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IMPROVED ERROR ESTIMATES OF A FINITE DIFFERENCE/SPECTRAL METHOD FOR TIME-FRACTIONAL DIFFUSION EQUATIONS

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Abstract. In this paper, we first consider the numerical method that Lin and Xu proposed and analyzed in [Finite difference/spectral approximations for the time-fractional diffusion equation, JCP 2007] for the time-fractional diffusion equation. It is a method basing on the combination of a finite different scheme in time and spectral method in space. The numerical analysis carried out in that paper showed that the scheme is of $(2-\alpha)$-order convergence in time and spectral accuracy in space for smooth solutions, where α is the time-fractional derivative order. The main purpose of this paper consists in refining the analysis and providing a sharper estimate for both time and space errors. More precisely, we improve the error estimates by giving a more accurate coefficient in the time error term and removing the factor in the space error term, which grows with decreasing time step. Then the theoretical results are validated by a number of numerical tests.

Key words. Error estimates, finite difference methods, spectral methods, time fractional diffusion equation.

1. Introduction

As a powerful tool in modelling the phenomenon related to nonlocality and spatial heterogeneity, the fractional partial differential equations (FPDE for short hereafter) has been attracting increasing attention in recent years. They are now finding its many applications in a broad range of fields such as control theory, biology, electrochemical processes, viscoelastic materials, polymer, finance, and etc; see, e.g.,[1, 2, 4, 5, 6, 8, 9, 12, 13, 19, 23, 25] and the references therein.

Similar to the role of the heat equation in traditional modelling, the time-fractional diffusion equation considered in this paper is of importance not only in its own right, but also it constitutes the kernel of many other more general FPDE. This model equation governs the evolution for the probability density function that describes anomalously diffusing particles. For some fractional models, we mention, e.g., the chaotic dynamics charge transport problem in amorphous semiconductors [26, 27], the NMR diffusometry in disordered materials [20], the dynamics of a bead in polymer network [3], and the propagation of mechanical diffusive waves in viscoelastic media [18]. For more applications where the time-fractional diffusion appears, we refer to a generalized diffusion equation which describes transport processes with long memory [10]; the physical model of water transport in soil, which is a generalized Richards' equation with time-fractional derivative [21]; the similarity problem of nonlinear integro-differential type [22], etc.

There have been a number of numerical methods constructed for the time-fractional diffusion equations. We mention, among others, the work [17] by Liu

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et al. on the finite difference method in both space and time, a finite difference scheme for the fractional diffusion-wave equation by Sun and Wu [29], a L1 scheme used to approximate the fractional order time derivative by Langlands and Henry [14], a particle tracking approach by Zhang et al. [30], an alternating direction implicit scheme by Zhang and Sun [31], finite difference schemes for a variable-order equation by Sun et al. [28], and convergence analysis of the finite element method in Jin et al. [11].

On one side, fractional derivatives are non-local operators, which explains one of their most significant uses in applications: they possess a memory effect which is present in several materials such as viscoelastic materials or polymers. On the other side, the nonlocality of the fractional derivatives makes the design of accurate and fast methods difficult. In particular, the fact that all previous solutions have to be saved to compute the solution at the current time point would make the storage very expensive if a low-order method is employed. This consideration has inspired some recent work [15, 16] on developing spectral methods for time-fractional differential equations. Particularly, Lin and Xu [16] proposed a finite difference scheme in time and Legendre spectral method in space for the time-fractional diffusion equation. A convergence rate of $(2-\alpha)$-order in time and spectral accuracy in space of the method was proved, where α is the time derivative order.

In this paper, we follow the work in [16] with an attempt to improve the error estimates obtained therein. The main contribution of the paper is as follows: Firstly, a sharper estimate for both time and space errors is derived by using different analysis techniques. Specifically, we obtain a more accurate coefficient in front of the time error term and remove the undesirable factor in the space error term, which grows with decreasing time step. Secondly, this new estimate is confirmed by a number of numerical tests carefully designed for the verification.

The outline of this paper is as follows. In the next section we first describe the time discretization for the time-fractional diffusion equation, then derive the truncation error. In Section 3 we describe two spectral methods for the space discretization, and derive the full discrete error estimates. Some numerical examples are given in Section 4. Finally we give some concluding remarks in Section 5.

2. A $2-\alpha$ order finite difference scheme in time

We first describe the problem of fractional differential equations that is studied in this paper. Let $T>0$, $\Lambda=(-1,1), I=(0,T]$, consider the time-fractional diffusion equation of the form

$$\partial_t^\alpha u(x,t)-\partial_x^2 u(x,t)=0,\quad x\in\Lambda,\ t\in I, \tag{1}$$

subject to the following initial and boundary conditions:

$$u(x,0)=g(x),\quad x\in\Lambda, \tag{2}$$

$$u(-1,t)=u(1,t)=0,\quad 0\le t\le T, \tag{3}$$

where α is the order of the time-fractional derivative. Here, we consider the case $0<\alpha<1$ and fractional derivative in the Caputo sense [23], defined by

$$\partial_t^\alpha u(x,t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t \partial_s u(x,s)\frac{ds}{(t-s)^\alpha},\quad 0<\alpha<1.$$

Let $t_k =: k\Delta t,\ k = 0, 1 \dots, K$, where $\Delta t =: \frac{T}{K}$ is the time step. We consider the following finite difference operator

$$L_t^\alpha u(x, t_{k+1}) := \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{k} b_j \frac{u(x, t_{k+1-j}) - u(x, t_{k-j})}{\Delta t^\alpha}, \tag{4}$$

where $b_j = (j+1)^{1-\alpha} - j^{1-\alpha},\ j = 0, 1, \dots k$. The time scheme we are going to investigate reads

$$L_t^\alpha u^{k+1}(x) = \partial_x^2 u^{k+1}(x),\ k = 0, 1, \dots, K-1, \tag{5}$$

where $u^{k+1}(x)$ is an approximation to $u(x, t_{k+1})$. The truncation error of this scheme, denoted by $r_{\Delta t}^{k+1}(x)$, is given by

$$r_{\Delta t}^{k+1}(x) = \partial_t^\alpha u(x, t_{k+1}) - L_t^\alpha u(x, t_{k+1}),\ \ 0 \le k \le K-1, \tag{6}$$

Then obviously we have

$$-\partial_x^2 u(x, t_{k+1}) + \frac{1}{\Delta t^\alpha \Gamma(2-\alpha)} \sum_{j=0}^{k} b_j \big(u(x, t_{k+1-j}) - u(x, t_{k-j}) \big) = -r_{\Delta t}^{k+1}(x),$$

or equivalently

$$u(t_{k+1}) - \alpha_0 \partial_x^2 u(t_{k+1}) = \sum_{j=0}^{k-1} (b_j - b_{j+1}) u(t_{k-j}) + b_k u(t_0) - \alpha_0 r_{\Delta t}^{k+1}, \tag{7}$$

where $\alpha_0 = \Gamma(2-\alpha)\Delta t^\alpha$, and the dependence on x has been omitted for notational convenience.

