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# ERROR ANALYSIS OF A HIGH ORDER METHOD FOR TIME-FRACTIONAL DIFFUSION EQUATIONS*

CHUNWAN LV† AND CHUANJU XU‡

**Abstract.** In this paper, we consider a numerical method for the time-fractional diffusion equation. The method uses a high order finite difference method to approximate the fractional derivative in time, resulting in a time stepping scheme for the underlying equation. Then the resulting equation is discretized in space by using a spectral method based on the Legendre polynomials. The main body of this paper is devoted to carry out a rigorous analysis for the stability and convergence of the time stepping scheme. As a by-product and direct extension of our previous work, an error estimate for the spatial discretization is also provided. The key contribution of the paper is the proof of the $(3-\alpha)$-order convergence of the time scheme, where $\alpha$ is the order of the time-fractional derivative. Then the theoretical result is validated by a number of numerical tests. To the best of our knowledge, this is the first proof for the stability of the $(3-\alpha)$-order scheme for the time-fractional diffusion equation.

**Key words.** time-fractional diffusion equation, time stepping scheme, spectral methods, error estimates

**AMS subject classifications.** 65M12, 65M06, 65M70, 35S10

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## 1. Introduction.

Fractional partial differential equations are attracting increasing attention as a tool in modeling the phenomenon related to nonlocality and spatial heterogeneity. They have applications in a broad range of fields; see, e.g., [16, 22, 13, 4, 24, 2, 3, 20, 5, 6, 11] and the references therein. As the basic and core of most fractional partial differential equations, the time-fractional diffusion equation (TFDE for short) considered in this paper is of importance not only in its own right, but also it reflects the main feature and difficulty of general fractional equations of its kind.

This equation was derived by using continuous time random walks [21, 14], with introduction of a fractional derivative term in time to represent the degree of memory in the diffusing material. A number of numerical methods have been proposed for solving this equation. For example, Liu et al. [19] presented a finite difference method in both space and time for the TFDE. Langlands and Henry [17] considered an L1 scheme for the discretization in time. Sun and Wu [27] proposed and analyzed a finite difference scheme for the fractional diffusion wave equation. Lin and Xu [18] investigated a finite difference scheme in time and Legendre spectral method in space for the TFDE. Deng [9] discussed a finite element method for the fractional Fokker–Planck equation. Ford, Xiao, and Yan [10] considered a time stepping method based

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†School of Mathematical Sciences and Fujian Provincial Key Laboratory of Mathematical Modeling and High Performance Scientific Computing, Xiamen University, 361005 Xiamen, China (lvchunwan@163.com).
‡Corresponding author. School of Mathematical Sciences and Fujian Provincial Key Laboratory of Mathematical Modeling and High Performance Scientific Computing, Xiamen University, 361005 Xiamen, China (cjxu@xmu.edu.cn).

on a quadrature formula approach for time-fractional partial differential equations. Zhang and Sun [29] proposed an alternating direction implicit scheme and Sun et al. [26] proposed finite difference schemes for a variable order time-fractional diffusion equation. Jin et al. [15] considered the initial boundary value problem for a time-fractional diffusion equation, and analyzed two semidiscrete schemes based on the Galerkin and lumped mass finite element methods. Almost optimal error estimates were obtained for right-hand side data. Yan, Pal, and Ford [28] proposed a $(3-\alpha)$-order method based on a direct discretization of the fractional differential operator.

The works most relevant to the present one are that of Sun and Wu [27], Lin and Xu [18], Cao, Xu, and Wang [8], Gao, Sun, and Zhang [12], and Alikhanov [1], which investigated, respectively, $(2-\alpha)$-order, $(3-\alpha)$-order, and second order schemes in time for the TFDE. In particular, numerical evidence has showed that the scheme proposed in [8] and [12] for the $\alpha$-order fractional derivative is of $(3-\alpha)$-order accuracy. In order to get a provable stability, Alikhanov [1] proposed a modified scheme, which is of second order accuracy. The stability of this second order scheme was then proved. The main goal of the present paper is to carry out a full analysis for the scheme constructed in [8] and [12], and provide some stability and error estimates for both time and space discretizations.

The rest of the paper is organized as follows: in the next section we first describe the time discretization for the time-fractional diffusion equation proposed in [8] and [12], then derive a sharp estimate for the truncation error. The stability analysis of the time discretization is carried out in section 3, together with an error estimate showing that the temporal accuracy is of $(3-\alpha)$-order. In section 4, we describe two spectral methods for the space discretization, and derive the full discrete error estimates. Some numerical examples are given in section 5.

## 2. Time discretization.

Let $T>0$, $\Lambda=(-1,1), I=(0,T]$. We consider the following time-fractional diffusion equation: for any $t\in I$, $u_0\in D(A)$, find $u(t)\in D(A)$ such that

$$\partial_t^\alpha u(t)+Au(t)=f \quad \text{with } u(0)=u_0, \tag{2.1}$$

where $A=-\partial_x^2, D(A)=H^2(\Lambda)\cap H_0^1(\Lambda)$, $\alpha\in(0,1)$ is the order of the time-fractional derivative, which is defined in the Caputo sense as follows [22]:

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

A preliminary result concerning the well-posedness of the initial value/boundary value problem (2.1) has been established by Sakamoto and Yamamoto [25], who proved that if $u_0\in D(A)$ and $f=0$, then $u\in C([0,T];D(A))$, $\partial_t^\alpha u\in C([0,T];L^2(\Lambda))\cap C((0,T];H_0^1(\Lambda))$. On the other side, if $f\in L^\infty((0,T);L^2(\Lambda))$ and $u_0=0$, then $u\in L^2((0,T);\,D(A))$, $\partial_t^\alpha u\in L^2((0,T)\times\Lambda)$. To our knowledge no more regularity result exists in the literature. However, throughout the paper, we will assume that the solution to the problem (2.1) has the necessary regularity. Furthermore, for ease of presentation and without loss of generality we will let $f=0$.

Now we describe the time stepping scheme that we are going to analyze. Let $t_k:=k\Delta t,\ k=0,1\ldots,K$, where $\Delta t:=\frac{T}{K}$ is the time step.

Starting with the definition of the fractional derivative at the first grid point, we have

$$\begin{aligned}\partial_t^\alpha u(t_1) &= \frac{1}{\Gamma(1-\alpha)}\int_0^{t_1}\partial_\tau u(\tau)\frac{d\tau}{(t_1-\tau)^\alpha}\\ &= \frac{1}{\Gamma(1-\alpha)}\frac{u(t_1)-u(t_0)}{\Delta t}\int_0^{t_1}\frac{d\tau}{(t_1-\tau)^\alpha}+r_{\Delta t}^1\\ &= \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha}\big(u(t_1)-u(t_0)\big)+r_{\Delta t}^1,\end{aligned} \tag{2.2}$$

where $r_{\Delta t}^1$ is the first step truncation error. Similarly, for $2 \le k \le K$, we have

$$\begin{aligned}&\partial_t^\alpha u(t_k)\\ &\quad= \frac{1}{\Gamma(1-\alpha)}\int_0^{t_k}\partial_\tau u(\tau)\frac{d\tau}{(t_k-\tau)^\alpha}\\ &\quad= \frac{1}{\Gamma(1-\alpha)}\left(\sum_{j=1}^{k-1}\int_{t_{j-1}}^{t_j}\partial_\tau u(\tau)\frac{d\tau}{(t_k-\tau)^\alpha}+\int_{t_{k-1}}^{t_k}\partial_\tau u(\tau)\frac{d\tau}{(t_k-\tau)^\alpha}\right)\\ &\quad= \frac{1}{\Gamma(1-\alpha)}\left(\sum_{j=1}^{k-1}\int_{t_{j-1}}^{t_j}\partial_\tau H_2^j(\tau)\frac{d\tau}{(t_k-\tau)^\alpha}+\int_{t_{k-1}}^{t_k}\partial_\tau H_2^{k-1}(\tau)\frac{d\tau}{(t_k-\tau)^\alpha}\right)+r_{\Delta t}^k\\ &\quad= \frac{1}{\Gamma(3-\alpha)\Delta t^\alpha}\left\{\sum_{j=1}^{k-1}\big(a_j u(t_{k-j-1})+b_j u(t_{k-j})+c_j u(t_{k-j+1})\big)\right.\\ &\qquad\qquad\left.+\frac{\alpha}{2}u(t_{k-2})-2u(t_{k-1})+\frac{4-\alpha}{2}u(t_k)\right\}+r_{\Delta t}^k,\end{aligned} \tag{2.3}$$

where

$$H_2^j(\tau) = u(t_j)-\frac{u(t_j)-u(t_{j-1})}{\Delta t}(t_j-\tau)-\frac{u(t_{j+1})-2u(t_j)+u(t_{j-1})}{\Delta t^2}\frac{(t_j-\tau)(\tau-t_{j-1})}{2}, \tag{2.4}$$

which interpolates the function $u$ at the 3 points $\{t_{j-1}, t_j, t_{j+1}\}, 1 \le j \le k-1$, i.e.,

$$H_2^j(t_{j-1}) = u(t_{j-1}),\ H_2^j(t_j) = u(t_j),\ H_2^j(t_{j+1}) = u(t_{j+1}), \tag{2.5}$$

$r_{\Delta t}^k$, $2 \le k \le K$, is the truncation error of the approximation, and

$$\begin{aligned}a_j &= -\frac{3}{2}(2-\alpha)(j+1)^{1-\alpha}+\frac{1}{2}(2-\alpha)j^{1-\alpha}+(j+1)^{2-\alpha}-j^{2-\alpha},\\ b_j &= 2(2-\alpha)(j+1)^{1-\alpha}-2(j+1)^{2-\alpha}+2j^{2-\alpha},\\ c_j &= -\frac{1}{2}(2-\alpha)\big((j+1)^{1-\alpha}+j^{1-\alpha}\big)+(j+1)^{2-\alpha}-j^{2-\alpha}.\end{aligned}$$

Before coming back to the truncation errors, let's first introduce the following finite difference operator: for all discrete functions $\{v^k\}_{k=0}^K$,

$$L_t^\alpha v^1 = \frac{1}{\Gamma(2-\alpha)\Delta t^\alpha}(v^1 - v^0),$$

$$L_t^\alpha v^k = \frac{1}{\Gamma(3-\alpha)\Delta t^\alpha}\left\{ \sum_{j=1}^{k-1} \left(a_j v^{k-j-1} + b_j v^{k-j} + c_j v^{k-j+1}\right) + \frac{\alpha}{2} v^{k-2} - 2v^{k-1} + \frac{4-\alpha}{2} v^k \right\},\ 2 \le k \le K. \tag{2.6}$$

Then we have

$$r_{\Delta t}^k = \partial_t^\alpha u(t_k) - L_t^\alpha u(t_k),\ 1 \le k \le K \tag{2.7}$$

or, equivalently,

$$L_t^\alpha u(t_k) + Au(t_k) = -r_{\Delta t}^k,\ 1 \le k \le K. \tag{2.8}$$

The above reformulation motivates the following time scheme:

$$\begin{cases} L_t^\alpha u^k + Au^k = 0,\ 1 \le k \le K, \\ u^0 = u_0, \end{cases} \tag{2.9}$$

where $u^k$ is an approximation of $u(t_k)$. Clearly the truncation term $r_{\Delta t}^k$ is an indicator of how accurate this approximation is, which we estimate below.

