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A SPACE-TIME SPECTRAL METHOD FOR THE TIME FRACTIONAL DIFFUSION EQUATION*

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Abstract. In this paper, we consider the numerical solution of the time fractional diffusion equation. Essentially, the time fractional diffusion equation differs from the standard diffusion equation in the time derivative term. In the former case, the first-order time derivative is replaced by a fractional derivative, making the problem global in time. We propose a spectral method in both temporal and spatial discretizations for this equation. The convergence of the method is proven by providing a priori error estimate. Numerical tests are carried out to confirm the theoretical results. Thanks to the spectral accuracy in both space and time of the proposed method, the storage requirement due to the "global time dependence" can be considerably relaxed, and therefore calculation of the long-time solution becomes possible.

Key words. space-time spectral method, time fractional diffusion equation, error estimate

AMS subject classifications. 35S10, 35A05, 65M70, 65M12

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1. Introduction.

Fractional partial differential equations (FPDEs) appear in the investigation of transport dynamics in complex systems which are governed by the anomalous diffusion and nonexponential relaxation patterns [21]. Related equations of importance are the space/time fractional diffusion equations, the fractional advection-diffusion equation [11, 12] for anomalous diffusion with sources and sinks, and the fractional Fokker–Planck equation [2] for anomalous diffusion in an external field, etc.

The time fractional diffusion equation (TFDE) considered in this paper is of interest not only in its own right, but also in that it constitutes the principal part in solving many other FPDEs (see next section for more details). This model equation governs the evolution for the probability density function that describes anomalously diffusing particles. Anomalous diffusion deviates from the standard Fichean description of Brownian motion, the main character of which is that its mean squared displacement is a nonlinear growth with respect to time, such as $\langle x^2(t)\rangle \sim t^\alpha$. The TFDE describes the anomalous subdiffusion corresponding to $0 < \alpha < 1$. Examples for subdiffusive transport include turbulent flow, chaotic dynamics charge transport in amorphous semiconductors [28, 29], NMR diffusometry in disordered materials [22], and dynamics of a bead in polymer network [1]. In [23], Nigmatullin used the fractional diffusion equation to describe diffusion in media with fractal geometry. Mainardi [20] pointed out that the propagation of mechanical diffusive wave in viscoelastic media can be modeled by TFDE.

The theoretical justification for this equation, together with the confirmation of physical and biological experiments, have led to an intensive investigation in recent years to design efficient numerical schemes. On one side, because of the integral in the

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definition of the noninteger order derivatives, it is apparent that these derivatives are nonlocal operators, which explains one of their most significant uses in applications: The noninteger derivatives possess a memory effect which it shares with several materials such as viscoelastic materials or polymers. On the other side, the feature of the fractional derivatives makes the design of accurate and fast methods difficult. Unlike the integer derivatives, which are local in the sense that the derivative of a function at a certain point in space or time depends only on the function in the vicinity of this point, presence of the integral in the noninteger order derivatives makes the problem global. In the TFDE, this means that 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 a low-order method is employed.

The TFDE as well as the fractional wave equation have been investigated in analytical and numerical frames by a number of authors [9, 17, 30, 39]. Some of these authors have tried to construct analytical solutions. For example, Schneider and Wyss [30] and Wyss [39] considered the time fractional diffusion-wave equations. The corresponding Green functions and their properties are obtained in terms of Fox functions. Gorenflo et al. [9, 10] used the similarity method and the method of Laplace transform to obtain the scale-invariant solution of TFDE in terms of the Wright function. However, the work done on the numerical solution of the TFDE is relatively sparse. Liu et al. [18] employed the finite difference method in both space and time, and analyzed the stability condition. Sun and Wu [32] proposed a finite difference scheme for the fractional diffusion-wave equation. Langlands and Henry [14] considered the implicit numerical scheme for a fractional diffusion equation in which the backward Euler approximation is used to discretize the first-order time derivative and the L1 scheme is used to approximate the fractional order time derivative. Lin and Xu [15] proposed a finite difference scheme in time and Legendre spectral method in space for TFDE. A convergence rate of $(2-\alpha)$-order in time and spectral accuracy in space of the method was rigorously proved. It is worthwhile noting that some of FPDEs, e.g., the time fractional wave equations, may be written in the form of integro-differential equations, for which there has been some work (see, for example, [13, 19, 27, 37] and the references therein).

However, all above mentioned papers dealt with the time discretization by finite difference methods. As we have known, any algorithm using a finite difference discretization of a fractional derivative has to take into account its nonlocal structure, which means a high storage requirement. Some techniques for handling this problem have been developed, e.g., by Ford and Simpson [7] and Diethelm and Freed [5], which was based on the so-called "fix memory principle". By choosing a storage length T depending on the mesh size h, i.e., $T = O(h^{-p/\alpha})$, schemes of order h^p can be constructed.

Our main motivation in this paper is to construct a spectral approximation in both space and time to the FPDEs considered. Since the time fractional derivative uses the global information, it is very natural to consider a global method, such as the spectral method. It is known that the spectral method has been an efficient tool for computing numerical solutions of differential equations because of its high-order accuracy. The use of the spectral method in the time discretization of FPDEs may significantly reduce the storage requirement because, as compared to low-order methods, much fewer time levels are needed to compute a smooth solution.

Generally speaking, the spectral method is employed for the spatial discretization. Compared to the spectral method in space, spectral method in time is relatively rare

for several reasons: firstly, for parabolic problems the time derivative is of first order, this makes the construction of efficient spectral methods quite troublesome; secondly, the spectral method is global, that is, the computation of the solution at an instant requires information about the solution at all other time levels. Nevertheless, there exists some work on the development of space-time spectral methods for integer-order PDEs [3, 8, 31, 33, 34, 35, 36, 38]. For parabolic problems, the time derivative is of first order; most existing time spectral methods were constructed based on the Petrov–Galerkin or Dual–Petrov–Galerkin formulation.

However, for FPDEs, the situation is quite different. As we will see in the paper, the fractional differential operator of order α, with $0 < \alpha < 1$, possesses some features of elliptic operators, as long as suitable spaces and norms are chosen. This makes us possible to use the standard Galerkin formulation. The main goal of this paper is to construct appropriate space-time spectral methods for FPDEs. Our main contribution is that we find suitable spaces and norms in which the time fractional differential problem can be formulated into an elliptic problem. Thanks to these spaces, the space-time spectral approximation can follow the Galerkin method for elliptic problems, and the optimal error estimate is then derived by using standard analysis techniques. We also give the implementation details which can be crucial for the efficiency of the method.

The outline of this paper is as follows. In the next section we introduce some notations and construct the weak formulation both in space and time directions for the time-fractional diffusion equation. The well-posedness of the problem is established. In section 3 we propose the space-time Galerkin spectral method and carry out the error analysis. In section 4, we give some implementation details and present the numerical results to support the theoretical prediction. In section 5, we give some concluding remarks. An appendix is given in the final section.

2. Problem and weak formulation. Let $\Lambda = (-1, 1), I = (0, T)$, be space and time domain, respectively. We denote $\Omega := \Lambda \times I$. The TFDE we consider in this paper reads

$$ {}_0\partial_t^\alpha u(x,t) - \partial_x^2 u(x,t) = f(x,t) \quad \forall (x,t) \in \Omega, \tag{2.1}$$

subject to the following initial and boundary conditions:

$$ u(x,0) = 0 \quad \forall x \in \Lambda, \tag{2.2}$$

$$ u(-1,t) = u(1,t) = 0 \quad \forall t \in I. \tag{2.3}$$

In the investigation of boundary value problems for TFDEs, there usually exist two ways to express the operator ${}_0\partial_t^\alpha$: Caputo and Riemann–Liouville definitions.

In the Caputo definition, the fractional derivative of order α, denoted by ${}_0^C\partial_t^\alpha u(x,t)$, is defined as

$$ {}_0^C\partial_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,\tau)}{\partial \tau} \frac{d\tau}{(t-\tau)^\alpha}, \quad 0 < \alpha < 1, \tag{2.4}$$

where $\Gamma(\cdot)$ denotes Gamma function.

