

# Finite difference/spectral approximations for the time-fractional diffusion equation <sup>☆</sup>

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## Abstract

In this paper, we consider the numerical resolution of a time-fractional diffusion equation, which is obtained from the standard diffusion equation by replacing the first-order time derivative with a fractional derivative (of order  $\alpha$ , with  $0 \leq \alpha \leq 1$ ). The main purpose of this work is to construct and analyze stable and high order scheme to efficiently solve the time-fractional diffusion equation. The proposed method is based on a finite difference scheme in time and Legendre spectral methods in space. Stability and convergence of the method are rigorously established. We prove that the full discretization is unconditionally stable, and the numerical solution converges to the exact one with order  $O(\Delta t^{2-\alpha} + N^{-m})$ , where  $\Delta t$ ,  $N$  and  $m$  are the time step size, polynomial degree, and regularity of the exact solution respectively. Numerical experiments are carried out to support the theoretical claims.

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## 1. Introduction

The use of fractional partial differential equations (FPDEs) in mathematical models has become increasingly popular in recent years. Different models using FPDEs have been proposed [4,14,16], and there has been significant interest in developing numerical schemes for their solution.

Roughly speaking, FPDEs can be classified into two principal kinds: space-fractional differential equation and time-fractional one. One of the simplest examples of the former is fractional order diffusion equations, which are generalizations of classical diffusion equations, treating super-diffusive flow processes. Much of

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the work published to date has been concerned with this kind of FPDEs (see e.g. [1,4–7,13,15,20] for a non-exhaustive list of references).

In this paper, we consider the time-fractional diffusion equation (TFDE), obtained from the standard diffusion equation by replacing the first-order time derivative with a fractional derivative of order  $\alpha$ , with  $0 \leq \alpha \leq 1$ . Time-fractional diffusion or wave equations are derived by considering continuous time random walk problems, which are in general non-Markovian processes. The physical interpretation of the fractional derivative is that it represents a degree of memory in the diffusing material [9]. These models have been investigated in analytical and numerical frames by a number of authors [8,11,18,19,21]. Some of these authors have tried to construct analytical solutions to problems of time-fractional differential equations. For example, Schneider and Wyss [18] and Wyss [21] considered the time-fractional diffusion-wave equations. The corresponding Green functions and their properties are obtained in terms of Fox functions. Gorenflo et al. [8,9] used the similarity method and the method of Laplace transform to obtain the scale-invariant solution of TFDE in terms of the Wright function. A similar construction of the solution to the time-fractional advection–dispersion equations or TFDE in whole-space and half-space has been given in [10,11] by using the Fourier–Laplace transforms.

However, published papers on the numerical solution of the TFDE equations are very sparse. Liu et al. [12] use a first-order finite difference scheme in both time and space directions for this equation, where some stability conditions are derived. Herein, we examine a practical finite difference/Legendre spectral method to solve the initial-boundary value time-fractional diffusion problem on a finite domain. An approach based on the backward differentiation combined with spatial collocation method is used to obtain estimates of  $(2-\alpha)$ -order convergence in time and exponential convergence in space. It is also shown that the time-stepping scheme is unconditionally stable for all  $\alpha \in [0, 1]$ . A series of numerical examples is presented and compared with the exact solutions to support the theoretical claims.

Let us emphasize that the computation of the numerical solution of time-fractional differential equations has been generally limited to simple cases (low spatial dimension or small time integration) due to the “global dependence” problem. Usually, by the definition of the fractional derivative, the solution at a time  $t_k$  depends on the solutions at all previous time levels  $t < t_k$ . The fact that all previous solutions have to be saved to compute the solution at the current time level would make the storage very expensive if low-order methods are employed for spatial discretization. Contrarily, use of the spectral method can relax this storage limit because, as compared to a low-order method, the spectral method needs fewer grid points to produce highly accurate solution. This is one of main advantages of the spectral method for FPDES. Another difficult point in solving TFDE lies in the discretization of the time-fractional derivative. The fact that the time-fractional derivative uses Caputo integral makes the standard schemes and corresponding numerical analysis not applicable. One of our main goals here is to propose an approach and provide an error analysis for this problem.

The outline of the paper is as follows: first, we provide in Section 2 an analytical solution of the TFDE in a bounded domain. Second, a finite difference scheme for temporal discretization of this problem is proposed in Section 3, where the stability and convergence analysis is given. A detailed error analysis is carried out for the semi-discrete problem, showing that the temporal accuracy is of  $(2-\alpha)$ -order. In Section 4, we construct a Legendre spectral collocation method for the spatial discretization of the TFDE. Error estimates are provided for the full discrete problem. Finally numerical experiments are presented in Section 5 which support the theoretical error estimates. Some concluding remarks are given in the final section.

## 2. Analytical solution of the TFDE in a bounded domain

In this section, we first describe the problem of fractional differential equation studied in this paper, and present some analytical solutions which will be found helpful in the comprehension of the nature of such a problem.

Let  $L > 0, T > 0, A = (0, L)$ , consider the time-fractional diffusion equation of the form

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} - \frac{\partial^2 u(x, t)}{\partial x^2} = f(x, t), \quad x \in A, \quad 0 < t \leq T \quad (2.1)$$

subject to the following initial and boundary conditions:

$$u(x, 0) = g(x), \quad x \in A, \tag{2.2}$$

$$u(0, t) = u(L, t) = 0, \quad 0 \leq t \leq T, \tag{2.3}$$

where  $\alpha$  is the order of the time-fractional derivative. Here, we consider the case  $0 \leq \alpha \leq 1$ .  $\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}$  in (2.1) is defined as the Caputo fractional derivatives of order  $\alpha$  [16], given by

$$\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{1}{\Gamma(1 - \alpha)} \int_0^t \frac{\partial u(x, s)}{\partial s} \frac{ds}{(t - s)^\alpha}, \quad 0 < \alpha < 1. \tag{2.4}$$

When  $\alpha = 1$ , Eq. (2.1) is the classical diffusion equation:

$$\frac{\partial u(x, t)}{\partial t} - \frac{\partial^2 u(x, t)}{\partial x^2} = f(x, t), \quad x \in A, \quad 0 < t \leq T, \tag{2.5}$$

while the case  $\alpha = 0$  corresponds to the classical Helmholtz elliptic equation. In fact the time derivative of integer order in (2.5) can be obtained by taking the limit  $\alpha \rightarrow 1$  in (2.4).

In the case  $0 < \alpha < 1$ , the definition of the Caputo fractional derivatives uses the information of the standard derivatives at all previous time levels (non-Markovian process).

If  $f \equiv 0$ , then by applying the finite sine and Laplace transforms to (2.1), the analytical solution for the problem (2.1)–(2.3) can be obtained [1] as

$$u(x, t) = \frac{2}{L} \sum_{n=0}^{\infty} E_\alpha(-a^2 n^2 t^\alpha) \sin( anx ) \int_0^L g(r) \sin( anr ) dr, \tag{2.6}$$

where  $a = \frac{\pi}{L}$  and

$$E_\alpha(z) = \sum_{m=0}^{\infty} \frac{z^m}{\Gamma(\alpha m + 1)}$$

is the Mittag–Leffler function.

We list here some special Mittag–Leffler-type functions having explicit expressions as follows:

$$E_1(-z) = e^{-z}, \quad E_2(z) = \cosh(\sqrt{z}), \quad E_{\frac{1}{2}}(z) = \sum_{m=0}^{\infty} \frac{z^m}{\Gamma(\frac{m}{2} + 1)} = e^{z^2} \operatorname{erfc}(-z),$$

where  $\operatorname{erfc}(z)$  is the error function complement defined by

$$\operatorname{erfc}(z) = \frac{1}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt.$$

Although expressed in a compact form, we note that using (2.6) to compute the exact solution is generally difficult (especially for large time) due to slow convergence of the series  $E_\alpha(z)$  for  $\alpha \in (0, 1)$  and big  $z$ . The exact solutions for a number of  $\alpha$  are plotted in Fig. 1, showing the smoothness of the solutions. The regularity of these solutions can be analyzed by using some properties of the Mittag–Leffler function [2].

In the analysis of the numerical method that follows, we will assume that problem (2.1)–(2.3) has a unique and sufficiently smooth solution.

### 3. Discretization in time: a finite difference scheme

In order to simplify the notations and without lose of generality, we consider the case  $f \equiv 0$  in the scheme construction and its numerical analysis.