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

$$|r_{\Delta t}^1| \le c_\alpha \widetilde{M}(u) \Delta t^{2-\alpha}\ \forall x \in \Lambda, \tag{2.10}$$

$$|r_{\Delta t}^k| \le c_\alpha M(u) \Delta t^{3-\alpha}\ \forall k = 2, 3, \dots, K\ \forall x \in \Lambda, \tag{2.11}$$

*where $c_\alpha$ depends only on $\alpha$, $\widetilde{M}(u) = \max_{t\in I} |\partial_t^2 u(t)|$, $M(u) = \max_{t \in I} |\partial_t^3 u(t)|$.*

*Proof.* (i) For the first step truncation error, we have from (2.2)

$$r_{\Delta t}^1 = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_1} \left( \partial_\tau u(\tau) - \frac{u(t_1) - u(t_0)}{\Delta t} \right) \frac{d\tau}{(t_1 - \tau)^\alpha}. \tag{2.12}$$

Using a Taylor expansion gives

$$\left| \partial_\tau u(\tau) - \frac{u(t_1) - u(t_0)}{\Delta t} \right| \le \frac{1}{2} \Delta t \max_{t \in (0, t_1)} |\partial_t^2 u(t)|,\ t_0 \le \tau \le t_1.$$

Thus (2.10) is proven.

(ii) Now we turn to prove (2.11). It follows from (2.7) and (2.6) that

$$r_{\Delta t}^k = R_1^k + R_2^k,\ 2 \le k \le K, \tag{2.13}$$

where

$$R_1^k = \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \left( \partial_\tau u(\tau) - \partial_\tau H_2^j(\tau) \right) \frac{d\tau}{(t_k - \tau)^\alpha}, \tag{2.14}$$

$$R_2^k = \frac{1}{\Gamma(1-\alpha)} \int_{t_{k-1}}^{t_k} \left( \partial_\tau u(\tau) - \partial_\tau H_2^{k-1}(\tau) \right) \frac{d\tau}{(t_k - \tau)^\alpha}. \tag{2.15}$$

First, we estimate $R_1^k$. Using integration by parts and (2.5) gives

$$R_1^k = \frac{-\alpha}{\Gamma(1-\alpha)} \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \left(u(\tau) - H_2^j(\tau)\right) \frac{d\tau}{(t_k-\tau)^{\alpha+1}}. \tag{2.16}$$

Using a Taylor expansion, we have

$$u(\tau) - H_2^j(\tau) = \frac{\partial_\tau^3 u(\xi)}{3!}(\tau - t_{j-1})(\tau - t_j)(\tau - t_{j+1}),\ t_{j-1} \le \xi \le t_{j+1}.$$

Thus

$$|R_1^k| = \frac{\alpha}{6\Gamma(1-\alpha)} \max_{t\in I} |\partial_t^3 u(t)| \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (\tau - t_{j-1})(t_j - \tau)(t_{j+1} - \tau) \frac{d\tau}{(t_k-\tau)^{\alpha+1}}.$$

Since $(\tau - t_{j-1})(t_j - \tau)(t_{j+1} - \tau)$ can be bounded by $\frac{2\sqrt{3}}{9}\Delta t^3$ for all $\tau \in (t_{j-1}, t_j)$, we have

$$\begin{aligned} |R_1^k| &\le \frac{\sqrt{3}\alpha}{27\Gamma(1-\alpha)} \max_{t\in I} |\partial_t^3 u(t)| \Delta t^3 \int_0^{t_{k-1}} (t_k - \tau)^{-\alpha-1} d\tau \\ &= \frac{\sqrt{3}\alpha}{27\Gamma(1-\alpha)} \max_{t\in I} |\partial_t^3 u(t)| \Delta t^3 \left( \frac{\Delta t^{-\alpha}}{\alpha} - \frac{t_k^{-\alpha}}{\alpha} \right) \\ &\le \frac{\sqrt{3}}{27\Gamma(1-\alpha)} \max_{t\in I} |\partial_t^3 u(t)| \Delta t^{3-\alpha}. \end{aligned} \tag{2.17}$$

Now we estimate $R_2^k$. A direct calculation shows that

$$|\partial_\tau u(\tau) - \partial_\tau H_2^{k-1}(\tau)| \le \frac{1}{6}\Delta t^2 \max_{t\in I} |\partial_t^3 u(t)| \ \forall \tau \in (t_{k-1}, t_k).$$

Hence

$$\begin{aligned} |R_2^k| &\le \frac{1}{6\Gamma(1-\alpha)} \max_{t\in I} |\partial_t^3 u(t)| \Delta t^2 \int_{t_{k-1}}^{t_k} \frac{d\tau}{(t_k-\tau)^\alpha} \\ &= \frac{1}{6\Gamma(2-\alpha)} \max_{t\in I} |\partial_t^3 u(t)| \Delta t^{3-\alpha}. \end{aligned} \tag{2.18}$$

Bringing (2.17) and (2.18) to (2.13), we obtain (2.11) and complete the proof. ∎

**3. Stability and convergence.** In order to analyze the scheme (2.9), we first introduce some notations to reformulate (2.9). We denote

$$\alpha_0 := \Gamma(3-\alpha)\Delta t^\alpha,\ \widetilde{\alpha}_0 := \Gamma(2-\alpha)\Delta t^\alpha,\ \beta_0 := c_1 + 2 - \frac{\alpha}{2}. \tag{3.1}$$

Then the scheme (2.9) can be rewritten into the following equivalent form:

for $k \geq 4$,

$$u^k + \alpha_0 \beta_0^{-1} A u^k = \beta_0^{-1} \Bigg( -(b_1 + c_2 - 2) u^{k-1} + \left(-a_1 - b_2 - c_3 - \frac{\alpha}{2}\right) u^{k-2} + \sum_{i=3}^{k-2} (-a_{i-1} - b_i - c_{i+1}) u^{k-i} + (-a_{k-2} - b_{k-1}) u^1 - a_{k-1} u^0 \Bigg). \tag{3.2}$$

For $k = 3, 2, 1$,

$$u^3 + \alpha_0 \beta_0^{-1} A u^3 = \beta_0^{-1} \left( -(b_1 + c_2 - 2) u^2 + \left(-a_1 - b_2 - \frac{\alpha}{2}\right) u^1 - a_2 u^0 \right), \tag{3.3}$$

$$u^2 + \alpha_0 \beta_0^{-1} A u^2 = \beta_0^{-1} \left( -(b_1 - 2) u^1 + \left(-a_1 - \frac{\alpha}{2}\right) u^0 \right), \tag{3.4}$$

$$u^1 + \widetilde{\alpha}_0 A u^1 = u^0. \tag{3.5}$$

In the above scheme, the dependence on $x$ has been omitted for the simplification of notation. The equations (3.2)–(3.5), subject to the homogeneous Dirichlet boundary conditions form the problem to be solved at each time step. To further simplify the notation, we introduce the coefficients as follows:

$$\begin{aligned}
&d_1^2 = -(b_1 - 2)\beta_0^{-1}, \quad d_0^2 = \left(-a_1 - \frac{\alpha}{2}\right)\beta_0^{-1}, \\
&d_2^3 = -(b_1 + c_2 - 2)\beta_0^{-1}, \quad d_1^3 = \left(-a_1 - b_2 - \frac{\alpha}{2}\right)\beta_0^{-1}, \quad d_0^3 = -a_2\beta_0^{-1},
\end{aligned}$$

and, for $k \geq 4$,

$$\begin{aligned}
d_{k-1}^k &= -(b_1 + c_2 - 2)\beta_0^{-1}, \quad d_{k-2}^k = \left(-a_1 - b_2 - c_3 - \frac{\alpha}{2}\right)\beta_0^{-1}, \\
d_{k-i}^k &= (-a_{i-1} - b_i - c_{i+1})\beta_0^{-1}, i = 3, 4, \ldots, k-2, \\
d_1^k &= (-a_{k-2} - b_{k-1})\beta_0^{-1}, \quad d_0^k = -a_{k-1}\beta_0^{-1}.
\end{aligned} \tag{3.6}$$

Then we have the scheme in a more compact form as follows:

$$u^k + \alpha_0 \beta_0^{-1} A u^k = \sum_{i=1}^{k} d_{k-i}^k u^{k-i}, \ 2 \leq k \leq K, \tag{3.7}$$

$$u^1 + \widetilde{\alpha}_0 A u^1 = u^0. \tag{3.8}$$

*Remark* 3.1. Differing from the $(2-\alpha)$-order scheme (see, e.g., [18, scheme (3.8)]), in which all coefficients in front of the discrete solutions are positive, the main difficulty in analyzing the new scheme (3.2)–(3.5) is related to the fact that the coefficients in the right-hand sides of (3.2)–(3.5) may change sign from one coefficient to another. Therefore the stability analysis of the new scheme will have to make use of a completely different technique.

Before carrying out the stability analysis for the time stepping problem (3.26), we first give two useful lemmas.

LEMMA 3.1. *For any* $0 < \alpha < 1$, $k \geq 4$, *the coefficients in the scheme* (3.7) *satisfy*

(1) $\beta_0 = \left(1 + \frac{\alpha}{2}\right) 2^{1-\alpha} > 0, \quad 0 < \alpha_0\beta_0^{-1} < \widetilde{\alpha}_0,$

(2) $\sum_{i=1}^{k} d_{k-i}^k = 1,$

(3) $d_{k-i}^k > 0, i = 3, 4, \ldots, k,$

(4) $0 < d_{k-1}^k < \frac{4}{3},$

(5) $-\frac{1}{2} < d_{k-2}^k < \frac{1}{3},$

(6) $\frac{1}{4}(d_{k-1}^k)^2 + d_{k-2}^k > 0.$

*Proof.* (1) can be checked directly. For example, we have

$$\alpha_0\beta_0^{-1} = \widetilde{\alpha}_0(2-\alpha)\left(1 + \frac{\alpha}{2}\right)^{-1} 2^{\alpha-1} = \widetilde{\alpha}_0\frac{2-\alpha}{2+\alpha}2^{\alpha} < \widetilde{\alpha}_0.$$

(2) can also be checked by a direct calculation using the definition of $d_{k-i}^k$ and summing them for all $i = 1, \ldots, k$. For example, for $k = 2$ we have

$$\begin{aligned} d_0^2 + d_1^2 &= \left(2 - b_1 - a_1 - \frac{\alpha}{2}\right)\beta_0^{-1} \\ &= \left(2 - (2-\alpha)2^{2-\alpha} + 2^{3-\alpha} - 2 + \frac{3}{2}(2-\alpha)2^{1-\alpha}\frac{1}{2}(2-\alpha) - 2^{2-\alpha} + 1 - \frac{\alpha}{2}\right)\beta_0^{-1} \\ &= \left(\left(1+\frac{\alpha}{2}\right)2^{1-\alpha}\right)\left(\left(1+\frac{\alpha}{2}\right)2^{1-\alpha}\right)^{-1} = 1. \end{aligned}$$

The case of other values of $k$ can be verified similarly.

