{1,j_1}, x_{2,j_2}, \cdots, x_{n,j_n})$. The exact function $u_J^k = u(\mathbf{x}_J, t_k)$ for $J \in \ddot{\psi}$ and $0 \leq k \leq K$. The corresponding numerical solutions of u at the point $(\mathbf{x}_J, t_k)$ are denoted by U_J^k.

2.1. The L2 formula for the temporal discretization

We establish an expression for the $L2$ formula in this subsection. First, we employ quadratic Lagrange interpolation with the nodes t_{j-1}, t_j, t_{j+1} to approximate $u(\cdot,t)$ on the subinterval $[t_j, t_{j+1}]$, which is given by:

$$L_{[t_j,t_{j+1}]}u(\cdot,t) = \varpi_{0,j}(t)u(\cdot,t_{j-1}) + \varpi_{1,j}(t)u(\cdot,t_j) + \varpi_{2,j}(t)u(\cdot,t_{j+1}), \tag{2.4}$$

where $\varpi_{i,j}(t), i = 0,1,2$ is denoted the quadratic Lagrangian interpolation basis functions at points t_{j-1}, t_j, t_{j+1}, which are defined as follows:

$$\varpi_{0,j}(t) = \frac{(t-t_j)(t-t_{j+1})}{2\Delta t^2},\ \varpi_{1,j}(t) = \frac{(t-t_{j-1})(t-t_{j+1})}{-\Delta t^2},\ \varpi_{2,j}(t) = \frac{(t-t_{j-1})(t-t_j)}{2\Delta t^2}.$$

Let $\Delta u(\cdot,t_k) = u(\cdot,t_k) - u(\cdot,t_{k-1})$, $\Delta u(\cdot,t_0) = u(\cdot,t_0)$ for all $k \geq 1$. When $k = 1,2$, we use ${}_0\partial_t^\theta\big(L_{[t_0,t_2]}u\big)(\cdot,t_1)$ and ${}_0\partial_t^\theta\big(L_{[t_0,t_2]}u\big)(\cdot,t_2)$ to approximate ${}_0\partial_t^\theta u(\cdot,t_1)$ and ${}_0\partial_t^\theta u(\cdot,t_2)$, respectively. We define $\omega_{1-\theta}(t) = \frac{1}{t^\theta\Gamma(1-\theta)}$, then

$$\begin{aligned}
{}_0\partial_t^\theta u(\cdot,t_1) &= \int_0^{t_1} \omega_{1-\theta}(t_1-s)\frac{\partial u(\cdot,s)}{\partial s}ds \\
&\approx \int_0^{t_1} \omega_{1-\theta}(t_1-s)\big[L_{[t_0,t_2]}u(\cdot,s)\big]'ds \\
&= \frac{1}{\Delta t^2}\int_0^{t_1} \omega_{1-\theta}(t_1-s)\Big[(s-t_{\frac{1}{2}})\Delta u(\cdot,t_2) - (s-t_{\frac{3}{2}})\Delta u(\cdot,t_1)\Big]ds \\
&= B_1^1\Delta u(\cdot,t_1) + B_1^2\Delta u(\cdot,t_2) \\
&\doteq {}_0^{L2}\partial_{\Delta t}^\theta u(\cdot,t_1),
\end{aligned} \tag{2.5}$$

$$\begin{aligned}
{}_0\partial_t^\theta u(\cdot,t_2) &= \int_0^{t_2} \omega_{1-\theta}(t_2-s)\frac{\partial u(\cdot,s)}{\partial s}ds \\
&\approx \int_0^{t_2} \omega_{1-\theta}(t_2-s)\big[L_{[t_0,t_2]}u(\cdot,s)\big]'ds \\
&= \frac{1}{\Delta t^2}\int_0^{t_2} \omega_{1-\theta}(t_2-s)\big[(s-t_{\frac{1}{2}})\Delta u(\cdot,t_2) - (s-t_{\frac{3}{2}})\Delta u(\cdot,t_1)\big]ds \\
&= B_2^1\Delta u(\cdot,t_1) + B_2^2\Delta u(\cdot,t_2) \\
&\doteq {}_0^{L2}\partial_{\Delta t}^\theta u(\cdot,t_2),
\end{aligned} \tag{2.6}$$

where $t_{\frac{k}{2}} = t_0 + \frac{k\Delta t}{2}$, and

$$B_j^1 = -\frac{1}{\Delta t^2}\int_0^{t_j} \omega_{1-\theta}(t_j-s)(s-t_{\frac{3}{2}})ds,\ B_j^2 = \frac{1}{\Delta t^2}\int_0^{t_j} \omega_{1-\theta}(t_j-s)(s-t_{\frac{1}{2}})ds, \quad j = 1,2.$$

When $k \geq 3$, we have

$$\begin{aligned}
&{}_0\partial_t^\theta u(\cdot,t_k) \\
&= \int_0^{t_1} \omega_{1-\theta}(t_k-s)\frac{\partial u(\cdot,s)}{\partial s}ds + \sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-s)\frac{\partial u(\cdot,s)}{\partial s}ds
\end{aligned}$$

$$\begin{aligned}
&\approx \int_0^{t_1} \omega_{1-\theta}(t_k-s)\big[L_{[t_0,t_2]}u(\cdot,s)\big]'ds + \sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-s)\big[L_{[t_j,t_{j+1}]}u(\cdot,s)\big]'ds \qquad (2.7)\\
&=\sum_{j=1}^{k} A_{k-j}^k \Delta u(\cdot,t_j)\\
&\doteq {}_0^{L2}\partial_{\Delta t}^{\theta} u(\cdot,t_k),
\end{aligned}$$

where the expression of the coefficient is as follows

$$\begin{aligned}
&A_0^k = \frac{1}{\Delta t^2}\int_{t_{k-1}}^{t_k} \omega_{1-\theta}(t_k-s)(s-t_{k-\frac{3}{2}})ds,\ A_{k-1}^k = -\frac{1}{\Delta t^2}\int_0^{t_2} \omega_{1-\theta}(t_k-s)(s-t_{\frac{3}{2}})ds,\\
&A_{k-2}^k = \frac{1}{\Delta t^2}\Big[\int_0^{t_2} \omega_{1-\theta}(t_k-s)(s-t_{\frac{1}{2}})ds - \int_{t_2}^{t_3} \omega_{1-\theta}(t_k-s)(s-t_{\frac{5}{2}})ds\Big], \qquad (2.8)\\
&A_{k-j}^k = \frac{1}{\Delta t^2}\Big[\int_{t_{j-1}}^{t_j} \omega_{1-\theta}(t_k-s)(s-t_{j-\frac{3}{2}})ds - \int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-s)(s-t_{j+\frac{1}{2}})ds\Big],\\
&\qquad j=3,\cdots,k-1.
\end{aligned}$$

Combining (2.5), (2.6) and (2.7), we have

$${}_0^{L2}\partial_{\Delta t}^{\theta} u(\cdot,t_k) = \begin{cases} B_1^1\Delta u(\cdot,t_1) + B_1^2\Delta u(\cdot,t_2), & k=1,\\ B_2^1\Delta u(\cdot,t_1) + B_2^2\Delta u(\cdot,t_2), & k=2,\\ \sum\limits_{j=1}^{k} A_{k-j}^k \Delta u(\cdot,t_j), & k\geq 3. \end{cases} \qquad (2.9)$$

To use the Grönwall inequality for the proof, we derive the relationship between this $L2$-type discrete scheme and the $L2$ scheme in [1] in the following description. First, we set the basic terms are defined for $l\geq 0$ as:

$$\begin{aligned}
&a_l^{(\theta)} = (l+1)^{1-\theta} - l^{1-\theta},\\
&b_l^{(\theta)} = \frac{1}{2-\theta}\Big[(l+1)^{2-\theta} - l^{2-\theta}\Big] - \frac{1}{2}\Big[(l+1)^{1-\theta} + l^{1-\theta}\Big].
\end{aligned} \qquad (2.10)$$

When $k=3$, according to formula (2.8), we have

$$\begin{aligned}
A_0^k &= \frac{1}{\Delta t^2}\int_{t_2}^{t_3} \omega_{1-\theta}(t_3-s)(s-t_{\frac{3}{2}})ds = \frac{1}{\Delta t^{\theta}\Gamma(2-\theta)}(a_0^{(\theta)} + b_0^{(\theta)}),\\
A_1^k &= \frac{1}{\Delta t^2}\int_0^{t_2} \frac{1}{(t_3-s)^{\theta}\Gamma(1-\theta)}(s-t_{\frac{1}{2}})ds - \frac{1}{\Delta t^2}\int_{t_2}^{t_3} \frac{1}{(t_3-s)^{\theta}\Gamma(1-\theta)}(s-t_{\frac{5}{2}})ds\\
&= \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\left(b_2^{(\theta)} + b_1^{(\theta)} + a_1^{(\theta)} - b_0^{(\theta)}\right),\\
A_2^k &= -\frac{1}{\Delta t^2}\int_0^{t_2} \omega_{1-\theta}(t_3-s)(s-t_{\frac{3}{2}})ds = \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\left(a_2^{(\theta)} - b_1^{(\theta)} - b_2^{(\theta)}\right),
\end{aligned}$$

it can be found that the discrete format is consistent with that of $j=2$ in paper [1].

By definition, for $k \geq 4$,

$$
\begin{aligned}
A_0^k &= \frac{1}{\Gamma(1-\theta)\Delta t^2}\int_{t_{k-1}}^{t_k}(t_k-s)^{-\theta}\big(s-t_{k-\frac{3}{2}}\big)\,ds = \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_0^{(\theta)}+b_0^{(\theta)}\big),\\
A_l^k &= \frac{1}{\Delta t^2}\Big[\int_{t_{k-l-1}}^{t_{k-l}}\omega_{1-\theta}(t_k-s)\big(s-t_{k-l-\frac{3}{2}}\big)ds - \int_{t_{k-l}}^{t_{k-l+1}}\omega_{1-\theta}(t_k-s)\big(s-t_{k-l+\frac{1}{2}}\big)ds\Big]\\
&= \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\left(a_l^{(\theta)}+b_l^{(\theta)}-b_{l-1}^{(\theta)}\right), \qquad 1\leq l\leq k-3,\\
A_{k-2}^k &= \frac{1}{\Delta t^2}\int_0^{t_2}\frac{1}{(t_k-s)^{\theta}\Gamma(1-\theta)}(s-t_{\frac{1}{2}})ds - \frac{1}{\Delta t^2}\int_{t_2}^{t_3}\frac{1}{(t_k-s)^{\theta}\Gamma(1-\theta)}(s-t_{\frac{5}{2}})ds\\
&= \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\left(a_{k-2}^{(\theta)}+b_{k-2}^{(\theta)}+b_{k-1}^{(\theta)}-b_{k-3}^{(\theta)}\right),\\
A_{k-1}^k &= -\frac{1}{\Delta t^2}\int_0^{t_2}\omega_{1-\theta}(t_k-s)(s-t_{\frac{3}{2}})ds = \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\left(a_{k-1}^{(\theta)}-b_{k-1}^{(\theta)}-b_{k-2}^{(\theta)}\right).
\end{aligned}
$$

By summarizing the above derived formulas, the coefficients A_l^k admit the following unified representation that when $k=3$,

$$
A_l^k = \begin{cases}
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_0^{(\theta)}+b_0^{(\theta)}\big), & l=0,\\
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_1^{(\theta)}+b_2^{(\theta)}+b_1^{(\theta)}-b_0^{(\theta)}\big), & l=1,\\
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_2^{(\theta)}-b_2^{(\theta)}-b_1^{(\theta)}\big), & l=2,
\end{cases} \tag{2.11}
$$

and for $k \geq 4$,

$$
A_l^k = \begin{cases}
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_0^{(\theta)}+b_0^{(\theta)}\big), & l=0,\\
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_l^{(\theta)}+b_l^{(\theta)}-b_{l-1}^{(\theta)}\big), & 1\leq l\leq k-3,\\
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_{k-2}^{(\theta)}+b_{k-1}^{(\theta)}+b_{k-2}^{(\theta)}-b_{k-3}^{(\theta)}\big), & l=k-2,\\
\dfrac{1}{\Gamma(2-\theta)\Delta t^{\theta}}\big(a_{k-1}^{(\theta)}-b_{k-1}^{(\theta)}-b_{k-2}^{(\theta)}\big), & l=k-1,
\end{cases} \tag{2.12}
$$

where the basis terms $a_l^{(\theta)}$ and $b_l^{(\theta)}$ are defined for (2.10).

It is straightforward to verify that for $k \geq 3$, the coefficients derived in this paper coincide with those given in [3]. Thus, the approach in [3] is employed for further validation. In contrast to [3], the $L2$ discrete scheme in this paper formulates the coupling form of the first two layers numerically; whereas [3] starts the analysis of $u(\cdot,t)$ from the second layer.

Properties of A_j^k are provided in Lemma 2.1.

Lemma 2.1. *For all $0<\theta<1$, $k \geqslant 3$ and $j=0,1,\cdots,k-1$,the following inequalities are valid:*

$$
A_0^k > A_2^k > A_3^k > \cdots > A_{k-1}^k > 0. \tag{2.13}
$$

Proof. According to Lemma 2.1 in [30], we have $A_2^k > A_3^k > \cdots > A_{k-1}^k > 0$,

$$A_0^k = \frac{a_0^{(\theta)} + b_0^{(\theta)}}{\Gamma(2-\theta)\Delta t^\theta} = \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big(2 - \frac{\theta}{2}\Big) > 0,$$

and the sign of A_1^k is uncertain. Since $\Gamma(2-\theta)\Delta t^\theta > 0$ throughout $0 < \theta < 1$, it suffices to show that the numerator of $A_0^k - A_2^k$ is positive.

When $k = 3$, one has

$$A_2^3 = \frac{a_2^{(\theta)} - b_2^{(\theta)} - b_1^{(\theta)}}{\Gamma(2-\theta)\Delta t^\theta},$$

so that

$$A_0^3 - A_2^3 = \frac{a_0^{(\theta)} + b_0^{(\theta)} - a_2^{(\theta)} + b_2^{(\theta)} + b_1^{(\theta)}}{\Gamma(2-\theta)\Delta t^\theta} = \frac{3^{2-\theta}\theta}{2\Gamma(3-\theta)\Delta t^\theta} > 0.$$

When $k = 4$, the coefficient reads

$$A_2^4 = \frac{a_2^{(\theta)} + b_3^{(\theta)} + b_2^{(\theta)} - b_1^{(\theta)}}{\Gamma(2-\theta)\Delta t^\theta},$$

and therefore

$$A_0^4 - A_2^4 = \frac{a_0^{(\theta)} + b_0^{(\theta)} - a_2^{(\theta)} - b_3^{(\theta)} - b_2^{(\theta)} + b_1^{(\theta)}}{\Gamma(2-\theta)\Delta t^\theta} = \frac{2^{1-2\theta}}{\Gamma(3-\theta)\Delta t^\theta}\big[(6-\theta)2^\theta - (6+\theta)\big].$$

Since $2^{1-2\theta}/(2-\theta) > 0$, it remains to check that $G(\theta) = (6-\theta)2^\theta - (6+\theta) > 0$ on $\theta \in (0,1)$. One has $G(0) = 0$ and

$$G'(\theta) = 2^\theta\big[(6-\theta)\ln 2 - 1\big] - 1.$$

For $0 < \theta < 1$, the bounds $6 - \theta > 5$ and $2^\theta > 1$ imply $G'(\theta) > 5\ln 2 - 2 > 0$, so G is strictly increasing and $G(\theta) > G(0) = 0$. Thus $A_0^4 > A_2^4$.