The scheme (5) was first proposed and analyzed in [16], where the unconditional stability and $2-\alpha$ order convergence were proved. The first goal of the current paper is to provide a more accurate error estimate for this scheme by using a new technique, as stated in the following lemma.

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

$$|r_{\Delta t}^{k+1}(x)| \le cM(u)\Delta t^{2-\alpha},\ \forall k = 0, 1, \dots, K-1, \forall x \in \Lambda \tag{8}$$

where c *is independent of* u *and* Δt, $M(u) = \max_{t \in I} |\partial_t^2 u(x, t)|$.

Proof. First a direct calculation shows

$$\begin{aligned} L_t^\alpha u(x, t_{k+1}) &= \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{k} \frac{u(x, t_{k+1-j}) - u(x, t_{k-j})}{\Delta t^\alpha} [(j+1)^{1-\alpha} - j^{1-\alpha}]. \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \frac{u(x, t_{k+1-j}) - u(x, t_{k-j})}{\Delta t} \int_{t_j}^{t_{j+1}} t^{-\alpha} dt \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \frac{u(x, t_{j+1}) - u(x, t_j)}{\Delta t} \int_{t_{k-j}}^{t_{k+1-j}} t^{-\alpha} dt \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \frac{u(x, t_{j+1}) - u(x, t_j)}{\Delta t} \int_{t_j}^{t_{j+1}} \frac{ds}{(t_{k+1} - s)^\alpha}. \end{aligned}$$

Then from definition (6) we have

$$
\begin{aligned}
& r_{\Delta t}^{k+1}(x) \\
= & \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} \partial_s u(x,s) \frac{ds}{(t_{k+1}-s)^{\alpha}} - L_t^{\alpha} u(x,t_{k+1}) \\
= & \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} \left[\partial_s u(x,s) - \frac{u(x,t_{j+1})-u(x,t_j)}{\Delta t} \right] \frac{ds}{(t_{k+1}-s)^{\alpha}}.
\end{aligned} \tag{9}
$$

By applying the following Taylor formula with the integral remainder

$$
f(t) = f(s) + \partial_t f(s)(t-s) + \int_s^t \partial_\tau^2 f(\tau)(t-\tau) d\tau, \quad \forall t, s \in I
$$

to the function $u(\cdot,t)$ at $t = t_j$ and $t = t_{j+1}$ respectively, we obtain, for all $s \in (t_j, t_{j+1})$,

$$
\begin{aligned}
& \partial_s u(x,s) - \frac{u(x,t_{j+1})-u(x,t_j)}{\Delta t} \\
= & -\frac{1}{\Delta t} \int_s^{t_{j+1}} \partial_\tau^2 u(x,\tau)(t_{j+1}-\tau) d\tau + \frac{1}{\Delta t} \int_s^{t_j} \partial_\tau^2 u(x,\tau)(t_j-\tau) d\tau.
\end{aligned}
$$

Inserting the above equality into (9) yields

$$
\begin{aligned}
r_{\Delta t}^{k+1}(x) = & \frac{1}{\Gamma(1-\alpha)\Delta t} \sum_{j=0}^{k} \Big[-\int_{t_j}^{t_{j+1}} \int_s^{t_{j+1}} \partial_\tau^2 u(x,\tau) \frac{t_{j+1}-s}{(t_{k+1}-s)^{\alpha}} d\tau ds \\
& + \int_{t_j}^{t_{j+1}} \int_s^{t_j} \partial_\tau^2 u(x,\tau) \frac{t_j-\tau}{(t_{k+1}-s)^{\alpha}} d\tau ds \Big] \\
= & \frac{1}{\Gamma(1-\alpha)\Delta t} \sum_{j=0}^{k} \Big[-\int_{t_j}^{t_{j+1}} \partial_\tau^2 u(x,\tau)(t_{j+1}-\tau) \int_{t_j}^{\tau} \frac{ds}{(t_{k+1}-s)^{\alpha}} d\tau \\
& - \int_{t_j}^{t_{j+1}} \partial_\tau^2 u(x,\tau)(t_j-\tau) \int_{\tau}^{t_{j+1}} \frac{ds}{(t_{k+1}-s)^{\alpha}} d\tau \Big] \\
= & \frac{1}{\Gamma(2-\alpha)\Delta t} \sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} \partial_\tau^2 u(x,\tau) \big[(t_{k+1}-\tau)^{1-\alpha} \Delta t \\
& - (t_{j+1}-\tau)(t_{k+1}-t_j)^{1-\alpha} + (t_j-\tau)(t_{k+1}-t_{j+1})^{1-\alpha} \big] d\tau.
\end{aligned} \tag{10}
$$

We denote

$$
\begin{aligned}
& R_j^{k+1}(\tau) \\
= & (t_{k+1}-\tau)^{1-\alpha} \Delta t - (t_{j+1}-\tau)(t_{k+1}-t_j)^{1-\alpha} + (t_j-\tau)(t_{k+1}-t_{j+1})^{1-\alpha}.
\end{aligned} \tag{11}
$$

It can be directly checked that $R_j^{k+1}(\tau) \geq 0$ for all $\tau \in [t_j, t_{j+1}]$ (also see [15]). Thus the Mean Value Theorem for Integrals can be applied to (10) to yield

$$
|r_{\Delta t}^{k+1}(x)| \leq \frac{M(u)}{\Gamma(2-\alpha)\Delta t} \sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} R_j^{k+1}(\tau) d\tau, \tag{12}
$$

where $M(u) = \max\limits_{\tau \in I} |\partial_\tau^2 u(x,\tau)|$. Now we turn to estimate the sum in the right-hand side of (12). Integrating $R_j^{k+1}(\tau)$ in the interval $[t_j, t_{j+1}]$ gives

$$\begin{aligned}
&\sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} R_j^{k+1}(\tau) d\tau \\
= \ & \frac{\Delta t^{3-\alpha}}{2(2-\alpha)} \sum_{j=0}^{k} \Big[2(k+1-j)^{2-\alpha} \\
& -2(k-j)^{2-\alpha} - (2-\alpha)\big((k+1-j)^{1-\alpha} + (k-j)^{1-\alpha}\big)\Big] \\
= \ & \frac{\Delta t^{3-\alpha}}{2(2-\alpha)} \sum_{l=0}^{k} \Big[2(l+1)^{2-\alpha} - 2l^{2-\alpha} - (2-\alpha)\big((l+1)^{1-\alpha} + l^{1-\alpha}\big)\Big] \\
= \ & \frac{\Delta t^{3-\alpha}}{2} \sum_{l=0}^{k} \Big[\frac{2}{2-\alpha}\big((l+1)^{2-\alpha} - l^{2-\alpha}\big) - \big((l+1)^{1-\alpha} + l^{1-\alpha}\big)\Big].
\end{aligned}$$