(3) It is observed that

$$\begin{aligned} &-a_{i-1} - b_i - c_{i+1} \\ &\quad = \frac{3}{2}(2-\alpha)i^{1-\alpha} - 3i^{2-\alpha} - \frac{1}{2}(2-\alpha)(i-1)^{1-\alpha} + (i-1)^{2-\alpha} \\ &\qquad - \frac{3}{2}(2-\alpha)(i+1)^{1-\alpha} + 3(i+1)^{2-\alpha} + \frac{1}{2}(2-\alpha)(i+2)^{1-\alpha} - (i+2)^{2-\alpha} \\ &\quad = \frac{3}{2}(2-\alpha)i^{1-\alpha} - 3i^{2-\alpha} - \frac{1}{2}(2-\alpha)i^{1-\alpha}\left(1-\frac{1}{i}\right)^{1-\alpha} + i^{2-\alpha}\left(1-\frac{1}{i}\right)^{2-\alpha} \\ &\qquad - \frac{3}{2}(2-\alpha)i^{1-\alpha}\left(1+\frac{1}{i}\right)^{1-\alpha} + 3i^{2-\alpha}\left(1+\frac{1}{i}\right)^{2-\alpha} \\ &\qquad + \frac{1}{2}(2-\alpha)i^{1-\alpha}\left(1+\frac{2}{i}\right)^{1-\alpha} - i^{2-\alpha}\left(1+\frac{2}{i}\right)^{2-\alpha}. \end{aligned}$$

For $i \geq 3$, using a Taylor expansion yields

$$
\begin{aligned}
&-a_{i-1} - b_i - c_{i+1} \\
&\quad = \frac{3}{2}(2-\alpha)i^{1-\alpha} - 3i^{2-\alpha} \\
&\qquad - \frac{1}{2}(2-\alpha)i^{1-\alpha}\left[1 - (1-\alpha)\frac{1}{i} + \frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{i}\right)^2 - \cdots\right] \\
&\qquad + i^{2-\alpha}\left[1 - (2-\alpha)\frac{1}{i} + \frac{(2-\alpha)(1-\alpha)}{2!}\left(\frac{1}{i}\right)^2\right. \\
&\qquad\qquad \left. - \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!}\left(\frac{1}{i}\right)^3 + \cdots\right] \\
&\qquad - \frac{3}{2}(2-\alpha)i^{1-\alpha}\left[1 + (1-\alpha)\frac{1}{i} + \frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{i}\right)^2\right. \\
&\qquad\qquad \left. + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{1}{i}\right)^3 + \cdots\right] \\
&\qquad + 3i^{2-\alpha}\left[1 + (2-\alpha)\frac{1}{i} + \frac{(2-\alpha)(1-\alpha)}{2!}\left(\frac{1}{i}\right)^2\right. \\
&\qquad\qquad \left. + \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!}\left(\frac{1}{i}\right)^3 + \cdots\right] \\
&\qquad + \frac{1}{2}(2-\alpha)i^{1-\alpha}\left[1 + (1-\alpha)\frac{2}{i} + \frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{2}{i}\right)^2\right. \\
&\qquad\qquad \left. + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{2}{i}\right)^3 + \cdots\right] \\
&\qquad - i^{2-\alpha}\left[1 + (2-\alpha)\frac{2}{i} + \frac{(2-\alpha)(1-\alpha)}{2!}\left(\frac{2}{i}\right)^2\right. \\
&\qquad\qquad \left. + \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!}\left(\frac{2}{i}\right)^3 + \cdots\right] \\
&\quad = -(2-\alpha)(1-\alpha)(-\alpha)i^{-\alpha-1} \\
&\qquad + \frac{1}{4!}(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)(-\alpha-3)i^{-\alpha-4} \\
&\qquad + \frac{12}{6!}(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)i^{-\alpha-5} \\
&\qquad + \frac{1}{7!}\frac{63}{2}(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)(-\alpha-5)i^{-\alpha-6} \\
&\qquad + \cdots \\
&\quad = -(2-\alpha)(1-\alpha)(-\alpha)i^{-\alpha-1}S_\alpha,
\end{aligned}
\tag{3.9}
$$

where

$$
\begin{aligned}
S_\alpha = {} & 1 - \frac{1}{4!}(-\alpha-1)(-\alpha-2)(-\alpha-3)i^{-3} \\
& - \frac{12}{6!}(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)i^{-4} \\
& - \frac{1}{7!}\frac{63}{2}(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)(-\alpha-5)i^{-5} + \cdots \\
\geq {} & 1 + \frac{(\alpha+1)(\alpha+2)(\alpha+3)}{4!}i^{-3} \\
& - \frac{12}{6!}(\alpha+1)(\alpha+2)(\alpha+3)(\alpha+4)i^{-4}\left(1 + \frac{1}{i} + \frac{1}{i^2} + \cdots\right).
\end{aligned}
$$

Noticing that $1 < 1 + \frac{1}{i} + \frac{1}{i^2} + \cdots = \frac{1}{1-\frac{1}{i}} \leq \frac{3}{2}$ for $i \geq 3$, we obtain

$$
S_\alpha \geq 1 + \frac{3!}{4!}i^{-3} - \frac{12}{6!}5!i^{-4}\frac{3}{2} = i^{-4}(i^4 - 3) + \frac{1}{4}i^{-3} > 0. \tag{3.10}
$$

Combining (3.9), (3.10), and (3.6), we have

$$
d_{k-i}^k = \frac{-a_{i-1} - b_i - c_{i+1}}{(1+\frac{\alpha}{2})2^{1-\alpha}} > 0,\ i = 3, 4, \ldots, k-2. \tag{3.11}
$$

Using the definition of $d_1^k$ and $d_0^k$ in (3.6), we can prove $d_1^k > 0,\ d_0^k > 0$ in a similar way.

(4) It follows from (3.6) that

$$
\begin{aligned}
d_{k-1}^k = -(b_1 + c_2 - 2)\beta_0^{-1} &= \frac{\left(3 + \frac{3}{2}\alpha\right)2^{1-\alpha} + \left(-\frac{\alpha}{2} - 2\right)3^{1-\alpha}}{\left(1 + \frac{\alpha}{2}\right)2^{1-\alpha}} \\
&\leq \frac{\left(3 + \frac{3}{2}\alpha\right)2^{1-\alpha} + \left(-\frac{\alpha}{2} - 2\right)2^{1-\alpha}}{\left(1 + \frac{\alpha}{2}\right)2^{1-\alpha}} = 1 + \frac{\frac{\alpha}{2}}{1 + \frac{\alpha}{2}} < \frac{4}{3} \quad \forall \alpha \in (0, 1).
\end{aligned} \tag{3.12}
$$

On the other hand, in virtue of the mean value theorem, we have

$$
3^{1-\alpha} \leq 2^{1-\alpha} + (1-\alpha)2^{-\alpha}.
$$

Thus

$$
\begin{aligned}
\left(3 + \frac{3}{2}\alpha\right)2^{1-\alpha} + \left(-\frac{\alpha}{2} - 2\right)3^{1-\alpha} &\geq \left(3 + \frac{3}{2}\alpha\right)2^{1-\alpha} - \left(\frac{\alpha}{2} + 2\right)\left[2^{1-\alpha} + (1-\alpha)2^{-\alpha}\right] \\
&= \alpha\left(\frac{\alpha}{2} + \frac{7}{2}\right)2^{-\alpha} > 0.
\end{aligned} \tag{3.13}
$$

This gives $d_{k-1}^k > 0$.

(5) Utilizing a Taylor expansion gives
(3.14)

$$
\begin{aligned}
& -a_1-b_2-c_3-\frac{\alpha}{2} \\
&\quad=\left(-3-\frac{3\alpha}{2}\right)2^{1-\alpha}+\left(6+\frac{3\alpha}{2}\right)3^{1-\alpha}-\left(3+\frac{\alpha}{2}\right)4^{1-\alpha} \\
&\quad=\left(-3-\frac{3\alpha}{2}\right)3^{1-\alpha}\left(1-\frac{1}{3}\right)^{1-\alpha}+\left(6+\frac{3\alpha}{2}\right)3^{1-\alpha}-\left(3+\frac{\alpha}{2}\right)3^{1-\alpha}\left(1+\frac{1}{3}\right)^{1-\alpha} \\
&\quad=\left(-3-\frac{3\alpha}{2}\right)3^{1-\alpha}\Bigg[1-(1-\alpha)\frac{1}{3}+\frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{3}\right)^2 \\
&\qquad\qquad -\frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{1}{3}\right)^3+\cdots\Bigg] \\
&\qquad+\left(6+\frac{3\alpha}{2}\right)3^{1-\alpha}-\left(3+\frac{\alpha}{2}\right)3^{1-\alpha}\Bigg[1+(1-\alpha)\frac{1}{3}+\frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{3}\right)^2 \\
&\qquad\qquad +\frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{1}{3}\right)^3+\cdots\Bigg] \\
&\quad=\left(-\frac{\alpha}{2}\right)3^{1-\alpha}+\alpha(1-\alpha)3^{-\alpha}+(-6-2\alpha)\frac{(1-\alpha)(-\alpha)}{2!}3^{-\alpha-1} \\
&\qquad+\alpha\frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}3^{-\alpha-2} \\
&\qquad+(-6-2\alpha)\frac{(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)}{4!}3^{-\alpha-3}+\cdots \\
&\qquad+\left((-1)^{k+1}\left(3+\frac{3}{2}\alpha\right)-\left(3+\frac{\alpha}{2}\right)\right)\frac{(1-\alpha)(-\alpha)\cdots(-\alpha-k+2)}{k!}3^{1-\alpha-k}+\cdots.
\end{aligned}
$$

It is seen that all terms except the first one on the right-hand side of (3.14) are positive. Thus we have

$$-a_1-b_2-c_3-\frac{\alpha}{2}\geq\left(-\frac{\alpha}{2}\right)3^{1-\alpha}+\alpha(1-\alpha)3^{-\alpha}.$$

Then it follows from the definition (3.6)

$$
\begin{aligned}
d_{k-2}^k &\geq \frac{(-\frac{\alpha}{2})3^{1-\alpha}+\alpha(1-\alpha)3^{-\alpha}}{(1+\frac{\alpha}{2})2^{1-\alpha}}=\frac{(-\frac{\alpha}{2}-\alpha^2)3^{-\alpha}}{(1+\frac{\alpha}{2})2^{1-\alpha}} \\
&\geq \frac{(-\frac{\alpha}{2}-\alpha^2)3^{-\alpha}}{(1+\frac{\alpha}{2})2\cdot 3^{-\alpha}}=-\left((\alpha+2)+\frac{3}{\alpha+2}\right)+\frac{7}{2}
\end{aligned}
$$

from which we get $d_{k-2}^k>-\frac{1}{2}$. On the other hand, some more calculation from (3.14) gives

$$
\begin{aligned}
& -a_1-b_2-c_3-\frac{\alpha}{2} \\
&\quad=\left(-\frac{\alpha}{2}\right)3^{1-\alpha}+\alpha(1-\alpha)3^{-\alpha}+(-6-2\alpha)\frac{(1-\alpha)(-\alpha)}{2!}3^{-\alpha-1} \\
&\qquad+\alpha\frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}3^{-\alpha-2} \\
&\qquad+(-6-2\alpha)\frac{(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)}{4!}3^{-\alpha-3}+\cdots
\end{aligned}
$$

$$\leq \left(-\frac{\alpha}{2}\right) 3^{1-\alpha} + \alpha(1-\alpha)3^{-\alpha} + 3^{-\alpha}\left(\frac{1}{3} + \left(\frac{1}{3}\right)^2 + \left(\frac{1}{3}\right)^3 + \cdots\right)$$
$$= \left(-\frac{\alpha}{2}\right) 3^{1-\alpha} + \alpha(1-\alpha)3^{-\alpha} + \frac{1}{2}3^{-\alpha}.$$