When $k \geq 5$, the coefficient lies in the bulk regime:

$$A_2^k = \frac{a_2^{(\theta)} + b_2^{(\theta)} - b_1^{(\theta)}}{\Gamma(2-\theta)\Delta t^\theta},$$

which gives

$$\begin{aligned} A_0^k - A_2^k &= \frac{1}{\Delta t^\theta \Gamma(3-\theta)}[(6-\theta)\cdot 2^{1-\theta} - \frac{8-\theta}{2}\cdot 3^{1-\theta}] \\ &\geq \frac{1}{\Delta t^\theta \Gamma(3-\theta)}[(6-\theta)\cdot 2^{1-\theta} - \frac{(8-\theta)}{2}\cdot(3-\theta)\cdot 2^{-\theta}] \\ &= \frac{2^{-1-\theta}}{\Delta t^\theta \Gamma(3-\theta)}\cdot\theta\cdot(7-\theta) \\ &> 0. \end{aligned}$$

Therefore $A_0^k > A_2^k$ for all $k \geq 5$.

Combining the above three cases, we conclude that $A_0^k > A_2^k > 0$ for every $k \geq 3$.

Therefore, we obtain the desired inequalities (2.13). □

Lemma 2.2. [4] *For $k = 1, 2, \cdots, K$, and a function $u(\cdot, t) \in C^3[0, T]$, we have*

$$ {}_0\partial_t^\theta u(\cdot, t_k) = {}_0^{L2}\partial_{\Delta t}^\theta u(\cdot, t_k) + O(\Delta t^{3-\theta}), \quad 0 < \theta < 1. \tag{2.14} $$

While the $L2$ formula (2.9) can be employed to approximate the Caputo derivatives in (1.1)-(1.2), equation (2.13) reveals that condition A1 in (2.2) originally proposed by Liao [16] fails to hold. Consequently, the theoretical framework established in [16] cannot be directly extended to the present discretization.

Therefore, we will construct an $L2$-type numerical scheme to satisfy the condition A1 in (2.2).

$$ \begin{aligned} {}_0^{L2}\partial_{\Delta t}^\theta u(\cdot, t_k) &= \sum_{j=1}^{k} A_{k-j}^k \Delta u(\cdot, t_j) \\ &= \sum_{j=1}^{k} A_{k-j}^k \left[u(\cdot, t_j) - u(\cdot, t_{j-1})\right] \\ &= q_0^{(\theta),k}\Delta u(\cdot, t_k) + q_1^{(\theta),k}\Delta u(\cdot, t_{k-1}) + \sum_{j=1}^{k} d_{k-j}^{(\theta)}\Delta u(\cdot, t_j) \\ &\triangleq q_0^{(\theta),k}\Delta u(\cdot, t_k) + q_1^{(\theta),k}\Delta u(\cdot, t_{k-1}) + {}_0^{L2}\overline{\partial}_{\Delta t}^\theta u(\cdot, t_k), \end{aligned} \tag{2.15} $$

where ${}_0^{L2}\overline{\partial}_{\Delta t}^\theta u(\cdot, t_k) = \sum_{j=1}^{k} d_{k-j}^{(\theta)}\Delta u(\cdot, t_j)$. According to the corresponding relation between the coefficients, the coefficients satisfy:

$$ \begin{aligned} &q_0^{(\theta),k} + d_0^{(\theta)} = A_0^k, \\ &q_1^{(\theta),k} + d_1^{(\theta)} = A_1^k, \\ &d_j^{(\theta)} = A_j^k, \ j = 2, 3, \cdots, k-1. \end{aligned} \tag{2.16} $$

Furthermore, we require the following inequality to hold

$$ d_0^{(\theta)} > d_1^{(\theta)} > d_2^{(\theta)} > d_3^{(\theta)} > \cdots > d_{k-1}^{(\theta)} > 0. \tag{2.17} $$

According to Lemma 2.1, we know only $d_0^{(\theta)} > d_1^{(\theta)} > d_2^{(\theta)}$ are true. For the purpose of the subsequent proof, we choose

$$ q_0^{(\theta),k} + 3q_1^{(\theta),k} = 0 \quad \text{and} \quad q_0^{(\theta),k} > 0, \ q_1^{(\theta),k} < 0. \tag{2.18} $$

Substituting (2.18) into (2.16), we obtain

$$ d_0^{(\theta)} + 3d_1^{(\theta)} = A_0^k + 3A_1^k = \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big[3(6-\theta)2^{-\theta} - 10 + \frac{5}{2}\theta\Big]. \tag{2.19} $$

Applying (2.19) and $d_1^{(\theta)} < d_0^{(\theta)}$, therefore

$$ d_0^{(\theta)} > \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big[\frac{3}{4}(6-\theta)2^{-\theta} - \frac{5}{2} + \frac{5}{8}\theta\Big]. \tag{2.20} $$

From (2.18), it is known that $q_0^{(\theta),k} > 0$, so there exists

$$d_0^{(\theta)} < A_0^k = \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big(2 - \frac{\theta}{2}\Big). \tag{2.21}$$

Let

$$\begin{aligned} 2 - \frac{\theta}{2} - \Big[\frac{3}{4}(6-\theta)2^{-\theta} - \frac{5}{2} + \frac{5}{8}\theta\Big] &= \frac{3}{8}\Big[12 - 3\theta - (6-\theta)\cdot 2^{1-\theta}\Big] \\ &\geq \frac{3}{8}\left[12 - 3\theta - (6-\theta)(2-\theta)\right] \\ &= \frac{3}{8}\theta(5-\theta) \\ &\geq 0. \end{aligned}$$

Therefore, (2.20) and (2.21) are not contradictory, they are compatible. So there exists such $d_0^{(\theta)}$.

Lemma 2.3. [1] *The operator ${}_0^{L2}\partial_{\Delta t}^\theta u(\cdot, t_k)$ defined in* (2.15) *satisfies the foregoing inequality. It serves as an alternative yet mathematically equivalent form of the L2 formulation in* (2.9)*:*

$$\begin{aligned} u(\cdot,t_k){}_0^{L2}\partial_{\Delta t}^\theta u(\cdot,t_k) &= u(\cdot,t_k)\Big[q_0^{(\theta),k}\Delta u(\cdot,t_k) + q_1^{(\theta),k}\Delta u(\cdot,t_{k-1}) + {}_0^{L2}\bar{\partial}_{\Delta t}^\theta u(\cdot,t_k)\Big] \\ &\geq E_k - E_{k-1} + \frac{1}{2}{}_0^{L2}\bar{\partial}_{\Delta t}^\theta u^2(\cdot,t_k), \end{aligned}$$

where

$$E_k = E_k(q_0^{(\theta),k}, q_1^{(\theta),k}) = \frac{1}{6}q_0^{(\theta),k}u^2(\cdot,t_k) + \frac{2}{3}q_0^{(\theta),k}\Big[u(\cdot,t_k) - \frac{1}{2}u(\cdot,t_{k-1})\Big]^2. \tag{2.22}$$

Remark 2.1. In Lemma 2.8 of Reference [1], equation (2.22) is written as:

$$E_k(q_0^{(\theta),k}, q_1^{(\theta),k}) = \frac{1}{6}q_0^{(\theta),k}u^2(\cdot,t_k) + \frac{1}{3}q_0^{(\theta),k}\Big[u(\cdot,t_k) - \frac{1}{2}u(\cdot,t_{k-1})\Big]^2.$$

After careful calculation, we found that the coefficient $\frac{2}{3}$ before $q_0^{(\theta),k}$ is correct, and the $\frac{1}{3}$ might be a typo.

Based on equations (2.16) and (2.20), we can obtain the final expression as follows:

$$d_0^{(\theta)} + 3d_1^{(\theta)} = A_0^k + 3A_1^k. \tag{2.23}$$

According to formula (2.17), we require $d_1^{(\theta)} > d_2^{(\theta)} = A_2^k$. If the term A_2^k is present in the $d_1^{(\theta)}$ part, then it is easier to compare $d_1^{(\theta)}$ and $d_2^{(\theta)}$. The relationship is given as follows:

$$d_0^{(\theta)} = \alpha_1(A_0^k + 3A_1^k) - \alpha_2 A_2^k, \tag{2.24}$$

$$3d_1^{(\theta)} = (1-\alpha_1)(A_0^k + 3A_1^k) + \alpha_2 A_2^k, \quad 0 < \alpha_1 < 1,\ \alpha_2 > 0. \tag{2.25}$$

To satisfy the inequality $d_0^{(\theta)} > d_1^{(\theta)}$ and $d_1^{(\theta)} > d_2^{(\theta)}$, we substitute Eqs. (2.24) and (2.25) to obtain:

$$3\alpha_1(A_0^k + 3A_1^k) - 3\alpha_2 A_2^k > (1-\alpha_1)(A_0^k + 3A_1^k) + \alpha_2 A_2^k,$$

$$(1-\alpha_1)(A_0^k+3A_1^k)+\alpha_2 A_2^k > 3A_2^k,$$

simplification yields the following two expressions:

$$(4\alpha_1-1)(A_0^k+3A_1^k-4A_2^k\frac{\alpha_2}{4\alpha_1-1})>0, \tag{2.26}$$

$$(1-\alpha_1)[A_0^k+3A_1^k-4A_2^k\frac{3-\alpha_2}{4(1-\alpha_1)}]>0. \tag{2.27}$$

Lemma 2.4. *For both* (2.26) *and* (2.27) *to hold, we utilize the fundamental inequality:*

$$A_0^k+3A_1^k-4A_2^k>0, \tag{2.28}$$

along with the parameter constraints:

$$\begin{aligned} &1/4<\alpha_1<1,\\ &0<\frac{\alpha_2}{4\alpha_1-1}\le 1,\\ &0<\frac{3-\alpha_2}{4(1-\alpha_1)}\le 1. \end{aligned} \tag{2.29}$$

Proof. To prove the validity of (2.26) and (2.27), we introduce the fundamental inequality (2.28), combined with the parameter constraint (2.29). The detailed derivations see Appendix A. □

2.2. Construction of the L2-compact difference scheme

The forthcoming lemma gives a detailed exposition of the high-order compact difference operator utilized in spatial discretization. The compact difference operators are defined as follows

$$H_l U_J=\begin{cases}\left(I+\dfrac{\Delta h_l^2}{12}\delta_{x_l}^2\right)u_J, & 1\le l\le n,\ J\in\psi,\\ u_J, & J\in\partial\ddot{\psi},\end{cases}$$

where I is the identity operator and $\delta_{x_l}^2$ is the second-order central difference operator in the x_l-direction.

The definitions of the discrete H^1 semi-norm and the H^1 norm for the grid function u in n dimensions are as follows:

$$\|\nabla_{\Delta h}u\|=\sqrt{\sum_{l=1}^{n}\|\delta_{x_l}u\|^2},\qquad \|u\|_{H^1}=\sqrt{\|u\|^2+\|\nabla_{\Delta h}u\|^2},$$

where $\|\cdot\|$ is the discrete L^2-norm defined by $\|w\|=(\sum\limits_{J\in\psi}\prod\limits_{l=1}^{n}\Delta h_l(w(\mathbf{x}_J))^2)^{\frac{1}{2}}$.

In the present study, instead of utilizing the aforementioned standard H^1 norm, we define the inner product and the $\bar{H}^1$-norm as follows, which will serve as the basic framework for our subsequent theoretical analysis:

$$(u,\bar{u})_{\bar{H}^1}=\sum_{l=1}^{n}\kappa_l(\prod_{m=1,m\neq l}^{n}H_m u,\prod_{m=1,m\neq l}^{n}H_m\bar{u})_{x_l},\ \|u\|_{\bar{H}^1}=\sqrt{\sum_{l=1}^{n}\kappa_l\|\prod_{m=1,m\neq l}^{n}H_m u\|_{x_l}^2},$$

where $||u||_{x_l} = \sqrt{\|\delta_{x_l} u\|^2 - \frac{\Delta h_l^2}{12}\|\delta_{x_l}^2 u\|^2}$, $l = 1, 2, \cdots, n$. The expressions $(u, \bar{u})_{x_l}$ and $(u, \bar{u})_{\bar{H}^1}$ define valid inner products, from which the corresponding norms are derived above.

A direct application of Lemma 1 in [4] shows that the $\|\cdot\|_{\bar{H}^1}$ norm and the classical $\|\cdot\|_{H^1}$ norm are equivalent.

Lemma 2.5. [4] *For $\forall\ u \in u_J^k$, the norm $\|u\|_{H^1}$ and $\|u\|_{\bar{H}^1}$ are equivalent and satisfy the following result:*

$$\sqrt{\Big(\frac{2}{3}\Big)^{2n-1} \min_l\{\kappa_l\}\Big(1+\frac{2}{3n}\Big)^{-1}}\|u\|_{H^1} \le ||u||_{\bar{H}^1} \le \Big(\frac{4}{3}\Big)^{n-1}\sqrt{\max_l\{\kappa_l\}}||u||_{H^1}.$$

Firstly, we introduce the properties of the compact finite difference operator in Lemma 2.6.

Lemma 2.6. [22] *Suppose that $g(x) \in C_x^6[a, b]$ and $\zeta(s) = 5(1-s)^3 - 3(1-s)^5$, then*

$$H_h g''(x_j) = \delta_x^2 g(x_j) + \frac{h^4}{360}\int_0^1 [g^{(6)}(x_j - sh) + g^{(6)}(x_j + sh)]\zeta(s)ds,$$

where $1 \le j \le M_l - 1$.