On the other side, the Riemann–Liouville definition, ${}_0^R\partial_t^\alpha$, reads

$$ {}_0^R\partial_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{u(x,\tau)}{(t-\tau)^\alpha} d\tau, \quad 0 < \alpha < 1. \tag{2.5}$$

The two definitions are linked by the following relationship, which can be verified by a direct calculation:

$$ {}_0^R\partial_t^\alpha u(x,t) = \frac{u(x,0)}{\Gamma(1-\alpha)t^\alpha} + {}_0^C\partial_t^\alpha u(x,t). \tag{2.6} $$

Many authors think that Caputo's version is more natural because it allows the handling of inhomogeneous initial conditions in an easier way. Nevertheless we will consider the Riemann–Liouville definition throughout this paper in order to simplify our discussion since most useful tools have been established by using the Riemann–Liouville definition. It is worthwhile to note, by virtue of (2.6), that for the homogeneous condition considered here the Riemann–Liouville definition coincides with the Caputo version.

Note that the TFDE (2.1) can also take the form as follows [14]:

$$ \partial_t u(x,t) - {}_0\partial_t^{1-\alpha}\partial_x^2 u(x,t) = {}_0\partial_t^{1-\alpha} f(x,t) \quad \forall (x,t) \in \Omega. \tag{2.7} $$

Here, we use the form (2.1) rather than (2.7) for the reason that the former facilitates the construction of our space-time spectral method. It should be emphasized that the method to be presented hereafter for (2.1) can be directly applied to the TFDE of form (2.7) through a simple partial integration transformation.

We are also aware that some of the FPDEs can be reformulated into a general form of integro-differential equations:

$$ \partial_t u(x,t) + \int_0^t K(t-s)Au(x,s)ds = f(x,t) \quad \forall (x,t) \in \Omega. $$

For example, the fractional wave equation

$$ \partial_t^2 u(x,t) - {}_0\partial_t^{1-\alpha}\partial_x^2 u(x,t) = f(x,t) \quad \forall (x,t) \in \Omega \tag{2.8} $$

corresponds to

$$ Au = -\partial_x^2 u, \quad K(s) = \frac{s^{\alpha-1}}{\Gamma(\alpha)}. $$

The Riemann–Liouville form of (2.8) is similar to (2.1) but with $1 < \alpha < 2$. We will not address this equation in the present paper, and leave this as a future work.

The TFDE (2.7) has been derived from continuous time random walks. The physical interpretation of the fractional derivative is that it represents a degree of memory in the diffusing material [10]. This equation is of interest not only in its own right, but also in that it represents the heart in many other important FPDEs. We mention, among others, the fractional Nernst–Planck equation describing the flux of ions through a diffusive membrane [2]:

$$ \partial_t C_k = {}_0\partial_t^{1-\alpha} D_{k,\alpha}\left[\triangle C_k + \nabla \cdot \left(\frac{C_k}{k_B T} z_k e \nabla V_m\right)\right], $$

where $C_k, D_{k,\alpha}$, and z_k are, respectively, the concentration, modified diffusion coefficient, and valence of the kth ionic species. e is the unit charge of an electron and k_B is Boltzmann's constant. T is the temperature. V_m is the membrane potential. The method presented below can be easily generalized to the fractional Nernst–Planck equation.

Now we turn to the model problems (2.1)–(2.3). For $0 < \alpha < 1$, the definition of the fractional derivative uses the information of the standard derivatives at all previous time levels. This makes the properties of the TFDE different from the well-known parabolic equations. However, we will see that, with the help of suitable inner products and norms, the TFDE can be considered as an elliptic problem in the corresponding Sobolev spaces.

In order to derive the variational formulation of problems (2.1)–(2.3) and prove its well-posedness, we need some preparation.

2.1. Preparation. First, we introduce some notations and define some functional spaces endowed with norms and inner products that are used hereafter. Let c be a generic positive constant independent of any functions and of any discretization parameters. We use the expression $A \lesssim B$ to mean that $A \leqslant cB$, and use the expression $A \cong B$ to mean that $A \lesssim B \lesssim A$. Let $\mathcal{O}$ be a domain which may stand for I, Λ, Ω, or $\mathbb{R}$. $L^2(\mathcal{O})$ is the space of measurable functions whose square is Lebesgue integrable in $\mathcal{O}$. The inner product and norm of $L^2(\mathcal{O})$ are defined by

$$(u, v)_{\mathcal{O}} = \int_{\mathcal{O}} uv \mathrm{d}\mathcal{O} \ , \quad \|u\|_{0,\mathcal{O}} = (u, u)_{\mathcal{O}}^{\frac{1}{2}}, \quad \forall u, v \in L^2(\mathcal{O}).$$

We also use $H^m(\mathcal{O})$ and $H_0^m(\mathcal{O})$ to denote the usual Sobolev spaces, whose norms are denoted by $\|\cdot\|_{m,\mathcal{O}}$.

Particularly, we will need to recall the definitions of some Sobolev spaces: for real $s \geqslant 0$, let

$$H^s(\mathbb{R}) = \left\{ v(t) | v \in L^2(\mathbb{R});\ \left(1 + |\omega|^2\right)^{\frac{s}{2}} \mathcal{F}(v)(\omega) \in L^2(\mathbb{R}) \right\},$$

endowed with the norm:

$$\|v\|_{s,\mathbb{R}} = \left\| \left(1 + |\omega|^2\right)^{\frac{s}{2}} \mathcal{F}(v)(\omega) \right\|_{0,\mathbb{R}},$$

where $\mathcal{F}(v)$ denotes the Fourier transform of v. For bounded domain I, we define space:

$$H^s(I) = \left\{ v \in L^2(I) | \exists\ \tilde{v} \in H^s(\mathbb{R}) \ \text{ such that } \tilde{v}|_I = v \right\},$$

with the norm:

$$\|v\|_{s,I} = \inf_{\tilde{v} \in H^s(\mathbb{R}), \tilde{v}|_I = v} \|\tilde{v}\|_{s,\mathbb{R}}.$$

Let $C_0^\infty(I)$ stand for the space of smooth functions with compact support in I, and $H_0^s(I)$ denote the closure of $C_0^\infty(I)$ with respect to norm $\|\cdot\|_{s,I}$. We also define the space

$${}_0C^\infty(I) = \{v | v \in C^\infty(I) \text{ with compact support in } (0, 1]\}.$$

The space ${}_0H^s(I)$ denotes the closure of ${}_0C^\infty(I)$ with respect to norm $\|\cdot\|_{s,I}$. For the Sobolev space X with norm $\|\cdot\|_X$, let

$$H^s(I; X) := \{v |\ \|v(\cdot, t)\|_X \in H^s(I)\},\ s \geqslant 0,$$

$${}_0H^s(I; X) := \{v |\ \|v(\cdot, t)\|_X \in {}_0H^s(I)\},\ s \geqslant 0,$$

endowed with the norm:

$$\|v\|_{H^s(I;X)} := \|\|v(\cdot,t)\|_X\|_{s,I}.$$

When X stands for $H^\sigma(\Lambda)$ or $H_0^\sigma(\Lambda), \sigma \geqslant 0$, the norm of the space $H^s(I;X)$ will be denoted by $\|\cdot\|_{\sigma,s,\Omega}$.

We define space:

$$B^s(\Omega) := {}_0H^s\left(I, L^2(\Lambda)\right) \cap L^2\left(I, H_0^1(\Lambda)\right)$$

equipped with the norm:

$$\|v\|_{B^s(\Omega)} := \left(\|v\|^2_{H^s(I,L^2(\Lambda))} + \|v\|^2_{L^2\left(I,H_0^1(\Lambda)\right)}\right)^{1/2}.$$

It can be verified that $B^s(\Omega)$ is a Banach space.