This gives

$$\begin{aligned} d_{k-2}^k &\leq \frac{(-\frac{\alpha}{2})3^{1-\alpha} + \alpha(1-\alpha)3^{-\alpha} + \frac{1}{2}3^{-\alpha}}{(1+\frac{\alpha}{2})2^{1-\alpha}} = \frac{-2\alpha^2-\alpha+1}{6+3\alpha}\left(\frac{3}{2}\right)^{1-\alpha} \\ &\leq \left|\frac{-2\alpha^2-\alpha+1}{6+3\alpha}\right|\frac{3}{2} = \left|\frac{7}{3} - \left(\frac{2}{3}(\alpha+2) + \frac{5}{3}\frac{1}{\alpha+2}\right)\right|\frac{3}{2} < \frac{1}{3} \quad \forall \alpha \in (0,1). \end{aligned}$$

(6) We derive from combining (3.12) and (3.13) that

$$d_{k-1}^k \geq \frac{\alpha(\frac{\alpha}{2}+\frac{7}{2})2^{-\alpha}}{(1+\frac{\alpha}{2})2^{1-\alpha}} = \frac{\alpha(\alpha+7)}{2(2+\alpha)} > 0, \tag{3.15}$$

and from (3.14) that

$$\begin{aligned} d_{k-2}^k &\geq \frac{(-\frac{\alpha}{2})3^{1-\alpha} + \alpha(1-\alpha)3^{-\alpha} + (-6-2\alpha)\frac{(1-\alpha)(-\alpha)}{2!}3^{-\alpha-1}}{(1+\frac{\alpha}{2})2^{1-\alpha}} \\ &= \frac{\alpha(-2\alpha^2-10\alpha+3)}{6(2+\alpha)}\frac{3^{-\alpha}}{2^{-\alpha}}. \end{aligned} \tag{3.16}$$

Using (3.15) and (3.16), we obtain

$$\begin{aligned} &\frac{1}{4}(d_{k-1}^k)^2 + d_{k-2}^k \\ &\quad\geq \frac{1}{4}\frac{\alpha^2(\alpha+7)^2}{4(\alpha+2)^2} + \frac{\alpha(-2\alpha^2-10\alpha+3)}{6(2+\alpha)}\frac{3^{-\alpha}}{2^{-\alpha}} \\ &\quad= \frac{3\alpha^2(\alpha+7)^2 2^{-\alpha} + 8\alpha(-2\alpha^2-10\alpha+3)(\alpha+2)3^{-\alpha}}{48(\alpha+2)^2 2^{-\alpha}} \\ &\quad\geq \frac{3\alpha^2(\alpha+7)^2(3^{-\alpha}+\alpha 3^{-\alpha-1}) + 8\alpha(-2\alpha^2-10\alpha+3)(\alpha+2)3^{-\alpha}}{48(\alpha+2)^2 2^{-\alpha}} \\ &\quad= \frac{\alpha 3^{-\alpha}(\alpha^4+\alpha^3+21(1-\alpha^2)+11\alpha+27)}{48(\alpha+2)^2 2^{-\alpha}} > 0. \end{aligned} \tag{3.17}$$

Note that in the above estimation we have used the inequality

$$2^{-\alpha} \geq 3^{-\alpha} + \alpha 3^{-\alpha-1} \quad \forall \alpha \in (0,1). \tag{3.18}$$

The proof of Lemma 3.1 is thus completed. ∎

*Remark* 3.2. We see from Lemma 3.1 that the coefficient $d_{k-2}^k$ can be negative. A more careful examination shows that the sign of $d_{k-2}^k$ depends on $\alpha$, and there exists $\alpha_0 \in (0,1)$ such that $d_{k-2}^k$ is positive for all $\alpha \in (\alpha_0, 1)$. In this interval, all the coefficients $\{d_{k-i}^k\}_{i=1}^k$ are positive. In this case the technique employed in [18] seems to be applicabe to prove the stability of the current scheme. However, in what follows we aim at providing a novel technique allowing us to establish the stability for all $\alpha$ in $(0,1)$.

Let's introduce the parameter

$$\eta := \frac{1}{2} d_{k-1}^k. \tag{3.19}$$

Through a recombination of the terms in (3.7), we obtain

$$\begin{aligned}
& u^k - \eta u^{k-1} + \alpha_0 \beta_0^{-1} A u^k \\
&\quad = \eta(u^{k-1} - \eta u^{k-2}) + (\eta^2 + d_{k-2}^k) u^{k-2} + d_{k-3}^k u^{k-3} + \cdots + d_0^k u^0 \\
&\quad = \eta(u^{k-1} - \eta u^{k-2}) + (\eta^2 + d_{k-2}^k)(u^{k-2} - \eta u^{k-3}) \\
&\qquad + (\eta^3 + d_{k-2}^k \eta + d_{k-3}^k) u^{k-3} + d_{k-4}^k u^{k-4} + \cdots + d_0^k u^0 \\
&\quad = \eta(u^{k-1} - \eta u^{k-2}) + (\eta^2 + d_{k-2}^k)(u^{k-2} - \eta u^{k-3}) \\
&\qquad + (\eta^3 + d_{k-2}^k \eta + d_{k-3}^k)(u^{k-3} - \eta u^{k-4}) \\
&\qquad + \cdots + (\eta^{k-2} + d_{k-2}^k \eta^{k-4} + \cdots + d_3^k \eta + d_2^k)(u^2 - \eta u^1) \\
&\qquad + (\eta^{k-1} + d_{k-2}^k \eta^{k-3} + \cdots + d_2^k \eta + d_1^k)(u^1 - \eta u^0) \\
&\qquad + (\eta^k + d_{k-2}^k \eta^{k-2} + \cdots + d_1^k \eta + d_0^k) u^0.
\end{aligned} \tag{3.20}$$

Now we denote

$$\overline{d}_{k-i}^k := \eta^i + \sum_{j=2}^{i} \eta^{i-j} d_{k-j}^k, i = 2, 3, \ldots, k, \tag{3.21}$$

$$\overline{u}^i := u^i - \eta u^{i-1}, i = 1, 2, \ldots, k. \tag{3.22}$$

Then we get the equivalent form of (3.7) as follows:

$$\overline{u}^k + \alpha_0 \beta_0^{-1} A u^k = \eta \overline{u}^{k-1} + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k \overline{u}^{k-i} + \overline{d}_0^k u^0. \tag{3.23}$$

The following lemma provides some good properties of the new coefficients.

LEMMA 3.2. *For $0 < \alpha < 1, k \geq 4$, the coefficients in the new scheme* (3.23) *satisfy*

(1) $0 < \eta < \dfrac{2}{3}$,

(2) $\overline{d}_{k-i}^k > 0,\ i = 2, 3, \ldots, k$,

(3) $\eta + \displaystyle\sum_{i=2}^{k-1} \overline{d}_{k-i}^k + \overline{d}_0^k \leq 1$,

(4) $\dfrac{1}{\overline{d}_0^k} < \dfrac{k^\alpha}{(2-\alpha)(1-\alpha)}$.

*Proof.* (1) Using Lemma 3.1(4) gives immediately the estimate for $\eta$.

(2) We derive from (3.21) and Lemma 3.1(6)

$$\overline{d}_{k-2}^k = \eta^2 + d_{k-2}^k = \frac{1}{4}(d_{k-1}^k)^2 + d_{k-2}^k > 0. \tag{3.24}$$

Furthermore, it can be verified that

$$\overline{d}_{k-i}^k = \overline{d}_{k-i+1}^k \eta + d_{k-i}^k,\ i = 3, 4, \ldots, k. \tag{3.25}$$

Then applying (3.24) and Lemma 3.1(3), and noticing $\eta > 0$, we get $\overline{d}_{k-i}^k > 0,\ i = 3, 4, \ldots, k$.

(3) Let $q_k := \eta + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k + \overline{d}_0^k$. It is observed from (3.21) that

$$\begin{aligned} q_k &= \eta(1 + \eta + \eta^2 + \cdots + \eta^{k-1}) + d_{k-2}^k(1 + \eta + \eta^2 + \cdots + \eta^{k-2}) \\ &\quad + \cdots + d_2^k(1 + \eta + \eta^2) + d_1^k(1 + \eta) + d_0^k \\ &= \eta\frac{1 - \eta^k}{1 - \eta} + d_{k-2}^k\frac{1 - \eta^{k-1}}{1 - \eta} + \cdots + d_2^k\frac{1 - \eta^3}{1 - \eta} + d_1^k\frac{1 - \eta^2}{1 - \eta} + d_0^k. \end{aligned}$$

That is

$$(1 - \eta)q_k = \eta(1 - \eta^k) + d_{k-2}^k(1 - \eta^{k-1}) + d_{k-3}^k + \cdots + d_1^k + d_0^k$$

$$- d_{k-3}^k\eta^{k-2} - \cdots - d_2^k\eta^3 - d_1^k\eta^2 - d_0^k\eta.$$

Then using Lemmas 3.1(3), 3.1(2), 3.1(6), and $\eta = \frac{1}{2}d_{k-1}^k$ gives

$$\begin{aligned} (1 - \eta)q_k &\leq \eta(1 - \eta^k) + d_{k-2}^k(1 - \eta^{k-1}) + d_{k-3}^k + \cdots + d_1^k + d_0^k \\ &= (\eta + d_{k-2}^k + d_{k-3}^k + \cdots + d_1^k + d_0^k) - \eta^{k-1}(\eta^2 + d_{k-2}^k) \\ &\leq (1 - \eta) - \eta^{k-1}(\eta^2 + d_{k-2}^k) \\ &= (1 - \eta) - \eta^{k-1}\left(\frac{1}{4}(d_{k-1}^k)^2 + d_{k-2}^k\right) < (1 - \eta). \end{aligned}$$

(4) First, obviously, we have $\overline{d}_0^k \geq d_0^k > 0$. For the second inequality, some manipulations give

$$\begin{aligned} d_0^k &= \frac{3}{2}(2-\alpha)k^{1-\alpha} - \frac{1}{2}(2-\alpha)(k-1)^{1-\alpha} - k^{2-\alpha} + (k-1)^{2-\alpha} \\ &= \frac{3}{2}(2-\alpha)k^{1-\alpha} - \frac{1}{2}(2-\alpha)k^{1-\alpha}\left(1 - \frac{1}{k}\right)^{1-\alpha} - k^{2-\alpha} + k^{2-\alpha}\left(1 - \frac{1}{k}\right)^{2-\alpha} \\ &= \frac{3}{2}(2-\alpha)k^{1-\alpha} - \frac{1}{2}(2-\alpha)k^{1-\alpha}\Bigg(1 - (1-\alpha)\frac{1}{k} + \frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{k}\right)^2 \\ &\qquad - \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{1}{k}\right)^3 + \cdots\Bigg) \\ &\quad - k^{2-\alpha} + k^{2-\alpha}\Bigg(1 - (2-\alpha)\frac{1}{k} + \frac{(2-\alpha)(1-\alpha)}{2!}\left(\frac{1}{k}\right)^2 \\ &\qquad - \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!}\left(\frac{1}{k}\right)^3 \\ &\qquad + \frac{(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)}{4!}\left(\frac{1}{k}\right)^4 - \cdots\Bigg) \\ &= (2-\alpha)(1-\alpha)k^{-\alpha} + \left(-\frac{1}{4} - \frac{1}{6}\right)(2-\alpha)(1-\alpha)(-\alpha)k^{-\alpha-1} \\ &\quad + \left(\frac{1}{2}\frac{1}{3!} + \frac{1}{4!}\right)(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)k^{-\alpha-2} + \cdots \\ &\geq (2-\alpha)(1-\alpha)k^{-\alpha}. \end{aligned}$$

That is

$$\frac{1}{\overline{d}_0^k} < \frac{k^\alpha}{(2-\alpha)(1-\alpha)}.$$

Thus the lemma is proved. ∎

It is seen from Lemma 3.2 that all the coefficients in the right-hand side of the scheme (3.23) are positive. Now we are in a position to establish the stability of the new time stepping scheme.