Let $s_l := \dfrac{2}{2-\alpha}\big((l+1)^{2-\alpha} - l^{2-\alpha}\big) - \big((l+1)^{1-\alpha} + l^{1-\alpha}\big)$, then $s_0 = \frac{\alpha}{2-\alpha}$, and it follows from the positivity of R_l^{k+1} that s_l is also positive for all l varying from 1 to k, and

$$\begin{aligned}
s_l \ = \ & l^{1-\alpha}\Big[\frac{2l}{2-\alpha}\Big(\big(1+\frac{1}{l}\big)^{2-\alpha} - 1\Big) - \big(1+\frac{1}{l}\big)^{1-\alpha} - 1\Big] \\
= \ & l^{1-\alpha}\Big[\frac{2l}{2-\alpha}\Big(-1+1+(2-\alpha)\frac{1}{l} + \frac{(2-\alpha)(1-\alpha)}{2!}\frac{1}{l^2} \\
& + \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!}\frac{1}{l^3} + \frac{(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)}{4!}\frac{1}{l^4} + \dots\Big) \\
& -1-1-(1-\alpha)\frac{1}{l} - \frac{(1-\alpha)(-\alpha)}{2!}\frac{1}{l^2} - \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\frac{1}{l^3} - \dots\Big] \\
= \ & l^{1-\alpha}\Big[\big(\frac{1}{2!} - \frac{2}{3!}\big)(1-\alpha)\alpha\frac{1}{l^2} + \big(\frac{1}{3!} - \frac{2}{4!}\big)(1-\alpha)\alpha(-\alpha-1)\frac{1}{l^3} + \dots\Big] \\
\le \ & l^{1-\alpha}\frac{1}{3!}(1-\alpha)\alpha\frac{1}{l^2}\Big[1 + \frac{2(\alpha+1)}{4}\frac{1}{l} + \frac{3(\alpha+1)(\alpha+2)}{20}\frac{1}{l^2} + \dots\Big] \\
\le \ & \frac{1}{3!}(1-\alpha)\alpha\frac{1}{l^{1+\alpha}}\Big[1 + \frac{1}{l} + \frac{1}{l^2} + \dots\Big] \\
\le \ & \frac{2}{3!}(1-\alpha)\alpha\frac{1}{l^{1+\alpha}} \\
\le \ & \frac{1}{l^{1+\alpha}}.
\end{aligned}$$

Therefore, the series $\sum_{l=0}^{k} s_l$ converges as $k \to \infty$ for all $\alpha > 0$. This means there exists a positive constant c, independent of k, such that

$$\sum_{j=0}^{k} \int_{t_j}^{t_{j+1}} R_j^{k+1}(\tau) d\tau \le c\Delta t^{3-\alpha}. \tag{13}$$

Finally, combining (12) and (13) gives (8). □

It is more convenient to rewrite the scheme (5) into the following equivalent form:

$$\begin{aligned} &b_0 u^{k+1} - \alpha_0 \partial_x^2 u^{k+1} \\ = \; &b_0 u^k - \sum_{j=0}^{k-1} b_{j+1} u^{k-j} + \sum_{j=1}^{k} b_j u^{k-j}, \; k = 0, 1, \dots, K-1, \end{aligned} \tag{14}$$

where the coefficients $b_j, j = 0, 1, \dots, k$, satisfy

$$\begin{aligned} &1 = b_0 > b_1 > \cdots > b_k > 0, \; b_k \to 0 \text{ as } k \to \infty; \\ &\sum_{j=0}^{k} (b_j - b_{j+1}) + b_{k+1} = 1. \end{aligned} \tag{15}$$

The equation (14), subject to the boundary conditions

$$u^{k+1}(-1) = u^{k+1}(1) = 0 \tag{16}$$

forms the problem to be solved at each time step.

Let $L^2(\Lambda), H^1(\Lambda)$, and $H_0^1(\Lambda)$ be usual Sobolev spaces, endowed with standard inner products and norms. The weak formulation of the equation (14) with the boundary conditions (16) reads: find $u^{k+1} \in H_0^1(\Lambda)$, $k \geq 0$, such that

$$\begin{aligned} &(u^{k+1}, v) + \alpha_0 \big(\partial_x u^{k+1}, \partial_x v\big) \\ = \; &\sum_{j=0}^{k-1} (b_j - b_{j+1})(u^{k-j}, v) + b_k (u^0, v), \; \forall v \in H_0^1(\Lambda), \end{aligned} \tag{17}$$

where $(\cdot,\cdot)$ is the usual L^2-inner product. For the sake of simplification, we define the H^1-inner product $(\cdot,\cdot)_1$ by:

$$(u, v)_1 := (u, v) + \alpha_0 (\partial_x u, \partial_x v),$$

and H^1-norm by

$$\|v\|_1 := (v, v)_1^{1/2}.$$

For the semi-discrete solution $\{u^k\}_{k=0}^K$, by following exactly the same lines as in [16] and using the lemma 2.1, we can derive the following error estimate.

Theorem 2.1. *Let u be the exact solution of (1)-(3), $\{u^k\}_{k=0}^K$ be the semi-discrete solution of* (17) *with the initial condition $u^0(x) = u(x, 0)$. Then the following error estimate holds:*

$$\|u(\cdot, t_k) - u^k\|_1 \leq c \max_{t \in I} \|\partial_t^2 u(\cdot, t)\|_0 T^\alpha \Delta t^{2-\alpha}, \; k = 1, 2, \cdots, K,$$

where c is independent of u, T, and Δt.

3. Spectral discretizations in space and error estimates

3.1. A Galerkin spectral method in space. Let $\mathbb{P}_N(\Lambda)$ be the space of all polynomials of degree less than or equal to N, and $\mathbb{P}_N^0(\Lambda) = H_0^1(\Lambda) \cap \mathbb{P}_N(\Lambda)$. We consider the Galerkin spectral discretization to the weak problem (17) as follows. For $k \geq 0$ find $u_N^{k+1} \in \mathbb{P}_N^0(\Lambda)$, such that for all $v_N \in \mathbb{P}_N^0(\Lambda)$

$$(u_N^{k+1}, v_N) + \alpha_0 \big(\partial_x u_N^{k+1}, \partial_x v_N\big) = \sum_{j=0}^{k-1} (b_j - b_{j+1})(u_N^{k-j}, v_N) + b_k (u_N^0, v_N). \tag{18}$$

For $\{u_N^j\}_{j=0}^k$ given, the existence and uniqueness of the solution u_N^{k+1} of (18) is guaranteed by the Lax-Milgram Lemma. The main purpose of this section is to derive an improvement estimate for the full discrete solution $\{u_N^k\}_{k=0}^K$ as compared to the one obtained in [16]. To this end, we define the H_0^1-orthogonal projection operator $\pi_N^{1,0}$ as follows. For all $\psi \in H_0^1(\Lambda)$, let $\pi_N^{1,0}\psi$ be in $P_N^0(\Lambda)$ such that

$$(\partial_x \pi_N^{1,0}\psi, \partial_x v_N) = (\partial_x \psi, \partial_x v_N), \ \forall v_N \in P_N^0(\Lambda). \tag{19}$$