First, we introduce a finite difference approximation to discretize the time-fractional derivative. Let  $t_k := k\Delta t$ ,  $k = 0, 1, \dots, K$ , where  $\Delta t := \frac{T}{K}$  is the time step. To motivate the construction of the scheme, we use the following formulation: for all  $0 \leq k \leq K - 1$ ,

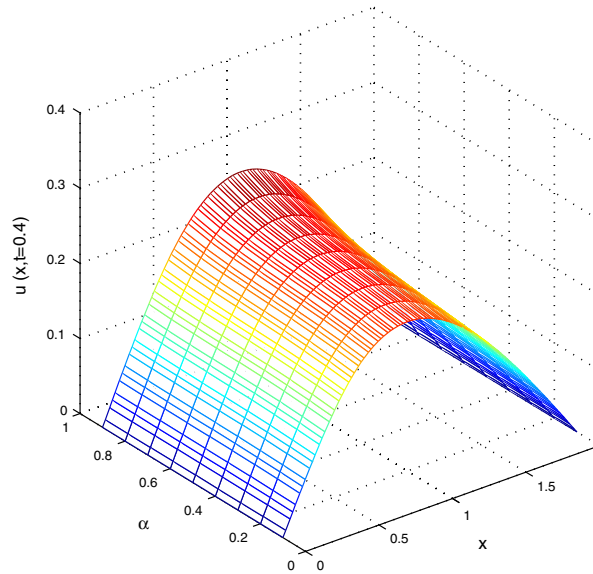


Fig. 1. Analytical solutions at  $t = 0.4$  for a number of  $\alpha$ .

$$\begin{aligned} \frac{\partial^\alpha u(x, t_{k+1})}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \int_{t_j}^{t_{j+1}} \frac{\partial u(x, s)}{\partial s} \frac{ds}{(t_{k+1}-s)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \frac{u(x, t_{j+1}) - u(x, t_j)}{\Delta t} \int_{t_j}^{t_{j+1}} \frac{ds}{(t_{k+1}-s)^\alpha} + r_{\Delta t}^{k+1}, \end{aligned} \tag{3.1}$$

where  $r_{\Delta t}^{k+1}$  is the truncation error. It can be verified that the truncation error takes the following form:

$$r_{\Delta t}^{k+1} \leq c_u \left[ \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \int_{t_j}^{t_{j+1}} \frac{t_{j+1} + t_j - 2s}{(t_{k+1}-s)^\alpha} ds + O(\Delta t^2) \right], \tag{3.2}$$

where  $c_u$  is a constant depending only on  $u$ .

For the first term in RHS of (3.2), we have

$$\begin{aligned} &\frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \int_{t_j}^{t_{j+1}} \frac{t_{j+1} + t_j - 2s}{(t_{k+1}-s)^\alpha} ds \\ &= -\frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \frac{1}{1-\alpha} (2j+1) \Delta t^{2-\alpha} [(k-j)^{1-\alpha} - (k+1-j)^{1-\alpha}] + \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \frac{2}{1-\alpha} \Delta t^{2-\alpha} [(j+1)(k-j)^{1-\alpha} \\ &\quad - j(k+1-j)^{1-\alpha}] + \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \frac{2}{(1-\alpha)(2-\alpha)} \Delta t^{2-\alpha} [(k-j)^{2-\alpha} - (k+1-j)^{2-\alpha}] \\ &= \frac{\Delta t^{2-\alpha}}{\Gamma(2-\alpha)} \left[ (k+1)^{1-\alpha} + 2(k^{1-\alpha} + (k-1)^{1-\alpha} + (k-2)^{1-\alpha} + \dots + 1^{1-\alpha}) \right] - \frac{2\Delta t^{2-\alpha}}{\Gamma(3-\alpha)} (k+1)^{2-\alpha} \\ &= \frac{\Delta t^{2-\alpha}}{\Gamma(2-\alpha)} \left[ (k+1)^{1-\alpha} + 2(k^{1-\alpha} + (k-1)^{1-\alpha} + (k-2)^{1-\alpha} + \dots + 1^{1-\alpha}) - \frac{2}{2-\alpha} (k+1)^{2-\alpha} \right]. \end{aligned}$$

Let

$$S(k) = (k+1)^{1-\alpha} + 2(k^{1-\alpha} + (k-1)^{1-\alpha} + (k-2)^{1-\alpha} + \dots + 1^{1-\alpha}) - \frac{2}{2-\alpha} (k+1)^{2-\alpha}.$$

Incidentally, we find that  $|S(k)|$  is bounded for all  $\alpha \in [0, 1]$  and all  $k \geq 1$ , as proven in the following lemma.

**Lemma 3.1.** For all  $\alpha \in [0, 1]$  and all  $K \geq 1$ , it holds

$$|S(K)| \leq c,$$

where  $c$  is a constant independent of  $\alpha, K$ .

**Proof.** First, for  $\alpha = 0$ , a direct calculation shows  $S(K) = 0$  for all  $K \geq 1$ . Now we prove the lemma for  $\alpha \in (0, 1]$ . It can be verified that

$$S(K) = (K + 1)^{1-\alpha} + 2(K^{1-\alpha} + (K - 1)^{1-\alpha} + (K - 2)^{1-\alpha} + \dots + 1^{1-\alpha}) - \frac{2}{2-\alpha} (K + 1)^{2-\alpha} = \sum_{k=0}^K a_k,$$

where

$$a_k = (k + 1)^{1-\alpha} + k^{1-\alpha} - \frac{2}{2-\alpha} ((k + 1)^{2-\alpha} - k^{2-\alpha}).$$

This observation leads us to prove that the series  $\sum_{k=0}^{\infty} a_k$  converges. It is well known that the series  $\sum_{k=1}^{\infty} \frac{1}{k^\beta}$  converges for all  $\beta > 1$ . By consequence, it suffices to prove  $|a_k| \leq \frac{1}{k^{1+\alpha}}$  for big enough  $k$ . In fact we have, for  $k \geq 2$ ,

$$\begin{aligned} |a_k| &= k^{1-\alpha} \left| \left(1 + \frac{1}{k}\right)^{1-\alpha} + 1 - \frac{2k}{2-\alpha} \left( \left(1 + \frac{1}{k}\right)^{2-\alpha} - 1 \right) \right| \\ &= k^{1-\alpha} \left| 1 + 1 + (1-\alpha)\frac{1}{k} + \frac{(1-\alpha)(-\alpha)}{2!} \frac{1}{k^2} + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!} \frac{1}{k^3} + \dots \right. \\ &\quad \left. - \frac{2k}{2-\alpha} \left( -1 + 1 + (2-\alpha)\frac{1}{k} + \frac{(2-\alpha)(1-\alpha)}{2!} \frac{1}{k^2} + \frac{(2-\alpha)(1-\alpha)(-\alpha)}{3!} \frac{1}{k^3} + \frac{(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)}{4!} \frac{1}{k^4} + \dots \right) \right| \\ &= k^{1-\alpha} \left| \left(\frac{1}{2!} - \frac{2}{3!}\right) (1-\alpha)(-\alpha) \frac{1}{k^2} + \left(\frac{1}{3!} - \frac{2}{4!}\right) (1-\alpha)(-\alpha)(-\alpha-1) \frac{1}{k^3} + \dots \right| \\ &\leq k^{1-\alpha} \frac{1}{3!} (1-\alpha)\alpha \frac{1}{k^2} \left( 1 + \frac{2(\alpha+1)}{4} \frac{1}{k} + \frac{3(\alpha+1)(\alpha+2)}{20} \frac{1}{k^2} + \dots \right) \\ &\leq \frac{1}{3!} (1-\alpha)\alpha \frac{1}{k^{1+\alpha}} \left( 1 + \frac{1}{k} + \frac{1}{k^2} + \dots \right) \leq \frac{2}{3!} (1-\alpha)\alpha \frac{1}{k^{1+\alpha}} \leq \frac{1}{k^{1+\alpha}}. \end{aligned}$$

The proof is completed.  $\square$

More precise bound of  $S(k)$  can be obtained by numerical computations. Indeed our numerical tests show that  $-1 \leq S(k) \leq 0 \forall 0 \leq \alpha \leq 1, k = 1, 2, \dots$ , as observed in Fig. 2, where evolution of  $S(k)$  as a function of  $k$  for several typical values of  $\alpha$  is plotted in the left figure, while limit of  $S(k)$  as  $k$  tends to infinity as a function of  $\alpha$  is shown in the right figure.

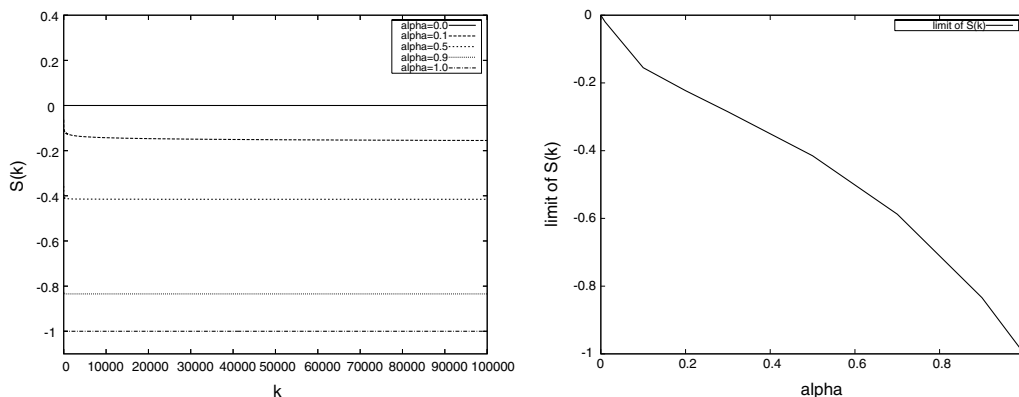


Fig. 2. (Left)  $S(k)$  as a function of  $k$  for several typical  $\alpha$ ; (right) limit of  $S(k)$  as a function of  $\alpha$ .