Let's consider the weak solution of (3.7), and derive stability estimates for the weak solution in some suitable norm. Since the first step equation is easier to treat, we will only consider (3.7) for $k \geq 2$. 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 (3.7) with the homogeneous boundary conditions reads find $u^k \in H_0^1(\Lambda)$, $2 \leq k \leq K$, such that

$$(u^k, v) + \alpha_0\beta_0^{-1}\big(\partial_x u^k, \partial_x v\big) = \sum_{i=1}^{k} d_{k-i}^k (u^{k-i}, v) \ \forall v \in H_0^1(\Lambda), \tag{3.26}$$

where $(\cdot,\cdot)$ is the usual $L^2$-inner product.

THEOREM 3.1. *The semidiscretized problem* (3.26) *is unconditionally stable and its solution satisfies the following estimate for all* $\Delta t > 0$*:*

$$\|u^k\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x u^k\|_0 \leq 4\|u^0\|_0,\ \ 1 \leq k \leq K. \tag{3.27}$$

*Proof.* By using Lemma 3.1(1), the proof for the case $k = 1$ is immediate. Next we will prove (3.27) for $k \geq 2$. It is readily seen from the above discussion that the problem (3.26) can be rewritten as follows:

$$(\overline{u}^k, v) + \alpha_0\beta_0^{-1}(\partial_x u^k, \partial_x v) = \eta(\overline{u}^{k-1}, v) + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k (\overline{u}^{k-i}, v) + \overline{d}_0^k (u^0, v) \ \forall v \in H_0^1(\Lambda). \tag{3.28}$$

Letting $v = 2\overline{u}^k$ in (3.28), we obtain

$$2\|\overline{u}^k\|_0^2 + 2\alpha_0\beta_0^{-1}(\partial_x u^k, \partial_x \overline{u}^k) = 2\eta(\overline{u}^{k-1}, \overline{u}^k) + 2\sum_{i=2}^{k-1} \overline{d}_{k-i}^k (\overline{u}^{k-i}, \overline{u}^k) + 2\overline{d}_0^k (u^0, \overline{u}^k). \tag{3.29}$$

In virtue of the identity $2(\partial_x u^k, \partial_x \overline{u}^k) = \|\partial_x \overline{u}^k\|_0^2 + \|\partial_x u^k\|_0^2 - \eta^2\|\partial_x u^{k-1}\|_0^2$, Lemma 3.2, and the Schwarz inequality, we obtain

$$\begin{aligned} &2\|\overline{u}^k\|_0^2 + \alpha_0\beta_0^{-1}\|\partial_x u^k\|_0^2 - \alpha_0\beta_0^{-1}\eta^2\|\partial_x u^{k-1}\|_0^2 \\ &\quad \leq \eta\|\overline{u}^{k-1}\|_0^2 + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k \|\overline{u}^{k-i}\|_0^2 + \overline{d}_0^k\|u^0\|_0^2 + \left(\eta + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k + \overline{d}_0^k\right)\|\overline{u}^k\|_0^2. \end{aligned}$$

Then from Lemmas 3.2(3) and 3.2(1), we get

(3.30)
$$\begin{aligned}\|\overline{u}^k\|_0^2 + \alpha_0\beta_0^{-1}\|\partial_x u^k\|_0^2 &\le \eta(\|\overline{u}^{k-1}\|_0^2 + \alpha_0\beta_0^{-1}\eta\|\partial_x u^{k-1}\|_0^2)\\ &\quad + \sum_{i=2}^{k-1}\overline{d}_{k-i}^k\|\overline{u}^{k-i}\|_0^2 + \overline{d}_0^k\|u^0\|_0^2\\ &\le \eta(\|\overline{u}^{k-1}\|_0^2 + \alpha_0\beta_0^{-1}\|\partial_x u^{k-1}\|_0^2)\\ &\quad + \sum_{i=2}^{k-1}\overline{d}_{k-i}^k(\|\overline{u}^{k-i}\|_0^2 + \alpha_0\beta_0^{-1}\|\partial_x u^{k-i}\|_0^2) + \overline{d}_0^k\|u^0\|_0^2.\end{aligned}$$

Now we want to prove the following estimate by induction:

$$\|\overline{u}^k\|_0^2 + \alpha_0\beta_0^{-1}\|\partial_x u^k\|_0^2 \le \|u^0\|_0^2, \quad 2 \le k \le K. \tag{3.31}$$

It is easy to check (3.31) for $k = 2$. Then assuming (3.31) is valid for $k = 2, \dots, j-1$, we deduce from (3.30)

$$\|\overline{u}^j\|_0^2 + \alpha_0\beta_0^{-1}\|\partial_x u^j\|_0^2 \le \left(\eta + \sum_{i=2}^{j-1}\overline{d}_{j-i}^j + \overline{d}_0^j\right)\|u^0\|_0^2 \le \|u^0\|_0^2 \quad \forall j = 1, 2, \dots, K.$$

Thus (3.31) is proven. Finally, we turn to estimate $\|u^k\|_0^2$ by using $\overline{u}^k = u^k - \eta u^{k-1}$. Applying the triangle inequality and (3.31) yields

$$\begin{aligned}\|u^k\|_0 = \|\overline{u}^k + \eta u^{k-1}\|_0 &\le \|\overline{u}^k\|_0 + \|\eta u^{k-1}\|_0 \le \|u^0\|_0 + \|\eta u^{k-1}\|_0\\ &\le (1+\eta)\|u^0\|_0 + \eta^2\|u^{k-2}\|_0\\ &\le (1 + \eta + \eta^2 + \cdots + \eta^k)\|u^0\|_0\\ &\le 3\|u^0\|_0.\end{aligned}$$

Combining the above estimate with (3.31) gives (3.27). The proof is completed. ∎

Now we carry out an error analysis for the solution of the semidiscretized problem. First, we realize from (2.10) that the first step solution $u^1$ has second order accuracy. In fact, from combining (2.10) and (2.9) for $k = 1$, we have

$$\frac{1}{\Gamma(2-\alpha)\Delta t^\alpha}(u(t_1) - u^1) + A(u(t_1) - u^1) = -r_{\Delta t}^1.$$

Thus

$$\|u(t_1) - u^1\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x(u(t_1) - u^1)\|_0 \le c_\alpha\|\partial_t^2 u\|_{L^\infty(L^2)}\Delta t^2,$$

where $\|v\|_{L^\infty(L^2)} := \sup_{t\in[0,t_1]}\|v(\cdot,t)\|_0$. In order to obtain a global $(3-\alpha)$-order accurate scheme, the first step solution will have to be computed with the same accuracy. To this end, we propose the substepping scheme within the interval $(0, t_1)$ as follows: let $n$ be the smallest integer such that $n \ge \frac{\Delta t}{\Delta t^{2-\alpha}}$, i.e.,

$$n = \left\lceil \frac{\Delta t}{\Delta t^{2-\alpha}} \right\rceil, \tag{3.32}$$

and set the substep size

$$\Delta t_1 = \frac{\Delta t}{n}. \tag{3.33}$$

Now we apply the first step scheme with the subtime step size $\Delta t_1$, i.e.,

$$\frac{1}{\Gamma(2-\alpha)\Delta t_1^\alpha}\sum_{j=0}^{m-1}(u^{1,(m-j)}-u^{1,(m-j-1)})b_j + Au^{1,(m)} = 0,\ m=1,2,\dots,n, \tag{3.34}$$

with $u^{1,(0)} = u_0$ to compute $u^{1,(n)}$, where $b_j = (j+1)^{-\alpha+1} - j^{-\alpha+1}$. Then set $u^1 := u^{1,(n)}$. In virtue of the above analysis, it is readily seen that $u^1$ is an approximation to $u(t_1)$ with accuracy

$$\begin{aligned}\|u(t_1)-u^1\|_0 + \sqrt{\alpha_1}\ \|\partial_x(u(t_1)-u^1)\|_0 &\le c\|\partial_t^2 u\|_{L^\infty(L^2)} n\Delta t_1^\alpha \Delta t_1^{2-\alpha}\\ &\le c\|\partial_t^2 u\|_{L^\infty(L^2)}\Delta t^{3-\alpha},\end{aligned} \tag{3.35}$$

where $\alpha_1 = \Gamma(2-\alpha)\Delta t_1^\alpha$.

THEOREM 3.2. *Let $u$ be the exact solution of* (2.1), *$\{u^k\}_{k=0}^K$ be the semidiscrete solution of* (3.26) *with the initial $u^0 = u(0)$, and $u^1$ by* (3.34). *Suppose $\partial_t^3 u \in L^\infty((0,T];L^2(\Lambda))$, then the following error estimate holds:*

$$\|u(t_k)-u^k\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x(u(t_k)-u^k)\|_0 \le c_{\alpha,T}\|\partial_t^3 u\|_{L^\infty(L^2)}\Delta t^{3-\alpha},\ 2\le k\le K, \tag{3.36}$$

*where $c_{\alpha,T}$ depends only on $\alpha$ and $T$.*

*Proof.* Let $e^k = u(t_k) - u^k$. By combining (2.8) and (2.9), we derive

$$(e^k,v) + \alpha_0\beta_0^{-1}(\partial_x e^k, \partial_x v) = \sum_{i=1}^k d_{k-i}^k (e^{k-i}, v) - \alpha_0\beta_0^{-1}(r_{\Delta t}^k, v)\quad \forall v\in H_0^1(\Lambda).$$

Taking $v = e^k$ and following the same line as in Theorem 3.1 allows us to get

$$\begin{aligned}&\|e^k\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x e^k\|_0\\ &\quad\le 4\left(\|e^0\|_0^2 + \|e^1\|_0^2 + \frac{4T^\alpha\Gamma(1-\alpha)}{\beta_0}\max_{2\le i\le K}\|r_{\Delta t}^i\|_0^2\right)^{\frac12},\ k=2,\dots,K.\end{aligned} \tag{3.37}$$