Hereafter, in cases where no confusion would arise, the domain symbols Λ, I, or Ω may be dropped from the notations.

We will also need to recall some definitions of fractional derivatives and related properties [24].

For real number $s \geqslant 0$, let n be the integer, such that $n-1 \leqslant s < n$. The left and right Riemann–Liouville derivatives of order s are, respectively, defined as:

left Riemann–Liouville derivative:

$${}_0D_t^s v(t) = \frac{1}{\Gamma(n-s)}\frac{d^n}{dt^n}\int_0^t \frac{v(\tau)d\tau}{(t-\tau)^{s-n+1}} \ \forall t \in [0,T],$$

right Riemann–Liouville derivative:

$${}_tD_T^s v(t) = \frac{(-1)^n}{\Gamma(n-s)}\frac{d^n}{dt^n}\int_t^T \frac{v(\tau)d\tau}{(\tau-t)^{s-n+1}} \ \forall t \in [0,T],$$

where $\frac{d^n}{dt^n}$ stands for the usual derivative of integer order n.

Let's remark that if function $v(t)$ has n order continuous derivative in $[0,T]$, then as s tends to n or $n-1$, the left Riemann–Liouville derivative becomes a conventional n or $n-1$ order derivative of function $v(t)$. In fact, a straightforward calculation shows

$$\begin{aligned}\lim_{s\to n} {}_0D_t^s v(t) &= \lim_{s\to n}\frac{d^n}{dt^n}\left(\frac{1}{\Gamma(n-s)}\int_0^t (t-\tau)^{n-s-1}v(\tau)d\tau\right)\\ &= \frac{d^n}{dt^n}{}_0D_t^0 v(t) = v^{(n)}(t),\\ \lim_{s\to n-1} {}_0D_t^s v(t) &= \lim_{s\to n-1}\frac{d^n}{dt^n}\left(\frac{1}{\Gamma(n-s)}\int_0^t (t-\tau)^{n-s-1}v(\tau)d\tau\right)\\ &= \frac{d^n}{dt^n}\int_0^t v(\tau)d\tau = v^{(n-1)}(t).\end{aligned}$$

For the reader's convenience, we list below a number of useful properties related to the Riemann–Liouville fractional derivative.

PROPERTY 2.1 (see [24]). *If* $0 < p < 1,\ 0 < q < 1,\ v(0) = 0,\ t > 0$, *then*

$${}_0D_t^{p+q}v(t) = {}_0D_t^p {}_0D_t^q v(t) = {}_0D_t^q {}_0D_t^p v(t).$$

PROPERTY 2.2 (see [24]). *(Fourier transform) For all real s, $v \in C_0^\infty(\mathbb{R})$, let $\mathcal{F}$ denote Fourier transform operator, then*

$$\mathcal{F}({}_{-\infty}D_t^s v(t)) = (i\omega)^s \mathcal{F}(v)(\omega),$$
$$\mathcal{F}({}_tD_{+\infty}^s v(t)) = (-i\omega)^s \mathcal{F}(v)(\omega).$$

One of the remarkable properties of the Riemann–Liouville fractional derivative is given in the following lemma. Note that the same identity with a slightly different condition can be found in [26]. Here, thanks to the modified condition given below we are able to prove the result in a simpler way.

LEMMA 2.1. *For real s, $0 < s < 1$, if $w(t) \in H^s(I), v(t) \in C_0^\infty(I)$, then*

$$({}_0D_t^s w(t),\ v(t))_I = (w(t),\ {}_tD_T^s v(t))_I\,. \tag{2.9}$$

Proof. By using integration by parts, we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}\int_\tau^T \frac{v(t)}{(t-\tau)^s}\,\mathrm{d}t &= \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\frac{v(t)(t-\tau)^{1-s}}{1-s}\bigg|_\tau^T - \frac{1}{1-s}\int_\tau^T v'(t)(t-\tau)^{1-s}\,\mathrm{d}t\right]\\ &= \frac{\mathrm{d}}{\mathrm{d}\tau}\left[\frac{v(T)(T-\tau)^{1-s}}{1-s}\right] - \frac{1}{1-s}\frac{\mathrm{d}}{\mathrm{d}\tau}\int_\tau^T v'(t)(t-\tau)^{1-s}\,\mathrm{d}t\\ &= \int_\tau^T \frac{v'(t)}{(t-\tau)^s}\,\mathrm{d}t. \end{aligned}\tag{2.10}$$

Employing again integration by parts, we obtain

$$\begin{aligned}({}_0D_t^s w(t),\ v(t))_I &= \frac{1}{\Gamma(1-s)}\int_0^T \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{w(\tau)}{(t-\tau)^s}\,\mathrm{d}\tau\ v(t)\,\mathrm{d}t\\ &= \frac{v(t)}{\Gamma(1-s)}\int_0^t \frac{w(\tau)}{(t-\tau)^s}\,\mathrm{d}\tau\bigg|_0^T - \frac{1}{\Gamma(1-s)}\int_0^T\int_0^t \frac{w(\tau)}{(t-\tau)^s}\,\mathrm{d}\tau\ v'(t)\,\mathrm{d}t\\ &= -\frac{1}{\Gamma(1-s)}\int_0^T\int_0^t \frac{w(\tau)}{(t-\tau)^s}\mathrm{d}\tau\ v'(t)\mathrm{d}t. \end{aligned}\tag{2.11}$$

Furthermore, by using (2.10), the right-hand side of (2.11) is reformulated into

$$\begin{aligned}&-\frac{1}{\Gamma(1-s)}\int_0^T\int_0^t \frac{w(\tau)}{(t-\tau)^s}\,\mathrm{d}\tau\ v'(t)\,\mathrm{d}t\\ &= -\frac{1}{\Gamma(1-s)}\int_0^T\int_\tau^T \frac{v'(t)}{(t-\tau)^s}\,\mathrm{d}t\ w(\tau)\,\mathrm{d}\tau\\ &= -\frac{1}{\Gamma(1-s)}\int_0^T \left(\frac{d}{d\tau}\int_\tau^T \frac{v(t)}{(t-\tau)^s}\,\mathrm{d}t\right) w(\tau)\mathrm{d}\tau\\ &= (w(\tau),\ {}_\tau D_T^s v(\tau))_I. \end{aligned}\tag{2.12}$$

Finally, combining (2.11) and (2.12) gives (2.9). The proof is completed. ∎

LEMMA 2.2. *For real $s > 0$, $v \in C_0^\infty(\mathbb{R})$, then*

$$({}_{-\infty}D_t^s v(t),\ {}_tD_\infty^s v(t))_{\mathbb{R}} = \cos(\pi s)\|{}_{-\infty}D_t^s v(t)\|^2_{L^2(\mathbb{R})}, \tag{2.13}$$

$$({}_{-\infty}D_t^s v(t),\ {}_tD_\infty^s v(t))_{\mathbb{R}} = \cos(\pi s)\|{}_tD_\infty^s v(t)\|^2_{L^2(\mathbb{R})}. \tag{2.14}$$

Proof. A proof of the identity (2.13) is given in [6]. The identity (2.14) can be proven by using (2.13) as follows. For $v \in C_0^\infty(\mathbb{R})$, let $w(t) = v(-t)$, then $w \in C_0^\infty(\mathbb{R})$. Applying (2.13) to w leads to

$$({}_{-\infty}D_t^s w(t),\ {}_tD_\infty^s w(t))_{\mathbb{R}} = \cos(\pi s)\|{}_{-\infty}D_t^s w(t)\|^2_{L^2(\mathbb{R})}. \tag{2.15}$$