By substituting the discrete grid points (x_J, t_k) into equation (1.1), we arrive at the following equation:

$$ {}_0\partial_t^\theta u(\mathbf{x}_J, t_k) - \sum_{l=1}^n \kappa_l \partial_{x_l}^2 u(\mathbf{x}_J, t_k) = f(\mathbf{x}_J, t_k, u(\mathbf{x}_J, t_k)). \tag{2.30}$$

Applying the high-dimensional spatial compact finite difference operator $\prod_{m=1}^n H_m$ to both sides of equation (2.30), we directly obtain the spatial semi-discretized formulation of the nonlinear time-fractional diffusion equations as follows:

$$\prod_{m=1}^n H_m \left({}_0^{L2}\partial_t^\theta u(\mathbf{x}_J, t_k)\right) - \prod_{m=1, m\ne l}^n H_m\Big(\sum_{l=1}^n \kappa_l \partial_{x_l}^2 u(\mathbf{x}_J, t_k)\Big) = \prod_{m=1}^n H_m f(\mathbf{x}_J, t_k, u(\mathbf{x}_J, t_k)).$$

Suppose $u(\mathbf{x}, t) \in C_{\mathbf{x},t}^{6,3}(\Omega \times [0, T])$, where $C_{\mathbf{x},t}^{\mathbf{6},3}(\Omega \times (0, T]) = \{\phi || \frac{\partial^6 \phi}{\partial x_i^6}| \le M, i = 1, 2, \cdots, n; |\frac{\partial^3 \phi}{\partial t^3}| \le M, \forall (\mathbf{x}, t) \in \Omega \times [0, T]\}$ and M is a positive constant. Based on Lemma 2.6 and (2.14), the full-discrete numerical scheme for equation (1.1) can be readily obtained:

$$\prod_{m=1}^n H_m \left({}_0^{L2}\partial_{\Delta t}^\theta u(\mathbf{x}_J, t_k)\right) - \sum_{l=1}^n \kappa_l \prod_{m=1, m\ne l}^n H_m \delta_{x_l}^2 u_J^k = \prod_{m=1}^n H_m f(\mathbf{x}_J, t_k, u_J^k) + R_J^k, \tag{2.31}$$

and R_J^k is the truncation error.

When $k \ge 3$, the construction of the difference scheme requires further approximation of the nonlinear term u_J^k within the source term f. A third-order piecewise extrapolation is adopted in the following form to meet the targeted convergence rate:

$$u_J^k = 3u_J^{k-1} - 3u_J^{k-2} + u_J^{k-3} + O(\Delta t^3). \tag{2.32}$$

We can easily confirm this approximation by means of Taylor's theorem. For the case $k \geq 3$, equation (2.31) is approximated by applying the formula given in (2.32), from which the corresponding discrete formulation is derived:

$$\begin{aligned}
&\prod_{m=1}^{n} H_m \left({}_0^{L2}\partial_{\Delta t}^{\theta} u(\mathbf{x}_J, t_k)\right) - \sum_{l=1}^{n} \kappa_l \prod_{\substack{m=1 \\ m\neq l}}^{n} H_m \delta_{x_l}^2 u_J^k = \prod_{m=1}^{n} H_m f(\mathbf{x}_J, t_k, u_J^k) + R_J^k, k = 1, 2, \\
&\prod_{m=1}^{n} H_m \left({}_0^{L2}\partial_{\Delta t}^{\theta} u(\mathbf{x}_J, t_k)\right) - \sum_{l=1}^{n} \kappa_l \prod_{\substack{m=1 \\ m\neq l}}^{n} H_m \delta_{x_l}^2 u_J^k \\
&= \prod_{m=1}^{n} H_m f\left(\mathbf{x}_J, t_k, 3u_J^{k-1} - 3u_J^{k-2} + u_J^{k-3}\right) + \bar{R}_J^k, \ k \geq 3.
\end{aligned} \tag{2.33}$$

According to formula (2.32), we know

$$\bar{R}_j^k = R_j^k + O(\Delta t^3), \tag{2.34}$$

so according to Lemmas 2.2 and 2.6, it can be concluded that the truncation error associated with numerical scheme (2.33) admits an upper bound of $O\big(\Delta t^{3-\theta} + \sum_{l=1}^{n} \Delta h_l^4\big)$.

Finally, we omit the truncation error R_J^k as $k = 1, 2$, $\bar{R}_J^k$ as $k \geq 3$ and substitute the function u_J^k by its numerical approximation U_J^k, We construct the $L2$-compact high-order difference scheme below to approximate the nonlinear high-dimensional time-fractional diffusion equations (1.1)-(1.2):

$$\begin{aligned}
&\prod_{m=1}^{n} H_m \left({}_0^{L2}\partial_{\Delta t}^{\theta} U_J^k\right) - \Lambda_{\Delta h} U_J^k = \prod_{m=1}^{n} H_m f(\mathbf{x}_J, t_k, U_J^k), \ k = 1, 2, \\
&\prod_{m=1}^{n} H_m \left({}_0^{L2}\partial_{\Delta t}^{\theta} U_J^k\right) - \Lambda_{\Delta h} U_J^k = \prod_{m=1}^{n} H_m f\left(\mathbf{x}_J, t_k, 3U_J^{k-1} - 3U_J^{k-2} + U_J^{k-3}\right), \ k \geq 3,
\end{aligned} \tag{2.35}$$

where $\Lambda_{\Delta h} U_J^k = \sum_{l=1}^{n} \kappa_l \prod_{\substack{m=1 \\ m\neq l}}^{n} H_m \delta_{x_l}^2 U_J^k$. The initial and boundary conditions are numerically discretized as follows:

$$\begin{aligned}
&U_J^0 = \varphi(\mathbf{x}_J, t_0), && J \in \ddot{\psi}, \\
&U_J^k = 0, && 0 < k \leq K, \ J \in \partial\ddot{\psi}.
\end{aligned} \tag{2.36}$$

3. Numerical analysis of the proposed compact difference method

To rigorously establish the convergence and stability of the proposed numerical scheme (2.35), we state the following Lemma 3.1.

Lemma 3.1. [4] *For the function $\{U_J^k \mid J \in \ddot{\psi},\ 0 \leq k \leq K\}$ that satisfies $U_J^k = 0$ on all boundaries $J \in \partial\ddot{\psi}$, the following equality holds:*

$$-\Big(\prod_{m=1}^{n} H_m U^k, \Lambda_{\Delta h} U^{\bar{k}}\Big) = \sum_{l=1}^{n} \kappa_l \Big(\prod_{m=1, m\neq l}^{n} H_m U^k, \prod_{m=1, m\neq l}^{n} H_m U^{\bar{k}}\Big)_{\mathbf{x}_l} = (U^k, U^{\bar{k}})_{\bar{H}^1}.$$

Especially, as $k=\bar{k}$,

$$-\Big(\prod_{m=1}^{n} H_m U^k, \Lambda_{\Delta h} U^k\Big) = \|U^k\|^2_{\tilde{H}^1}.$$

The discrete fractional Grönwall inequality given below lays the foundation for analyzing the convergence of our established method.

Lemma 3.2. [13] (Discrete fractional Grönwall-type inequality for the $L1$ discretization scheme) *Let* $\{U^k, g^k \mid k=0,1,2,\cdots\}$ *denote nonnegative sequences where* U^0 *is a given initial value. Let* η *be a positive constant independent of the time step* Δt. *If*

$${}_0^{L1}\partial^{\theta}_{\Delta t} U^k \le \eta U^k + g^k, \quad k \ge 1,$$

then there exists a positive constant $\Delta t^{(*)} = \frac{1}{\sqrt[\theta]{2\Gamma(2-\theta)\eta}}$ *such that whenever* $\Delta t \leqslant \Delta t^{(*)}$, *the following inequality holds:*

$$U^k \le 2\Big(U^0 + \frac{t_k^{\theta}}{\Gamma(1+\theta)} \max_{0\le i\le k} g^i\Big) E_{\theta}\big(2\eta t_k^{\theta}\big), 2 \le k \le K, \tag{3.1}$$

where $E_{\theta}(z) = \sum\limits_{j=0}^{\infty} \frac{z^j}{\Gamma(j\theta+1)}$ *is the Mittag-Leffler function.*

Lemma 3.3. [3] *For all* $\theta \in (0,1)$, *and* $l = 1,2,3,\cdots$, *exists*

$$\begin{aligned} &\frac{1-\theta}{(l+1)^{\theta}} < a_l^{(\theta)} < \frac{1-\theta}{l^{\theta}}, \quad \frac{\theta(1-\theta)}{(l+2)^{\theta+1}} < a_l^{(\theta)} - a_{l+1}^{(\theta)} < \frac{\theta(1-\theta)}{l^{\theta+1}}, \\ &\frac{\theta(1-\theta)}{12(l+1)^{\theta+1}} < b_l^{(\theta)} < \frac{\theta(1-\theta)}{12 l^{\theta+1}}. \end{aligned} \tag{3.2}$$

Lemma 3.4. *In order to satisfy the conditions* $\frac{1}{3}q_0^{(\theta),k} + d_0^{(\theta)} - \sigma \bar{a}_0^{(\theta)} \ge 0$ *and* $d_j^{(\theta)} - \sigma \bar{a}_j^{(\theta)} \ge 0$, $j = 1,2,\cdots,k-1$, *the parameter* σ *must satisfy*

$$\sigma \le \min_{1\le j\le k-1} \left\{ \frac{\frac{1}{3}q_0^{(\theta),k} + d_0^{(\theta)}}{\bar{a}_0^{(\theta)}}, \frac{d_j^{(\theta)}}{\bar{a}_j^{(\theta)}} \right\}. \tag{3.3}$$

Moreover, such a parameter σ *can be chosen explicitly.*

Proof. For a detailed proof, see Appendix B. □

Theorem 3.1. (Convergence) *Suppose the nonlinear term in* (1.1) *satisfies the Lipschitz condition* (1.4). *There exists* $\Delta t^{(*)} > 0$ *such that the compact difference scheme formulated in* (2.35)-(2.36) *admits the a priori estimate when* $\Delta t < \Delta t^{(*)}$:

$$\sum_{k=0}^{K} \|e^k\|^2 \Delta t \le C\Big(\Delta t^{3-\theta} + \sum_{l=1}^{n} \Delta h_l^4\Big)^2, \tag{3.4}$$

where $e_J^k = U_J^k - u_J^k$ *and* $C > 0$ *does not depend on* $\Delta h_l, l = 1,2,\cdots,n$ *and* Δt.

Proof. For $k=1,2$, by subtracting (2.35) from (2.33), the following can be obtained:

$$\prod_{m=1}^{n} H_m \left({}_0^{L2}\partial_{\Delta t}^{\theta} e_J^k\right) - \Lambda_{\Delta h} e_J^k = \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_k, U_J^k) - f(\mathbf{x}_J, t_k, u_J^k)\right] + R_J^k. \tag{3.5}$$

According to (2.9), (3.5) can be rewritten as:

$$\begin{aligned}
&- B_1^1 \prod_{m=1}^{n} H_m e_J^0 + (B_1^1 - B_1^2) \prod_{m=1}^{n} H_m e_J^1 + B_1^2 \prod_{m=1}^{n} H_m e_J^2 - \Lambda_{\Delta h} e_J^1 \\
&= \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_1, U_J^1) - f(\mathbf{x}_J, t_1, u_J^1)\right] + R_J^1, \\
&- B_2^1 \prod_{m=1}^{n} H_m e_J^0 + (B_2^1 - B_2^2) \prod_{m=1}^{n} H_m e_J^1 + B_2^2 \prod_{m=1}^{n} H_m e_J^2 - \Lambda_{\Delta h} e_J^2 \\
&= \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_2, U_J^2) - f(\mathbf{x}_J, t_2, u_J^2)\right] + R_J^2.
\end{aligned}$$

By direct calculation (2.9), the coefficients at the first two time levels are given by

$$(B_1^1, B_1^2, B_2^1, B_2^2) = \frac{\Delta t^{-\theta}}{\Gamma(3-\theta)} \left(\frac{4-3\theta}{2},\ \frac{\theta}{2},\ 2^{-\theta}(2-3\theta),\ 2^{-\theta}(2+\theta)\right). \tag{3.6}$$

Let

$$\begin{aligned}
&-B_1^1 = \Delta t^{-\theta} \bar{G}_0^1, \quad B_1^1 - B_1^2 = \Delta t^{-\theta} \bar{G}_1^1, \quad B_1^2 = \Delta t^{-\theta} \bar{G}_2^1, \\
&-B_2^1 = \Delta t^{-\theta} G_0^1, \quad B_2^1 - B_2^2 = \Delta t^{-\theta} G_1^1, \quad B_2^2 = \Delta t^{-\theta} G_2^1.
\end{aligned} \tag{3.7}$$

Substituting (3.6) into (3.7), we obtain

$$\begin{aligned}
&\bar{G}_0^1 = -\frac{4-3\theta}{2\Gamma(3-\theta)}, \quad \bar{G}_1^1 = \frac{2(1-\theta)}{\Gamma(3-\theta)}, \quad \bar{G}_2^1 = \frac{\theta}{2\Gamma(3-\theta)}, \\
&G_0^1 = -\frac{2^{-\theta}(2-3\theta)}{\Gamma(3-\theta)}, \quad G_1^1 = -\frac{4\theta\, 2^{-\theta}}{\Gamma(3-\theta)}, \quad G_2^1 = \frac{2^{-\theta}(2+\theta)}{\Gamma(3-\theta)}.
\end{aligned} \tag{3.8}$$

For $0<\theta<1$, it follows that $\bar{G}_0^1<0, \bar{G}_1^1>0, \bar{G}_2^1>0, G_1^1<0, G_2^1>0$.
It is easy to obtain by calculation and $e_J^0=0$, we have

$$\begin{aligned}
&\Delta t^{-\theta} \sum_{k=1}^{2} \bar{G}_k^1 \prod_{m=1}^{n} H_m e_J^k - \Lambda_{\Delta h} e_J^1 = \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_1, U_J^1) - f(\mathbf{x}_J, t_1, u_J^1)\right] + R_J^1, \\
&\Delta t^{-\theta} \sum_{k=1}^{2} G_k^1 \prod_{m=1}^{n} H_m e_J^k - \Lambda_{\Delta h} e_J^2 = \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_2, U_J^2) - f(\mathbf{x}_J, t_2, u_J^2)\right] + R_J^2.
\end{aligned} \tag{3.9}$$

We first consider the nonlinear source term $f(\mathbf{x}, t, u)$, which is assumed to satisfy the differential mean value theorem, and there exist positive constants L_k for $k=1,2$ such that

$$f(\mathbf{x}_J, t_k, U_J^k) - f(\mathbf{x}_J, t_k, u_J^k) = L_k\big(U_J^k - u_J^k\big) = L_k e_J^k, \quad \forall k = 1,2, \tag{3.10}$$

and $|L_k| \le \bar{L},\ \forall k = 1, 2.$

Among (3.10), then (3.9) can get

$$\Delta t^{-\theta}\bar{G}_1^1 \prod_{m=1}^{n} H_m e_J^1 + \Delta t^{-\theta}\bar{G}_2^1 \prod_{m=1}^{n} H_m e_J^2 - \Lambda_{\Delta h} e_J^1 = L_1 \prod_{m=1}^{n} H_m e_J^1 + R_J^1, \tag{3.11}$$

$$\Delta t^{-\theta}G_1^1 \prod_{m=1}^{n} H_m e_J^1 + \Delta t^{-\theta}G_2^1 \prod_{m=1}^{n} H_m e_J^2 - \Lambda_{\Delta h} e_J^2 = L_2 \prod_{m=1}^{n} H_m e_J^2 + R_J^2. \tag{3.12}$$