Finally, using Lemma 2.1 and (3.35) gives (3.36). The proof is complete. ∎

## 4. Spectral discretization in space and error estimates.

Let $\mathbb{P}_N(\Lambda)$ be the space of all polynomials of degree less than or equal to $N$, and $\mathbb{P}_N^0(\Lambda) = H_0^1(\Lambda)\cap\mathbb{P}_N(\Lambda)$. The error estimation for $u_N^k$ will make use of the $H_0^1$-orthogonal projection operator $\pi_N^{1,0}$, defined by for all $\psi\in H_0^1(\Lambda)$, let $\pi_N^{1,0}\psi$ be in $\mathbb{P}_N^0(\Lambda)$ such that

$$(\partial_x\pi_N^{1,0}\psi, \partial_x v_N) = (\partial_x\psi, \partial_x v_N)\ \forall v_N\in\mathbb{P}_N^0(\Lambda). \tag{4.1}$$

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

$$\|\psi - \pi_N^{1,0}\psi\|_l \le cN^{l-m}\|\psi\|_m\quad \forall\psi\in H^m(\Lambda)\cap H_0^1(\Lambda),\ m\ge 1, l=0,1. \tag{4.2}$$

We first consider the first step full discrete solution, which is obtained by the spectral approximation to the subtime stepping problems (3.34), i.e., for all $m = 1,2,\dots,n$, with $n$ given in (3.32), find $u_N^{1,(m)}\in\mathbb{P}_N^0(\Lambda)$ such that for all $v_N\in\mathbb{P}_N^0(\Lambda)$,

$$\frac{1}{\Gamma(2-\alpha)\Delta t_1^\alpha}\sum_{j=0}^{m-1} b_j(u_N^{1,(m-j)} - u_N^{1,(m-j-1)}, v_N) + (\partial_x u_N^{1,(m)}, \partial_x v_N) = 0 \tag{4.3}$$

with $u_N^{1,(0)} = \pi_N^{1,0}u^0$. Then set $u_N^1 := u_N^{1,(n)}$. The following error estimate can be derived for this first step solution:

$$\begin{aligned}\|u(t_1) - u_N^1\|_0 &+ \sqrt{\alpha_1}\ \|\partial_x(u(t_1) - u_N^1)\|_0 \\ &\le c\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^2 u\|_{L^\infty(H^m)} \\ &\quad + \Delta t^{3-\alpha}\|\partial_t^2 u\|_{L^\infty(L^2)} + N^{1-m}\|u\|_{L^\infty(H^m)}\big),\end{aligned} \tag{4.4}$$

where $\|v\|_{L^\infty(H^m)} := \sup_{t\in[0,t_1]}\|v(\cdot,t)\|_m$, $\alpha_1$ was given in (3.35).

For the sake of simplification, we omit the proof of the above estimate, and only derive the error estimate of the spectral method for the time steps $k \ge 2$.

The spectral discretization of the weak problem (3.26) reads find $u_N^k \in \mathbb{P}_N^0(\Lambda)$ such that

$$(u_N^k, v_N) + \alpha_0\beta_0^{-1}\big(\partial_x u_N^k, \partial_x v_N\big) = \sum_{i=1}^k d_{k-i}^k(u_N^{k-i}, v_N) \quad \forall v_N \in \mathbb{P}_N^0(\Lambda). \tag{4.5}$$

Obviously, for $\{u_N^j\}_{j=0}^{k-1}$ given, the existence and uniqueness of the solution $u_N^k$ to (4.5) is guaranteed by the Lax–Milgram lemma.

THEOREM 4.1. *Let $u$ be the exact solution of* (2.1), *$\{u_N^k\}_{k=2}^K$ be the solution of the problem* (4.5) *with the first step solution $u_N^1$ given by* (4.3) *and the initial condition $u_N^0 = \pi_N^{1,0}u^0$. Suppose $\partial_t^3 u \in L^\infty((0,T]; H^m(\Lambda)), m \ge 1$. Then for $k = 2,\dots,K$, we have*

$$\begin{aligned}\|u(t_k) - u_N^k\|_0 &+ \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x(u(t_k) - u_N^k)\|_0 \\ &\le c_{\alpha,T}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)} \\ &\quad + \Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)} + N^{1-m}\|u\|_{L^\infty(H^m)}\big),\end{aligned} \tag{4.6}$$

*where $c_{\alpha,T}$ is a constant, which may depend on $\alpha$ and $T$.*

*Proof.* First we obtain from (2.8)

$$\begin{aligned}(u(t_k), v_N) + \alpha_0\beta_0^{-1}(\partial_x u(t_k), \partial_x v_N) &- \sum_{i=1}^k d_{k-i}^k(u(t_{k-i}), v_N) \\ &= -\alpha_0\beta_0^{-1}(r_{\Delta t}^k, v_N) \quad \forall v_N \in \mathbb{P}_N^0(\Lambda).\end{aligned} \tag{4.7}$$

Let $e_N^k := u_N^k - \pi_N^{1,0}u(t_k)$. It follows from (4.5) and (4.7)

$$(e_N^k, v_N) + \alpha_0\beta_0^{-1}(\partial_x e_N^k, \partial_x v_N) = \sum_{i=1}^k d_{k-i}^k(e_N^{k-i}, v_N) + \alpha_0\beta_0^{-1}(\delta_N^k, v_N),\ k \ge 2, \tag{4.8}$$

where

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

with $I_d$ the identity operator. From (2.7), we have

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

Using the triangle inequality, we obtain

$$\|\delta_N^k\|_0 \le \|(I_d-\pi_N^{1,0})\partial_t^\alpha u(t_k)\|_0 + \|(I_d-\pi_N^{1,0})r_{\Delta t}^k\|_0 + \|r_{\Delta t}^k\|_0. \tag{4.9}$$

To estimate the right-hand side, we apply (2.13) and (2.16). Then

$$\begin{aligned}
\|r_{\Delta t}^k\|_0 \le{}& \left\| \frac{-\alpha}{\Gamma(1-\alpha)} \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (u(\tau)-H_2^j(\tau)) \frac{d\tau}{(t_k-\tau)^{\alpha+1}} \right\|_0 \\
&+ \left\| \frac{1}{\Gamma(1-\alpha)} \int_{t_{k-1}}^{t_k} (\partial_\tau u(\tau) - \partial\tau H_2^{k-1}(\tau)) \frac{d\tau}{(t_k-\tau)^\alpha} \right\|_0, \\
\|(I_d-\pi_N^{1,0})r_{\Delta t}^k\|_0 \le{}& \left\| \frac{-\alpha}{\Gamma(1-\alpha)} \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} (I_d-\pi_N^{1,0})(u(\tau)-H_2^j(\tau)) \frac{d\tau}{(t_k-\tau)^{\alpha+1}} \right\|_0 \\
&+ \left\| \frac{1}{\Gamma(1-\alpha)} \int_{t_{k-1}}^{t_k} (I_d-\pi_N^{1,0})(\partial_\tau u(\tau) - \partial\tau H_2^{k-1}(\tau)) \frac{d\tau}{(t_k-\tau)^\alpha} \right\|_0.
\end{aligned}$$

It follows from a similar procedure as in the proof of Lemma 2.1:

$$\|r_{\Delta t}^k\|_0 \le c_\alpha \max_{t\in I} \|\partial_t^3 u(\cdot,t)\|_0 \Delta t^{3-\alpha}, \tag{4.10}$$

$$\|(I_d-\pi_N^{1,0})r_{\Delta t}^k\|_0 \le c_\alpha \max_{t\in I} \|(I_d-\pi_N^{1,0})\partial_t^3 u(\cdot,t)\|_0 \Delta t^{3-\alpha}. \tag{4.11}$$

Bringing (4.10), (4.11), and (4.2) to (4.9) gives

$$\begin{aligned}
\|\delta_N^k\|_0 \le{}& c_\alpha\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)} \\
&+ \Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)}\big),\ k\ge 2.
\end{aligned} \tag{4.12}$$

Let $\overline{e}_N^i = e_N^i - \eta e_N^{i-1},\ i=2,\dots,k$, where $\eta$ is given in (3.19). It is observed that (4.8) can be rewritten equivalently under the following form

$$\begin{aligned}
&(\overline{e}_N^k, v_N) + \alpha_0\beta_0^{-1}(\partial_x e_N^k, \partial_x v_N) \\
&\qquad = \eta(\overline{e}_N^{k-1}, v_N) + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k(\overline{e}_N^{k-i}, v_N) + \overline{d}_0^k(e_N^0, v_N) + \alpha_0\beta_0^{-1}(\delta_N^k, v_N),
\end{aligned}$$

where $\overline{d}_j^k$ is defined in (3.21). Then following the similar procedure as in Theorem 3.1, we derive

$$\begin{aligned}
\|e_N^k\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x e_N^k\|_0 &\le 4\left(\|e_N^0\|_0^2 + \|e_N^1\|_0^2 + \frac{4T^\alpha\Gamma(1-\alpha)}{\beta_0}\max_{2\le i\le K}\|\delta_N^i\|_0^2\right)^{\frac12} \\
&\le c_{\alpha,T}\left(\|e_N^1\|_0 + \max_{2\le i\le K}\|\delta_N^i\|_0\right).
\end{aligned}$$

Applying (4.4), the triangle inequality, and (4.12) to the right-hand side leads to

$$\begin{aligned}
&\|e_N^k\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x e_N^k\|_0 \\
&\quad\le c_{\alpha,T}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)} \\
&\qquad + \Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)}\big),\ 2\le k\le K.
\end{aligned}$$

Finally, we use the following triangle inequalities

$$\|u(t_k) - u_N^k\|_0 \leq \|e_N^k\|_0 + \|u(t_k) - \pi_N^{1,0} u(t_k)\|_0,$$
$$\|\partial_x(u(t_k) - u_N^k)\|_0 \leq \|\partial_x e_N^k\|_0 + \|\partial_x(u(t_k) - \pi_N^{1,0} u(t_k))\|_0,$$

and the estimate (4.2) to conclude

$$\begin{aligned}&\|u(t_k) - u_N^k\|_0 + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x(u(t_k) - u_N^k)\|_0 \\ &\quad\leq c_{\alpha,T}\big(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)} \\ &\qquad + \Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)} + N^{1-m}\|u\|_{L^\infty(H^m)}\big).\end{aligned}$$

The proof of the theorem is complete. ∎

**Influence of numerical quadratures and forcing function.** Now we consider the influence on the errors if the forcing function $f$ is present in the right-hand side of (2.1) and the Gauss–Lobatto numerical quadratue is used to evaluate the integrals in space. Let $L_N(x)$ denote the Legendre polynomial of degree $N$, $\{\xi_j,\ j = 0, 1, \ldots, N\}$ are the Legendre–Gauss–Lobatto (LGL) 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 estimates are well known [7, 23]:

$$\|\varphi\|_0 \leq \|\varphi\|_N \leq \sqrt{3}\|\varphi\|_0\ \forall\varphi \in \mathbb{P}_N(\Lambda), \tag{4.13}$$

$$|(\varphi, v_N) - (\varphi, v_N)_N| \leq cN^{-m}\|\varphi\|_m\|v_N\|_0\ \forall\varphi \in H^m(\Lambda), \quad \forall v_N \in \mathbb{P}_N(\Lambda),\ m \geq 1. \tag{4.14}$$

Now we analyze the spectral collocation approximation in space to the weak problem (3.26) with the additional forcing term $f$. We first consider the first step full discrete problem: for $m = 1, 2, \ldots, n$, find $u_N^{1,(m)} \in \mathbb{P}_N^0(\Lambda)$ such that

$$\widetilde{a}_N(u_N^{1,(m)}, v_N) = \widetilde{\mathcal{F}}_N(v_N)\ \forall v_N \in \mathbb{P}_N^0(\Lambda), \tag{4.15}$$

where the bilinear form $\widetilde{a}_N(\cdot,\cdot)$ is defined by

$$\widetilde{a}_N(u_N^{1,(m)}, v_N) := (u_N^{1,(m)}, v_N)_N + \alpha_1(\partial_x u_N^{1,(m)}, \partial_x v_N)_N,$$

and the functional $\widetilde{\mathcal{F}}_N(\cdot)$ is given by

(4.16)
$$\widetilde{\mathcal{F}}_N(v_N) := \sum_{i=0}^{m-2}(b_i - b_{i+1})(u_N^{1,(m-i-1)}, v_N)_N + b_{m-1}(u_N^{1,(0)}, v_N)_N + \alpha_1(f(\cdot, m\Delta t_1), v_N)_N.$$

Then set $u_N^1 = u_N^{1,(n)}$.