On the other hand, a direct calculation shows

$$\begin{aligned}
{}_{-\infty}D_t^s w(t) &= \frac{1}{\Gamma(n-s)}\frac{d^n}{dt^n}\int_{-\infty}^{t}\frac{w(\tau)d\tau}{(t-\tau)^{s-n+1}} \\
&= \frac{1}{\Gamma(n-s)}\frac{d^n}{dt^n}\int_{-\infty}^{t}\frac{v(-\tau)d\tau}{(t-\tau)^{s-n+1}} \\
&= \frac{1}{\Gamma(n-s)}\frac{d^n}{dt^n}\int_{-t}^{\infty}\frac{v(\zeta)d\zeta}{(\zeta-(-t))^{s-n+1}} \\
&\overset{y=-t}{=} \frac{(-1)^n}{\Gamma(n-s)}\frac{d^n}{dy^n}\int_{y}^{\infty}\frac{v(\zeta)d\zeta}{(\zeta-y)^{s-n+1}} \\
&= {}_yD_\infty^s v(y). \quad \{\text{by definition}\}
\end{aligned} \tag{2.16}$$

Similarly, we have

$${}_tD_\infty^s w(t) \overset{y=-t}{=} {}_{-\infty}D_y^s v(y). \tag{2.17}$$

Finally, combining (2.16), (2.17) and (2.15) yields

$$({}_{-\infty}D_y^s v(y),\ {}_yD_\infty^s v(y))_{\mathbb{R}} = \cos(\pi s)\|{}_yD_\infty^s v(y)\|^2_{L^2(\mathbb{R})}.$$

This proves (2.14). ∎

Remark 2.1. In the particular case $s = k + 1/2$ with nonnegative integers k, the identities (2.13) and (2.14) can be proved in a simpler way. In fact, in these cases the right-hand sides of both identities are zero for all $v \in C_0^\infty(\mathbb{R})$. On the other side, by composite formula and Lemma 2.1, we have

$$\begin{aligned}
\left({}_{-\infty}D_t^{k+\frac{1}{2}}v(t),\ {}_tD_\infty^{k+\frac{1}{2}}v(t)\right)_{\mathbb{R}} &= \left({}_{-\infty}D_t^{\frac{1}{2}}D^k v(t),\ {}_tD_\infty^{\frac{1}{2}}D^k v(t)\right)_{\mathbb{R}} \\
&= \left(DD^k v(t),\ D^k v(t)\right)_{\mathbb{R}} \\
&= \frac{1}{2}\left(D^k v(t)\right)^2\Big|_{-\infty}^{\infty} \\
&= 0.
\end{aligned}$$

This proves (2.13) and (2.14).

Now we aim at establishing a relationship between Riemann–Liouville derivatives and fractional Sobolev spaces on bounded domains. Note that similar relationships between fractional derivatives and fractional Sobolev spaces have been derived in [6], where the authors first defined the fractional Sobolev spaces on the whole line and then confined them on bounded intervals. Here, we choose to define the spaces directly on bounded domains by the Riemann–Liouville fractional derivatives. This will enable us to deduce some useful results for bounded domains more simply. First we introduce several definitions, which are generalizations of the ones for the whole line.

DEFINITION 2.1. *Let $s > 0$, we define the seminorm:*

$$|v|_{H_l^s(I)} := \|{}_0D_t^s v\|_{L^2(I)},$$

and norm:

$$\|v\|_{H_l^s(I)} := \left(\|v\|^2_{L^2(I)} + |v|^2_{H_l^s(I)}\right)^{\frac{1}{2}}.$$

We then define $H_l^s(I)$ as the closure of $C_0^\infty(I)$ with respect to norm $\|\cdot\|_{H_l^s(I)}$.

DEFINITION 2.2. *Let $s > 0$, we define the seminorm:*

$$|v|_{H_r^s(I)} := \|{}_tD_T^s v\|_{L^2(I)},$$

and norm:

$$\|v\|_{H_r^s(I)} := \left(\|v\|^2_{L^2(I)} + |v|^2_{H_r^s(I)}\right)^{\frac{1}{2}}.$$

Let $H_r^s(I)$ denote the closure of $C_0^\infty(I)$ with respect to norm $\|\cdot\|_{H_r^s(I)}$.

DEFINITION 2.3. *Let $s > 0$, $s \neq n + \frac{1}{2}$, we define the seminorm:*

$$|v|_{H_c^s(I)} := |({}_0D_t^s v,\ {}_tD_T^s v)_{L^2(I)}|^{\frac{1}{2}},$$

and norm:

$$\|v\|_{H_c^s(I)} := \left(\|v\|^2_{L^2(I)} + |v|^2_{H_c^s(I)}\right)^{\frac{1}{2}}.$$

Then we define $H_c^s(I)$ as the closure of $C_0^\infty(I)$ with respect to norm $\|\cdot\|_{H_c^s(I)}$.

We would like to indicate that if the domain I in the Definitions 2.1–2.3 is replaced by the whole line $\mathbb{R}$, then the seminorms of the spaces $H_l^s(\mathbb{R}), H_r^s(\mathbb{R})$, and $H_c^s(\mathbb{R})$ should be defined, respectively, by

$$|v|_{H_l^s(\mathbb{R})} := \|{}_{-\infty}D_t^s v\|_{L^2(\mathbb{R})},\ |v|_{H_r^s(\mathbb{R})} := \|{}_tD_\infty^s v\|_{L^2(\mathbb{R})},$$
$$|v|_{H_c^s(\mathbb{R})} := |({}_{-\infty}D_t^s v,\ {}_tD_\infty^s v)_{L^2(\mathbb{R})}|^{\frac{1}{2}}.$$

For these spaces, thanks to Lemma 2.2, the following equivalence holds.

LEMMA 2.3. *Let $s > 0$, $s \neq n + \frac{1}{2}$, the spaces $H_l^s(\mathbb{R})$, $H_r^s(\mathbb{R})$, and $H_c^s(\mathbb{R})$ are equal in the sense that their seminorms as well as norms are equivalent.*

This result is generalized to the bounded interval I in the following lemma.

LEMMA 2.4. *Let $s > 0$, $s \neq n + \frac{1}{2}$, the spaces $H_l^s(I)$, $H_r^s(I)$, and $H_c^s(I)$ are equal in the sense that their seminorms as well as norms are equivalent.*

Proof. It suffices to prove that the three seminorms $|\cdot|_{H_l^s(I)}, |\cdot|_{H_c^s(I)}$, and $|\cdot|_{H_r^s(I)}$ are equivalent in the space $C_0^\infty(I)$. For all v in $C_0^\infty(I)$, let $\tilde{v}$ be the extension of v by zero outside I. From the definition of fractional derivative, we know that left (right) Riemann–Liouville derivative at the time t uses the information earlier (later) than t. This means that

$$\begin{cases} {}_{-\infty}D_t^s \tilde{v} = 0 & t \leqslant 0 \\ {}_tD_\infty^s \tilde{v} = 0 & t \geqslant T. \end{cases} \tag{2.18}$$

Thus

$$\operatorname{supp}({}_{-\infty}D_t^s \tilde{v}\ {}_tD_\infty^s \tilde{v}) \subset I,$$

which implies

$$|v|_{H_c^s(I)} = |\tilde{v}|_{H_c^s(\mathbb{R})}. \tag{2.19}$$

On the other hand, by Lemma 2.3, using (2.19) and Hölder inequality, we obtain

$$|v|_{H_l^s(I)} \leqslant |\tilde{v}|_{H_l^s(\mathbb{R})} \cong |\tilde{v}|_{H_c^s(\mathbb{R})} = |v|_{H_c^s(I)} \lesssim |v|^{\frac{1}{2}}_{H_l^s(I)} |v|^{\frac{1}{2}}_{H_r^s(I)}.$$

Thus

$$|v|_{H_l^s(I)} \lesssim |v|_{H_r^s(I)}.$$

Similarly we can prove

$$|v|_{H_r^s(I)} \lesssim |v|_{H_l^s(I)}.$$

This gives

$$|v|_{H_r^s(I)} \cong |v|_{H_l^s(I)} \cong |v|_{H_c^s(I)}. \qquad \square$$

LEMMA 2.5. *Let $s > 0$, $s \neq n + \frac{1}{2}$, the spaces $H_c^s(I)$ and $H_0^s(I)$ are equal with seminorms and norms.*