Multiplying $G_1^1 \prod_{l=1}^{n} \Delta h_l \Lambda_{\Delta h} e_J^1$ in equation (3.11) and $-\bar{G}_2^1 \prod_{l=1}^{n} \Delta h_l \Lambda_{\Delta h} e_J^2$ in equation (3.12), by summing over $J \in \psi$ and adding them, we have

$$\begin{aligned}
&\Delta t^{-\theta}\bar{G}_1^1 G_1^1 (\prod_{m=1}^{n} H_m e^1, \Lambda_{\Delta h} e^1) - \Delta t^{-\theta}\bar{G}_2^1 G_2^1 (\prod_{m=1}^{n} H_m e^2, \Lambda_{\Delta h} e^2) \\
&- G_1^1(\Lambda_{\Delta h} e^1, \Lambda_{\Delta h} e^1) + \bar{G}_2^1(\Lambda_{\Delta h} e^2, \Lambda_{\Delta h} e^2) \\
=& G_1^1(L_1 \prod_{m=1}^{n} H_m e^1, \Lambda_{\Delta h} e^1) + G_1^1(R^1, \Lambda_{\Delta h} e^1) \\
&- \bar{G}_2^1(L_2 \prod_{m=1}^{n} H_m e^2, \Lambda_{\Delta h} e^2) - \bar{G}_2^1(R^2, \Lambda_{\Delta h} e^2).
\end{aligned} \tag{3.13}$$

According to Lemma 3.1, equation (3.13) can be rewritten as

$$\begin{aligned}
&-\Delta t^{-\theta}\bar{G}_1^1 G_1^1 \|e^1\|_{\bar{H}^1}^2 + \Delta t^{-\theta}\bar{G}_2^1 G_2^1 \|e^2\|_{\bar{H}^1}^2 - G_1^1 \|\Lambda_{\Delta h} e^1\|^2 + \bar{G}_2^1 \|\Lambda_{\Delta h} e^2\|^2 \\
=& -G_1^1 L_1 \|e^1\|_{\bar{H}^1}^2 + \bar{G}_2^1 L_2 \|e^2\|_{\bar{H}^1}^2 - G_1^1[-(R^1, \Lambda_{\Delta h} e^1)] + \bar{G}_2^1[-(R^2, \Lambda_{\Delta h} e^2)] \\
\le& -G_1^1 \bar{L} \|e^1\|_{\bar{H}^1}^2 + \bar{G}_2^1 \bar{L} \|e^2\|_{\bar{H}^1}^2 - \frac{1}{2} G_1^1 \big(\|R^1\|^2 + \|\Lambda_{\Delta h} e^1\|^2\big) \\
&+ \frac{1}{2} \bar{G}_2^1 \big(\|R^2\|^2 + \|\Lambda_{\Delta h} e^2\|^2\big),
\end{aligned} \tag{3.14}$$

where the above inequality uses $-G_1^1$ and $\bar{G}_2^1$ are all positive numbers depending on θ, and (3.10), (3.14) rearrange, then multiplying both sides of (3.14) by 2, we obtain

$$\begin{aligned}
&-2\Delta t^{-\theta}\bar{G}_1^1 G_1^1 \|e^1\|_{\bar{H}^1}^2 + 2\Delta t^{-\theta}\bar{G}_2^1 G_2^1 \|e^2\|_{\bar{H}^1}^2 - G_1^1 \|\Lambda_{\Delta h} e^1\|^2 + \bar{G}_2^1 \|\Lambda_{\Delta h} e^2\|^2 \\
\le& -2G_1^1 \bar{L} \|e^1\|_{\bar{H}^1}^2 + 2\bar{G}_2^1 \bar{L} \|e^2\|_{\bar{H}^1}^2 - G_1^1 \|R^1\|^2 + \bar{G}_2^1 \|R^2\|^2.
\end{aligned} \tag{3.15}$$

Because $-2\Delta t^{-\theta}\bar{G}_1^1 G_1^1$, $2\Delta t^{-\theta}\bar{G}_2^1 G_2^1$, $-G_1^1$, $\bar{G}_2^1$ are all positive, (3.15) becomes

$$(-2\Delta t^{-\theta}\bar{G}_1^1 G_1^1 + 2G_1^1 \bar{L}) \|e^1\|_{\bar{H}^1}^2 + (2\Delta t^{-\theta}\bar{G}_2^1 G_2^1 - 2\bar{G}_2^1 \bar{L}) \|e^2\|_{\bar{H}^1}^2 \le -G_1^1 \|R^1\|^2 + \bar{G}_2^1 \|R^2\|^2.$$

Let

$$\lambda_1 = \min\left\{-2\Delta t^{-\theta}\bar{G}_1^1 G_1^1 + 2G_1^1 \bar{L}, 2\Delta t^{-\theta}\bar{G}_2^1 G_2^1 - 2\bar{G}_2^1 \bar{L}\right\},\ \lambda_2 = \max\left\{-G_1^1,\ \bar{G}_2^1\right\}. \tag{3.16}$$

For sufficiently small $\Delta t > 0$, by using (3.16) and (3.17) can be rewritten as

$$\|e^1\|_{\bar{H}^1}^2 + \|e^2\|_{\bar{H}^1}^2 \le \frac{\lambda_2}{\lambda_1} \left(\|R^1\|^2 + \|R^2\|^2\right). \tag{3.17}$$

Therefore, we have

$$\|e^k\|_{\bar{H}^1} \leq C\big(\Delta t^{3-\theta} + \sum_{l=1}^{n} \Delta h_l^4\big), \quad k = 1, 2. \tag{3.18}$$

Next, we will prove (3.4) as $k \geq 3$. By subtracting (2.35) from (2.33) for the second row, the following can be obtained:

$$\prod_{m=1}^{n} H_m \left({}_0^{L2}\partial_{\Delta t}^{\theta} e_J^k\right) - \Lambda_{\Delta h} e_J^k = \prod_{m=1}^{n} H_m \rho_J^k + \bar{R}_J^k, \tag{3.19}$$

in which

$$\rho_J^k = f\big(\mathbf{x}_J, t_k, 3U_J^{k-1} - 3U_J^{k-2} + U_J^{k-3}\big) - f\big(\mathbf{x}_J, t_k, 3u_J^{k-1} - 3u_J^{k-2} + u_J^{k-3}\big).$$

Considering the key equality (2.15), we multiply each side of (3.19) by the scalar $-\prod_{l=1}^{n} \Delta h_l \Lambda_{\Delta h} e_J^k$, this yields

$$\begin{aligned} &-\big(\prod_{m=1}^{n} H_m({}_0^{L2}\partial_{\Delta t}^{\theta} e^k), \Lambda_{\Delta h} e^k\big) + \big(\Lambda_{\Delta h} e^k,\ \Lambda_{\Delta h} e^k\big) \\ =&-\big(\prod_{m=1}^{n} H_m \rho^k,\ \Lambda_{\Delta h} e^k\big) - \big(\bar{R}^k,\ \Lambda_{\Delta h} e^k\big). \end{aligned} \tag{3.20}$$

The second term in equality (3.20) is estimated in the following way:

$$\big(\Lambda_{\Delta h} e^k,\ \Lambda_{\Delta h} e^k\big) = \|\Lambda_{\Delta h} e^k\|^2. \tag{3.21}$$

Next, we will estimate the first term on the right of (3.20). Using the inverse estimate $\|\delta_{x_m}^2 v\| \leq \frac{2}{\Delta h_m}\|\delta_{x_m} v\| \leq \frac{4}{\Delta h_m^2}\|v\|, m = 1, 2, \cdots, n$, we have

$$\|H_m v\| = \|(I + \frac{\Delta h_m^2}{12}\delta_{x_m}^2)v\| \leq \|v\| + \frac{\Delta h_m^2}{12}\|\delta_{x_m}^2 v\| \leq \frac{4}{3}\|v\|.$$

Applying this estimate successively gives

$$\|\prod_{m=1}^{n} H_m v\| = \|H_1(\prod_{m=2}^{n} H_m v)\| \leq \frac{4}{3}\|\prod_{m=2}^{n} H_m v\| \leq \cdots \leq \Big(\frac{4}{3}\Big)^n \|v\|.$$

Thus, we have

$$\|\prod_{m=1}^{n} H_m v\| \leq C_H \|v\|,$$

where $C_H = (\frac{4}{3})^n$ is independent of the mesh sizes.

Consequently, by applying the Cauchy–Schwarz inequality and Young's inequality successively, we obtain

$$-(\prod_{m=1}^{n} H_m \rho^k, \Lambda_{\Delta h} e^k) \leq |(\prod_{m=1}^{n} H_m \rho^k, \Lambda_{\Delta h} e^k)|$$

$$\begin{aligned}&\le C_H\|\rho^k\|\,\|\Lambda_{\Delta h}e^k\|\\&\le \frac{1}{2}\|\Lambda_{\Delta h}e^k\|^2+\frac{C_H^2}{2}\|\rho^k\|^2.\end{aligned}\tag{3.22}$$

By the Lipschitz assumption (1.4),

$$\begin{aligned}\|\rho^k\|^2&=\left\|f\big(\mathbf{x}_J,t_k,3U^{k-1}-3U^{k-2}+U^{k-3}\big)-f\big(\mathbf{x}_J,t_k,3u^{k-1}-3u^{k-2}+u^{k-3}\big)\right\|^2\\&\le L^2\left\|3e^{k-1}-3e^{k-2}+e^{k-3}\right\|^2\\&\le 2L^2\|e^{k-3}\|^2+2L^2\|-3e^{k-2}+3e^{k-1}\|^2\\&\le 36L^2\|e^{k-1}\|^2+36L^2\|e^{k-2}\|^2+2L^2\|e^{k-3}\|^2.\end{aligned}$$

According to Lemma 2.5,

$$\|e^j\|\le\|e^j\|_{H^1}\le C_P\|e^j\|_{\bar{H}^1},$$

where $C_P=\frac{1}{\sqrt{\left(\frac{2}{3}\right)^{2n-1}\min_l\{\kappa_l\}\left(1+\frac{2}{3n}\right)^{-1}}}$. We further have

$$\|\rho^k\|^2\le 36C_P^2L^2\|e^{k-1}\|^2_{\bar{H}^1}+36C_P^2L^2\|e^{k-2}\|^2_{\bar{H}^1}+2C_P^2L^2\|e^{k-3}\|^2_{\bar{H}^1}.\tag{3.23}$$

The last term in (3.20) is estimated as

$$-\big(\bar{R}^k,\ \Lambda_{\Delta h}e^k\big)\le\frac{1}{2}\|\bar{R}^k\|^2+\frac{1}{2}\|\Lambda_{\Delta h}e^k\|^2.\tag{3.24}$$

Substituting (3.21), (3.22) and (3.24) into (3.20), we obtain

$$-\big(\prod_{m=1}^{n}H_m({}_0^{L2}\partial^{\theta}_{\Delta t}e^k),\,\Lambda_{\Delta h}e^k\big)\le\frac{C_H^2}{2}\|\rho^k\|^2+\frac{1}{2}\|\bar{R}^k\|^2.\tag{3.25}$$

Since different values of k correspond to different discrete schemes, we discuss the different values of k separately. When $k=3$, substituting the discrete scheme in (2.9), the first term of (3.25) can be expanded in discrete form as follows:

$$\begin{aligned}&-\big(\prod_{m=1}^{n}H_m({}_0^{L2}\partial^{\theta}_{\Delta t}e^3),\,\Lambda_{\Delta h}e^3\big)\\&=\Big({}_0^{L2}\partial^{\theta}_{\Delta t}e^3,\,e^3\Big)_{\bar{H}^1}\\&=\big(A_2^3(e^1-e^0)+A_1^3(e^2-e^1)+A_0^3(e^3-e^2),\,e^3\big)_{\bar{H}^1}\\&=-A_2^3(e^0,e^3)_{\bar{H}^1}+(A_2^3-A_1^3)(e^1,e^3)_{\bar{H}^1}+(A_1^3-A_0^3)(e^2,e^3)_{\bar{H}^1}+A_0^3(e^3,e^3)_{\bar{H}^1}.\end{aligned}\tag{3.26}$$

Substitute (3.26) into (3.25) and rearranging the terms, we obtain

$$\begin{aligned}A_0^3(e^3,e^3)_{\bar{H}^1}\le{}&A_2^3(e^0,e^3)_{\bar{H}^1}+(A_1^3-A_2^3)(e^1,e^3)_{\bar{H}^1}+(A_0^3-A_1^3)(e^2,e^3)_{\bar{H}^1}\\&+\frac{C_H^2}{2}\|\rho^k\|^2+\frac{1}{2}\|\bar{R}^k\|^2.\end{aligned}\tag{3.27}$$

It follows from Lemma 2.1 that $A_0^3 > 0$. Setting $A_0^3 = \frac{4-\theta}{2\,\Gamma(3-\theta)\Delta t^\theta} \doteq \frac{1}{g_0}$, we define

$$g_1 = g_0 A_2^3, \quad g_2 = g_0(A_1^3 - A_2^3), \quad g_3 = g_0(A_0^3 - A_1^3).$$

Because of $g_0 = \frac{1}{A_0^3} = \frac{2\,\Gamma(3-\theta)\Delta t^\theta}{4-\theta}$, dividing both sides of (3.27) by A_0^3, we obtain

$$(e^3, e^3)_{\bar{H}^1} \le g_1(e^0, e^3)_{\bar{H}^1} + g_2(e^1, e^3)_{\bar{H}^1} + g_3(e^2, e^3)_{\bar{H}^1} + \frac{1}{2} g_0 C_H^2 \|\rho^k\|^2 + \frac{g_0}{2}\|\bar{R}^k\|^2. \quad (3.28)$$

According to [4], we know $g_1 = \frac{4-\theta-3^{2-\theta}\theta}{4-\theta}, g_2 = \frac{-12+3\theta+4(1+\theta)3^{1-\theta}}{4-\theta}, g_3 = \frac{12-3\theta-(4+\theta)3^{1-\theta}}{4-\theta}$. Therefore, We can calculate that $g_i (i = 1, 2, 3)$ are bounded constants depending only on θ Applying the Cauchy–Schwarz inequality and Young's inequality successively to each cross term of the historical levels, we have

$$g_1(e^0, e^3)_{\bar{H}^1} \le |g_1| \cdot \|e^0\|_{\bar{H}^1} \cdot \|e^3\|_{\bar{H}^1} \le |g_1|^2 \|e^0\|_{\bar{H}^1}^2 + \frac{1}{4}\|e^3\|_{\bar{H}^1}^2, \quad (3.29)$$

$$g_2(e^1, e^3)_{\bar{H}^1} \le |g_2| \cdot \|e^1\|_{\bar{H}^1} \cdot \|e^3\|_{\bar{H}^1} \le |g_2|^2 \|e^1\|_{\bar{H}^1}^2 + \frac{1}{4}\|e^3\|_{\bar{H}^1}^2, \quad (3.30)$$

$$g_3(e^2, e^3)_{\bar{H}^1} \le |g_3| \cdot \|e^2\|_{\bar{H}^1} \cdot \|e^3\|_{\bar{H}^1} \le |g_3|^2 \|e^2\|_{\bar{H}^1}^2 + \frac{1}{4}\|e^3\|_{\bar{H}^1}^2. \quad (3.31)$$