It is known that the following estimate holds [7]:

$$\|\psi - \pi_N^{1,0}\psi\|_l \le cN^{l-m}\|\psi\|_m, \quad \forall \psi \in H^m(\Lambda) \cap H_0^1(\Lambda), \ m \ge 1, l = 0, 1. \tag{20}$$

Theorem 3.1. *Let u be the exact solution of (1)-(3), $\{u_N^k\}_{k=0}^K$ be the solution of problem (18) with the initial condition $u_N^0 = \pi_N^1 u^0$. Suppose $\partial_t^2 u \in L^\infty((0,T]; H^m(\Lambda))$, $m \ge 1$. Then for $0 \le \alpha < 1, k = 0, 1, \dots, K$, we have*

$$\begin{aligned} \|u(t_k) - u_N^k\|_1 \quad \le \quad & \frac{cT^\alpha}{1-\alpha}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)} \\ & + \Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)}\big) + cN^{1-m}\|u\|_{L^\infty(H^m)}, \end{aligned} \tag{21}$$

where $\|v\|_{L^\infty(H^m)} := \sup_{t\in(0,T)} \|v(\cdot,t)\|_m$, and c is a constant independent of α, T, Δt and N. Furthermore, the estimate for the case α close to 1 can be improved by

$$\begin{aligned} \|u(t_k) - u_N^k\|_1 \quad \le \quad & cT\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)} \\ & + \Delta t\|\partial_t^2 u\|_{L^\infty(L^2)}\big) + cN^{1-m}\|u\|_{L^\infty(H^m)}. \end{aligned} \tag{22}$$

Proof. First we obtain from (7)

$$\begin{aligned} & (u(t_{k+1}), v_N) + \alpha_0(\partial_x u(t_{k+1}), \partial_x v_N) - \sum_{j=0}^{k-1}(b_j - b_{j+1})(u(t_{k-j}), v_N) - b_k(u(t_0), v_N) \\ & = -\alpha_0(r_{\Delta t}^{k+1}, v_N), \quad \forall v_N \in \mathbb{P}_N^0(\Lambda). \end{aligned}$$

This can be reformulated as follows by using the definition of $\pi_N^{1,0}$:

$$\begin{aligned} & (\pi_N^{1,0}u(t_{k+1}), v_N) + \alpha_0(\partial_x \pi_N^{1,0}u(t_{k+1}), \partial_x v_N) \\ & -\sum_{j=0}^{k-1}(b_j - b_{j+1})(\pi_N^{1,0}u(t_{k-j}), v_N) - b_k(\pi_N^{1,0}u(t_0), v_N) \\ = \quad & -\Big(\big(I_d - \pi_N^{1,0}\big)\big(u(t_{k+1}) \\ & -\sum_{j=0}^{k-1}(b_j - b_{j+1})u(t_{k-j}) - b_k u(t_0)\big), v_N\Big) - \alpha_0(r_{\Delta t}^{k+1}, v_N) \\ = \quad & -\alpha_0\big((I_d - \pi_N^{1,0})L_t^\alpha u(t_{k+1}), v_N\big) - \alpha_0(r_{\Delta t}^{k+1}, v_N), \end{aligned} \tag{23}$$

where I_d is the identity operator. Let $e_N^k := u_N^k - \pi_N^{1,0}u(t_k)$. Subtracting (23) from (18) gives

$$\begin{aligned} & (e_N^{k+1}, v_N) + \alpha_0(\partial_x e_N^{k+1}, \partial_x v_N) \\ = \quad & \sum_{j=0}^{k-1}(b_j - b_{j+1})(e_N^{k-j}, v_N) + b_k(e_N^0, v_N) + \alpha_0(\delta_N^{k+1}, v_N), \end{aligned} \tag{24}$$

where

$$\delta_N^{k+1} = (I_d - \pi_N^{1,0})L_t^\alpha u(t_{k+1}) + r_{\Delta t}^{k+1}.$$

From (6), we have

$$\delta_N^{k+1} = (I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_{k+1}) - r_{\Delta t}^{k+1}) + r_{\Delta t}^{k+1}.$$

Using triangle inequality, we obtain

$$\|\delta_N^{k+1}\|_0 \leq \|(I_d - \pi_N^{1,0})\partial_t^\alpha u(t_{k+1})\|_0 + \|(I_d - \pi_N^{1,0})r_{\Delta t}^{k+1}\|_0 + \|r_{\Delta t}^{k+1}\|_0.$$

According to (10), we have

$$r_{\Delta t}^{k+1}(x) = \frac{1}{\Gamma(2-\alpha)\Delta t}\sum_{j=0}^{k}\int_{t_j}^{t_{j+1}} \partial_\tau^2 u(x,\tau)R_j^{k+1}(\tau)d\tau,$$

where R_j^{k+1} is defined in (11). We know from the proof of Lemma 2.1 that $R_j^{k+1}(\tau) \geq 0$ for all $\tau \in [t_j, t_{j+1}]$, and

$$\frac{1}{\Gamma(2-\alpha)\Delta t}\sum_{j=0}^{k}\int_{t_j}^{t_{j+1}} R_j^{k+1}(\tau)d\tau \leq c\Delta t^{2-\alpha}.$$

Consequently, we get

$$\left\|r_{\Delta t}^{k+1}\right\|_0 \leq c\Delta t^{2-\alpha}\max_{\tau\in I}\left\|\partial_\tau^2 u(\cdot,\tau)\right\|_0.$$

Furthermore, it is an easy task to verify that

$$\left\|(I_d - \pi_N^{1,0})r_{\Delta t}^{k+1}\right\|_0 = \left\|\frac{1}{\Gamma(2-\alpha)\Delta t}\sum_{j=0}^{k}\int_{t_j}^{t_{j+1}} (I_d - \pi_N^{1,0})\partial_\tau^2 u(\cdot,\tau)R_j^{k+1}(\tau)d\tau\right\|_0,$$

from which we get

$$\left\|(I_d - \pi_N^{1,0})r_{\Delta t}^{k+1}\right\|_0 \leq c\Delta t^{2-\alpha}\max_{\tau\in I}\left\|(I_d - \pi_N^{1,0})\partial_\tau^2 u(\cdot,\tau)\right\|_0.$$

Then by using (20), we deduce from the above estimates:

(25)
$$\begin{aligned}
\|\delta_N^{k+1}\|_0 \quad \leq \quad & \left\|(I_d - \pi_N^{1,0})\partial_t^\alpha u(\cdot,t_{k+1})\right\|_0 + c\Delta t^{2-\alpha}\max_{\tau\in I}\left\|(I_d - \pi_N^{1,0})\partial_\tau^2 u(\cdot,\tau)\right\|_0 \\
& + c\Delta t^{2-\alpha}\max_{\tau\in I}\left\|\partial_\tau^2 u(\cdot,\tau)\right\|_0 \\
\leq \quad & cN^{-m}\|\partial_t^\alpha u(\cdot,t_{k+1})\|_m + c\Delta t^{2-\alpha}N^{-m}\max_{\tau\in I}\left\|\partial_\tau^2 u(\cdot,\tau)\right\|_m \\
& + c\Delta t^{2-\alpha}\max_{\tau\in I}\left\|\partial_\tau^2 u(\cdot,\tau)\right\|_0 \\
\leq \quad & cN^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + c\Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)} \\
& + c\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)}.
\end{aligned}$$