Using Lemma 3.1, and taking into account the fact that  $\frac{1}{\Gamma(2-\alpha)} \leq 2$  for all  $\alpha \in [0, 1]$ , we have

$$\left| \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \int_{t_j}^{t_{j+1}} \frac{t_{j+1} + t_j - 2s}{(t_{k+1} - s)^\alpha} ds \right| \leq 2\Delta t^{2-\alpha}.$$

As a result, it holds

$$r_{\Delta t}^{k+1} \lesssim c_u \Delta t^{2-\alpha}. \tag{3.3}$$

On the other side, a straightforward calculation of the first term in RHS of (3.1) gives

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

For the sake of simplification, let us introduce the notations  $b_j := (j+1)^{1-\alpha} - j^{1-\alpha}, j = 0, 1, \dots, k$ , and define the discrete fractional differential operator  $L_t^\alpha$  by

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

Then (3.1) reads

$$\frac{\partial^\alpha u(x, t_{k+1})}{\partial t^\alpha} = L_t^\alpha u(x, t_{k+1}) + r_{\Delta t}^{k+1}. \tag{3.4}$$

Using  $L_t^\alpha u(x, t_{k+1})$  as an approximation of  $\frac{\partial^\alpha u(x, t_{k+1})}{\partial t^\alpha}$  leads to the following finite difference scheme to (2.1):

$$L_t^\alpha u^{k+1}(x) = \frac{\partial^2 u^{k+1}(x)}{\partial x^2}, \quad k = 0, 1, \dots, K-1, \tag{3.5}$$

where  $u^{k+1}(x)$  is an approximation to  $u(x, t_{k+1})$ . By virtue of (3.3), this scheme is formally of  $(2-\alpha)$ -order accuracy. A rigorous analysis of the convergence rate will be provided later for both semi-discrete and full-discrete cases, where we will prove that the temporal accuracy of the scheme (3.5) is globally of order  $2-\alpha$ .

Scheme (3.5) can be rewritten into, with simplification by omitting the dependence of  $u^{k+1}(x)$  on  $x$ :

$$b_0 u^{k+1} - \Gamma(2-\alpha) \Delta t^\alpha \frac{\partial^2 u^{k+1}}{\partial x^2} = b_0 u^k - \sum_{j=1}^k b_j [u^{k+1-j} - u^{k-j}] = b_0 u^k - \sum_{j=0}^{k-1} b_{j+1} u^{k-j} + \sum_{j=1}^k b_j u^{k-j}. \tag{3.6}$$

It is worthwhile to noting that the second term in the RHS of (3.6) automatically vanishes when  $k \leq 1$ , while the last two terms of (3.6) vanish when  $k = 0$ .

It is direct to check that

$$\begin{aligned} b_j &> 0, \quad j = 0, 1, \dots, k, \\ 1 &= b_0 > b_1 > \dots > b_k, \quad b_k \rightarrow 0 \quad \text{as } k \rightarrow \infty, \\ \sum_{j=0}^k (b_j - b_{j+1}) + b_{k+1} &= (1 - b_1) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) + b_k = 1. \end{aligned} \tag{3.7}$$

Let us introduce the parameter  $\alpha_0$ :

$$\alpha_0 := \Gamma(2-\alpha) \Delta t^\alpha,$$

and note that  $b_0 = 1$ , then by reformulating the right-hand side of (3.6), we obtain an equivalent form to scheme (3.5):

$$u^{k+1} - \alpha_0 \frac{\partial^2 u^{k+1}}{\partial x^2} = (1 - b_1)u^k + \sum_{j=1}^{k-1} (b_j - b_{j+1})u^{k-j} + b_k u^0, \quad k \geq 1. \tag{3.8}$$

Here again, when  $k = 1$  scheme (3.8) becomes

$$u^2 - \alpha_0 \frac{\partial^2 u^2}{\partial x^2} = (1 - b_1)u^1 + b_1 u^0.$$

For the special case  $k = 0$ , that is the first time step, the scheme simply reads

$$u^1 - \alpha_0 \frac{\partial^2 u^1}{\partial x^2} = u^0. \tag{3.9}$$

Eqs. (3.8) and (3.9), together with the boundary conditions

$$u^{k+1}(0) = u^{k+1}(L) = 0, \quad k \geq 0, \tag{3.10}$$

and the initial condition

$$u^0(x) = g(x), \quad x \in A \tag{3.11}$$

form a complete set of the semi-discrete problem.

It will be useful to define the error term  $r^{k+1}$  by

$$r^{k+1} := \alpha_0 \left[ \frac{\partial^2 u(x, t_{k+1})}{\partial t^2} - L_t^2 u(x, t_{k+1}) \right]. \tag{3.12}$$

Then we have from (3.3) and (3.4)

$$|r^{k+1}| = \Gamma(2 - \alpha) \Delta t^\alpha |r_{\Delta t}^{k+1}| \leq c_u \Delta t^2. \tag{3.13}$$

To introduce the variational formulation of the problem (3.8), we define some functional spaces endowed with standard norms and inner products that will be used hereafter.

$$\begin{aligned} H^1(A) &:= \left\{ v \in L^2(A), \frac{dv}{dx} \in L^2(A) \right\}, \\ H_0^1(A) &:= \{ v \in H^1(A), v|_{\partial A} = 0 \}, \\ H^m(A) &:= \left\{ v \in L^2(A), \frac{d^k v}{dx^k} \in L^2(A) \text{ for all positive integer } k \leq m \right\}, \end{aligned}$$

where  $L^2(A)$  is the space of measurable functions whose square is Lebesgue integrable in  $A$ . The inner products of  $L^2(A)$  and  $H^1(A)$  are defined, respectively, by

$$(u, v) = \int_A uv \, dx, \quad (u, v)_1 = (u, v) + \left( \frac{du}{dx}, \frac{dv}{dx} \right)$$

and the corresponding norms by

$$\|v\|_0 = (v, v)^{1/2}, \quad \|v\|_1 = (v, v)_1^{1/2}.$$

The norm  $\|\cdot\|_m$  of the space  $H^m(A)$  is defined by

$$\|v\|_m = \left( \sum_{k=0}^m \left\| \frac{d^k v}{dx^k} \right\|_0^2 \right)^{1/2}.$$

In this paper, instead of using the above standard  $H^1$ -norm, we prefer to define  $\|\cdot\|_1$  by

$$\|v\|_1 = \left( \|v\|_0^2 + \alpha_0 \left\| \frac{du}{dx} \right\|_0^2 \right)^{1/2}. \tag{3.14}$$

It is well known that the standard  $H^1$ -norm and the norm defined by (3.14) are equivalent, the latter will be used in what follows.

The variational (weak) formulation of the Eq. (3.8) subject to the boundary condition (3.10) reads: find  $u^{k+1} \in H_0^1(A)$ , such that

$$(u^{k+1}, v) + \alpha_0 \left( \frac{\partial u^{k+1}}{\partial x}, \frac{\partial v}{\partial x} \right) = (1 - b_1)(u^k, v) + \sum_{j=1}^{k-1} (b_j - b_{j+1})(u^{k-j}, v) + b_k(u^0, v), \quad \forall v \in H_0^1(A). \tag{3.15}$$

For this weak semi-discretized problem, we have the following stability result.

**Theorem 3.1.** *The semi-discretized problem (3.15) is unconditionally stable in the sense that for all  $\Delta t > 0$ , it holds*

$$\|u^{k+1}\|_1 \leq \|u^0\|_0, \quad k = 0, 1, \dots, K - 1.$$

**Proof.** We will prove the result by induction. First when  $k = 0$ , we have

$$(u^1, v) + \alpha_0 \left( \frac{\partial u^1}{\partial x}, \frac{\partial v}{\partial x} \right) = (u^0, v) \quad \forall v \in H_0^1(A).$$

Taking  $v = u^1$  and using the inequality  $\|v\|_0 \leq \|v\|_1$  and Schwarz inequality, we obtain immediately

$$\|u^1\|_1 \leq \|u^0\|_0.$$

Suppose now we have proven

$$\|u^j\|_1 \leq \|u^0\|_0, \quad j = 1, 2, \dots, k, \tag{3.16}$$

we want to prove  $\|u^{k+1}\|_1 \leq \|u^0\|_0$ . Taking  $v = u^{k+1}$  in (3.15) gives

$$(u^{k+1}, u^{k+1}) + \alpha_0 \left( \frac{\partial u^{k+1}}{\partial x}, \frac{\partial u^{k+1}}{\partial x} \right) = (1 - b_1)(u^k, u^{k+1}) + \sum_{j=1}^{k-1} (b_j - b_{j+1})(u^{k-j}, u^{k+1}) + b_k(u^0, u^{k+1}).$$

Hence, by using (3.16), we have

$$\begin{aligned} \|u^{k+1}\|_1^2 &\leq (1 - b_1)\|u^k\|_0\|u^{k+1}\|_0 + \sum_{j=1}^{k-1} (b_j - b_{j+1})\|u^{k-j}\|_0\|u^{k+1}\|_0 + b_k\|u^0\|_0\|u^{k+1}\|_0 \\ &\leq [(1 - b_1) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) + b_k]\|u^0\|_0\|u^{k+1}\|_1. \end{aligned}$$

Finally, the last equality of (3.7) yields

$$\|u^{k+1}\|_1 \leq \|u^0\|_0. \quad \square$$

Now we carry out an error analysis for the solution of the semi-discretized problem. We denote from now by  $c$  a generic constant which may not be the same at different occurrences.