For simplicity, set $C_0 = C_H^2 C_P^2$, which is also independent of the mesh sizes. Substituting (3.23) for $k = 3$, (3.29)–(3.31) into Eq. (3.28) and collecting the dominant terms on the left-hand side, we obtain

$$\begin{aligned}\frac{1}{4}\|e^3\|_{\bar{H}^1}^2 \le\ & |g_1|^2 \|e^0\|_{\bar{H}^1}^2 + |g_2|^2 \|e^1\|_{\bar{H}^1}^2 + |g_3|^2 \|e^2\|_{\bar{H}^1}^2 \\ & + g_0\Big[C_0\big(18L^2\|e^2\|_{\bar{H}^1}^2 + 18L^2\|e^1\|_{\bar{H}^1}^2 + L^2\|e^0\|_{\bar{H}^1}^2\big) + \frac{1}{2}\|\bar{R}^3\|^2\Big].\end{aligned}$$

According to $\|e^0\|_{\bar{H}^1} = 0$ and rearranging into the standard recurrence form,

$$\|e^3\|_{\bar{H}^1}^2 \le C\left(\|e^1\|_{\bar{H}^1}^2 + \|e^2\|_{\bar{H}^1}^2\right) + 2g_0\|\bar{R}^3\|^2. \quad (3.32)$$

Using (2.34) and (3.18), we finally arrive at

$$\|e^3\|_{\bar{H}^1}^2 \le \bar{C}_1\Big(\Delta t^{3-\theta} + \sum_{l=1}^{n} \Delta h_l^4\Big)^2, \quad (3.33)$$

where this recurrence structure holds for $k = 3$.

Following the same derivation for $k = 3$, the corresponding results for $k = 4$ and $k = 5$ are obtained, respectively,

$$\begin{aligned}\|e^4\|_{\bar{H}^1}^2 &\le \bar{C}_2\Big(\Delta t^{3-\theta} + \sum_{l=1}^{n} \Delta h_l^4\Big)^2, \quad k = 4, \\ \|e^5\|_{\bar{H}^1}^2 &\le \bar{C}_3\Big(\Delta t^{3-\theta} + \sum_{l=1}^{n} \Delta h_l^4\Big)^2, \quad k = 5.\end{aligned} \quad (3.34)$$

When $k \geq 6$, we derive the estimates for each term in equality (3.20). Regarding the first term, in view of the definition and Lemma 3.1, we have

$$\begin{aligned} &-\Big(\prod_{m=1}^{n} H_m\left({}_0^{L2}\partial_{\Delta t}^{\theta} e^k\right), \Lambda_{\Delta h} e^k\Big) \\ &= \big({}_0^{L2}\partial_{\Delta t}^{\theta} e^k,\ e^k\big)_{\bar{H}^1} \\ &= \big(q_0^{(\theta),k}\Delta e^k + q_1^{(\theta),k}\Delta e^{k-1},\ e^k\big)_{\bar{H}^1} + \big({}_0^{L2}\bar{\partial}_{\Delta t}^{\theta} e^k,\ e^k\big)_{\bar{H}^1} \\ &\geq E_k - E_{k-1} + \frac{1}{2}{}_0^{L2}\bar{\partial}_{\Delta t}^{\theta}\|e^k\|_{\bar{H}^1}^2, \end{aligned} \tag{3.35}$$

where

$$E_k = \frac{1}{6}q_0^{(\theta),k}\|e^k\|_{\bar{H}^1}^2 + \frac{2}{3}q_0^{(\theta),k}\Big\|e^k - \frac{1}{2}e^{k-1}\Big\|_{\bar{H}^1}^2,$$

here this conclusion can be deduced from Lemma 2.3.

Substituting (3.35) into (3.25), we get

$$E_k - E_{k-1} + \frac{1}{2}{}_0^{L2}\bar{\partial}_{\Delta t}^{\theta}\|e^k\|_{\bar{H}^1}^2 \leq \frac{C_H^2}{2}\|\rho^k\|^2 + \frac{1}{2}\|\bar{R}^k\|^2. \tag{3.36}$$

In the proof process, we denote C_k, $k = 1, 2, 3, \cdots$, as a positive constant that is independent of Δt and $\Delta h_l, i = 1, 2, \cdots, n$. Multiplying inequality (3.36) by Δt, we replace the index k with j and carry out summation for j ranging from 6 to k. Then substitute (3.23) into this inequality, after simplification, we obtain

$$\begin{aligned} &\Delta t\Big[\sum_{j=6}^{k}(E_j - E_{j-1}) + \frac{1}{2}\sum_{j=6}^{k}{}_0^{L2}\bar{\partial}_{\Delta t}^{\theta}\|e^j\|_{\bar{H}^1}^2\Big] \\ &\leq \Delta t\sum_{j=6}^{k}\Big[C_0(18L^2\|e^{j-1}\|_{\bar{H}^1}^2 + 18L^2\|e^{j-2}\|_{\bar{H}^1}^2 + L^2\|e^{j-3}\|_{\bar{H}^1}^2) + \frac{1}{2}\|\bar{R}^j\|^2\Big]. \end{aligned} \tag{3.37}$$

For the first term of the equality (3.37), we have

$$\begin{aligned} &\Delta t\sum_{j=6}^{k}(E_j - E_{j-1}) \\ &= \Delta t(E_k - E_5) \\ &= \Delta t\Big(\frac{1}{6}q_0^{(\theta),k}\|e^k\|_{\bar{H}^1}^2 + \frac{2}{3}q_0^{(\theta),k}\|e^k - \frac{1}{2}e^{k-1}\|_{\bar{H}^1}^2 - \frac{1}{6}q_0^{(\theta),5}\|e^5\|_{\bar{H}^1}^2 - \frac{2}{3}q_0^{(\theta),5}\|e^5 - \frac{1}{2}e^4\|_{\bar{H}^1}^2\Big). \end{aligned} \tag{3.38}$$

It follows from Appendix A that, for $k \geq 5$, $q_0^{(\theta),k}$ is the same expression and remains unchanged.

For the second term of the equality (3.37), we get

$$\begin{aligned} \frac{1}{2}\Delta t\sum_{j=6}^{k}{}_0^{L2}\bar{\partial}_{\Delta t}^{\theta}\|e^j\|_{\bar{H}^1}^2 &= \frac{1}{2}\Delta t\sum_{j=6}^{k}\sum_{n=1}^{j} d_{j-n}^{(\theta)}\left(\|e^n\|_{\bar{H}^1}^2 - \|e^{n-1}\|_{\bar{H}^1}^2\right) \\ &= \frac{1}{2}\Delta t\Big(\sum_{j=1}^{k} d_{k-j}^{(\theta)}\|e^j\|_{\bar{H}^1}^2 - \sum_{i=1}^{5} d_{5-i}^{(\theta)}\|e^i\|_{\bar{H}^1}^2\Big), \end{aligned} \tag{3.39}$$

where we use $\|e^0\|^2_{\bar{H}^1}=0$ in (3.39).

Plugging (3.38) and (3.39) into (3.37), reformulate (3.37) as

$$\begin{aligned}
&\Delta t\Big(\frac{1}{6}q_0^{(\theta),k}\|e^k\|^2_{\bar{H}^1}+\frac{2}{3}q_0^{(\theta),k}\Big\|e^k-\frac{1}{2}e^{k-1}\Big\|^2_{\bar{H}^1}+\frac{1}{2}\sum_{j=1}^{k}d_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}\Big)\\
&\le \Delta t\Big[\frac{1}{6}q_0^{(\theta),5}\|e^5\|^2_{\bar{H}^1}+\frac{2}{3}q_0^{(\theta),5}\Big\|e^5-\frac{1}{2}e^4\Big\|^2_{\bar{H}^1}+\frac{1}{2}\sum_{i=1}^{5}d_{5-i}^{(\theta)}\|e^i\|^2_{\bar{H}^1}\Big]\\
&\quad+\Delta t\sum_{j=6}^{k}\Big[C_0(18L^2\|e^{j-1}\|^2_{\bar{H}^1}+18L^2\|e^{j-2}\|^2_{\bar{H}^1}+L^2\|e^{j-3}\|^2_{\bar{H}^1})+\frac{1}{2}\|\bar{R}^j\|^2\Big]\\
&\le C_1\Big(\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t+\sum_{j=6}^{k}\|\bar{R}^j\|^2\Delta t\Big).
\end{aligned}\tag{3.40}$$

In order to proceed with the proof, a bound on $\sum\limits_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}$ on the right-hand side of (3.40) is required. To this end, we neglect some positive terms and rearrange (3.40) as

$$\Delta t\Big(\frac{1}{6}q_0^{(\theta),k}\|e^k\|^2_{\bar{H}^1}+\frac{1}{2}\sum_{j=1}^{k}d_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}\Big)\le C_1\Big(\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t+\sum_{j=6}^{k}\|\bar{R}^j\|^2\Delta t\Big).\tag{3.41}$$

With the aim of utilizing the Grönwall inequality, we transform (3.41) into the following form:

$$\begin{aligned}
&\Delta t\Big(\frac{1}{3}q_0^{(\theta),k}\|e^k\|^2_{\bar{H}^1}+d_0^{(\theta)}\|e^k\|^2_{\bar{H}^1}+\sum_{j=1}^{k-1}d_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}\Big)\\
&=\Delta t\Big[\Big(\frac{1}{3}q_0^{(\theta),k}+d_0^{(\theta)}\Big)\|e^k\|^2_{\bar{H}^1}+\sum_{j=1}^{k-1}d_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}\Big]\\
&=\Delta t\Big[\Big(\frac{1}{3}q_0^{(\theta),k}+d_0^{(\theta)}-\sigma\bar{a}_0^{(\theta)}\Big)\|e^k\|^2_{\bar{H}^1}+\sum_{j=1}^{k-1}\Big(d_{k-j}^{(\theta)}-\sigma\bar{a}_{k-j}^{(\theta)}\Big)\|e^j\|^2_{\bar{H}^1}+\sigma\sum_{j=1}^{k}\bar{a}_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}\Big]\\
&\le C_2\Big(\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t+\sum_{j=6}^{k}\|\bar{R}^j\|^2\Delta t\Big).
\end{aligned}\tag{3.42}$$

According to Lemma 3.4, we omit some positive terms and reformulate (3.42) as

$$\Delta t\sigma\sum_{j=1}^{k}\bar{a}_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}\le C_2\Big(\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t+\sum_{j=6}^{k}\|\bar{R}^j\|^2\Delta t\Big).\tag{3.43}$$

Denote $\xi^k=\sum\limits_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t$, then $\|e^k\|^2_{\bar{H}^1}=\frac{\xi^k-\xi^{k-1}}{\Delta t}\ge 0$. The left-hand side of (3.43) becomes

$$\Delta t\sigma\sum_{j=1}^{k}\bar{a}_{k-j}^{(\theta)}\|e^j\|^2_{\bar{H}^1}=\sigma\sum_{j=1}^{k}\bar{a}_{k-j}^{(\theta)}(\xi^j-\xi^{j-1}).$$

Because $\sum_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t=\sum_{j=1}^{k}(\xi^j-\xi^{j-1})=\xi^k$, therefore (3.43) can be rewritten as

$$\sigma\sum_{j=1}^{k}\bar{a}^{(\theta)}_{k-j}(\xi^j-\xi^{j-1})\le C_2\Big(\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\xi^k+\sum_{j=6}^{k}\|\bar{R}^j\|^2\Delta t\Big). \tag{3.44}$$

Combining (2.1), (3.44) is equivalent as follows

$${}^{L1}_{0}\partial^{\theta}_{\Delta t}\xi^k\le C_3\xi^k+C_3\Big(\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum_{j=6}^{k}\|\bar{R}^j\|^2\Delta t\Big). \tag{3.45}$$

Applying the discrete Grönwall inequality stated in Lemma 3.2 to (3.45) yields

$$\xi^k\le 2\Big(\xi^0+\frac{t^{\theta}_k}{\Gamma(1+\theta)}\max_{0\le i\le k}g^i\Big)E_{\theta}(2C_3t^{\theta}_k), \tag{3.46}$$

where $g^i=C_3\Big(\sum\limits_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum\limits_{j=6}^{i}\|\bar{R}^j\|^2\Delta t\Big)$.

According to the definition of ξ^k, we know $\xi^0=0$. Using (3.46), we have

$$\begin{aligned}\xi^k&=\sum_{j=1}^{k}\|e^j\|^2_{\bar{H}^1}\Delta t\\&\le\Big(2\frac{t^{\theta}_k}{\Gamma(1+\theta)}\max_{0\le i\le k}C_3\big[\sum_{i=1}^{5}\|e^i\|^2_{\bar{H}^1}+\sum_{j=6}^{i}\|\bar{R}^j\|^2\Delta t\big]\Big)E_{\theta}(2C_3t^{\theta}_k)\\&\le C_4(\Delta t^{3-\theta}+\sum_{l=1}^{n}\Delta h_l^4)^2.\end{aligned} \tag{3.47}$$

If the step size satisfies $\Delta t\le\frac{1}{\sqrt[\theta]{2\Gamma(2-\theta)C_3}}$, now from relation (3.47) and $\sum\limits_{k=0}^{K}\|e^k\|^2\Delta t\le\sum\limits_{k=0}^{K}\|e^k\|^2_{\bar{H}^1}\Delta t$, one can complete the proof of Theorem 3.1. □

Theorem 3.2. (Stability) *The proposed L2-compact difference scheme* (2.35)-(2.36) *is conditionally stable with respect to initial condition perturbations, provided that the conditions presented in Theorem 3.1 hold.*

Proof. Let $\tilde{U}^k_J$ be the numerical solution corresponding to the perturbed initial data $\tilde{\varphi}$, and define the error $\varepsilon^k_J=U^k_J-\tilde{U}^k_J$. By the discretization of the initial and boundary conditions, $\varepsilon^0_J=\varphi-\tilde{\varphi}$. Then $\varepsilon^k_J=0$ for $J\in\partial\ddot{\psi}$.