Taking $v_N = e_N^{k+1}$ in (24), we obtain

$$\|e_N^{k+1}\|_1 \leq \sum_{j=0}^{k-1}(b_j - b_{j+1})\|e_N^{k-j}\|_0 + b_k\|e_N^0\|_0 + \alpha_0\|\delta_N^{k+1}\|_0. \tag{26}$$

In the following we are going to prove

$$\|e_N^k\|_1 \leq b_{k-1}^{-1}\alpha_0\max_{0\leq j\leq k}\|\delta_N^j\|_0,\ k = 1,2,\ldots,K. \tag{27}$$

by using mathematical induction. When $k=1$, we deduce from (26)

$$\|e_N^1\|_1 \leq b_0\|e_N^0\|_0 + \alpha_0\|\delta_N^1\|_0 = \alpha_0\|\delta_N^1\|_0 \leq b_0^{-1}\alpha_0\max_{0\leq j\leq 1}\|\delta_N^j\|_0.$$

Assuming the estimate

$$\|e_N^i\|_1 \leq b_{i-1}^{-1}\alpha_0 \max_{0\leq j\leq i}\|\delta_N^j\|_0,\ i=0,1\dots,k \tag{28}$$

is true, we want to prove that it also holds for $i=k+1$. It can be done by combining (26), (28), and (15)

$$\begin{aligned}
\|e_N^{k+1}\|_1 &\leq \Big[(1-b_1)+\sum_{j=1}^{k-1}(b_j-b_{j+1})+b_k\Big]b_k^{-1}\alpha_0 \max_{0\leq j\leq k+1}\|\delta_N^j\|_0\\
&= b_k^{-1}\alpha_0 \max_{0\leq j\leq k+1}\|\delta_N^j\|_0.
\end{aligned}$$

This completes the proof of (27). Then inserting (25) into (26), and noticing $b_{k-1}^{-1}\leq \dfrac{k^\alpha}{1-\alpha}$, we obtain

$$\begin{aligned}
\|e_N^k\|_1 &\leq b_{k-1}^{-1}\alpha_0 \max_{0\leq j\leq k}\|\delta_N^j\|_0\\
&\leq b_{k-1}^{-1}k^{-\alpha}k^\alpha\Delta t^\alpha\Delta t^{-\alpha}\Gamma(2-\alpha)\Delta t^\alpha \max_{0\leq j\leq k}\|\delta_N^k\|_0\\
&\leq \frac{cT^\alpha}{1-\alpha}\Gamma(2-\alpha)\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)}+\Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}\\
&\quad +\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)}\big).
\end{aligned}$$

Finally, we use the following triangle inequality

$$\|u(k)-u_N^k\|_1 \leq \|e_N^k\|_1+\|u(t_k)-\pi_N^1 u(t_k)\|_1$$

and the estimate (20) to conclude

$$\begin{aligned}
\|u(k)-u_N^k\|_1 &\leq \frac{cT^\alpha}{1-\alpha}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)}+\Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}\\
&\quad +\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)}\big)+cN^{1-m}\|u\|_{L^\infty(H^m)}.
\end{aligned}$$

Thus (21) is proved.

Now we consider the case $\alpha\to 1$. Note that in this case, the coefficient $\frac{T^\alpha}{1-\alpha}$ in the estimate (21) blows up as $\alpha\to 1$. Therefore, we seek an improved estimate for α close to 1. First we can prove by induction the following estimate:

$$\|e_N^k\|_1 \leq \alpha_0\sum_{j=0}^{k}\|\delta_N^j\|_0,\ k=1,2,\dots,K. \tag{29}$$

This statement is trivially true when $k=1$. Now we want to prove if the estimate (29) is true for $i=0,1,\dots,k$, then it is also true for $i=k+1$. In fact, we have

$$\|e_N^{k+1}\|_1 \leq \Big[\sum_{j=0}^{k-1}(b_j-b_{j+1})+b_k\Big]\sum_{j=0}^{k}\alpha_0\|\delta_N^j\|_0+\alpha_0\|\delta_N^{k+1}\|_0\leq\sum_{j=0}^{k+1}\alpha_0\|\delta_N^j\|_0.$$

This proves (29). Then we obtain from (29):

$$\begin{aligned}
\|e_N^k\|_1 &\leq c\Delta t\sum_{j=0}^{k}\|\delta_N^j\|_0\leq cT\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)}\\
&\quad +\Delta t N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}+\Delta t\|\partial_t^2 u\|_{L^\infty(L^2)}\big).
\end{aligned}$$

Finally we get (22) by using the triangle inequality. The proof of the theorem is complete. □

3.2. A Legendre collocation method in space. Let $L_N(x)$ denotes the Legendre polynomial of degree N. $\{\xi_j,\ j=0,1,\ldots,N\}$ are the Legendre-Gauss-Lobatto (GLL) points, i.e., zeros of $(1-x^2)L_N'(x)$; $\{\omega_j,\ j=0,1,\ldots,N\}$ are the weights such that the following quadrature holds

$$\int_{-1}^{1}\varphi(x)dx=\sum_{j=0}^{N}\varphi(\xi_j)\omega_j,\ \forall\varphi\in\mathbb{P}_{2N-1}(\Lambda).$$

We define the discrete inner product:

$$(\phi,\psi)_N:=\sum_{i=0}^{N}\phi(\xi_i)\psi(\xi_i)\omega_i,$$

and let $\|\phi\|_N:=(\phi,\phi)_N^{1/2}$. Then the following inequality is well known:

$$\|\phi\|_0\le\|\phi\|_N\le\sqrt{3}\|\phi\|_0,\ \forall\varphi\in\mathbb{P}_N(\Lambda). \tag{30}$$

Now we consider the Legendre collocation approximation as follows: find $u_N^{k+1}\in P_N^0(\Lambda)$, such that

$$A_N(u_N^{k+1},v_N)=F_N(v_N),\ \forall v_N\in P_N^0(\Lambda), \tag{31}$$

where the bilinear form $A_N(\cdot,\cdot)$ is defined by

$$A_N(u_N^{k+1},v_N):=(u_N^{k+1},v_N)_N+\alpha_0(\partial_x u_N^{k+1},\partial_x v_N)_N,$$

and the functional $F_N(\cdot)$ is given by

$$F_N(v_N):=\sum_{j=0}^{k-1}(b_j-b_{j+1})(u_N^{k-j},v_N)_N+b_k(u_N^0,v_N)_N.$$

We denote by $\|\cdot\|_{1,N}$ the norm associated to the bilinear form $A_N(\cdot,\cdot)$:

$$\|\psi_N\|_{1,N}:=A_N^{1/2}(\psi_N,\psi_N),\ \forall\psi_N\in P_N(\Lambda).$$

According to (30), the norm $\|\cdot\|_{1,N}$ is equivalent to the usual $\|\cdot\|_1$ norm.