**Theorem 3.2.** *Let  $u$  be the exact solution of (2.1)–(2.3),  $\{u^k\}_{k=0}^K$  be the time-discrete solution of (3.15) with the initial condition  $u^0(x) = u(x, 0)$ , then we have the following error estimates:*

(1) when  $0 \leq \alpha < 1$ ,

$$\|u(t_k) - u^k\|_1 \leq c_{u,\alpha} T^\alpha \Delta t^{2-\alpha}, \quad k = 1, 2, \dots, K, \tag{3.17}$$

where  $c_{u,\alpha} := c_u / (1 - \alpha)$ , with  $c_u$ : constant defined in (3.3);

(2) when  $\alpha \rightarrow 1$ ,

$$\|u(t_k) - u^k\|_1 \leq c_u T \Delta t, \quad k = 1, 2, \dots, K. \tag{3.18}$$



**Proof.** (1) First consider the case  $0 \leq \alpha < 1$ . We start by proving the following estimate:

$$\|u(t_j) - u^j\|_1 \leq c_u b_{j-1}^{-1} \Delta t^2, \quad j = 1, 2, \dots, K. \tag{3.19}$$

As in the proof of **Theorem 3.1**, we will use the mathematical induction. Let  $\bar{e}^k = u(x, t_k) - u^k(x)$ . For  $j = 1$ , we have, by combining (2.1), (3.9) and (3.12), the error equation:

$$(\bar{e}^1, v) + \alpha_0 \left( \frac{\partial \bar{e}^1}{\partial x}, \frac{\partial v}{\partial x} \right) = (\bar{e}^0, v) + (r^1, v) = (r^1, v) \quad \forall v \in H_0^1(A).$$

Taking  $v = \bar{e}^1$  yields

$$\|\bar{e}^1\|_1^2 \leq \|r^1\|_0 \|\bar{e}^1\|_0.$$

This, together with (3.13), gives

$$\|u(t_1) - u^1\|_1 \leq c_u b_0^{-1} \Delta t^2.$$

Therefore, (3.19) is proven for the case  $j = 1$ .

Suppose now (3.19) holds for all  $j = 1, 2, \dots, k$ , we need then to prove that it holds also for  $j = k + 1$ .

By combining (2.1), (3.12) and (3.15), we derive,  $\forall v \in H_0^1(A)$

$$(\bar{e}^{k+1}, v) + \alpha_0 \left( \frac{\partial \bar{e}^{k+1}}{\partial x}, \frac{\partial v}{\partial x} \right) = (1 - b_1)(\bar{e}^k, v) + \sum_{j=1}^{k-1} (b_j - b_{j+1})(\bar{e}^{k-j}, v) + b_k(\bar{e}^0, v) + (r^{k+1}, v). \tag{3.20}$$

Let  $v = \bar{e}^{k+1}$  in (3.20), then

$$\|\bar{e}^{k+1}\|_1^2 \leq (1 - b_1)\|\bar{e}^k\|_0 \|\bar{e}^{k+1}\|_0 + \sum_{j=1}^{k-1} (b_j - b_{j+1})\|\bar{e}^{k-j}\|_0 \|\bar{e}^{k+1}\|_0 + b_k\|\bar{e}^0\|_0 \|\bar{e}^{k+1}\|_0 + \|r^{k+1}\|_0 \|\bar{e}^{k+1}\|_0.$$

Dividing by  $\|\bar{e}^{k+1}\|_1$  at both sides, using the induction assumption and the fact that  $\frac{b_j^{-1}}{b_{j+1}^{-1}} < 1$  for all non-negative integer  $j$ , we obtain

$$\|\bar{e}^{k+1}\|_1 \leq \left[ (1 - b_1)b_{k-1}^{-1} + \sum_{j=1}^{k-1} (b_j - b_{j+1})b_{k-j-1}^{-1} \right] c_u \Delta t^2 + c_u \Delta t^2 \leq \left[ (1 - b_1) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) + b_k \right] c_u b_k^{-1} \Delta t^2.$$

Using (3.7) in the above inequality gives

$$\|\bar{e}^{k+1}\|_1 \leq c_u b_k^{-1} \Delta t^2.$$

The estimate (3.19) is proved.

Now, by the definition of  $b_k$ , a direct computation shows that

$$k^{-\alpha} b_{k-1}^{-1} = \frac{k^{-\alpha}}{k^{1-\alpha} - (k-1)^{1-\alpha}} \rightarrow \frac{1}{1-\alpha}, \quad \text{as } k \rightarrow \infty,$$

and the function  $\phi(x) := \frac{x^{-\alpha}}{x^{1-\alpha} - (x-1)^{1-\alpha}}$  is increasing on  $x$  for all  $x > 1$  since

$$\phi'(x) = \frac{1}{x(x-1)^\alpha} \left[ 1 - \left( 1 - \frac{1}{x} \right)^\alpha - \frac{\alpha}{x} \right] \geq 0 \quad \forall x > 1, \quad 0 \leq \alpha \leq 1.$$

This means  $k^{-\alpha} b_{k-1}^{-1}$  increasingly tends to  $\frac{1}{1-\alpha}$  as  $1 < k \rightarrow \infty$ . Note that  $k^{-\alpha} b_{k-1}^{-1} = 1$  when  $k = 1$ , hence we have

$$k^{-\alpha} b_{k-1}^{-1} \leq \frac{1}{1-\alpha}, \quad k = 1, 2, \dots, K. \tag{3.21}$$

Consequently we obtain, for all  $k$  such that  $k\Delta t \leq T$ ,

$$\|u(t_k) - u^k\|_1 \leq c_u b_{k-1}^{-1} \Delta t^2 = c_u k^{-\alpha} b_{k-1}^{-1} k^\alpha \Delta t^2 \leq c_u \frac{1}{1-\alpha} (k\Delta t)^\alpha \Delta t^{2-\alpha} \leq c_{u,\alpha} T^\alpha \Delta t^{2-\alpha}.$$

(2) Now we consider the case  $\alpha \rightarrow 1$ . Note that in this case, the estimate (3.17) has no meaning since  $c_{u,\alpha}$  tends to infinity as  $\alpha \rightarrow 1$ . Therefore, we need to look for an estimate of other form.

Taking into account the fact  $j\Delta t \leq T$  for all  $j = 1, 2, \dots, K$ , we are led to establish:

$$\|u(t_j) - u^j\|_1 \leq c_u j \Delta t^2, \quad j = 1, 2, \dots, K. \tag{3.22}$$

Once again, we derive this estimate by induction.

(3.22) is obvious for  $j = 1$ . Suppose now (3.22) holds for  $j = 1, 2, \dots, k$ , we want to prove that it remains true for  $j = k + 1$ . A similar procedure as in case (1) leads to

$$\begin{aligned} \|\bar{e}^{k+1}\|_1 &\leq (1 - b_1) \|\bar{e}^k\|_0 + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \|\bar{e}^{k-j}\|_0 + b_k \|\bar{e}^0\|_0 + \|r^{k+1}\|_0 \\ &\leq (1 - b_1) [c_u k \Delta t^2] + \sum_{j=1}^{k-1} (b_j - b_{j+1}) [c_u (k - j) \Delta t^2] + c_u \Delta t^2 \\ &= \left[ (1 - b_1) \frac{k}{k+1} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \frac{k-j}{k+1} + \frac{1}{k+1} \right] c_u (k+1) \Delta t^2 \\ &= \left[ (1 - b_1) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) - (1 - b_1) \frac{1}{k+1} - \sum_{j=1}^{k-1} (b_j - b_{j+1}) \frac{j+1}{k+1} + \frac{1}{k+1} \right] c_u (k+1) \Delta t^2. \end{aligned} \tag{3.23}$$

It is observed that

$$(1 - b_1) \frac{1}{k+1} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \frac{j+1}{k+1} + b_k \geq \frac{1}{k+1} \left[ (1 - b_1) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) + b_k \right] = \frac{1}{k+1},$$

which is equivalent to

$$-(1 - b_1) \frac{1}{k+1} - \sum_{j=1}^{k-1} (b_j - b_{j+1}) \frac{j+1}{k+1} + \frac{1}{k+1} \leq b_k.$$

Bringing this inequality into (3.23) gives

$$\|\bar{e}^{k+1}\|_1 \leq \left[ (1 - b_1) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) + b_k \right] c_u (k+1) \Delta t^2 = c_u (k+1) \Delta t^2.$$

Hence (3.22) is proven, i.e. (3.18) holds. The proof is completed.  $\square$

### 4. Full discretization

#### 4.1. A Galerkin spectral method in space

To simplify the notations, we let  $A = (-1, 1)$  hereafter. The Galerkin spectral discretization proceeds by approximating the solution by the polynomials of high degree. To this end, we define  $\mathbb{P}_N(A)$  the space of all polynomials of degree  $\leq N$  with respect to  $x$ . Then the discrete space, denoted by  $\mathbb{P}_N^0(A)$ , is defined as follows:  $\mathbb{P}_N^0(A) := H_0^1(A) \cap \mathbb{P}_N(A)$ .

Now consider the spectral discretization to the problem (3.15) as follows: find  $u_N^{k+1} \in \mathbb{P}_N^0(A)$ , such that for all  $v_N \in \mathbb{P}_N^0(A)$

$$(u_N^{k+1}, v_N) + \alpha_0 \left( \frac{\partial}{\partial x} u_N^{k+1}, \frac{\partial}{\partial x} v_N \right) = (1 - b_1) (u_N^k, v_N) + \sum_{j=1}^{k-1} (b_j - b_{j+1}) (u_N^{k-j}, v_N) + b_k (u_N^0, v_N). \tag{4.1}$$

For  $\{u_N^j\}_{j=0}^k$  given, the well-posedness of the problem (4.1) is guaranteed by the well-known Lax–Milgram Lemma. We are interested in this section in deriving an error estimate for the full-discrete solution  $\{u_N^k\}_{k=0}^K$ .