Subtracting the two sets of discrete schemes in (2.35) yields the error equations:

$$\begin{aligned}&\prod_{m=1}^{n}H_m\big({}^{L2}_{0}\partial^{\theta}_{\Delta t}\varepsilon^k_J\big)-\Lambda_{\Delta h}\varepsilon^k=\prod_{m=1}^{n}H_m\big[f(\mathbf{x}_J,t_k,U^k)-f(\mathbf{x}_J,t_k,\tilde{U}^k)\big],\quad k=1,2,\\&\prod_{m=1}^{n}H_m\big({}^{L2}_{0}\partial^{\theta}_{\Delta t}\varepsilon^k_J\big)-\Lambda_{\Delta h}\varepsilon^k=\prod_{m=1}^{n}H_m\,\bar{\rho}^k_J,\qquad\qquad k\ge 3,\end{aligned} \tag{3.48}$$

where $\bar{\rho}_J^k = f(\mathbf{x}_J, t_k, 3U^{k-1} - 3U^{k-2} + U^{k-3}) - f(\mathbf{x}_J, t_k, 3\tilde{U}^{k-1} - 3\tilde{U}^{k-2} + \tilde{U}^{k-3})$.

For $k = 1, 2$, expanding the fractional time difference operator gives

$$\begin{aligned}
&\Delta t^{-\theta} \sum_{k=0}^{2} \bar{G}_k^1 \prod_{m=1}^{n} H_m \varepsilon_J^k - \Lambda_{\Delta h} \varepsilon_J^1 = \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_1, U_J^1) - f(\mathbf{x}_J, t_1, \tilde{U}_J^1) \right], \\
&\Delta t^{-\theta} \sum_{k=0}^{2} G_k^1 \prod_{m=1}^{n} H_m \varepsilon_J^k - \Lambda_{\Delta h} \varepsilon_J^2 = \prod_{m=1}^{n} H_m \left[f(\mathbf{x}_J, t_2, U_J^2) - f(\mathbf{x}_J, t_2, \tilde{U}_J^2) \right].
\end{aligned} \tag{3.49}$$

Multiplying the first equation in (3.49) by $G_1^1 \Lambda_{\Delta h} \varepsilon^1$ and the second by $-\bar{G}_2^1 \Lambda_{\Delta h} \varepsilon^2$, and adding the resulting identities.

$$\begin{aligned}
&\Delta t^{-\theta} \bar{G}_1^1 G_1^1 \Big(\prod_{m=1}^{n} H_m \varepsilon^1, \Lambda_{\Delta h} \varepsilon^1 \Big) - \Delta t^{-\theta} \bar{G}_2^1 G_2^1 \Big(\prod_{m=1}^{n} H_m \varepsilon^2, \Lambda_{\Delta h} \varepsilon^2 \Big) \\
&- G_1^1 \left(\Lambda_{\Delta h} \varepsilon^1, \Lambda_{\Delta h} \varepsilon^1 \right) + \bar{G}_2^1 \left(\Lambda_{\Delta h} \varepsilon^2, \Lambda_{\Delta h} \varepsilon^2 \right) \\
= &\, G_1^1 \Big(L_1 \prod_{m=1}^{n} H_m \varepsilon^1, \Lambda_{\Delta h} \varepsilon^1 \Big) - \Delta t^{-\theta} \bar{G}_0^1 G_1^1 \Big(\prod_{m=1}^{n} H_m \varepsilon^0, \Lambda_{\Delta h} \varepsilon^1 \Big) \\
&- \bar{G}_2^1 \Big(L_2 \prod_{m=1}^{n} H_m \varepsilon^2, \Lambda_{\Delta h} \varepsilon^2 \Big) + \Delta t^{-\theta} G_0^1 \bar{G}_2^1 \Big(\prod_{m=1}^{n} H_m \varepsilon^0, \Lambda_{\Delta h} \varepsilon^2 \Big),
\end{aligned} \tag{3.50}$$

where L_1, L_2 is derived similarly to (3.10) using the differential mean value theorem.

According to Lemma 3.1, equation (3.50) can be rewritten as

$$\begin{aligned}
&-\Delta t^{-\theta} \bar{G}_1^1 G_1^1 \|\varepsilon^1\|_{\bar{H}^1}^2 + \Delta t^{-\theta} \bar{G}_2^1 G_2^1 \|\varepsilon^2\|_{\bar{H}^1}^2 - G_1^1 \|\Lambda_{\Delta h} \varepsilon^1\|^2 + \bar{G}_2^1 \|\Lambda_{\Delta h} \varepsilon^2\|^2 \\
= &-G_1^1 L_1 \|\varepsilon^1\|_{\bar{H}^1}^2 + \bar{G}_2^1 L_2 \|\varepsilon^2\|_{\bar{H}^1}^2 + \Delta t^{-\theta} \bar{G}_0^1 G_1^1 (\varepsilon^0, \varepsilon^1)_{\bar{H}^1} - \Delta t^{-\theta} G_0^1 \bar{G}_2^1 (\varepsilon^0, \varepsilon^2)_{\bar{H}^1} \\
= &-G_1^1 L_1 \|\varepsilon^1\|_{\bar{H}^1}^2 + \bar{G}_2^1 L_2 \|\varepsilon^2\|_{\bar{H}^1}^2 \\
&+ \Delta t^{-\theta} \Big(\frac{\bar{G}_0^1 G_1^1}{\sqrt{-\bar{G}_1^1 G_1^1}} \varepsilon^0, \sqrt{-\bar{G}_1^1 G_1^1} \varepsilon^1 \Big)_{\bar{H}^1} + \Delta t^{-\theta} \Big(\frac{-G_0^1 \bar{G}_2^1}{\sqrt{\bar{G}_2^1 G_2^1}} \varepsilon^0, \sqrt{\bar{G}_2^1 G_2^1} \varepsilon^2 \Big)_{\bar{H}^1} \\
\le &-G_1^1 \bar{L} \|\varepsilon^1\|_{\bar{H}^1}^2 + \bar{G}_2^1 \bar{L} \|\varepsilon^2\|_{\bar{H}^1}^2 + \frac{1}{2} \Delta t^{-\theta} \Big[\frac{(\bar{G}_0^1)^2 G_1^1}{-\bar{G}_1^1} \|\varepsilon^0\|_{\bar{H}^1}^2 - \bar{G}_1^1 G_1^1 \|\varepsilon^1\|_{\bar{H}^1}^2 \Big] \\
&+ \frac{1}{2} \Delta t^{-\theta} \Big[\frac{(G_0^1)^2 \bar{G}_2^1}{G_2^1} \|\varepsilon^0\|_{\bar{H}^1}^2 + \bar{G}_2^1 G_2^1 \|\varepsilon^2\|_{\bar{H}^1}^2 \Big].
\end{aligned}$$

Following the same arguments as those used in (3.14)-(3.17), the terms involving $\|\varepsilon^1\|_{\bar{H}^1}^2$ and $\|\varepsilon^2\|_{\bar{H}^1}^2$ on the right-hand side can be absorbed into the left-hand side for sufficiently small Δt. Consequently,

$$\|\varepsilon^1\|_{\bar{H}^1}^2 + \|\varepsilon^2\|_{\bar{H}^1}^2 \le C \|\varepsilon^0\|_{\bar{H}^1}^2. \tag{3.51}$$

For $k \ge 3$, following the same arguments as in (3.20) the expression reads

$$-\big(\prod_{m=1}^{n} H_m \big({}_0^{L2}\partial_{\Delta t}^{\theta} \varepsilon^k \big), \Lambda_{\Delta h} \varepsilon^k \big) + \big(\Lambda_{\Delta h} \varepsilon^k, \Lambda_{\Delta h} \varepsilon^k \big) = -\big(\prod_{m=1}^{n} H_m \bar{\rho}^k, \Lambda_{\Delta h} \varepsilon^k \big). \tag{3.52}$$

Substituting (3.21) and (3.22) and applying the Cauchy–Schwarz inequality and Young's inequality, we obtain

$$-\Big(\prod_{m=1}^{n} H_m\big({}_0^{L2}\partial_{\Delta t}^{\theta}\varepsilon^k\big),\, \Lambda_{\Delta h}\varepsilon^k\Big) \le \frac{C_H^2}{2}\|\bar{\rho}^k\|^2. \tag{3.53}$$

A derivation process similar to (3.33) and (3.34), we finally arrive at the unified estimate

$$\|\varepsilon^k\|_{\bar{H}^1}^2 \le C\|\varepsilon^0\|_{\bar{H}^1}^2, \qquad k = 3, 4, 5. \tag{3.54}$$

When $k \ge 6$, similar to (3.36), we obtain

$$\tilde{E}_k - \tilde{E}_{k-1} + \frac{1}{2}\,{}_0^{L2}\bar{\partial}_{\Delta t}^{\theta}\|\varepsilon^k\|_{\bar{H}^1}^2 \le \frac{C_H^2}{2}\|\bar{\rho}^k\|^2, \tag{3.55}$$

where $\tilde{E}_k = \frac{1}{6}q_0^{(\theta),k}\|\varepsilon^k\|_{\bar{H}^1}^2 + \frac{2}{3}q_0^{(\theta),k}\Big\|\varepsilon^k - \frac{1}{2}\varepsilon^{k-1}\Big\|_{\bar{H}^1}^2$.

Following the derivation in (3.47), we can also conclude that

$$\sum_{k=1}^{K}\|\varepsilon^k\|_{\bar{H}^1}^2\Delta t \le C\|\varepsilon^0\|_{\bar{H}^1}^2, \quad k \ge 6.$$

Theorem 3.2 has been completed. □

4. Numerical examples

This section presents three numerical examples of nonlinear time-fractional diffusion equations in different spatial dimensions, so as to validate theoretical conclusions and illustrate the efficiency of the proposed schemes.

These numerical experiments are designed to validate our theoretical convergence results, and further demonstrate the error bounds with respect to the time step Δt and spatial mesh size Δh for the proposed hybrid scheme.

Set $\Delta h = \Delta h_l, l = 1, 2, \cdots, n$, and define

$$e(\Delta t, \Delta h) = \Big(\sum_{k=1}^{K}\|u(\mathbf{x}, t_k) - u_J^k\|^2\Delta t\Big)^{\frac{1}{2}}.$$

The temporal and spatial convergence rates are defined, respectively, by

$$\mathbf{Order}_{\Delta t} = \log_2\left(\frac{e(2\Delta t, \Delta h)}{e(\Delta t, \Delta h)}\right), \qquad \mathbf{Order}_{\Delta h} = \log_2\left(\frac{e(\Delta t, 2\Delta h)}{e(\Delta t, \Delta h)}\right).$$

To investigate the temporal convergence order, we choose a sufficiently small spatial mesh size Δh such that the spatial compact difference discretization error is negligible. Conversely, when studying the spatial convergence behavior, we employ a sufficiently small time step Δt to minimize the influence of temporal $L2$ discretization errors.

Example 4.1. Suppose that $u(\mathbf{x},t) = t^4(x_1-1)^4(x_1+1)^4$ is the smooth exact solution of (1.1) and (1.2), for $\Omega=[-1,1]$. The corresponding source term $f(\mathbf{x},t)$ can be easily derived as follows:

$$\begin{aligned} f(\mathbf{x},t,u(\mathbf{x},t)) = {} & \frac{\Gamma(5)}{\Gamma(5-\theta)}t^{4-\theta}(x_1-1)^4(x_1+1)^4 \\ & -t^4[12(x_1+1)^2(x_1-1)^4+32(x_1+1)^3(x_1-1)^3+12(x_1+1)^4(x_1-1)^2] \\ & +t^{12}(x_1-1)^{12}(x_1+1)^{12}-t^4(x_1-1)^4(x_1+1)^4-u^3(\mathbf{x},t)+u(\mathbf{x},t). \end{aligned}$$

In order to examine the temporal accuracy, we set $K=2^k, k=6,\cdots,9$ and fix $M_1=2^{11}$ for various values of θ, as listed in Table 1. Numerical results show that the convergence orders approach 2.2, 2.4 and 2.6 corresponding to $\theta=0.8,0.6,0.4$, respectively. It is obvious that the temporal accuracy reaches $3-\theta$, which coincides with the conclusion in Theorem 3.1.

Table 1. Temporal errors and convergence rates for $\theta=0.4$, 0.6, 0.8.

Δt	$\theta=0.4$	$\mathbf{Order}_{\Delta t}$	$\theta=0.6$	$\mathbf{Order}_{\Delta t}$	$\theta=0.8$	$\mathbf{Order}_{\Delta t}$
$\frac{1}{64}$	1.118782×10^{-5}	–	2.603670×10^{-5}	–	8.435651×10^{-5}	–
$\frac{1}{128}$	1.693088×10^{-6}	2.72420	4.941835×10^{-6}	2.39743	1.880155×10^{-5}	2.16565
$\frac{1}{256}$	2.596252×10^{-7}	2.70516	9.372152×10^{-7}	2.39859	4.146819×10^{-6}	2.18078
$\frac{1}{512}$	4.033075×10^{-8}	2.68648	1.776480×10^{-7}	2.39936	9.092097×10^{-7}	2.18932

For the spatial accuracy, we take $M_1=2^m, m=3,4,5,6$ for $K=2^{11}$. Numerical simulations of Table 2 reveal that the spatial convergence order is close to 4 for $\theta=0.4,0.6,0.8$.

Table 2. Spatial errors and convergence rates for $\theta=0.4$, 0.6, 0.8.

Δh	$\theta=0.4$	$\mathbf{Order}_{\Delta h}$	$\theta=0.6$	$\mathbf{Order}_{\Delta h}$	$\theta=0.8$	$\mathbf{Order}_{\Delta h}$
$\frac{1}{8}$	4.622451×10^{-3}	–	4.297787×10^{-3}	–	3.937382×10^{-3}	–
$\frac{1}{16}$	3.034842×10^{-4}	3.92896	2.817789×10^{-4}	3.93096	2.575344×10^{-4}	3.93440
$\frac{1}{32}$	1.916536×10^{-5}	3.98505	1.778214×10^{-5}	3.98606	1.621773×10^{-5}	3.98912
$\frac{1}{64}$	1.200140×10^{-6}	3.99723	1.109993×10^{-6}	4.00181	9.912159×10^{-7}	4.03223

Example 4.2. Let $u(\mathbf{x},t)=t^4(x_1-1)^4(x_1+1)^4(x_2-1)^4(x_2+1)^4$ be the smooth exact solution of (1.1) and (1.2), for $\Omega=[-1,1]\times[-1,1]$. The corresponding source term $f(\mathbf{x},t)$ can be easily derived as follows:

$$f(\mathbf{x},t,u(\mathbf{x},t))$$

$$
\begin{aligned}
&= \frac{\Gamma(5)}{\Gamma(5-\theta)} t^{4-\theta}(x_1-1)^4(x_1+1)^4(x_2-1)^4(x_2+1)^4 \\
&\quad -t^4[12(x_1-1)^2(x_1+1)^4(x_2-1)^4(x_2+1)^4 + 32(x_1+1)^3(x_1-1)^3(x_2-1)^4(x_2+1)^4 \\
&\quad +12(x_1+1)^2(x_1-1)^4(x_2-1)^4(x_2+1)^4 + 12(x_1+1)^4(x_1-1)^4(x_2-1)^2(x_2+1)^4 \\
&\quad +32(x_1+1)^4(x_1-1)^4(x_2-1)^3(x_2+1)^3 + 12(x_1+1)^4(x_1-1)^4(x_2-1)^4(x_2+1)^2] \\
&\quad +t^{12}(x_1-1)^{12}(x_1+1)^{12}(x_2-1)^{12}(x_2+1)^{12} - t^4(x_1-1)^4(x_1+1)^4(x_2-1)^4(x_2+1)^4 \\
&\quad -u^3(\mathbf{x},t) + u(\mathbf{x},t).
\end{aligned}
$$

For the temporal accuracy, we choose $K = 2^k, k = 4, \cdots, 7$ with $M_1 = M_2 = 2^{10}$. Numerical results of Table 3 show that the convergence orders approach 2.2, 2.4 and 2.6 corresponding to $\theta = 0.8, 0.6, 0.4$, respectively. It is obvious that the temporal accuracy reaches $3-\theta$, which coincides with the conclusion in Theorem 3.1.