Theorem 3.2. *Let u be the exact solution of (1)-(3), $\{u_N^k\}_{k=0}^K$ be the solution of problem (31) with the initial condition $u_N^0=\pi_N^{1,0}u^0$. Suppose $\partial_t^2 u\in L^\infty((0,T];H^m(\Lambda))$, $m\ge 1$. Then for $0\le\alpha<1, k=1,2,\ldots,K$, we have*

$$\begin{aligned}\|u(t_k)-u_N^k\|_{1,N}\ &\le\ cN^{1-m}\|u\|_{L^\infty(H^m)}+\frac{cT^\alpha}{1-\alpha}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)}\\&\qquad+\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)}+\Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}\big),\end{aligned} \tag{32}$$

where c is a constant independent of α, T, Δt, and N. Furthermore, a better estimate holds for the case $\alpha\to 1$ as follows:

$$\begin{aligned}\|u(t_k)-u_N^k\|_{1,N}\ &\le\ cN^{1-m}\|u\|_{L^\infty(H^m)}+cT\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)}\\&\qquad+\Delta t\|\partial_t^2 u\|_{L^\infty(L^2)}+\Delta tN^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}\big).\end{aligned} \tag{33}$$

Proof. Let $e_N^{k+1}=u_N^{k+1}-\pi_N^{1,0}u(t_{k+1})$, then a straightforward calculation shows

$$\begin{aligned}A_N(e_N^{k+1},v_N)\ &=\ (e_N^{k+1},v_N)_N+\alpha_0(\partial_x e_N^{k+1},\partial_x v_N)_N\\&=\ (u_N^{k+1},v_N)_N+\alpha_0(\partial_x u_N^{k+1},\partial_x v_N)_N-(\pi_N^{1,0}u(t_{k+1}),v_N)_N\\&\qquad-\alpha_0(\partial_x\pi_N^{1,0}u(t_{k+1}),\partial_x v_N)_N.\end{aligned}$$

Using (31), we obtain

(34)
$$\begin{aligned}
&(e_N^{k+1}, v_N)_N + \alpha_0(\partial_x e_N^{k+1}, \partial_x v_N)_N\\
= \;& \sum_{j=0}^{k-1}(b_j - b_{j+1})(e_N^{k-j}, v_N)_N + b_k(e_N^0, v_N)_N + (\varepsilon_1^{k+1}, v_N)_N + (\varepsilon_2^{k+1}, v_N)_N,
\end{aligned}$$

where

$$\begin{aligned}
&(\varepsilon_1^{k+1}, v_N)_N\\
= \;& (u(t_{k+1}) - \pi_N^{1,0}u(t_{k+1}), v_N)_N - \sum_{j=0}^{k-1}(b_j - b_{j+1})\big(u(t_{k-j}) - \pi_N^{1,0}u(t_{k-j}), v_N\big)_N\\
& -b_k\big(u(t_0) - \pi_N^{1,0}u(t_0), v_N\big)_N,
\end{aligned}$$

and

$$\begin{aligned}
&(\varepsilon_2^{k+1}, v_N)_N\\
= \;& -(u(t_{k+1}) - \pi_N^{1,0}u(t_{k+1}), v_N)_N + \sum_{j=0}^{k-1}(b_j - b_{j+1})(u(t_{k-j}), v_N)_N\\
& +b_k(u(t_0), v_N)_N - (\pi_N^{1,0}u(t_{k+1}), v_N)_N - \alpha_0(\partial_x \pi_N^{1,0}u(t_{k+1}), \partial_x v_N)_N.
\end{aligned}$$

Next we estimate $(\varepsilon_1^{k+1}, v_N)_N$ and $(\varepsilon_2^{k+1}, v_N)_N$. Firstly, it is observed that

$$\begin{aligned}
(\varepsilon_1^{k+1}, v_N)_N &= \Big((I_d - \pi_N^{1,0})(u(t_{k+1}) - \sum_{j=0}^{k-1}(b_j - b_{j+1})u(t_{k-j}) - b_k u(t_0)), v_N\Big)_N\\
&= \alpha_0\Big((I_d - \pi_N^{1,0})\frac{1}{\Gamma(2-\alpha)}\sum_{j=0}^{k} b_j \frac{u(t_{k+1-j}) - u(t_{k-j})}{\Delta t^\alpha}, v_N\Big)_N\\
&= \alpha_0\Big((I_d - \pi_N^{1,0})\big(\partial_t^\alpha u(t_{k+1}) + r_{\Delta t}^{k+1}\big), v_N\Big)_N.
\end{aligned}$$

By using the following inequality [7, 24]: $\forall \varphi \in H^m(\Lambda),\ m \geq 1$,

(35)
$$(\varphi, v_N) - (\varphi, v_N)_N \leq cN^{-m}\|\varphi\|_m\|v_N\|_0,$$

we obtain

$$\begin{aligned}
|(\varepsilon_1^{k+1}, v_N)_N| &\leq \alpha_0\Big[\big((I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_{k+1}) + r_{\Delta t}^{k+1}), v_N\big)_0\\
&\quad +cN^{-1}\big\|(I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_{k+1}) + r_{\Delta t}^{k+1})\big\|_1\|v_N\|_0\Big]\\
&\leq \alpha_0\Big[\big\|(I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_{k+1}) + r_{\Delta t}^{k+1})\big\|_0\|v_N\|_0\\
&\quad +cN^{-1}\big\|(I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_{k+1}) + r_{\Delta t}^{k+1})\big\|_1\|v_N\|_0\Big].
\end{aligned}$$

Using the estimate (20) once again and following a similar procedure as in Theorem 3.1, we get

$$|(\varepsilon_1^{k+1}, v_N)_N| \leq c\alpha_0(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)})\|v_N\|_{0,N}.$$

On the other hand, we have

$$\begin{aligned}
&(\varepsilon_2^{k+1}, v_N)_N \\
= \quad & -\Big(u(t_{k+1}) + \sum_{j=0}^{k-1}(b_j - b_{j+1})u(t_{k-j}) + b_k u(t_0), v_N\Big)_N - \alpha_0(\partial_x \pi_N^{1,0} u(t_{k+1}), \partial_x v_N)_N \\
= \quad & -\alpha_0\Big(\frac{1}{\Gamma(2-\alpha)}\sum_{j=0}^{k} b_j \frac{u(t_{k+1-j}) - u(t_{k-j})}{\Delta t^\alpha}, v_N\Big)_N - \alpha_0(\partial_x \pi_N^{1,0} u(t_{k+1}), \partial_x v_N).
\end{aligned}$$