Let  $\pi_N^1$  be the  $H^1$ -orthogonal projection operator from  $H_0^1(\mathcal{A})$  into  $\mathbb{P}_N^0(\mathcal{A})$ , associated to the norm  $\|\cdot\|_1$  defined in (3.14), that is, for all  $\psi \in H_0^1(\mathcal{A})$ , define  $\pi_N^1\psi \in \mathbb{P}_N^0(\mathcal{A})$ , such that,  $\forall v_N \in \mathbb{P}_N^0(\mathcal{A})$ ,

$$(\pi_N^1\psi, v_N) + \alpha_0 \left( \frac{d}{dx} \pi_N^1\psi, \frac{d}{dx} v_N \right) = (\psi, v_N) + \alpha_0 \left( \frac{d}{dx} \psi, \frac{d}{dx} v_N \right). \tag{4.2}$$

It is known that the following projection estimate holds [3]:

$$\|\psi - \pi_N^1\psi\|_1 \leq cN^{1-m}\|\psi\|_m, \quad \text{if } \psi \in H^m(\mathcal{A}) \cap H_0^1(\mathcal{A}), \quad m \geq 1. \tag{4.3}$$

**Theorem 4.1.** Let  $\{u_N^k\}_{k=0}^K$  is the solution of the problem (4.1) with the initial condition  $u_N^0$  taken to be  $\pi_N^1u^0$ ,  $\{u^k\}_{k=0}^K$  the solution of the problem (3.15). Suppose  $u^k \in H^m(\mathcal{A}) \cap H_0^1(\mathcal{A}), m > 1$ , then

- For  $0 \leq \alpha < 1$ ,

$$\|u^k - u_N^k\|_1 \leq c_\alpha \Delta t^{-\alpha} N^{1-m} \max_{0 \leq j \leq k} \|u^j\|_m, \quad k = 1, 2, \dots, K, \tag{4.4}$$

where  $c_\alpha = \frac{c}{1-\alpha}$ , with  $c$  depends only on  $T^\alpha$ .

- For  $\alpha \rightarrow 1$ ,

$$\|u^k - u_N^k\|_1 \leq cN^{1-m} \sum_{j=0}^k \|u^j\|_m, \quad k = 1, 2, \dots, K, \tag{4.5}$$

where  $c$  depends only on  $T$ .

**Proof.** By the definition of  $\pi_N^1$ , (4.2), we have, for the solution  $u^{k+1}$  of (3.15),

$$(\pi_N^1u^{k+1}, v_N) + \alpha_0 \left( \frac{\partial}{\partial x} \pi_N^1u^{k+1}, \frac{\partial}{\partial x} v_N \right) = \left( (1 - b_1)u^k + \sum_{j=1}^{k-1} (b_j - b_{j+1})u^{k-j} + b_ku^0, v_N \right). \quad \forall v_N \in \mathbb{P}_N^0(\mathcal{A}). \tag{4.6}$$

Let  $\tilde{e}_N^{k+1} = \pi_N^1u^{k+1} - u_N^{k+1}, e_N^{k+1} = u^{k+1} - u_N^{k+1}$ , by subtracting (4.1) from (4.6), we obtain

$$(\tilde{e}_N^{k+1}, v_N) + \alpha_0 \left( \frac{\partial}{\partial x} \tilde{e}_N^{k+1}, \frac{\partial}{\partial x} v_N \right) = a_k(e_N^k, v_N) + \sum_{j=1}^{k-1} a_{k-j}(e_N^{k-j}, v_N) + a_0(e_N^0, v_N) \quad \forall v_N \in \mathbb{P}_N^0(\mathcal{A}), \tag{4.7}$$

where

$$a_k = 1 - b_1, \quad a_{k-j} = b_j - b_{j+1}, \quad j = 1, 2, \dots, k - 1, \quad a_0 = b_k.$$

Taking  $v_N = \tilde{e}_N^{k+1}$  in (4.7) results in

$$\|\tilde{e}_N^{k+1}\|_1 \leq a_k\|e_N^k\|_0 + \sum_{j=1}^{k-1} a_{k-j}\|e_N^{k-j}\|_0 + a_0\|e_N^0\|_0.$$

Using the triangular inequality  $\|e_N^{k+1}\|_1 \leq \|\tilde{e}_N^{k+1}\|_1 + \|u^{k+1} - \pi_N^1u^{k+1}\|_1$ , we have

$$\|e_N^{k+1}\|_1 \leq a_k\|e_N^k\|_0 + \sum_{j=1}^{k-1} a_{k-j}\|e_N^{k-j}\|_0 + a_0\|e_N^0\|_0 + \|u^{k+1} - \pi_N^1u^{k+1}\|_1. \tag{4.8}$$

Now, by applying a similar argument as in Theorem 3.2 to (4.8) and noting that  $\sum_{j=0}^k a_j = 1, a_j > 0 \forall j$ , we obtain

- For  $0 \leq \alpha < 1$ ,

$$\|e_N^k\|_1 \leq b_{k-1}^{-1} \max_{0 \leq j \leq k} \|u^j - \pi_N^1u^j\|_1, \quad k = 1, 2, \dots, K. \tag{4.9}$$

- For  $\alpha \rightarrow 1$ ,

$$\|e_N^k\|_1 \leq \sum_{j=0}^k \|u^j - \pi_N^1 u^j\|_1, \quad k = 1, 2, \dots, K. \tag{4.10}$$

Finally, (4.4) is obtained by applying (3.21) and (4.3) to (4.9), while (4.5) is given by applying (4.3) to (4.10).  $\square$

**Remark 4.1.** (1) (4.9) is better than the usual estimate obtained by using the standard Gronwall lemma to (4.8).

(2) Estimate (4.5) can be rewritten into an alternative form:

$$\|u^k - u_N^k\|_1 \leq c\Delta t^{-1} N^{1-m} \sum_{j=0}^k \Delta t \|u^j\|_m, \quad k = 1, 2, \dots, K,$$

where  $\sum_{j=0}^k \Delta t \|u^j\|_m$  has a clearer meaning to be a discrete form of  $\int_0^{t_k} \|u(t)\|_m dt$ .

(3) By using the well-known Aubin–Nitche trick, it is possible to derive an error estimate in the  $L^2$ -norm as follows:

- For  $0 \leq \alpha < 1$ ,

$$\|u^k - u_N^k\|_0 \leq c_\alpha \Delta t^{-\alpha} N^{-m} \max_{0 \leq j \leq k} \|u^j\|_m, \quad k = 1, 2, \dots, K,$$

- For  $\alpha \rightarrow 1$ ,

$$\|u^k - u_N^k\|_0 \leq c\Delta t^{-1} N^{-m} \sum_{j=0}^k \Delta t \|u^j\|_m, \quad k = 1, 2, \dots, K.$$

Now we aim at deriving an estimate for  $\|u(t_k) - u_N^k\|_1$ , which is given in the following theorem.

**Theorem 4.2.** Let  $u$  be the exact solution of (2.1)–(2.3),  $\{u_N^k\}_{k=0}^K$  the solution of the problem (4.1) with the initial condition  $u_N^0 = \pi_N^1 u^0$ . Suppose  $u \in H^1([0, T], H^m(\Lambda) \cap H_0^1(\Lambda))$ ,  $m > 1$ , then we have

- (1) when  $0 \leq \alpha < 1$ ,

$$\|u(t_k) - u_N^k\|_1 \leq \frac{T^\alpha}{1 - \alpha} (c_u \Delta t^{2-\alpha} + c\Delta t^{-\alpha} N^{1-m} \|u\|_{L^\infty(H^m)}), \quad k \leq K; \tag{4.11}$$

- (2) when  $\alpha \rightarrow 1$ ,

$$\|u(t_k) - u_N^k\|_1 \leq T(c_u \Delta t + c\Delta t^{-1} N^{1-m} \|u\|_{L^\infty(H^m)}), \quad k \leq K, \tag{4.12}$$

where  $\|u\|_{L^\infty(H^m)} := \sup_{t \in (0, T)} \|u(x, t)\|_m$ ,  $c_u$  depends on  $\|u\|_{H^1(L^\infty)}$ , and  $c$  and  $c_u$  are independent of  $T, \Delta t$ , and  $N$ .

**Proof.** Since the proof follows a standard procedure as above, we omit the details by giving only the sketch.

From (3.12),  $\{u(t_j)\}_{j=1}^K$  satisfy  $\forall v \in H_0^1(\Lambda)$ ,

$$(u(t_{k+1}), v) + \alpha_0 \left( \frac{\partial u(t_{k+1})}{\partial x}, \frac{\partial v}{\partial x} \right) = \left( (1 - b_1)u(t_k) + \sum_{j=1}^{k-1} (b_j - b_{j+1})u(t_{k-j}) + b_k u(t_0), v \right) + (r^{k+1}, v). \tag{4.13}$$

By projecting  $u(t_{k+1})$  into  $\pi_N^1 u(t_{k+1}) \in \mathbb{P}_N^0(\Lambda)$ , and using (4.2), we have for all  $v_N \in \mathbb{P}_N^0(\Lambda)$

$$(\pi_N^1 u(t_{k+1}), v_N) + \alpha_0 \left( \frac{\partial}{\partial x} \pi_N^1 u(t_{k+1}), \frac{\partial}{\partial x} v_N \right) = \left( (1 - b_1)u(t_k) + \sum_{j=1}^{k-1} (b_j - b_{j+1})u(t_{k-j}) + b_k u(t_0), v_N \right) + (r^{k+1}, v_N). \tag{4.14}$$