The collocation version of (4.5) for $k \geq 2$ is find $u_N^k \in \mathbb{P}_N^0(\Lambda)$ such that

$$a_N(u_N^k, v_N) = \mathcal{F}_N(v_N) \ \forall v_N \in \mathbb{P}_N^0(\Lambda), \tag{4.17}$$

where

$$a_N(u_N^k, v_N) := (u_N^k, v_N)_N + \alpha_0\beta_0^{-1}(\partial_x u_N^k, \partial_x v_N)_N, \tag{4.18}$$

$$\mathcal{F}_N(v_N) := \sum_{i=1}^{k} d_{k-i}^k (u_N^{k-i}, v_N)_N + \alpha_0\beta_0^{-1}(f(\cdot, t_k), v_N)_N. \tag{4.19}$$

For the sake of simplification, we only give the error estimate for the problem (4.17).

THEOREM 4.2. *Let $u$ be the exact solution of (2.1), $\{u_N^k\}_{k=2}^K$ be the solution of problem (4.17) with the first step solution $u_N^1$ given by (4.15). Suppose $\partial_t^3 u \in L^\infty((0,T]; H^m(\Lambda)), m \geq 1$, and $f \in L^\infty((0,T]; H^\sigma(\Lambda)), \sigma \geq 1$ . Then for $k = 2, \dots, K$, we have*

$$\begin{aligned} &\|u(t_k) - u_N^k\| + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x(u(t_k) - u_N^k)\| \\ &\quad \leq c_{\alpha,T}\big(\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)} + N^{-\sigma}\|f\|_{L^\infty(H^\sigma)} + N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} \\ &\qquad + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)} + N^{1-m}\|u\|_{L^\infty(H^m)}\big). \end{aligned} \tag{4.20}$$

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

$$\begin{aligned} a_N(e_N^k, v_N) &= (e_N^k, v_N)_N + \alpha_0\beta_0^{-1}(\partial_x e_N^k, \partial_x v_N)_N \\ &= (u_N^k, v_N)_N + \alpha_0\beta_0^{-1}(\partial_x u_N^k, \partial_x v_N)_N - (\pi_N^{1,0}u(t_k), v_N)_N \\ &\quad - \alpha_0\beta_0^{-1}(\partial_x \pi_N^{1,0} u(t_k), \partial_x v_N)_N \ \forall v_N \in \mathbb{P}_N^0(\Lambda). \end{aligned}$$

Using (4.17), we obtain

$$(e_N^k, v_N)_N + \alpha_0\beta_0^{-1}(\partial_x e_N^k, \partial_x v_N)_N = \sum_{i=1}^{k} d_{k-i}^k (e_N^{k-i}, v_N)_N + (\varepsilon_1^k, v_N)_N + (\varepsilon_2^k, v_N)_N, \tag{4.21}$$

where

$$(\varepsilon_1^k, v_N)_N = (u(t_k) - \pi_N^{1,0}u(t_k), v_N)_N - \sum_{i=1}^{k} d_{k-i}^k \big(u(t_{k-i}) - \pi_N^{1,0}u(t_{k-i}), v_N\big)_N$$

and

$$\begin{aligned} (\varepsilon_2^k, v_N)_N = &-(u(t_k), v_N)_N + \sum_{i=1}^{k} d_{k-i}^k (u(t_{k-i}), v_N)_N + \alpha_0\beta_0^{-1}(f(\cdot, t_k), v_N)_N \\ &- \alpha_0\beta_0^{-1}(\partial_x \pi_N^{1,0} u(t_k), \partial_x v_N)_N. \end{aligned}$$

Next we estimate $(\varepsilon_1^k, v_N)_N$ and $(\varepsilon_2^k, v_N)_N$. First, it is observed that

$$\begin{aligned}(\varepsilon_1^k, v_N)_N &= \left((I_d - \pi_N^{1,0})(u(t_k) - \sum_{i=1}^{k} d_{k-i}^k u(t_{k-i})), v_N\right)_N \\ &= \Big((I_d - \pi_N^{1,0})\alpha_0\beta_0^{-1} L_t^\alpha u(t_k), v_N\Big)_N \\ &= \alpha_0\beta_0^{-1}\Big((I_d - \pi_N^{1,0})\big(\partial_t^\alpha u(t_k) - r_{\Delta t}^k\big), v_N\Big)_N.\end{aligned}$$

By using the estimate (4.14), we obtain

$$\begin{aligned}|(\varepsilon_1^k, v_N)_N| &\le \alpha_0\beta_0^{-1}\big|\big((I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_k) - r_{\Delta t}^k), v_N\big)\big| \\ &\quad + c\alpha_0\beta_0^{-1}N^{-1}\big\|(I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_k) - r_{\Delta t}^k)\big\|_1\|v_N\|_0 \\ &\le \alpha_0\beta_0^{-1}\Big[\big\|(I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_k) - r_{\Delta t}^k)\big\|_0 \\ &\qquad + cN^{-1}\big\|(I_d - \pi_N^{1,0})(\partial_t^\alpha u(t_k) - r_{\Delta t}^k)\big\|_1\Big]\|v_N\|_0.\end{aligned}$$

Using the estimate (4.2) once again and following a similar procedure as in Theorem 4.1, we get

$$|(\varepsilon_1^k, v_N)_N| \le c_\alpha\alpha_0\beta_0^{-1}(N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + \Delta t^{3-\alpha}N^{-m}\|\partial_t^3 u\|_{L^\infty(H^m)})\|v_N\|_0. \tag{4.22}$$

On the other hand, we have

$$\begin{aligned}(\varepsilon_2^k, v_N)_N = -\alpha_0\beta_0^{-1}\big(L_t^\alpha u(t_k), v_N\big)_N \\ + \alpha_0\beta_0^{-1}(f(\cdot, t_k), v_N)_N - \alpha_0\beta_0^{-1}(\partial_x\pi_N^{1,0}u(t_k), \partial_x v_N).\end{aligned}$$

Note that in the equality above we have used the fact that

$$(\partial_x\pi_N^{1,0}u(t_k), \partial_x v_N)_N = (\partial_x\pi_N^{1,0}u(t_k), \partial_x v_N)\ \forall v_N \in \mathbb{P}_N^0(\Lambda).$$

Furthermore, we get from (2.1)

$$(\partial_x u(t_k), \partial_x v_N) = -(\partial_t^\alpha u(t_k), v_N) + (f(\cdot, t_k), v_N).$$

Using this equality and (4.1) we obtain

$$\begin{aligned}(\varepsilon_2^k, v_N)_N &= \alpha_0\beta_0^{-1}\big(L_t^\alpha u(t_k), v_N\big) - \alpha_0\beta_0^{-1}\big(L_t^\alpha u(t_k), v_N\big)_N \\ &\quad + \alpha_0\beta_0^{-1}\big(\partial_t^\alpha u(t_k) - L_t^\alpha u(t_k), v_N\big) \\ &\quad + \alpha_0\beta_0^{-1}\big(f(\cdot, t_k), v_N\big)_N - \alpha_0\beta_0^{-1}\big(f(\cdot, t_k), v_N\big).\end{aligned}$$

Applying (4.14) to the above result gives

$$\begin{aligned}\big|(\varepsilon_2^k, v_N)_N\big| &\le \alpha_0\beta_0^{-1}\big(\|r_{\Delta t}^k\|_0 + cN^{-m}\|f(\cdot, t_k)\|_m + cN^{-m}\|\partial_t^\alpha u(t_k) - r_{\Delta t}^k\|_m\big)\|v_N\|_0 \\ &\le \alpha_0\beta_0^{-1}c_\alpha\big(\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)} + N^{-\sigma}\|f\|_{L^\infty(H^\sigma)} \\ &\quad + N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)}\big)\|v_N\|_0.\end{aligned} \tag{4.23}$$

Combining (4.22) and (4.23) yields

$$\begin{aligned}\big|(\varepsilon_1^k, v_N)_N\big| + \big|(\varepsilon_2^k, v_N)_N\big| &\le \alpha_0\beta_0^{-1}c_\alpha\big(\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)} + N^{-\sigma}\|f\|_{L^\infty(H^\sigma)} \\ &\quad + N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)}\big)\|v_N\|_0.\end{aligned} \tag{4.24}$$

Let $\overline{e}_N^i := e_N^i - \eta e_N^{i-1},\ i = 2, \ldots, k$. It is observed that (4.21) can be rewritten under the following equivalent form:

$$\begin{aligned}
&(\overline{e}_N^k, v_N)_N + \alpha_0\beta_0^{-1}(\partial_x e_N^k, \partial_x v_N)_N \\
&\quad = \eta(\overline{e}_N^{k-1}, v_N)_N + \sum_{i=2}^{k-1} \overline{d}_{k-i}^k (\overline{e}_N^{k-i}, v_N)_N + \overline{d}_0^k (e_N^0, v_N)_N \\
&\qquad + (\varepsilon_1^k, v_N)_N + (\varepsilon_2^k, v_N)_N.
\end{aligned}$$

Thus using (4.13), (4.24), and a similar technique as in Theorem 4.1 allows us to obtain

$$\begin{aligned}
\|e_N^k\| + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x e_N^k\| &\le \|e_N^k\|_N + \sqrt{\alpha_0\beta_0^{-1}}\ \|\partial_x e_N^k\|_N \\
&\le c_{\alpha,T}\big(\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(L^2)} + N^{-\sigma}\|f\|_{L^\infty(H^\sigma)} \\
&\qquad + N^{-m}\|\partial_t^\alpha u\|_{L^\infty(H^m)} + N^{-m}\Delta t^{3-\alpha}\|\partial_t^3 u\|_{L^\infty(H^m)}\big).
\end{aligned}$$

Finally, by using (4.2) and the following triangle inequalities

$$\begin{aligned}
\|u(t_k) - u_N^k\|_0 &\le \|e_N^k\|_0 + \|u(t_k) - \Pi_N^{1,0} u(t_k)\|_0, \\
\|\partial_x(u(t_k) - u_N^k)\|_0 &\le \|\partial_x e_N^k\|_0 + \|\partial_x(u(t_k) - \Pi_N^{1,0} u(t_k))\|_0,
\end{aligned}$$

we get (4.20). ∎

## 5. Numerical results.

**5.1. Implementation.** The full discrete problem for the first time step (4.15) is implemented by using the Lagrangian polynomial $\{h_j\}_{j=1}^{N-1}$ based on the LGL points as the basis functions, we arrive at each time substep $m = 1, \ldots, n$ at a linear system as follows:

$$(B + \alpha_1 A)\underline{u}^{1,(m)} = \underline{\widetilde{f}}, \tag{5.1}$$

where $B$ is the mass matrix with the entries $B_{ij} := \omega_i\delta_{ij}, i, j = 1, \ldots, N-1$, $\alpha_1$ was given in (3.35), and $A$ is the stiffness matrix having the entries

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

$\underline{u}^{1,(m)}$ is the nodal unknown vector $(u_N^{1,(m)}(\xi_j))_{j=1}^{N-1}$, and $\underline{\widetilde{f}} = (\widetilde{\mathcal{F}}_N(h_j))_{j=1}^{N-1}$ with $\widetilde{\mathcal{F}}_N$ defined in (4.16).