Table 3. Temporal errors and convergence rates for $\theta = 0.4$, 0.6, 0.8.

Δt	$\theta = 0.4$	$\mathbf{Order}_{\Delta t}$	$\theta = 0.6$	$\mathbf{Order}_{\Delta t}$	$\theta = 0.8$	$\mathbf{Order}_{\Delta t}$
$\frac{1}{16}$	9.094856×10^{-5}	–	4.796561×10^{-4}	–	4.935981×10^{-4}	–
$\frac{1}{32}$	1.490327×10^{-5}	2.60942	9.492779×10^{-5}	2.28842	1.173203×10^{-4}	2.07288
$\frac{1}{64}$	2.418199×10^{-6}	2.62362	1.842424×10^{-6}	2.32684	2.686658×10^{-5}	2.12657
$\frac{1}{128}$	3.776326×10^{-7}	2.67888	3.539550×10^{-6}	2.37002	6.000670×10^{-5}	2.16262

For the spatial accuracy, we take $M_1 = M_2 = M = 2^m$, $m = 3, 4, 5$ and set $K = 2^{12}$ in Table 4. Numerical simulations reveal that the spatial convergence order is close to 4 for $\theta = 0.4, 0.6, 0.8$.

Table 4. Spatial errors and convergence rates for $\theta = 0.4$, 0.6, 0.8.

Δh	$\theta = 0.4$	$\mathbf{Order}_{\Delta h}$	$\theta = 0.6$	$\mathbf{Order}_{\Delta h}$	$\theta = 0.8$	$\mathbf{Order}_{\Delta h}$
$\frac{1}{8}$	3.466733×10^{-3}	–	3.273728×10^{-3}	–	3.055873×10^{-3}	–
$\frac{1}{16}$	2.131397×10^{-4}	4.02371	2.009993×10^{-4}	4.02371	1.872741×10^{-4}	4.02836
$\frac{1}{32}$	1.303284×10^{-5}	4.03158	1.228435×10^{-5}	4.03158	1.143660×10^{-5}	4.03342

Example 4.3. We take $u(\mathbf{x},t) = t^4 \sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3)$ as the smooth exact solution of (1.1) and (1.2), for $\Omega = [-1,1]\times[-1,1]\times[-1,1]$. The corresponding source term $f(\mathbf{x},t)$ can be easily derived as follows:

$$f(\mathbf{x},t,u(\mathbf{x},t))$$

$$
\begin{aligned}
&= \frac{\Gamma(5)}{\Gamma(5-\theta)} t^{4-\theta} \sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3) \\
&\quad +12\pi^2 t^4 \sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3) + t^{12}(\sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3))^3 \\
&\quad -t^4 \sin(2\pi x_1)\sin(2\pi x_2)\sin(2\pi x_3) - u^3(\mathbf{x},t) + u(\mathbf{x},t).
\end{aligned}
$$

In order to examine the temporal accuracy, we use a grid refinement strategy with $K = 2^m$, $m = 4, 5, 6$ and fix the spatial grid number $M_1 = M_2 = M_3 = 2^6$, as listed in Table 5. Numerical results show that the convergence orders approach 2.2, 2.4 and 2.6 corresponding to $\theta = 0.8, 0.6, 0.4$, respectively. It is obvious that the temporal accuracy reaches $3 - \theta$, which coincides with the conclusion in Theorem 3.1.

Table 5. Temporal errors and convergence rates for $\theta = 0.4$, 0.6, 0.8.

Δt	$\theta = 0.4$	$\mathbf{Order}_{\Delta t}$	$\theta = 0.6$	$\mathbf{Order}_{\Delta t}$	$\theta = 0.8$	$\mathbf{Order}_{\Delta t}$
$\frac{1}{16}$	5.449342×10^{-4}	–	9.2670838×10^{-5}	–	1.773613×10^{-4}	–
$\frac{1}{32}$	9.330038×10^{-5}	2.54613	1.787688×10^{-5}	2.37402	3.951182×10^{-5}	2.16634
$\frac{1}{64}$	1.546712×10^{-6}	2.59268	3.371133×10^{-5}	2.40679	8.638811×10^{-6}	2.19338

For the spatial accuracy, we take $M_1 = M_2 = M_3 = 2^k$, $k = 3, 4, 5$ and set $K = 2^{10}$ in Table 6, which ensures the temporal error is dominated by the spatial error. Numerical simulations reveal that the spatial convergence order is close to 4 for $\theta = 0.4, 0.6, 0.8$.

Table 6. Spatial errors and convergence rates for $\theta = 0.4$, 0.6, 0.8.

Δh	$\theta = 0.4$	$\mathbf{Order}_{\Delta h}$	$\theta = 0.6$	$\mathbf{Order}_{\Delta h}$	$\theta = 0.8$	$\mathbf{Order}_{\Delta h}$
$\frac{1}{8}$	9.607807×10^{-3}	–	9.563847×10^{-3}	–	9.509576×10^{-3}	–
$\frac{1}{16}$	5.647641×10^{-4}	4.08849	5.621233×10^{-4}	4.08863	5.588264×10^{-4}	4.08891
$\frac{1}{32}$	3.464962×10^{-5}	4.02674	3.448839×10^{-5}	4.02670	3.428954×10^{-5}	4.02656

5. Concluding remarks

This paper proposes an improved numerical scheme for high-dimensional time-fractional nonlinear diffusion equations, combining an improved $L2$-type temporal discretization scheme with locally uniform $3 - \theta$ order and a high-dimensional compact finite differences in space. By equivalently reformulating the high-order temporal scheme, we rigorously establish the convergence of the proposed method. This reformulation enables the direct application of the discrete fractional Grönwall inequality. Theoretical analysis demonstrates that the scheme achieves a

temporal convergence order of $3-\theta$ and a spatial convergence order of four. Numerical experiments corroborate the theoretical predictions, confirming both the accuracy and stability of the scheme. Future work will focus on extending this numerical framework to optimal control problems governed by high-dimensional time-fractional nonlinear diffusion equations based on the sum-of-exponentials approximation to develop a fast algorithm.

Appendix A: The proof of Lemma 2.4.

Proof. We first prove that (2.28) holds. Based on the proof of Lemma 2.3 in [3], we can see that the cases $k=3,4$ have already been proven. We now prove the case $k\geq 5$:

$$\begin{aligned}
A_0^k+3A_1^k-4A_2^k &= \frac{1}{\Gamma(2-\theta)\Delta t^\theta}\Big\{a_0^{(\theta)}+b_0^{(\theta)}+3(b_1^{(\theta)}+a_1^{(\theta)}-b_0^{(\theta)})-4(b_2^{(\theta)}+a_2^{(\theta)}-b_1^{(\theta)})\Big\}\\
&= \frac{1}{\Gamma(3-\theta)\Delta t^\theta}\Big\{\frac{9}{2}\theta-18+(33-\frac{11}{2}\theta)2^{1-\theta}+(2\theta-16)3^{1-\theta}\Big\}\\
&\geqslant \frac{1}{2\Gamma(3-\theta)\Delta t^\theta}\Big\{9(\theta-4)+2^{1-\theta}(-2\theta^2+11\theta+18)\Big\}\\
&\doteq \frac{\Delta t^{-\theta}}{2\Gamma(3-\theta)}\tilde{f}(\theta),
\end{aligned}$$

where $\tilde{f}(\theta)=9(\theta-4)+2^{1-\theta}\left(-2\theta^2+11\theta+18\right)$.

We now prove $\tilde{f}(\theta)\geq 0$. Through computational analysis, it can be derived that $\tilde{f}(0)=0,\tilde{f}(1)=0$, we get

$$\begin{aligned}
&\tilde{f}'(\theta)=9+2^{1-\theta}(-4\theta+11)+2^{1-\theta}\left(-2\theta^2+11\theta+18\right)(-\ln 2),\tilde{f}'(0)>0,\tilde{f}'(1)<0,\\
&\tilde{f}''(\theta)=2^{1-\theta}\left[-4+2(-4\theta+11)(-\ln 2)+\left(-2\theta^2+11\theta+18\right)(-\ln 2)^2\right]\doteq 2^{1-\theta}g(\theta),
\end{aligned}$$

where $g(\theta)=-4+2(-4\theta+11)(-\ln 2)+(-2\theta^2+11\theta+18)(-\ln 2)^2$. In what follows, we prove that $g(\theta)\leq 0$.

Since $g'(\theta)=8\ln 2+(11-4\theta)(\ln 2)^2>0$, $g(\theta)$ is monotonically increasing, so $g(0)<g(\theta)<g(1)$. Substituting the boundary values $g(0)<0$ and $g(1)<0$ yields $g(\theta)<0$ for all θ in the interval.

This implies $\tilde{f}''(\theta)<0$, so $\tilde{f}'(\theta)$ is monotonically decreasing with $\tilde{f}'(1)=-2.7150$ and $\tilde{f}'(0)=6.0467$. Hence, $\tilde{f}(\theta)$ first increases and then decreases, attaining its minimum at the endpoints $\tilde{f}(0)=\tilde{f}(1)=0$. We conclude $\tilde{f}(\theta)\geq 0$, which completes the proof.

We next prove that $q_0^{(\theta),k}>0$. According to equation (2.16), we have:

$$q_0^{(\theta),k}=A_0^k-d_0^{(\theta)}=A_0^k-\alpha_1\left(A_0^k+3A_1^k\right)+\alpha_2A_2^k=(1-\alpha_1)A_0^k-3\alpha_1A_1^k+\alpha_2A_2^k. \quad \text{(A.1)}$$

Substituting the above coefficients into equation (2.12) and expanding yield: For $k=3$,

$$\begin{aligned}
q_0^{(\theta),3} &= \frac{1}{\Delta t^\theta\Gamma(2-\theta)}\Big\{(1-\alpha_1)\Big(a_0^{(\theta)}+b_0^{(\theta)}\Big)-3\alpha_1\Big(a_1^{(\theta)}+b_1^{(\theta)}+b_2^{(\theta)}-b_0^{(\theta)}\Big)\\
&\quad+\alpha_2\Big(a_2^{(\theta)}-b_1^{(\theta)}-b_2^{(\theta)}\Big)\Big\}\\
&= \frac{1}{\Delta t^\theta\Gamma(2-\theta)}\Big\{(1-\alpha_1)a_0^{(\theta)}-3\alpha_1a_1^{(\theta)}+\alpha_2a_2^{(\theta)}\\
&\quad+\Big[(1+2\alpha_1)b_0^{(\theta)}-(3\alpha_1+\alpha_2)\Big(b_1^{(\theta)}+b_2^{(\theta)}\Big)\Big]\Big\}.
\end{aligned} \quad \text{(A.2)}$$

For $k=4$, we have

$$\begin{aligned} q_0^{(\theta),4} &= \frac{1}{\Delta t^\theta \Gamma(2-\theta)}\Big\{(1-\alpha_1)\left(a_0^{(\theta)}+b_0^{(\theta)}\right)-3\alpha_1\left(b_1^{(\theta)}-b_0^{(\theta)}+a_1^{(\theta)}\right) \\ &\quad +\alpha_2\left(b_3^{(\theta)}+b_2^{(\theta)}-b_1^{(\theta)}+a_2^{(\theta)}\right)\Big\} \\ &= \frac{1}{\Delta t^\theta \Gamma(2-\theta)}\Big\{(1-\alpha_1)a_0^{(\theta)}-3\alpha_1 a_1^{(\theta)}+\alpha_2 a_2^{(\theta)}+(1+2\alpha_1)b_0^{(\theta)} \\ &\quad -(3\alpha_1+\alpha_2)b_1^{(\theta)}+\alpha_2\left(b_2^{(\theta)}+b_3^{(\theta)}\right)\Big\}. \end{aligned} \tag{A.3}$$

For $k\geq 5$, we get

$$\begin{aligned} q_0^{(\theta),k} &= \frac{1}{\Delta t^\theta \Gamma(2-\theta)}\Big\{(1-\alpha_1)\Big(a_0^{(\theta)}+b_0^{(\theta)}\Big)-3\alpha_1\Big(b_1^{(\theta)}+a_1^{(\theta)}-b_0^{(\theta)}\Big)+\alpha_2\Big(b_2^{(\theta)}+a_2^{(\theta)}-b_1^{(\theta)}\Big)\Big\} \\ &= \frac{1}{\Delta t^\theta \Gamma(2-\theta)}\Big\{(1-\alpha_1)a_0^{(\theta)}-3\alpha_1 a_1^{(\theta)}+\alpha_2 a_2^{(\theta)}+(1+2\alpha_1)b_0^{(\theta)} \\ &\quad -(3\alpha_1+\alpha_2)b_1^{(\theta)}+\alpha_2 b_2^{(\theta)}\Big\}. \end{aligned} \tag{A.4}$$

An analysis is performed on the parameter combinations α_1,α_2 that satisfy (2.29). Clearly, there are many pairs α_1,α_2 such that $q_0^{(\theta),k}>0$ holds for all $\theta\in(0,1)$, and Eqs. (A.2)-(A.4) are all positive.

To verify the above conclusion, we select a typical parameter pair $\alpha_1=\frac{1}{3}$, $\alpha_2=\frac{1}{3}$, and substitute it into Eqs. (A.2)-(A.4) for verification.