Let  $\tilde{\epsilon}_N^{k+1} = \pi_N^1 u(t_{k+1}) - u_N^{k+1}$ ,  $\epsilon_N^{k+1} = u(t_{k+1}) - u_N^{k+1}$ , by subtracting (4.1) from (4.14), we obtain

$$(\tilde{\epsilon}_N^{k+1}, v_N) + \alpha_0 \left( \frac{\partial}{\partial x} \tilde{\epsilon}_N^{k+1}, \frac{\partial}{\partial x} v_N \right) = \left( a_k \epsilon_N^k + \sum_{j=1}^{k-1} a_{k-j} \epsilon_N^{k-j} + a_0 \epsilon_N^0, v_N \right) + (r^{k+1}, v_N), \quad \forall v_N \in \mathbb{P}_N^0(\mathcal{A}), \quad (4.15)$$

where

$$a_k = 1 - b_1, \quad a_{k-j} = b_j - b_{j+1}, \quad j = 1, 2, \dots, k-1, a_0 = b_k.$$

Taking  $v_N = \tilde{\epsilon}_N^{k+1}$  in (4.15) and using the triangular inequality  $\|\tilde{\epsilon}_N^{k+1}\|_1 \leq \|\epsilon_N^{k+1}\|_1 + \|u(t_{k+1}) - \pi_N^1 u(t_{k+1})\|_1$ , we have

$$\begin{aligned} \|\tilde{\epsilon}_N^{k+1}\|_1 &\leq a_k \|\epsilon_N^k\|_0 + \sum_{j=1}^{k-1} a_{k-j} \|\epsilon_N^{k-j}\|_0 + a_0 \|\epsilon_N^0\|_0 + \|r^{k+1}\|_0 + \|u(t_{k+1}) - \pi_N^1 u(t_{k+1})\|_1 \\ &\leq a_k \|\epsilon_N^k\|_0 + \sum_{j=1}^{k-1} a_{k-j} \|\epsilon_N^{k-j}\|_0 + a_0 \|\epsilon_N^0\|_0 + c_u \Delta t^2 + cN^{1-m} \|u(t_{k+1})\|_m. \end{aligned} \quad (4.16)$$

It is at this point we distinguish two cases for  $\alpha$ , and follow the same lines as in Theorem 3.2 to obtain:

(1)  $0 \leq \alpha < 1$ ,

$$\|\epsilon_N^k\|_1 \leq b_{k-1}^{-1} (c_u \Delta t^2 + cN^{1-m} \|u\|_{L^\infty(H^m)}) \leq \frac{T^\alpha}{1-\alpha} (c_u \Delta t^{2-\alpha} + c \Delta t^{-\alpha} N^{1-m} \|u\|_{L^\infty(H^m)}), \quad k = 0, 1, \dots, K.$$

(2)  $\alpha \rightarrow 1$ ,

$$\|\epsilon_N^k\|_1 \leq k (c_u \Delta t^2 + cN^{1-m} \|u\|_{L^\infty(H^m)}) \leq T (c_u \Delta t + c \Delta t^{-1} N^{1-m} \|u\|_{L^\infty(H^m)}), \quad k = 0, 1, \dots, K.$$

The proof of the theorem is completed.  $\square$

**Remark 4.2.** In the estimates (4.11) and (4.12), the error contribution from the spatial approximation (second terms in the right-hand sides) is affected by the inverse of the time step. It is worthwhile noting that similar results are also found for the standard diffusion equation. However for regular enough (in space) solution,  $N^{1-m}$  can be much smaller than  $\Delta t$ , therefore this affection generally would not reduce the global accuracy.

#### 4.2. A Legendre collocation method in space

The Galerkin method proposed in Section 4.1 itself is of interest in its own right. It offers some advantage in the numerical analysis, and could be implemented once a suitable basis for the space  $\mathbb{P}_N^0(\mathcal{A})$  is chosen. However, the Galerkin method is generally computational expensive and difficult to extend to more complex geometries and higher spatial dimension. An alternative is offered by the Legendre collocation spectral method, which consists in approximating the integrals by using the Legendre Gauss-type quadratures.

We need some more notations to define such an alternative method. Let  $L_N(x)$  denotes the Legendre polynomial of degree  $N$ .  $\xi_j, j = 0, 1, \dots, N$ , are the Legendre–Gauss–Lobatto (GLL) points, i.e. zeros of  $(1-x^2)L'_N(x)$ ;  $\omega_j, j = 0, 1, \dots, N$ , the Legendre weights defined such that the following quadrature holds

$$\int_{-1}^1 \varphi(x) dx = \sum_{j=0}^N \varphi(\xi_j) \omega_j \quad \forall \varphi(x) \in \mathbb{P}_{2N-1}(\mathcal{A}). \quad (4.17)$$

Define the discrete inner product as follow, for any continuous functions  $\phi$  and  $\psi$ ,

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

and the associated discrete norm  $\|\phi\|_N := (\phi, \phi)_N^{1/2}$ . It is well known that the discrete norm  $\|\cdot\|_N$  is equivalent to the standard  $L^2$ -norm in  $\mathbb{P}_N(\mathcal{A})$ :

$$\|\phi\|_0 \leq \|\phi\|_N \leq \sqrt{3}\|\phi\|_0 \quad \forall \phi \in \mathbb{P}_N(A). \tag{4.18}$$

Let  $I_N$  is the interpolation operator based on the  $N + 1$  GLL points, i.e.,  $\forall \psi \in C^0(\bar{A}), I_N \psi \in \mathbb{P}_N(A)$ , such that  $I_N \psi(\xi_j) = \psi(\xi_j), j = 0, \dots, N$ .

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

$$A_N(u_N^{k+1}, v_N) = F_N(v_N), \quad \text{for all } v_N \in \mathbb{P}_N^0(A), \tag{4.19}$$

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

$$A_N(u_N^{k+1}, v_N) := (u_N^{k+1}, v_N)_N + \alpha_0 \left( \frac{\partial}{\partial x} u_N^{k+1}, \frac{\partial}{\partial x} v_N \right)_N$$

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

$$F_N(v_N) := (1 - b_1)(u_N^k, v_N)_N + \sum_{j=1}^{k-1} (b_j - b_{j+1})(u_N^{k-j}, v_N)_N + b_k(u_N^0, v_N)_N.$$

Taking into account the norm equivalence (4.18), the well-posedness of the problem (4.19) is immediate with the help of the Lax–Milgram Lemma. However, rigorous error estimation for the solution of (4.19) is less evident, and requires much more detailed analysis.

For the sake of simplification, let us also introduce  $A(\cdot, \cdot)$  and  $F(\cdot)$  as follows:

$$A(u^{k+1}, v) := (u^{k+1}, v) + \alpha_0 \left( \frac{\partial}{\partial x} u^{k+1}, \frac{\partial}{\partial x} v \right),$$

$$F(v) := (1 - b_1)(u^k, v) + \sum_{j=1}^{k-1} (b_j - b_{j+1})(u^{k-j}, v) + b_k(u^0, v).$$

Then the semi-discretized problem (3.15) can be rewritten in the compact form: find  $u^{k+1} \in H_0^1(A)$ , such that

$$A(u^{k+1}, v) = F(v), \quad \text{for all } v \in H_0^1(A). \tag{4.20}$$

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

$$\|\psi_N\|_{1,N} := A_N^{1/2}(\psi_N, \psi_N) \quad \forall \psi_N \in \mathbb{P}_N(A).$$

It is readily seen, from (4.17) and (4.18), that the norm  $\|\cdot\|_{1,N}$  is equivalent to the norm  $\|\cdot\|_1$  defined in (3.14).

**Theorem 4.3.** *Let  $\{u_N^k\}_{k=0}^K$  is the solution of the problem (4.19) with the initial condition  $u_N^0$  taken to be  $I_N u(0)$ ,  $\{u^k\}_{k=0}^K$  the solution of the problem (3.15). Suppose  $u^k \in H^m(A) \cap H_0^1(A), m > 1$ , then*

- For  $0 \leq \alpha < 1$ ,

$$\|u^k - u_N^k\|_{1,N} \leq c_\alpha \Delta t^{-\alpha} N^{1-m} \max_{0 \leq j \leq k} \|u^j\|_m, \quad k = 1, 2, \dots, K, \tag{4.21}$$

where  $c_\alpha = \frac{c}{1-\alpha}$

- For  $\alpha \rightarrow 1$ ,

$$\|u^k - u_N^k\|_{1,N} \leq c \Delta t^{-1} N^{1-m} \max_{0 \leq j \leq k} \|u^j\|_m, \quad k = 1, 2, \dots, K, \tag{4.22}$$

where  $c$  depends only on  $T$ .