Note that in the last equality above we have used the fact that $(\partial_x \pi_N^{1,0} u(t_{k+1}), \partial_x v_N)_N = (\partial_x \pi_N^{1,0} u(t_{k+1}), \partial_x v_N)$. From (1), we have $(\partial_t^\alpha u(t_{k+1}), v_N) = -(\partial_x u(t_{k+1}), \partial_x v_N)$. Then by using (19), (20), and the above equality, we obtain

$$\begin{aligned}
&(\varepsilon_2^{k+1}, v_N)_N \\
= \quad & \alpha_0(L_t^\alpha u(t_{k+1}), v_N) - \alpha_0(L_t^\alpha u(t_{k+1}), v_N)_N + \alpha_0(\partial_t^\alpha u(t_{k+1}) - L_t^\alpha u(t_{k+1}), v_N).
\end{aligned}$$

Now we use (6), (8), and (35) to yield

$$\begin{aligned}
|(\varepsilon_2^{k+1}, v_N)_N| \quad \le \quad & c\alpha_0\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} \\
& +\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} + \Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}\big)\|v_N\|_{0,N}.
\end{aligned}$$

Taking $v_N = e_N^{k+1}$ in (34), and combining all above estimates together, we obtain

$$\begin{aligned}
& A_N(e_N^{k+1}, e_N^{k+1}) = \|e_N^{k+1}\|_{1,N}^2 \\
\le \quad & \sum_{j=0}^{k-1}(b_j - b_{j+1})\|e_N^{k-j}\|_{0,N}\|e_N^{k+1}\|_{1,N} + b_k\|e_N^0\|_{0,N}\|e_N^{k+1}\|_{1,N} \\
& +c\alpha_0(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} \\
& +\Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)})\|e_N^{k+1}\|_{1,N},
\end{aligned}$$

which gives

$$\begin{aligned}
\|e_N^{k+1}\|_{1,N} \quad \le \quad & \sum_{j=0}^{k-1}(b_j - b_{j+1})\|e_N^{k-j}\|_{0,N} + b_k\|e_N^0\|_{0,N} \\
& +c\alpha_0(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} \\
& +\Delta t^{2-\alpha N^{-m}}\|\partial_t^2 u\|_{L^\infty(H^m)}).
\end{aligned}$$

Finally, following the same lines as in Theorem 3.1 allows us to get first

$$\begin{aligned}
\|e_N^k\|_{1,N} \quad \le \quad & cb_{k-1}^{-1}\alpha_0(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} \\
& +N^{-m}\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(H^m)}) \\
\le \quad & \frac{cT^\alpha}{1-\alpha}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} \\
& +\Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}\big),
\end{aligned}$$

then, by the triangle inequality

$$\begin{aligned}
\|u(t_k) - u_N^k\|_{1,N} \quad \le \quad & \|u(t_k) - \pi_N^{1,0}u(t_k)\|_{1,N} + \|u_N^k - \pi_N^{1,0}u(t_k)\|_{1,N} \\
\le \quad & cN^{1-m}\|u\|_{L^\infty(H^m)} + \frac{cT^\alpha}{1-\alpha}(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} \\
& +\Delta t^{2-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} + \Delta t^{2-\alpha}N^{-m}\|\partial_t^2 u\|_{L^\infty(H^m)}).
\end{aligned}$$

The estimate (33) for the case $\alpha \to 1$ can be obtained in a similar way as in Theorem 3.1 for the same case. This completes the proof of the theorem.

4. Numerical results

The full scheme (31) is implemented exactly as in [16]: by choosing the Lagrangian polynomial $\{h_j\}_{j=1}^{N-1}$ based on the LGL points as the basis functions, we arrive at each time step at a linear system as follows:

$$(B + \alpha_0 A)\underline{u}^{k+1} = \underline{f}, \tag{36}$$

where B is the mass matrix with the entries $B_{ij} := \omega_i \delta_{ij},\ i, j = 1, \ldots, N-1$, and A is the stiffness matrix with the entries:

$$A_{ij} := \sum_{q=0}^{N} D_{qi} D_{qj} \omega_q, \quad D_{ij} := h_j'(\xi_i),\ i, j = 1, \ldots, N-1.$$

$\underline{u}^{k+1}$ is the nodal unknown vector $(u_N^{k+1}(\xi_j))_{j=1}^{N-1}$, the right hand side vector $\underline{f}$ is given by $(F_N(h_i))_{j=1}^{N-1}$.

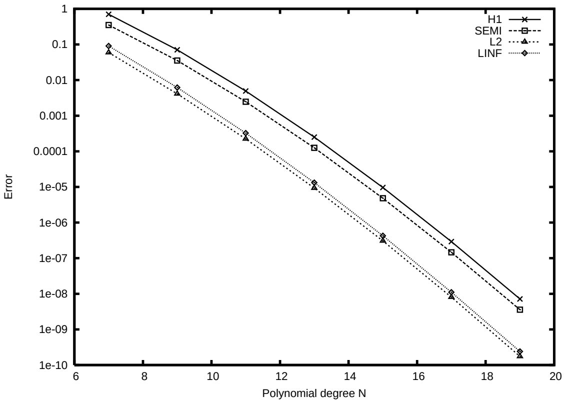

FIGURE 1. Errors for the smooth solution as a function of the polynomial degree N for $\alpha = 0.1$.

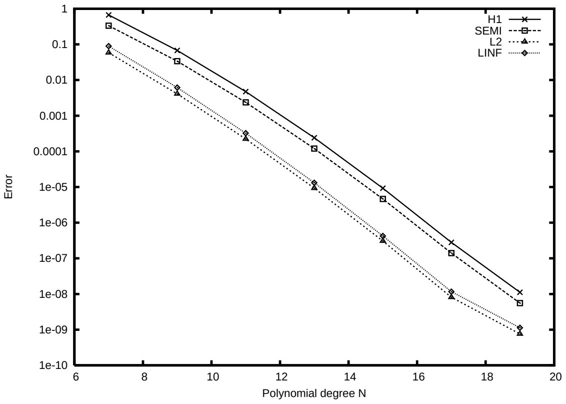

FIGURE 2. Errors for the smooth solution as a function of the polynomial degree N for $\alpha = 0.5$.

The system (36) is symmetric positive definite, thus can be solved by employing the conjugate gradient method.

We now present some numerical results to verify the error estimates. The numerical test is carried out in the same framework as in [16]. Our focus here is to confirm that the error behavior obeys the rate law $O(\Delta t^{2-\alpha}) + O(N^{1-m})$ predicted in Theorem 3.2 rather than $O(\Delta t^{2-\alpha}) + O(\Delta t^{-1}N^{1-m})$ derived in [16]. To this end, we consider the problem (1)-(3) with an additional forcing term $f(x,t) := \frac{3}{\Gamma(2-\alpha)}t^{3-\alpha}\sin(2\pi x) + 4\pi^2 t^3 \sin(2\pi x)$ and initial condition $g(x) := 0$, such that the exact solution is $u(x,t) = t^3\sin(2\pi x)$. For this smooth solution the convergence in space is expected to be exponential.