For $k=3$, substitute the specific values $\alpha_1=\frac{1}{3}$, $\alpha_2=\frac{1}{3}$ into (A.2),

$$\begin{aligned} q_0^{(\theta),3} &= \frac{1}{3\Delta t^\theta \Gamma(2-\theta)}\Big\{5-4\cdot 2^{1-\theta}+3^{1-\theta}+\frac{5}{2-\theta}-\frac{5}{2}-\frac{4\left(3^{2-\theta}-1\right)}{2-\theta}+4\cdot 2^{1-\theta}+2\cdot 3^{1-\theta}+2\Big\} \\ &= \frac{1}{3\Delta t^\theta \Gamma(3-\theta)}\left[18-\frac{9}{2}\theta-(6+3\theta)3^{1-\theta}\right] \\ &\geq 0. \end{aligned} \tag{A.5}$$

For $k=4$, evaluate (A.3) at the specific values $\alpha_1=\frac{1}{3}$ and $\alpha_2=\frac{1}{3}$.

$$\begin{aligned} q_0^{(\theta),4} &= \frac{1}{3\Delta t^\theta \Gamma(3-\theta)}\Big\{18-\frac{9}{2}\theta+\Big(\frac{5}{2}\theta-15\Big)\cdot 2^{1-\theta}+\Big(3+\frac{1}{2}\theta\Big)\cdot 4^{1-\theta}\Big\} \\ &\doteq \frac{1}{3\Delta t^\theta \Gamma(3-\theta)}\tilde{f}(\theta), \end{aligned} \tag{A.6}$$

where $\tilde{f}(\theta)=18-\frac{9}{2}\theta+\big(\frac{5}{2}\theta-15\big)\cdot 2^{1-\theta}+\big(3+\frac{1}{2}\theta\big)\cdot 4^{1-\theta}$, $\tilde{f}(0)=0$, $\tilde{f}(1)>0$.

By using the method of differentiation, we can prove that $\tilde{f}''(\theta)<0$, $\tilde{f}'(\theta)$ is decreasing, so $0<\tilde{f}'(1)<\tilde{f}'(\theta)<\tilde{f}'(0)$. Thus, $\tilde{f}(\theta)$ is increasing. Combining with $\tilde{f}(0)=0$, we conclude $\tilde{f}(\theta)\geq\tilde{f}(0)\geq 0$. Therefore $q_0^{(\theta),4}\geq 0$. The proof that equation (A.6) is greater than or equal to zero is completed.

For $k\geq 5$, by setting $\alpha_1=\frac{1}{3}$ and $\alpha_2=\frac{1}{3}$ in (A.4), we obtain:

$$q_0^{(\theta),k}=\frac{1}{3\Delta t^\theta \Gamma(2-\theta)}\Big\{2-3\left(2^{1-\theta}-1\right)+\left(3^{1-\theta}-2^{1-\theta}\right)+5\left(\frac{1}{2-\theta}-\frac{1}{2}\right)$$

$$
\begin{aligned}
&- 4\Big[\frac{1}{2-\theta}\big(2^{2-\theta}-1\big) - \frac{1}{2}\Big(2^{1-\theta}+1\Big)\Big] \\
&+ \frac{1}{2-\theta}\big(3^{2-\theta}-2^{2-\theta}\big) - \frac{1}{2}\big(3^{1-\theta}+2^{1-\theta}\big)\Big\} \\
&= \frac{1}{3\Delta t^{\theta}\Gamma(3-\theta)}\Big\{18 - \frac{9}{2}\theta + \big(\frac{5}{2}\theta - 15\big)\cdot 2^{1-\theta} + \big(4 - \frac{1}{2}\theta\big)\cdot 3^{1-\theta}\Big\}. \qquad \text{(A.7)}
\end{aligned}
$$

From the Lagrange Mean Value Theorem, we have $3^{1-\theta}-2^{1-\theta} = (1-\theta)\xi^{-\theta}, \xi \in (2,3)$. Thus,

$$
2^{1-\theta} = 3^{1-\theta} - (1-\theta)\xi^{-\theta} \le 3^{1-\theta} - (1-\theta)3^{-\theta} = (\frac{2}{3} + \frac{1}{3}\theta)3^{1-\theta}.
$$

Then we obtain:

$$
\begin{aligned}
q_0^{(\theta),k} &\ge \frac{1}{3\Delta t^{\theta}\Gamma(3-\theta)}\Big\{18 - \frac{9}{2}\theta + (\frac{5}{2}\theta - 15)(\frac{2}{3} + \frac{1}{3}\theta)3^{1-\theta} + (4 - \frac{1}{2}\theta)3^{1-\theta}\Big\} \\
&\doteq \frac{1}{3\Delta t^{\theta}\Gamma(3-\theta)}\tilde{f}(\theta),
\end{aligned}
$$

where $\tilde{f}(\theta) = 18 - \frac{9}{2}\theta + \big(\frac{5}{2}\theta - 15\big)\big(\frac{2}{3} + \frac{1}{3}\theta\big)\,3^{1-\theta} + \big(4 - \frac{1}{2}\theta\big)\,3^{1-\theta}$.

By using the method of differentiation, we can prove that $\tilde{f}''(\theta)$ changes from positive to negative, meaning $\tilde{f}'(\theta)$ first increases then decreases. Hence,

$$
\tilde{f}'(\theta) \ge \min\{\tilde{f}'(0), \tilde{f}'(1)\}.
$$

Direct computation shows that $\tilde{f}'(0) \approx 3.775 > 0$ and $\tilde{f}'(1) \approx 3.220 > 0$, so $\tilde{f}'(\theta) > 0$ for all $\theta \in (0,1)$. Consequently, $\tilde{f}(\theta)$ is strictly monotonically increasing. Thus,

$$
\tilde{f}(\theta) \ge \tilde{f}(0) = 0 \quad \text{for all } \theta \in (0,1).
$$

Therefore, $q_0^{(\theta),k} \ge 0$, which completes the proof. In summary, the proof of Lemma 2.4 is completed. □

Appendix B: The proof of Lemma 3.4.

Proof. The expression of $a_l^{(\theta)}$ is shown in (2.1), and $\bar{a}_l^{(\theta)} = \frac{1}{\Gamma(2-\theta)\Delta t^{\theta}} \cdot a_l^{(\theta)}$. Therefore, the expression of $\bar{a}_0^{(\theta)}$ is $\bar{a}_0^{(\theta)} = \frac{1}{\Delta t^{\theta}\Gamma(2-\theta)}$.

Substituting Eqs. (2.16) and (2.23) into (2.18), we obtain

$$
\frac{1}{3}q_0^{(\theta),k} + d_0^{(\theta)} = \frac{1}{3}\Big(A_0^k - d_0^{(\theta)}\Big) + d_0^{(\theta)} = \frac{1}{3}\Big[(1+2\alpha_1)A_0^k + 6\alpha_1 A_1^k - 2\alpha_2 A_2^k\Big]. \qquad \text{(B.1)}
$$

For $k = 3$,

$$
\begin{aligned}
\frac{\frac{1}{3}q_0^{(\theta),3} + d_0^{(\theta)}}{\bar{a}_0^{(\theta)}} = \frac{1}{3}\Big\{&(1+2\alpha_1)a_0^{(\theta)} + 6\alpha_1 a_1^{(\theta)} - 2\alpha_2 a_2^{(\theta)} + (1-4\alpha_1)b_0^{(\theta)} \\
&+ (6\alpha_1 + 2\alpha_2)\Big(b_1^{(\theta)} + b_2^{(\theta)}\Big)\Big\}.
\end{aligned} \qquad \text{(B.2)}
$$

Substitute $\alpha_1 = \frac{1}{3}$ and $\alpha_2 = \frac{1}{3}$ into (B.2). It can be verified by calculation that the expression is a decreasing function. Therefore, formula (B.2) attains its minimum value when $\theta = 1$. That is

$$\frac{\frac{1}{3}q_0^{(\theta),3} + d_0^{(\theta)}}{\bar{a}_0^{(\theta)}} \geq \frac{\frac{1}{3}q_0^{(1)} + d_0^{(1)}}{\bar{a}_0^{(1)}} = \frac{1}{2}.$$

For $k = 4$,

$$\begin{aligned}\frac{\frac{1}{3}q_0^{(\theta),4} + d_0^{(\theta)}}{\bar{a}_0^{(\theta)}} =& \frac{1}{3}\Big\{(1+2\alpha_1)a_0^{(\theta)} + 6\alpha_1 a_1^{(\theta)} - 2\alpha_2 a_2^{(\theta)} \\ &+ (1-4\alpha_1)b_0^{(\theta)} + (6\alpha_1 + 2\alpha_2)b_1^{(\theta)} - 2\alpha_2\left(b_2^{(\theta)} + b_3^{(\theta)}\right)\Big\}.\end{aligned}$$

Substituting $\alpha_1 = \frac{1}{3}$ and $\alpha_2 = \frac{1}{3}$, we calculate that the minimum value is $\frac{1}{2}$ when $k = 4$. For $k \geq 5$,

$$\begin{aligned}\frac{\frac{1}{3}q_0^{(\theta),k} + d_0^{(\theta)}}{\bar{a}_0^{(\theta)}} =& \frac{1}{3}\Big\{(1+2\alpha_1)a_0^{(\theta)} + 6\alpha_1 a_1^{(\theta)} - 2\alpha_2 a_2^{(\theta)} + (1-4\alpha_1)b_0^{(\theta)} \\ &+ (6\alpha_1 + 2\alpha_2)b_1^{(\theta)} - 2\alpha_2 b_2^{(\theta)}\Big\}.\end{aligned}$$

Substituting $\alpha_1 = \frac{1}{3}$ and $\alpha_2 = \frac{1}{3}$, we calculate that when $k \geq 5$, the minimum value is $\frac{1}{2}$. That is, when $k \geq 3$,

$$\frac{\frac{1}{3}q_0^{(\theta),k} + d_0^{(\theta)}}{\bar{a}_0^{(\theta)}} \geq \frac{1}{2}.$$

Next, we attempt to find the minimum value of $\frac{d_j^{(\theta)}}{\bar{a}_j^{(\theta)}}$. Substituting $l = 1, 2$ into equation (2.10), we obtain

$$\bar{a}_1^{(\theta)} = \frac{\Delta t^{-\theta}}{\Gamma(2-\theta)}\left(2^{1-\theta} - 1\right), \quad \bar{a}_2^{(\theta)} = \frac{\Delta t^{-\theta}}{\Gamma(2-\theta)}\left(3^{1-\theta} - 2^{1-\theta}\right).$$

For $k = 3$, $j = 1, 2$,

$$\begin{aligned}\frac{d_1^{(\theta)}}{\bar{a}_1^{(\theta)}} &= \frac{1}{3a_1^{(\theta)}}\Big\{\frac{2}{3}\Big(a_0^{(\theta)} + b_0^{(\theta)}\Big) + 2\Big(a_1^{(\theta)} + b_1^{(\theta)} + b_2^{(\theta)} - b_0^{(\theta)}\Big) + \frac{1}{3}\Big(a_2^{(\theta)} - b_1^{(\theta)} - b_2^{(\theta)}\Big)\Big\} \\ &\geq \frac{1}{9a_1^{(\theta)}} \cdot 6a_1^{(\theta)} \\ &= \frac{2}{3}. \end{aligned} \tag{B.3}$$

Since $d_2^{(\theta)} = A_2^k$, $\bar{a}_2^{(\theta)} = \frac{\Delta t^{-\theta}}{\Gamma(2-\theta)}\left(3^{1-\theta} - 2^{1-\theta}\right)$, directly using the original (A.7) of [1], we have

$$\frac{d_2^{(\theta)}}{\bar{a}_2^{(\theta)}} = \frac{1}{3^{1-\theta} - 2^{1-\theta}}\left(a_2^{(\theta)} - b_1^{(\theta)} - b_2^{(\theta)}\right) \geq \frac{11}{16}. \tag{B.4}$$

For $k=4$ and $j=1,2,3$, the ratio of $d_1^{(\theta)}$ to $\bar{a}_1^{(\theta)}$ is presented in (B.5):

$$\frac{d_1^{(\theta)}}{\bar{a}_1^{(\theta)}}=\frac{1}{9a_1^{(\theta)}}\left\{2a_0^{(\theta)}+6a_1^{(\theta)}+a_2^{(\theta)}-4b_0^{(\theta)}+5b_1^{(\theta)}+b_2^{(\theta)}+b_3^{(\theta)}\right\}\geq\frac{1}{9a_1^{(\theta)}}\cdot 6a_1^{(\theta)}=\frac{2}{3}. \tag{B.5}$$

Correspondingly, using (A.6) in [1], the ratio of $d_j^{(\theta)}$ to $\bar{a}_j^{(\theta)}, j=2,3$ can be expressed as

$$\frac{d_2^{(\theta)}}{\bar{a}_2^{(\theta)}}=\frac{1}{3^{1-\theta}-2^{1-\theta}}\left(b_3^{(\theta)}+b_2^{(\theta)}-b_1^{(\theta)}+a_2^{(\theta)}\right)\geq\frac{3}{4}, \tag{B.6}$$

$$\frac{d_3^{(\theta)}}{\bar{a}_3^{(\theta)}}=\frac{1}{4^{1-\theta}-3^{1-\theta}}\left(a_3^{(\theta)}-b_2^{(\theta)}-b_3^{(\theta)}\right)\geq\frac{11}{16}. \tag{B.7}$$

For $k\geq 5$, and $j=1,2,\cdots k-1$,

$$\begin{aligned}\frac{d_1^{(\theta)}}{\bar{a}_1^{(\theta)}}&=\frac{1}{3\left(2^{1-\theta}-1\right)}\Big\{(1-\alpha_1)\left(a_0^{(\theta)}+b_0^{(\theta)}\right)+3(1-\alpha_1)\left(b_1^{(\theta)}+a_1^{(\theta)}-b_0^{(\theta)}\right)\\&\quad+\alpha_2\left(b_2^{(\theta)}+a_2^{(\theta)}-b_1^{(\theta)}\right)\Big\}\\&\geq\frac{2}{3},\end{aligned} \tag{B.8}$$

$$\frac{d_2^{(\theta)}}{\bar{a}_2^{(\theta)}}=\frac{1}{3^{1-\theta}-2^{1-\theta}}\left(b_2^{(\theta)}+a_2^{(\theta)}-b_1^{(\theta)}\right)\geq\frac{3}{4}. \tag{B.9}$$

According to Lemma 3.3 and Eqs. (A.5)–(A.7) in [1], we have

$$\frac{d_l^{(\theta)}}{\bar{a}_l^{(\theta)}}\geq\frac{3}{4},\ l=1,\cdots,k-2,\quad\frac{d_{k-1}^{(\theta)}}{\bar{a}_{k-1}^{(\theta)}}\geq\frac{11}{16}. \tag{B.10}$$

Therefore, according to formulas (B.3)-(B.10), we obtain $d_j^{(\theta)}/\bar{a}_j^{(\theta)}\geq\frac{1}{2}$. So when $\sigma=\frac{1}{2}$, the condition is satisfied. □

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