**Proof.** Let  $w_N$  be any function in  $\mathbb{P}_N^0(A)$ , denote  $\sigma_N := u_N^{k+1} - w_N$ . Then a straightforward calculation shows

$$A_N(\sigma_N, \sigma_N) = A(u^{k+1} - w_N, \sigma_N) + A(w_N, \sigma_N) - A_N(w_N, \sigma_N) + F_N(\sigma_N) - F(\sigma_N).$$

This gives

$$\|\sigma_N\|_{1,N}^2 \leq \|u^{k+1} - w_N\|_1 \|\sigma_N\|_1 + |A(w_N, \sigma_N) - A_N(w_N, \sigma_N)| + |F(\sigma_N) - F_N(\sigma_N)| \quad \forall w_N \in \mathbb{P}_N^0(A).$$

Obviously, for all  $w_N \in \mathbb{P}_{N-1}^0(\mathcal{A})$ , we have, by virtue of (4.17),

$$A(w_N, \sigma_N) = A_N(w_N, \sigma_N).$$

Hence

$$\|\sigma_N\|_{1,N}^2 \leq \|u^{k+1} - w_N\|_1 \|\sigma_N\|_1 + |F(\sigma_N) - F_N(\sigma_N)| \quad \forall w_N \in \mathbb{P}_{N-1}^0(\mathcal{A}). \tag{4.23}$$

Now we estimate the last term above. By definition, we have

$$\begin{aligned} |F(\sigma_N) - F_N(\sigma_N)| &= |(1 - b_1)[(u^k, \sigma_N) - (u_N^k, \sigma_N)_N] + \sum_{j=1}^{k-1} (b_j - b_{j+1})[(u^{k-j}, \sigma_N) - (u_N^{k-j}, \sigma_N)_N] \\ &\quad + b_k[(u^0, \sigma_N) - (u_N^0, \sigma_N)_N]|. \end{aligned} \tag{4.24}$$

It is known that the following result holds (see e.g. [3,17]):  $\forall g \in H^m(\mathcal{A})$ ,  $m \geq 1$ ,  $\forall g_N \in \mathbb{P}_N(\mathcal{A})$ ,

$$\begin{aligned} (g, \sigma_N) - (g_N, \sigma_N)_N &\leq (2\|g - I_N g\|_0 + \|g - I_{N-1} g\|_0) \|\sigma_N\|_0 + \|g - g_N\|_{0,N} \|\sigma_N\|_{0,N} \\ &\leq (cN^{-m} \|g\|_m + \|g - g_N\|_{0,N}) \|\sigma_N\|_{0,N}. \end{aligned}$$

Applying this result to  $g = u^j$ ,  $g_N = u_N^j$  for all  $j = 1, 2, \dots, k$ , we obtain from (4.24):

$$\begin{aligned} |F(\sigma_N) - F_N(\sigma_N)| &\leq \left\{ (1 - b_1)[cN^{-m} \|u^k\|_m + \|u^k - u_N^k\|_{0,N}] + \sum_{j=1}^{k-1} (b_j - b_{j+1})[cN^{-m} \|u^{k-j}\|_m \right. \\ &\quad \left. + \|u^{k-j} - u_N^{k-j}\|_{0,N}] + b_k[cN^{-m} \|u^0\|_m + \|u^0 - u_N^0\|_{0,N}] \right\} \|\sigma_N\|_{0,N}. \end{aligned}$$

Let  $\varepsilon_N^j := u^j - u_N^j$ , then using (3.7) yields

$$|F(\sigma_N) - F_N(\sigma_N)| \leq \left[ (1 - b_1) \|\varepsilon_N^k\|_{0,N} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \|\varepsilon_N^{k-j}\|_{0,N} + b_k \|\varepsilon_N^0\|_{0,N} + cN^{-m} \max_{0 \leq j \leq k} \|u^j\|_m \right] \|\sigma_N\|_{0,N}. \tag{4.25}$$

Combining (4.23) and (4.25), and using the norm equivalence, we have

$$\begin{aligned} \|\sigma_N\|_{1,N} &\leq (1 - b_1) \|\varepsilon_N^k\|_{0,N} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \|\varepsilon_N^{k-j}\|_{0,N} + b_k \|\varepsilon_N^0\|_{0,N} + cN^{-m} \max_{0 \leq j \leq k} \|u^j\|_m \\ &\quad + c \|u^{k+1} - w_N\|_{1,N} \quad \forall w_N \in \mathbb{P}_{N-1}^0(\mathcal{A}). \end{aligned}$$

Now using the following triangular inequality

$$\|\varepsilon_N^{k+1}\|_{1,N} \leq \|\sigma_N\|_{1,N} + \|u^{k+1} - w_N\|_{1,N},$$

we obtain

$$\begin{aligned} \|\varepsilon_N^{k+1}\|_{1,N} &\leq (1 - b_1) \|\varepsilon_N^k\|_{0,N} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \|\varepsilon_N^{k-j}\|_{0,N} + b_k \|\varepsilon_N^0\|_{0,N} + cN^{-m} \max_{0 \leq j \leq k} \|u^j\|_m \\ &\quad + c \|u^{k+1} - w_N\|_{1,N} \quad \forall w_N \in \mathbb{P}_{N-1}^0(\mathcal{A}). \end{aligned}$$

The above estimate specially holds for  $w_N = \pi_{N-1}^0 u^{k+1}$ , which implies

$$\begin{aligned} \|\varepsilon_N^{k+1}\|_{1,N} &\leq (1 - b_1) \|\varepsilon_N^k\|_{0,N} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \|\varepsilon_N^{k-j}\|_{0,N} + b_k \|\varepsilon_N^0\|_{0,N} + cN^{-m} \max_{0 \leq j \leq k} \|u^j\|_m + cN^{1-m} \|u^{k+1}\|_m \\ &\leq (1 - b_1) \|\varepsilon_N^k\|_{0,N} + \sum_{j=1}^{k-1} (b_j - b_{j+1}) \|\varepsilon_N^{k-j}\|_{0,N} + b_k \|\varepsilon_N^0\|_{0,N} + cN^{1-m} \max_{0 \leq j \leq k+1} \|u^j\|_m. \end{aligned}$$

Finally, following a similar procedure as in Theorem 3.2 to distinguish the two cases for  $\alpha$ , we obtain (4.21) and (4.22).  $\square$

**Remark 4.3.** Similar to the Theorem 4.2, some error estimates for  $\|u(t_k) - u_N^k\|_{1,N}$  for the solution of the Legendre collocation approximation (4.19) can be derived. We omit the details here.

### 5. Numerical validation

#### 5.1. Implementation

For completeness sake, the implementation is briefly described here. Considering problem (4.19), we express the function  $u_N^{k+1}$  in terms of the Lagrangian interpolants based on the Legendre–Gauss–Lobatto points  $\xi_j; j = 0, 1, \dots, N$ ,

$$u_N^{k+1}(x) = \sum_{j=0}^N u_j^{k+1} h_j(x), \tag{4.26}$$

where  $u_j^{k+1} := u_N^{k+1}(\xi_j)$ , unknowns of the discrete solution.  $h_j$  is the Lagrangian polynomial defined in  $\mathcal{A}$ , i.e.

$$h_j \in \mathbb{P}_N(\mathcal{A}), h_j(\xi_i) = \delta_{ij} \quad \forall i, j \in \{0, 1, \dots, N\},$$

with  $\delta_{ij}$ : the Kronecker-delta symbol.

By bringing (4.26) into (4.19), and taking into account the homogeneous Dirichlet boundary condition (i.e.,  $u_0^{k+1} = u_N^{k+1} = 0$ ), then choosing each test function  $v_N$  to be  $h_i(x), i = 1, 2, \dots, N - 1$ , we obtain

$$\left( \sum_{j=1}^{N-1} u_j^{k+1} h_j, h_i \right)_N + \alpha_0 \left( \frac{d}{dx} \sum_{j=1}^{N-1} u_j^{k+1} h_j, \frac{d}{dx} h_i \right)_N = F_N(h_i), \quad i = 1, 2, \dots, N - 1.$$

Using the definition of the discrete inner product  $(\cdot, \cdot)_N$  to the above system gives

$$\sum_{j=1}^{N-1} u_j^{k+1} \sum_{q=0}^N h_j(\xi_q) h_i(\xi_q) \omega_q + \alpha_0 \sum_{j=1}^{N-1} u_j^{k+1} \sum_{q=0}^N \frac{dh_j}{dx}(\xi_q) \frac{dh_i}{dx}(\xi_q) \omega_q = F_N(h_i), \quad i = 1, 2, \dots, N - 1.$$

Thus, we arrive at the following matrix statement of problem (4.19)

$$\sum_{j=1}^{N-1} H_{ij} u_j^{k+1} = F_i, \quad i = 1, 2, \dots, N - 1, \tag{4.27}$$

where  $F_i = F_N(h_i)$ , and for all  $i, j \in \{0, 1, \dots, N\}$ ,

$$H_{ij} = A_{ij} + \alpha_0 B_{ij}, \quad A_{ij} = \sum_{q=0}^N D_{qi} D_{qj} \omega_q,$$

$$B_{ij} = \omega_i \delta_{ij}, \quad D_{ij} = \frac{dh_j}{dx}(\xi_i).$$

We remember that  $\alpha_0$  is the positive constant defined just below (3.7).

Therefore, at each time step, we obtain a system of linear algebraic equations with different right-hand-side vector  $\{F_i\}_{i=1}^{N-1}$ . Since the matrix  $H$  is symmetric positive definite, we choose the conjugate gradient method to solve (4.27); see, for example, [22] for some details.

#### 5.2. Numerical results

We carry out in this section a series of numerical experiments and present some results to confirm our theoretical statements. The main purpose is to check the convergence behavior of the numerical solution with respect to the time step  $\Delta t$  and polynomial degree  $N$  used in the calculation.