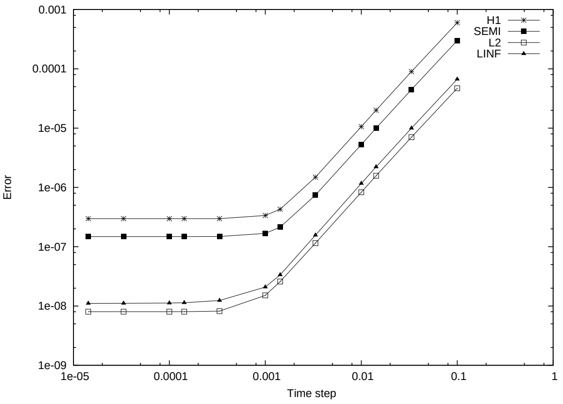

FIGURE 3. Error for the smooth solution versus the time step size Δt for $\alpha = 0.1, N = 17$.

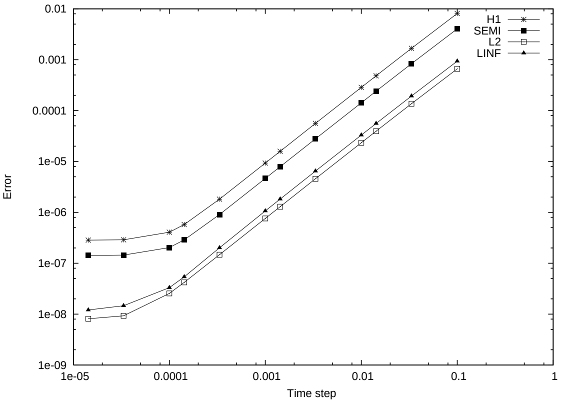

FIGURE 4. Error for the smooth solution versus the time step size Δt for $\alpha = 0.5, N = 17$.

To check the spatial accuracy, we compute the errors $\|u(T) - u_N^k\|$ in the discrete H^1, L^2, and L^∞ norms, and investigate the error behavior with respect to the polynomial degree N for a small enough time step size. In Fig. 1 and Fig. 2, we present the errors as a function of the polynomial degree N for $\Delta t = 10^{-4}$ and

$\alpha = 0.1, 0.5$ respectively. We can draw a number of conclusions from these two figures: 1) The straight lines in the semi-log coordinates indicate that the errors decay exponentially; 2) Although the accuracy of the numerical solutions slightly decreases when the order of the fractional derivative increases, the latter does not effect the exponential convergence rate of the proposed method; 3) The straight lines equally indicate that for $\Delta t = 10^{-4}$ and $N \leq 17$ the temporal error is negligible as compared to the spatial error. That is, the spatial error term dominates the temporal error term in the error estimate for $\Delta t \leq 10^{-4}$ and $N \leq 17$.

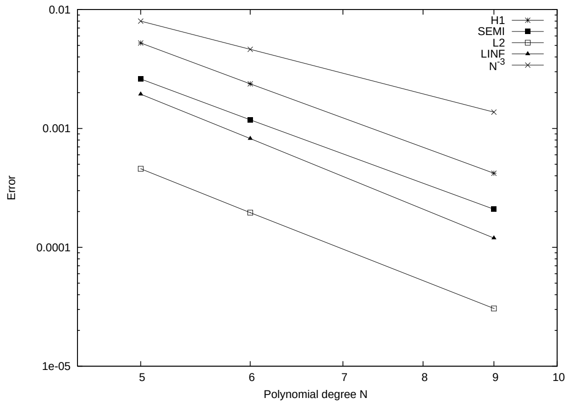

FIGURE 5. Errors for the solution of limited regularity as a function of the polynomial degree N for $\alpha = 0.1$.

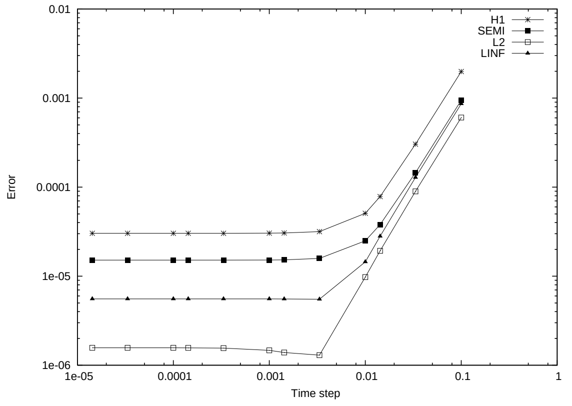

FIGURE 6. Error for the solution of limited regularity versus the time step size Δt for $\alpha = 0.1, N = 17$.

Keeping the third point above in mind, we now fix $N = 17$ and let Δt vary from 10^{-1} to 10^{-5}, and the results obtained are plotted in Fig. 3 and Fig. 4. Obviously in the ranges $\Delta t > 10^{-3}$ for $\alpha = 0.1$ and $\Delta t > 10^{-4}$ for $\alpha = 0.5$, the error stemming from the time discretization dominates the spatial discretization error. Therefore the total error decreases when the time stepping size decreases in these ranges until it reaches a size Δt_c such that the spatial error becomes dominant. The error decay rate is indeed of order $2-\alpha$, which is in a very good agreement with the theoretical prediction. It is observed in Fig. 3 and Fig. 4 that the size Δt_c for $\alpha = 0.1$ and $\alpha = 0.5$ are approximately 10^{-3} and 10^{-4} respectively. What we want to emphasize here is the error behavior after $\Delta t = \Delta t_c$. Fig. 3 and Fig. 4 show that the error stops decreasing when $\Delta t < \Delta t_c$ because the spatial error term now becomes dominant. But it is interesting to see that the error converges to a constant as Δt tends to 0, which clearly indicates that the error behaves like $O(\Delta t^{2-\alpha})+O(N^{1-m})$ as predicted in Theorem 3.2 rather than $O(\Delta t^{2-\alpha}) + O(\Delta t^{-1}N^{1-m})$ as given in [16].

The convergence behavior is further verified by testing a solution of limited regularity. That is, we check the convergence rate of the proposed method for the exact solution with limited regularity in $I \times (0, 2)$ as follows: $u(x, t) = t^3(x-2)x^{\frac{5}{2}}$. In Fig. 5, we present the errors versus the polynomial degrees N in a log-log plot for $\alpha = 0.1$ with fixed $\Delta t = 10^{-4}$. The N^{-3} decay rate is also shown for comparison reason. We observe here the algebraic convergence rates, which is conform to the spatial regularity of the exact solution.

The errors versus the time step for fixed $N = 17$ are plotted in Fig. 6 to investigate the error decay rate with respect to Δt. It is observed that the error keeps decreasing when Δt decreases in a range of relatively large time step sizes until the spatial error becomes the leading error. Then this spatial leading error remains unchanged when Δt continues to decrease. This observation once again confirms the error estimate established in Theorem 3.2.

5. Concluding remarks

In this paper we considered the numerical analysis of a known scheme for the time-fractional diffusion equation. We derived a sharper estimate for the time and space errors of this scheme by providing a more accurate coefficient in the time error term and removing the undesirable factor in the space error term. This new error estimate was then confirmed through a series of numerical tests.

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