Then the first step solution is obtained by setting $\underline{u}^1 = \underline{u}^{1,(n)}$.

Similarly, the nodal unknown $\underline{u}^k$ for $k \ge 2$ satisfies the linear system as follows:

$$(B + \alpha_0\beta_0^{-1} A)\underline{u}^k = \underline{f}, \tag{5.2}$$

where the right-hand side vector $\underline{f}$ is given by $(\mathcal{F}_N(h_j))_{j=1}^{N-1}$ with $\mathcal{F}_N$ being defined in (4.19).

Both systems (5.1) and (5.2) are symmetric positive definite, and will be solved by employing the conjugate gradient method.

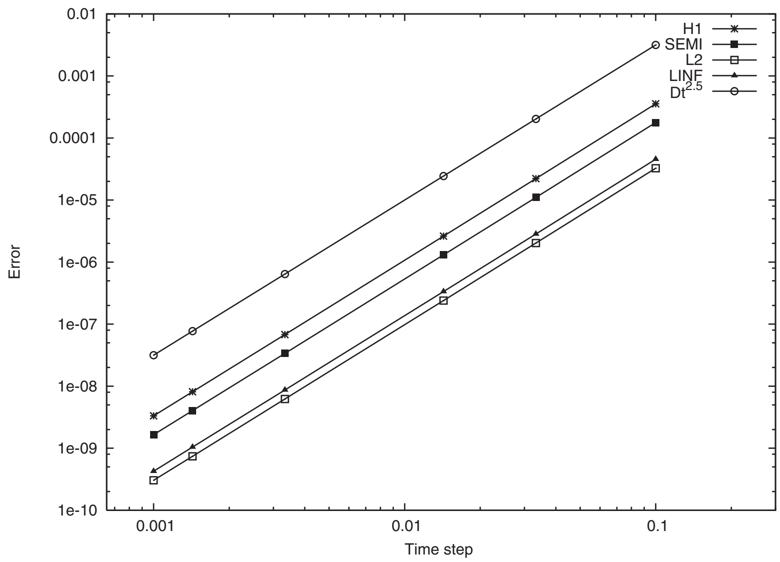


FIG. 1. *Errors as a function of the time step $\Delta t$ for $\alpha = 0.5$.*

**5.2. Numerical results.** In this subsection, we present numerical results to validate the error estimates obtained in Theorem 4.2 for the proposed time stepping/spectral method. Theorem 4.2 indicates that the convergence of numerical solutions would be of $(3-\alpha)$-order in time and exponential in space with respect to the polynomial degree if the exact solution is smooth enough. To this end, we choose the following forcing term and initial condition

$$f(x,t) = 3t^{1-\alpha}E_{1,2-\alpha}(3t)\cos\left(2\pi x + \frac{\pi}{2}\right) + 4\pi^2 e^{3t}\cos\left(2\pi x + \frac{\pi}{2}\right),$$
$$u_0(x) = \cos\left(2\pi x + \frac{\pi}{2}\right),$$

such that the problem (2.1) admits the smooth exact solution

$$u(x,t) = e^{3t}\cos\left(2\pi x + \frac{\pi}{2}\right),$$

where $E_{\mu,\nu}(z)$ is the Mittag–Leffler function

$$E_{\mu,\nu}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\mu n + \nu)}.$$

We first investigate the convergence rate of the time stepping scheme. To this end the polynomial degree $N$ is chosen big enough such that the spatial error is negligible as compared to the temporal error. In Figures 1–2, we plot the errors at $t = 1$ in the $H^1$, semi-$H^1$, $L^2$, and $L^\infty$ norms as a function of the time step sizes for $N = 28$. A logarithmic scale has been used for both the $\Delta t$-axis and error-axis in these figures, As predicted by the theoretical estimates, the proposed time scheme yields a temporal approximation order close to $3-\alpha$, i.e., the slopes of the error curves in these log-log plots are 2.5 and 2.01, respectively, for $\alpha = 0.5$ and 0.99.

It is interesting to see the impact of the first step error on the long time solution. We list in Table 1 the errors at the time $t = 1$, computed from the full discrete problem

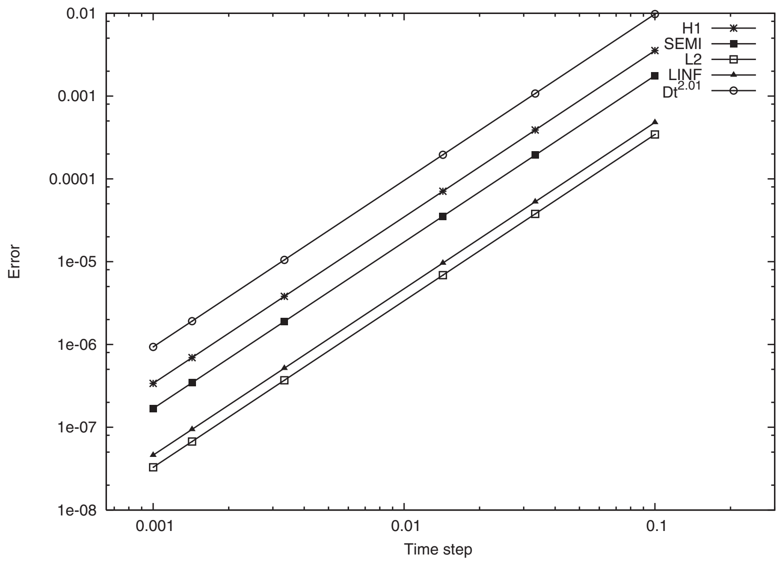


FIG. 2. *Errors as a function of the time step* $\Delta t$ *for* $\alpha = 0.99$.

TABLE 1
*Comparison on the errors at the end time without and with first time subcycling.*

| $\alpha$ | $\Delta t$ | Error without subcycling | Order | Error with subcycling | order |
|---|---|---|---|---|---|
| 0.3 | $\frac{1}{20}$ | $0.15884737E-03$ | | $0.15880081E-03$ | |
| | $\frac{1}{40}$ | $0.24345575E-04$ | 2.70 | $0.24338796E-04$ | 2.70 |
| | $\frac{1}{80}$ | $0.36206737E-05$ | 2.74 | $0.36196583E-05$ | 2.74 |
| | $\frac{1}{160}$ | $0.53168998E-06$ | 2.76 | $0.53153568E-06$ | 2.76 |
| | $\frac{1}{320}$ | $0.77833516E-07$ | 2.77 | $0.77809947E-07$ | 2.77 |
| | $\frac{1}{640}$ | $0.11416560E-07$ | 2.76 | $0.11413228E-07$ | 2.76 |
| | $\frac{1}{1280}$ | $0.16839934E-08$ | 2.76 | $0.16830342E-08$ | 2.76 |
| 0.7 | $\frac{1}{20}$ | $0.20876050E-02$ | | $0.20871967E-02$ | |
| | $\frac{1}{40}$ | $0.44554159E-03$ | 2.23 | $0.44545574E-03$ | 2.23 |
| | $\frac{1}{80}$ | $0.92573200E-04$ | 2.27 | $0.92556254E-04$ | 2.27 |
| | $\frac{1}{160}$ | $0.18987644E-04$ | 2.29 | $0.18984001E-04$ | 2.29 |
| | $\frac{1}{320}$ | $0.38712140E-05$ | 2.29 | $0.38704436E-05$ | 2.29 |
| | $\frac{1}{640}$ | $0.78710005E-06$ | 2.30 | $0.78693657E-06$ | 2.30 |
| | $\frac{1}{1280}$ | $0.15978074E-06$ | 2.30 | $0.15974607E-06$ | 2.30 |

(4.17) with and without the first step subcycling (4.15), respectively. It is found that the errors without and with the first step subcycling are essentially the same. This means that the first step error has decaying impact on the solution when the time increases. Indeed a closer look at the scheme (3.7) shows that the coefficient $d_1^k$ in front of the first step solution $u^1$ is decreasing as $k$ increases. This test implies that the first step subcycling (3.34) would not be really necessary if we are only interested in approximating the long time solution.

Finally the spatial accuracy is tested and shown in Figure 3, in which the errors with respect to the polynomial degree are plotted by fixing a time step size sufficiently

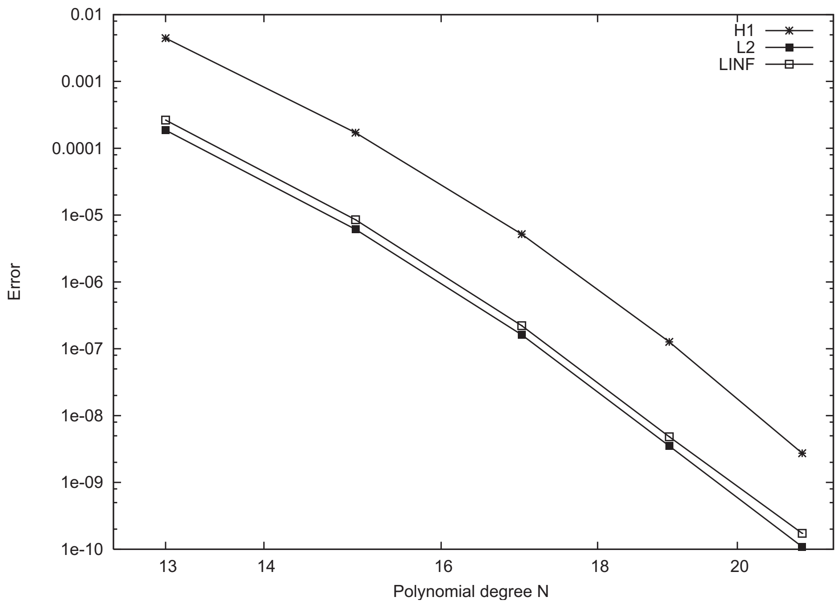


FIG. 3. *Errors as a function of the polynomial degree $N$ for $\alpha = 0.5$ and $\Delta t = 10^{-4}$.*

small. It is seen that the convergence rate is exponential as expected since the exact solution is a smooth function with respect to the space variable.

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