Proof. Once again, we just need to prove that the seminorms $|\cdot|_{H_c^s(I)}$ and $|\cdot|_{H^s(I)}$ are equivalent in $C_0^\infty(I)$. To this end, for all $v \in C_0^\infty(I)$, let $\tilde{v}$ be the extension of v by zero outside I. Then, in virtue of equality (2.19), Lemma 2.3, Plancherel theorem, and Property 2.2, we have

$$\begin{aligned} |v|_{H_c^s(I)} &= |\tilde{v}|_{H_c^s(\mathbb{R})} \cong |\tilde{v}|_{H_l^s(\mathbb{R})} = \|\mathcal{F}({}_0D_t^s \tilde{v})\|_0 \\ &= \|(i\omega)^s \mathcal{F}(\tilde{v})\|_0 \cong |\tilde{v}|_{H^s(\mathbb{R})} \cong |v|_{H^s(I)}. \qquad \square \end{aligned}$$

It is well known that it holds

$$H_0^s(I) \subset H_0^q(I) \quad \text{if } q \leq s.$$

Therefore, a direct consequence of Lemmas 2.4 and 2.5 is that the following embeddings hold:

$$H_l^s(I) \subset H_l^q(I), \quad H_r^s(I) \subset H_r^q(I), \quad H_c^s(I) \subset H_c^q(I) \quad \text{if } q \leq s.$$

2.2. Variational formulation. Now we consider the weak formulation of problem (2.1) as follows: for $f \in L^2(\Omega)$, find $u \in B^{\frac{\alpha}{2}}(\Omega)$ such that

$$\mathcal{A}(u, v) = \mathcal{F}(v) \quad \forall v \in B^{\frac{\alpha}{2}}(\Omega), \tag{2.20}$$

where the bilinear form $\mathcal{A}(\cdot, \cdot)$ is defined by

$$\mathcal{A}(u, v) := \left({}_0\partial_t^{\frac{\alpha}{2}} u, {}_t\partial_T^{\frac{\alpha}{2}} v\right)_\Omega + (\partial_x u, \partial_x v)_\Omega,$$

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

$$\mathcal{F}(v) := (f, v)_\Omega.$$

Formally, the variational formulation (2.20) can be derived from (2.1) by using the following lemma.

LEMMA 2.6. *For all $0 < \alpha < 1$, if $w \in {}_0H^1(I), v \in {}_0H^{\frac{\alpha}{2}}(I)$, then*

$$({}_0D_t^\alpha w, v)_I = \left({}_0D_t^{\frac{\alpha}{2}} w, {}_tD_T^{\frac{\alpha}{2}} v\right)_I. \tag{2.21}$$

In fact, by multiplying (2.1) with $v \in B^{\frac{\alpha}{2}}(\Omega)$, and integrating the resulting equation over Ω, we have

$$({}_0\partial_t^\alpha u, v)_\Omega + \left(\partial_x^2 u, v\right)_\Omega = (f, v)_\Omega \quad \forall v \in B^{\frac{\alpha}{2}}(\Omega).$$

Then (2.20) is obtained by employing Lemma 2.6 with respect to t to the first term, and classical integration by parts with respect to x to the second term.

Reciprocally, if a regular enough function u is the solution of (2.20), we can prove, by following the standard procedure, that u is also the solution of (2.1) in the distribution sense.

Now we turn to prove Lemma 2.6.

Proof of Lemma 2.6. First, it is known (see [16]) that

$$H_0^s(I) = H^s(I) = {}_0H^s(I) \quad \text{if } 0 < s < \frac{1}{2}. \tag{2.22}$$

Hence for any $0 < \alpha < 1$, $v \in {}_0H^{\frac{\alpha}{2}}(I)$ implies $v \in H_0^{\frac{\alpha}{2}}(I)$, and by the definition of $H_0^{\frac{\alpha}{2}}(I)$, there exists a sequence $v_n \in C_0^\infty(I)$, such that

$$\|v_n - v\|_{H^{\frac{\alpha}{2}}(I)} \to 0 \quad \text{as } n \to +\infty.$$

For all $w \in H^1(I)$ with $w(0) = 0$, by virtue of Property 2.1 and Lemma 2.1, we have

$$({}_0D_t^\alpha w, v_n)_I = \left({}_0D_t^{\frac{\alpha}{2}}\, {}_0D_t^{\frac{\alpha}{2}} w, v_n\right)_I = \left({}_0D_t^{\frac{\alpha}{2}} w, {}_tD_T^{\frac{\alpha}{2}} v_n\right)_I. \tag{2.23}$$

On one side, it holds

$$|({}_0D_t^\alpha w, v_n)_I - ({}_0D_t^\alpha w, v)_I| \leqslant \|{}_0D_t^\alpha w\|_0 \|v - v_n\|_0 \to 0 \quad \text{as } n \to +\infty,$$

which implies

$$({}_0D_t^\alpha w, v_n)_I \to ({}_0D_t^\alpha w, v)_I \quad \text{as } n \to +\infty. \tag{2.24}$$

On the other side, applying Lemmas 2.4 and 2.5 yields

$$\begin{aligned} &\left|\left({}_0D_t^{\frac{\alpha}{2}} w, {}_tD_T^{\frac{\alpha}{2}} v_n\right)_I - \left({}_0D_t^{\frac{\alpha}{2}} w, {}_tD_T^{\frac{\alpha}{2}} v\right)_I\right| \\ &\leqslant \left\|{}_0D_t^{\frac{\alpha}{2}} w\right\|_0 |v - v_n|_{H_r^{\frac{\alpha}{2}}(I)} \lesssim \left\|{}_0D_t^{\frac{\alpha}{2}} w\right\|_0 \|v - v_n\|_{H^{\frac{\alpha}{2}}(I)} \to 0 \quad \text{as } n \to +\infty. \end{aligned}$$

This gives

$$\left({}_0D_t^{\frac{\alpha}{2}} w, {}_tD_T^{\frac{\alpha}{2}} v_n\right)_I \to \left({}_0D_t^{\frac{\alpha}{2}} w, {}_tD_T^{\frac{\alpha}{2}} v\right)_I \quad \text{as } n \to +\infty. \tag{2.25}$$

Finally, by taking limit on both sides of (2.23) as $n \to +\infty$, and using (2.24) and (2.25), we obtain (2.21). ∎

THEOREM 2.1. *For all* $0 < \alpha < 1$ *and* $f \in L^2(\Omega)$, *problem* (2.20) *is well-posed. Furthermore, if* u *is the solution of* (2.20), *then it holds*

$$\|u\|_{B^{\frac{\alpha}{2}}(\Omega)} \lesssim \|f\|_{0,\Omega}. \tag{2.26}$$

Proof. The well-posedness of problem (2.20) is guaranteed by the well-known Lax–Milgram lemma. The continuity of the bilinear form $\mathcal{A}$ and the functional $\mathcal{F}$

is obvious. We only need to prove the coercivity of $\mathcal{A}$ in the space $B^{\frac{\alpha}{2}}(\Omega)$. By Lemmas 2.4 and 2.5, we have, for all $v \in B^{\frac{\alpha}{2}}(\Omega)$,

$$\mathcal{A}(v,v) \gtrsim \left({}_0D_t^{\frac{\alpha}{2}} v,\ {}_0D_t^{\frac{\alpha}{2}} v\right)_\Omega + (\partial_x v, \partial_x v)_\Omega \gtrsim \|v\|^2_{B^{\frac{\alpha}{2}}(\Omega)}. \tag{2.27}$$

Thus the well-posedness of problem (2.20) is proved. In order to derive the stability (2.26), we take $v = u$ in (2.20), then use (2.27) to get

$$\|u\|^2_{B^{\frac{\alpha}{2}}(\Omega)} \lesssim (f,u)_\Omega. \tag{2.28}$$

The estimate (2.26) is now a direct consequence of (2.28) and the Schwarz inequality and Poincaré inequality. ∎

Remark 2.2. We emphasize that the solution of the problem (2.20) does not imply the homogeneous initial condition imposed upon the strong solution of (2.1) for the reason that there is no trace at time $t = 0$ for functions in $B^{\frac{\alpha}{2}}(\Omega)$ with $\frac{\alpha}{2} < \frac{1}{2}$. In fact, there is no sense to define values at a given time of a function in $B^{\frac{\alpha}{2}}(\Omega)$ with $\frac{\alpha}{2} < \frac{1}{2}$; see, e.g., (2.22). Thus the equivalence between the problem under strong formulation (2.1) and the problem under variational formulation (2.20) should be understood in the following sense: first it is obvious that a solution of (2.1) is also a solution (unique in the weak sense) of (2.20); inversely, a regular enough solution (in this case, defining initial values at $t = 0$ makes sense) is also a solution of (2.1).