**Example 1.** We consider the problem (2.1)–(2.3) with an exact analytical solution:

$$u(x, t) = t^2 \sin(2\pi x).$$

It can be checked that the corresponding forcing term and initial condition are respectively

$$f(x, t) = \frac{2}{\Gamma(3 - \alpha)} t^{2-\alpha} \sin(2\pi x) + 4\pi^2 t^2 \sin(2\pi x), \quad g(x) = 0.$$

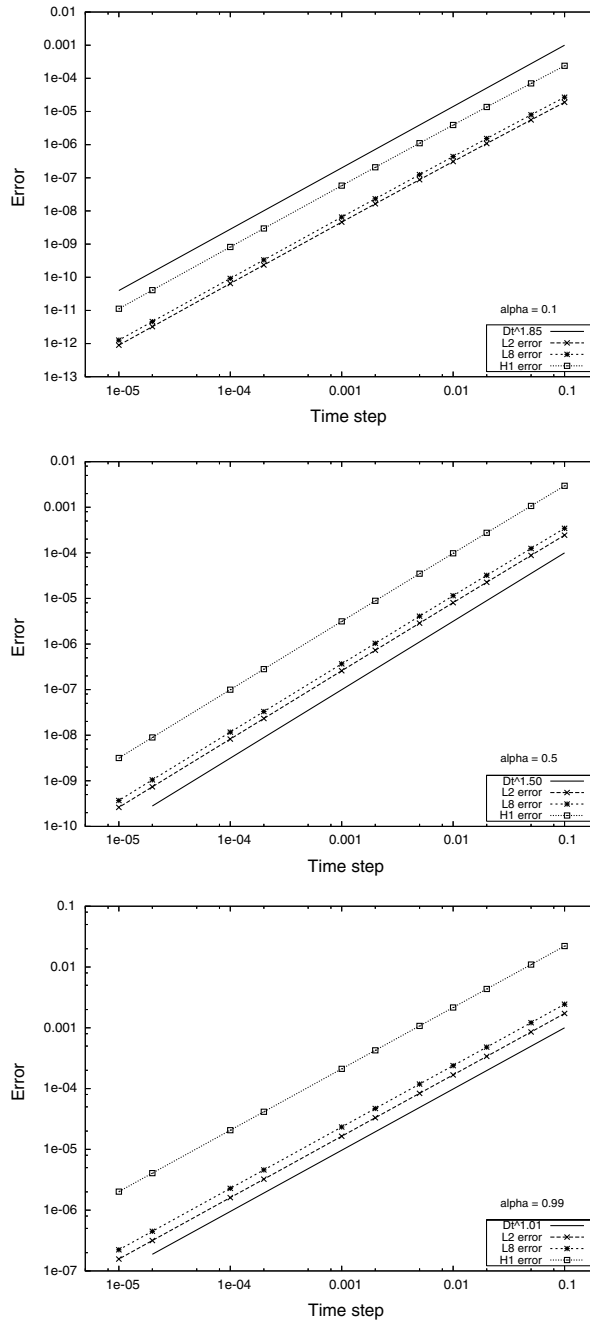


Fig. 3. Errors as a function of the time step  $\Delta t$  for several  $\alpha$ .

For the purpose of accuracy investigation, we compute the errors  $\|u(T) - u_N^K\|$  in three discrete norms:  $L^2$ ,  $H^1$ , and  $L^\infty$ . All the numerical results reported in the figures below have been evaluated at  $T = 1$ .

We first investigate the temporal convergence rate. To this end, polynomial  $N$  is chosen big enough such that the errors stemming from the spatial approximation is negligible. In Fig. 3, we plot the errors in the  $L^2$ ,  $H^1$ , and  $L^\infty$  norms as a function of the time step sizes for  $N = 24$ . A logarithmic scale has been used for both  $\Delta t$ -axis and error-axis in these figures. As predicted by the theoretical estimates, the finite difference

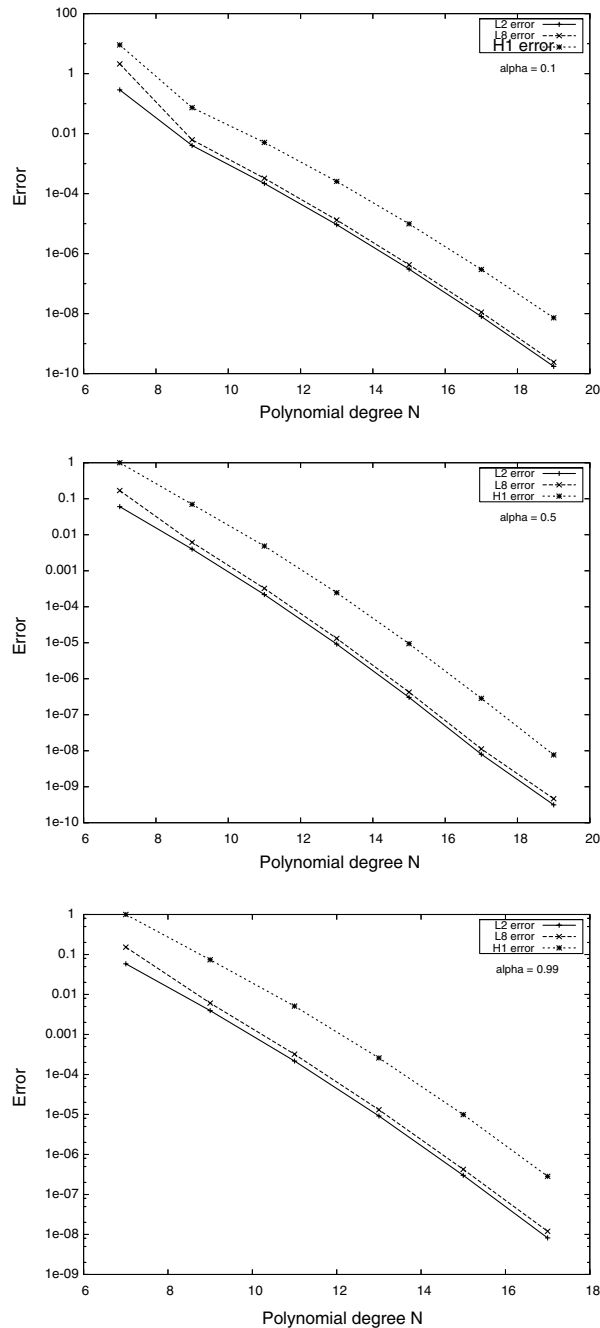


Fig. 4. Errors as a function of the polynomial degree  $N$  for several  $\alpha$ .

scheme yields a temporal approximation order close to  $2-\alpha$ , i.e. the slopes of the error curves in these log-log plots are 1.85, 1.5, and 1.01 respectively for  $\alpha = 0.1, 0.5$ , and  $0.99$ .

Now we check the spatial accuracy with respect to the polynomial degree by fixing the time step sufficiently small to avoid contamination of the temporal error. In Fig. 4, we present the errors as a function of the polynomial degree  $N$  for three values of  $\alpha$ : 0.1, 0.5, and 0.99. A logarithmic scale is now used for the error-axis. Clearly, the errors show an exponential decay, since in these semi-log representations one observes that the error variations are essentially linear versus the polynomial degrees for all three  $\alpha$ . That is the so-called spectral accuracy as expected since the exact solution is smooth.

**Example 2.** The advantage of the spectral method depends on the regularity of the solution. In this example, we take the following exact solution with limit regularity in  $A := (0, 2)$ :

$$u(x, t) = t^2[x(1-x)(2-x)]^{16/3}, \tag{4.28}$$

and investigate the spatial accuracy of the proposed method when  $N$  increases. In Fig. 5, we show the error decay rates in different norms with respect to polynomials degree with  $\alpha = 0.5, \Delta t = 10^{-4}$ . The  $N^{-4}$  and  $N^{-5}$  decay rates are also shown in order to make a close comparison. It is observed that the errors in all three norms decay with a rate between  $N^{-4}$  and  $N^{-5}$ . This result seems reasonable since it can be verified that the solution (4.28) belongs to  $H^5(\Omega)$ .

### 6. Concluding remarks

In this work, we have developed and analyzed efficient numerical methods for the time-fractional diffusion equations. In particular, we analyzed the convergence properties of the classical backward differentiation scheme (in time) for the time-fractional derivative. Incidentally, we found, first by numerical tests then by rigorous proof (see Lemma 3.1), that application of the standard first-order backward differentiation to the time derivative in the integral of the time-fractional derivative (3.1) leads to globally  $2-\alpha$ -order accuracy in time. To date we are not aware of any similar results in published papers which offer estimate better than first-order accuracy. Regarding the spatial discretization, use of the Legendre spectral collocation method results in exponential convergence in space. Some error estimates in different contexts are derived, showing that the combination of the backward differentiation in time and Legendre spectral method in space leads to an approximation of order  $\Delta t^{2-\alpha} + N^{-m}$  for smooth enough solution. Our numerical experiments are in perfect agreement with the theoretical results.

It should be mentioned that the estimates given in the paper are valid also in two and three dimensional cases. Beyond these theoretical results, thanks to the high resolution feature of the spectral approximation, the proposed method is well adapted to treat the TFDE in higher spatial dimension. It remains however that

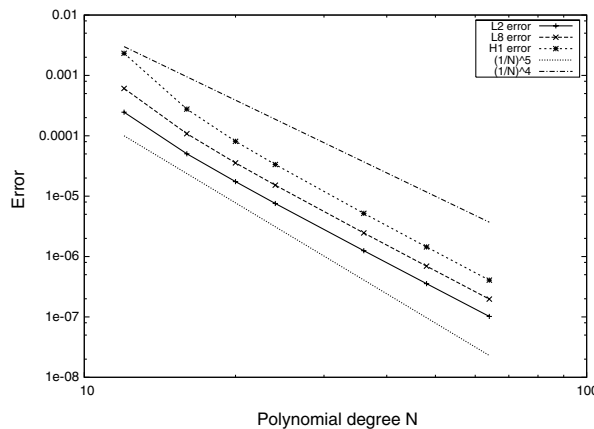


Fig. 5. Errors as a function of the polynomial degree  $N$  for example 2.

in 3D case the storage requirement to save the solution for all time levels may not be acceptable in practical applications. One of the future works along this direction is therefore to investigate possible methods which allow to reduce the storage requirement by overcoming the so-called “global dependence” problem, as mentioned in the introduction. Other future works include improving the temporal accuracy by constructing uniformly second-order schemes for all  $\alpha \in [0, 1]$  by using, for example, appropriate graded meshes. Also in the future we would like to investigate fractional derivatives in both space and time.

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