3. Spectral Galerkin method. In this section we propose a spectral Galerkin method to numerically solve the initial boundary value problem of TFDE expressed in weak form (2.20). Our goal here is first to introduce some approximation operators and derive the corresponding approximation results, then establish an error estimate for the numerical solution.

In order to discretize problem (2.20), we define $P_M(\Lambda)$ (*respectively*, $P_N(I)$) as the polynomials spaces of degree less than or equal to M (*resp.* N), with respect to x (*resp.* t). For spectral approximations in space, we introduce the space:

$$P_M^0(\Lambda) := P_M(\Lambda) \cap H_0^1(\Lambda).$$

Since the initial value $u(x,0) = 0$, it is natural to construct the approximation space (in time):

$$P_N^E(I) := \{v \in P_N(I) | v(0) = 0\}.$$

For a pair of positive integers M, N, let $L := (M,N)$, and

$$S_L := P_M^0(\Lambda) \otimes P_N^E(I).$$

Our space-time spectral Galerkin approximation to problem (2.20) reads as: find $u_L \in S_L$, such that

$$\mathcal{A}(u_L, v_L) = \mathcal{F}(v_L) \quad \forall v_L \in S_L. \tag{3.1}$$

Since S_L is a subspace of $B^{\frac{\alpha}{2}}(\Omega)$, the well-posedness of the Galerkin formulation (3.1) can be established similarly as in the continuous case (2.20).

THEOREM 3.1. *For all* $0 < \alpha < 1$ *and* $f \in L^2(\Omega)$, *discrete problem* (3.1) *is well-posed. Furthermore, if* u_L *is the solution of* (3.1), *then* u_L *satisfies*

$$\|u_L\|_{B^{\frac{\alpha}{2}}(\Omega)} \lesssim \|f\|_{0,\Omega}. \tag{3.2}$$

In the purpose of carrying out an error analysis to the spectral Galerkin method, we introduce two approximation operators as follows. We define the orthogonal projector $\Pi_M^{1,0} : H_0^1(\Lambda) \to P_M^0(\Lambda)$ by $\forall v \in H_0^1(\Lambda), \Pi_M^{1,0} v \in P_M^0(\Lambda)$, such that

$$\left(\left(\Pi_M^{1,0} v - v \right)', \phi' \right)_\Lambda = 0 \quad \forall \phi \in P_M^0(\Lambda).$$

Then, for all $v \in H^m(\Lambda) \cap H_0^1(\Lambda), m \geqslant 1$, the following optimal error estimates hold (see Theorem 1.7 in [4]):

$$\left| \Pi_M^{1,0} v - v \right|_{1,\Lambda} \lesssim M^{1-m} \|v\|_{m,\Lambda}, \tag{3.3}$$

$$\left\| \Pi_M^{1,0} v - v \right\|_{0,\Lambda} \lesssim M^{-m} \|v\|_{m,\Lambda}. \tag{3.4}$$

We let Π_N denote the classical $L^2(I)$ orthogonal projection operator in time. For the projector Π_N, the error estimate is well known (Theorem 1.2 in [4]):

$$\|\Pi_N v - v\|_{0,I} \lesssim N^{-m} \|v\|_{m,I} \quad \forall v \in H^m(I), m \geqslant 0. \tag{3.5}$$

Now, we construct the projection operator $\Pi_N^E : {}_0H^1(I) \to P_N^E(I)$ by $\forall v \in {}_0H^1(I)$,

$$\Pi_N^E v := \int_0^t \Pi_{N-1} v'(\tau) d\tau.$$

Then we have by (3.5):

$$\left| \Pi_N^E v - v \right|_{1,I} = \|\Pi_{N-1} v' - v'\|_{0,I} \lesssim N^{1-m} \|v\|_{m,I} \; \forall v \in H^m(I) \cap {}_0H^1(I), m \geqslant 1. \tag{3.6}$$

An estimate for the L^2-error of Π_N^E can be deduced by using the Aubin–Nitsche trick, as stated in the following lemma.

LEMMA 3.1. *It holds*

$$\left\| \Pi_N^E v - v \right\|_{0,I} \lesssim N^{-m} \|v\|_{m,I} \quad \forall v \in H^m(I) \cap {}_0H^1(I), m \geqslant 1. \tag{3.7}$$

Proof. First, it is well known that the Poincaré inequality holds in the space ${}_0H^1(I)$. As a result, we can use the standard Aubin–Nitche's trick to obtain:

$$\left\| \Pi_N^E v - v \right\|_{0,I} \lesssim N^{-1} \left| \Pi_N^E v - v \right|_{1,I} \quad \forall v \in H^m(I) \cap {}_0H^1(I), m \geqslant 1.$$

Then combining (3.6) and the above estimate yields (3.7). ∎

For $0 < s < 1$, we can derive, by applying the standard space interpolation technique [16], the H^s-error estimate as follows:

$$\left\| \Pi_N^E v - v \right\|_{s,I} \lesssim N^{s-m} \|v\|_{m,I} \quad \forall v \in H^m(I) \cap {}_0H^1(I), m \geqslant 1. \tag{3.8}$$

In the next lemma, we study properties of the composite approximation operator $\Pi_N^E \Pi_M^{1,0}$.

LEMMA 3.2. *Let* $0 < s < 1, \gamma > 1, \sigma \geqslant 1$. *If* $v \in {}_0H^s(I; H^\sigma(\Lambda)) \cap H^\gamma(I; H_0^1(\Lambda))$, *then we have*

$$\left\| \partial_x \left(v - \Pi_N^E \Pi_M^{1,0} v \right) \right\|_{0,0} \lesssim M^{1-\sigma} \|v\|_{\sigma,0} + N^{-\gamma} \|v\|_{1,\gamma},$$

$$\left\| {}_0\partial_t^s \left(v - \Pi_N^E \Pi_M^{1,0} v \right) \right\|_{0,0} \lesssim N^{s-\gamma} \|v\|_{0,\gamma} + N^{s-\gamma} M^{-\sigma} \|v\|_{\sigma,\gamma} + M^{-\sigma} \|v\|_{\sigma,s}.$$

Proof. Let I_d denote identity operator, and then by using estimates (3.3), (3.4), and (3.8), we get

$$\begin{aligned}\left\|\partial_x\left(v-\Pi_N^E\Pi_M^{1,0}v\right)\right\|_{0,0} &\lesssim \left\|\partial_x\left(v-\Pi_M^{1,0}v\right)\right\|_{0,0}+\left\|\Pi_M^{1,0}v-\Pi_M^{1,0}\Pi_N^E v\right\|_{1,0}\\ &\lesssim M^{1-\sigma}\|v\|_{\sigma,0}+\left\|v-\Pi_N^E v\right\|_{1,0}\\ &\lesssim M^{1-\sigma}\|v\|_{\sigma,0}+N^{-\gamma}\|v\|_{1,\gamma},\\ \left\|{}_0\partial_t^s\left(v-\Pi_N^E\Pi_M^{1,0}v\right)\right\|_{0,0} &\lesssim \left\|v-\Pi_N^E v\right\|_{0,s}+\left\|\Pi_N^E v-\Pi_N^E\Pi_M^{1,0}v\right\|_{0,s}\\ &\lesssim N^{s-\gamma}\|v\|_{0,\gamma}+\left\|\left(\Pi_N^E-I_d\right)\left(v-\Pi_M^{1,0}v\right)\right\|_{0,s}+\left\|v-\Pi_M^{1,0}v\right\|_{0,s}\\ &\lesssim N^{s-\gamma}\|v\|_{0,\gamma}+N^{s-\gamma}M^{-\sigma}\|v\|_{\sigma,\gamma}+M^{-\sigma}\|v\|_{\sigma,s}. \qquad \square\end{aligned}$$

We are now in a position to derive the error estimate for the solution of the space-time spectral approximation.

THEOREM 3.2. *Let $0<\alpha<1$, $\gamma>1$, $\sigma\geqslant 1$, and let u, u_L be, respectively, the solutions of* (2.1) *and* (3.1). *If $u\in {}_0H^{\frac{\alpha}{2}}(I;H^\sigma(\Lambda))\cap H^\gamma(I;H_0^1(\Lambda))$, then we have*

$$\begin{aligned}\|u-u_L\|_{B^{\frac{\alpha}{2}}(\Omega)} \lesssim\ & N^{\frac{\alpha}{2}-\gamma}\|u\|_{0,\gamma}+N^{\frac{\alpha}{2}-\gamma}M^{-\sigma}\|u\|_{\sigma,\gamma}+M^{-\sigma}\|u\|_{\sigma,\frac{\alpha}{2}}\\ &+M^{1-\sigma}\|u\|_{\sigma,0}+N^{-\gamma}\|u\|_{1,\gamma}.\end{aligned} \tag{3.9}$$

Proof. In virtue of the standard error estimate for the Galerkin method of elliptic problems, we have

$$\|u-u_L\|_{B^{\frac{\alpha}{2}}(\Omega)}\leqslant \inf_{v_L\in S_L}\|u-v_L\|_{B^{\frac{\alpha}{2}}(\Omega)}.$$

By taking $v_L=\Pi_N^E\Pi_M^{1,0}u$ and employing Lemma 3.2 we obtain immediately the estimate (3.9). $\square$

4. Numerical results.

4.1. Implementation. We start with some implementation details. In order to make problem (3.1) practical, all the integrals involved in (3.1) are evaluated by using suitable numerical quadratures. For the reason that the integrands in the left-hand side of (3.1) are polynomials in space, we choose as usual the Gauss–Lobatto–Legendre (GLL) quadrature to approximate the integrations in the space direction. On the other hand, the evaluation of the time integrations is more delicate for the reason that the definition of the time fractional derivative makes the integrands non polynomial in time. Thus we will introduce an exact Gauss–Lobatto–Jacobi (GLJ) quadrature to evaluate the integrations in the time direction.

To this end, we first introduce some notations. Let's denote by L_M the Legendre polynomial of degree M. The points of the GLL quadrature formula, denoted by x_k, are defined by

$$x_0=-1, x_M=1, L_M^{'}(x_k)=0, k=1,\ldots,M-1,$$

where $x_0<x_1<\cdots<x_M$. The associated weights of the GLL quadrature formula are denoted by ρ_k, $0\leq k\leq M$.

We now consider the space-time spectral method with numerical quadratures as follows: find $u_L\in S_L$ such that

$$\left({}_0\partial_t^{\frac{\alpha}{2}}u_L,{}_t\partial_T^{\frac{\alpha}{2}}v_L\right)_L+\left(\partial_x u_L,\partial_x v_L\right)_L=(f,v_L)_L\quad\forall v_L\in S_L, \tag{4.1}$$

where $(\cdot,\cdot)_L$ is defined by

$$(u,v)_L = \sum_{k=0}^{M} \int_0^T u(x_k,t)v(x_k,t)\rho_k \mathrm{d}t, \quad \forall u,v \in C^0(\Omega). \tag{4.2}$$

It is noted that in (4.1) the integrations in space have been approximated by the GLL quadrature while in the time direction the integrations remain exact. In the following, we will present a method to efficiently compute the integrations in time.

First, we need to choose a suitable basis. In order for the method to be more efficient, we choose to use the tensor product basis that combines a 1D basis for $P_M^0(\Lambda)$ and one for $P_N^E(I)$. It is natural to use the Lagrangian polynomials as basis in space. Let $\{h_i(x) : i = 0,\dots,M\}$ be the Lagrangian polynomials associated with GLL points $\{x_i : i = 0,\dots,M\}$. That is, $h_i(x) \in P_M(\Lambda)$, such that $h_i(x_k) = \delta_{ik}$, with δ denoting the Kronecker symbol. Obviously, we have

$$P_M^0(\Lambda) = \mathrm{span}\{h_i; i = 1,2,\dots,M-1\}.$$

For 1D basis in time variable, in order to derive an exact numerical quadrature for integrations in time as we are going to see later, we will need to use different bases to express the trial functions and test functions. For this purpose, we construct the functions $\phi_j(t)$ and $\psi_n(t)$ as follows:

$$\phi_j(t) = J_j^{-\alpha/2,0}\left(\frac{2t}{T}-1\right) + J_{j-1}^{-\alpha/2,0}\left(\frac{2t}{T}-1\right),\ j = 1,2,\dots,N,$$
$$\psi_n(t) = \frac{n}{n-\alpha/2} J_n^{0,-\alpha/2}\left(\frac{2t}{T}-1\right) + J_{n-1}^{0,-\alpha/2}\left(\frac{2t}{T}-1\right),\ n = 1,2,\dots,N,$$

where $J_k^{\alpha,\beta}$ is the Jacobi polynomial of degree k. The choice of the Jacobi weights with the exponent pairs $(-\alpha/2,0)$ and $(0,-\alpha/2)$ is motivated by the consideration of efficiently computing the integral $\int_0^T {}_0\partial_t^{\alpha/2}\phi_j(t)\ {}_t\partial_T^{\alpha/2}\psi_n(t)\mathrm{d}t$, needed to form the stiffness matrix; see (4.5). As shown in the appendix, with this choice, the integrand ${}_0\partial_t^{\alpha/2}\phi_j(t)\ {}_t\partial_T^{\alpha/2}\psi_n(t)$ can be transformed to a polynomial multiplied by a weight function $t^{-\alpha/2}(T-t)^{-\alpha/2}$; see (A.8). As a consequence, use of the standard Gauss–Lobatto rule with Jacobi weights for evaluating $\int_0^T {}_0\partial_t^{\alpha/2}\phi_j(t)\ {}_t\partial_T^{\alpha/2}\psi_n(t)\mathrm{d}t$ becomes possible.

It can be directly verified that both sets $\{\phi_j; j = 1,2,\dots,N\}$ and $\{\psi_n; n = 1,2,\dots,N\}$ are linear independent, and moreover

$$\phi_j(0) = J_j^{-\alpha/2,0}(-1) + J_{j-1}^{-\alpha/2,0}(-1) = (-1)^j + (-1)^{j-1} = 0,$$

$$\begin{aligned}\psi_n(0) &= \frac{n}{n-\alpha/2} J_n^{0,-\alpha/2}(-1) + J_{n-1}^{0,-\alpha/2}(-1)\\ &= (-1)^n \frac{n}{n-\alpha/2}\frac{\Gamma(n-\alpha/2+1)}{\Gamma(1-\alpha/2)n!} + (-1)^{n-1}\frac{\Gamma(n-\alpha/2)}{\Gamma(1-\alpha/2)(n-1)!}\\ &= 0.\end{aligned}$$

Thus both sets $\{\phi_j; j = 1,2,\dots,N\}$ and $\{\psi_n; n = 1,2,\dots,N\}$ form the space $P_N^E(I)$:

$$\begin{aligned}P_N^E(I) &= \mathrm{span}\{\phi_j; j = 1,2,\dots,N\},\\ &= \mathrm{span}\{\psi_n; n = 1,2,\dots,N\}.\end{aligned}$$

Now we construct the following bases for the space $P_M^0(\Lambda) \otimes P_N^E(I)$:

$$P_M^0(\Lambda) \otimes P_N^E(I) = span\{h_i(x)\phi_j(t),\ i = 1, \ldots, M-1; j = 1, \ldots, N\}. \tag{4.3}$$

$$P_M^0(\Lambda) \otimes P_N^E(I) = span\{h_m(x)\psi_n(t),\ m = 1, \ldots, M-1; n = 1, \ldots, N\}. \tag{4.4}$$

By expressing u_L in the basis (4.3)

$$u_L(x,t) = \sum_{i=1}^{M-1} \sum_{j=1}^{N} u_{ij} h_i(x) \phi_j(t),$$

and let the test function v_L go through all basis functions in (4.4), we arrive at the matrix statement of (4.1):

$$\mathbf{A}\mathbf{u} = \mathbf{f}, \tag{4.5}$$

where $\mathbf{u} = (u_{ij})_{(M-1)N}$ is the unknown vector, $\mathbf{A} = (a_{mn,ij})_{((M-1)N))^2}$ with

$$a_{mn,ij} = \left(h_i\ {}_0\partial_t^{\frac{\alpha}{2}} \phi_j,\ h_m\ {}_t\partial_T^{\frac{\alpha}{2}} \psi_n\right)_L + (\partial_x h_i \phi_j, \partial_x h_m \psi_n)_L,$$

and $\mathbf{f} = (f_{mn})_{(M-1)N}$ with

$$f_{mn} = (f, h_m \psi_n)_L.$$

By definition (4.2), $a_{mn,ij}$ can be rewritten into

$$\begin{aligned} a_{mn,ij} &= \sum_{k=0}^{M} h_i(x_k) h_m(x_k) \rho_k \int_0^T {}_0\partial_t^{\frac{\alpha}{2}} \phi_j(t)\ {}_t\partial_T^{\frac{\alpha}{2}} \psi_n(t) \mathrm{d}t \\ &\quad + \sum_{k=0}^{M} h_i'(x_k) h_m'(x_k) \rho_k \int_0^T \phi_j(t) \psi_n(t) \mathrm{d}t \\ &= \delta_{im} \rho_m \int_0^T {}_0\partial_t^{\frac{\alpha}{2}} \phi_j(t)\ {}_t\partial_T^{\frac{\alpha}{2}} \psi_n(t) \mathrm{d}t + \sum_{k=0}^{M} D_{ki} D_{km} \rho_k \int_0^T \phi_j(t) \psi_n(t) \mathrm{d}t, \end{aligned} \tag{4.6}$$

where $D_{ij} = h_j'(x_i)$, and $D := (D_{ij})$ is the usual derivative matrix in space. Similarly, we have

$$f_{mn} = \sum_{k=0}^{M} \int_0^T f(x_k, t) h_m(x_k) \psi_n(t) \rho_k \mathrm{d}t = \rho_m \int_0^T f(x_m, t) \psi_n(t) \mathrm{d}t. \tag{4.7}$$

Note that (4.5) is a nonsymmetric positive definite system, we use Bi-CG [25] to solve it.

It remains, however, to compute the integrals involved in (4.6) and (4.7). The presence of the time fractional derivatives makes the computations nontrivial. We will present in the appendix a method to efficiently calculate the integrations in time.

4.2. Numerical results. In this subsection, we present numerical results obtained by the proposed space-time spectral method. Estimate (3.9) indicates that the convergence of numerical solutions is exponential if the exact solution is smooth. To

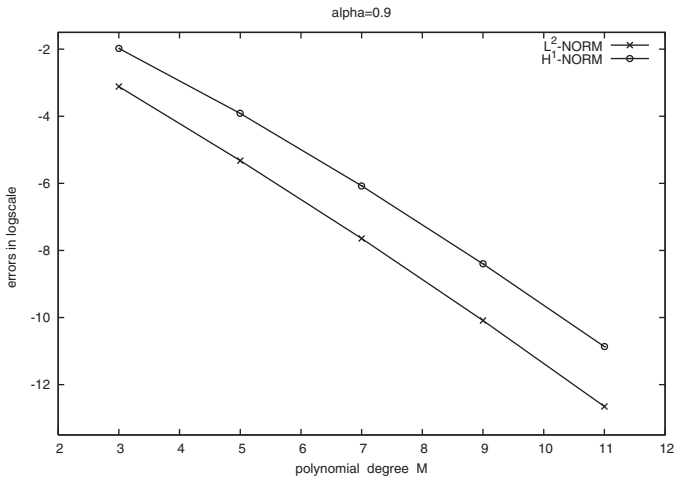

FIG. 4.1. *H^1- and L^2-errors versus M with $N = 16, \alpha = 0.9$.*

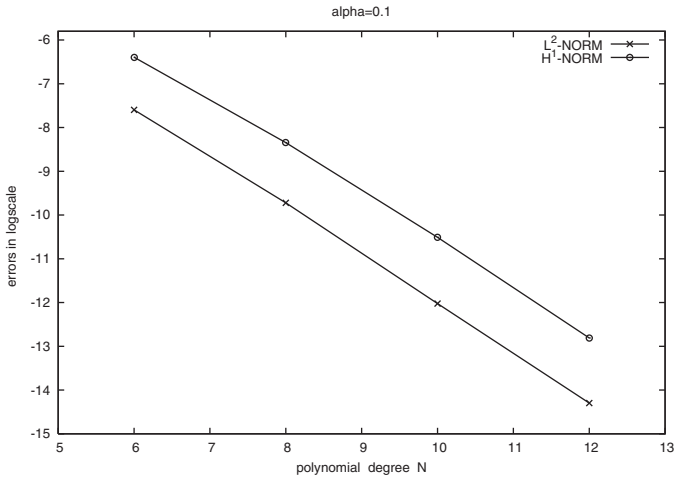

FIG. 4.2. *H^1- and L^2-errors versus N with $M = 15, \alpha = 0.1$.*

confirm the theoretical prediction, a numerical experiment is carried out by considering the problem with the exact analytical solution:

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

The main purpose is to check the convergence behavior of numerical solutions with respect to the polynomial degrees M and N for several α. In Figures 4.1–4.4, we plot the L^2-errors and H^1-errors in semilog scale. The first computational investigation is concerned with the spatial errors. In this first test, we fix $N = 16$, a value large enough such that the time discretization errors are negligible as compared with the space errors. In Figure 4.1, we plot the errors as functions of the polynomial degrees M for $\alpha = 0.9$. As expected, the errors show an exponential decay, since in this semilog representation one observes that the error variations are essentially linear versus the degrees of polynomial.

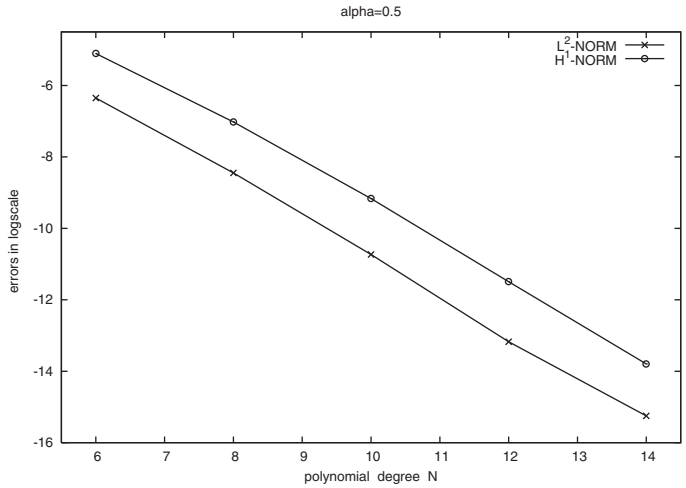

FIG. 4.3. *H^1- and L^2-errors versus N with $M = 15, \alpha = 0.5$.*

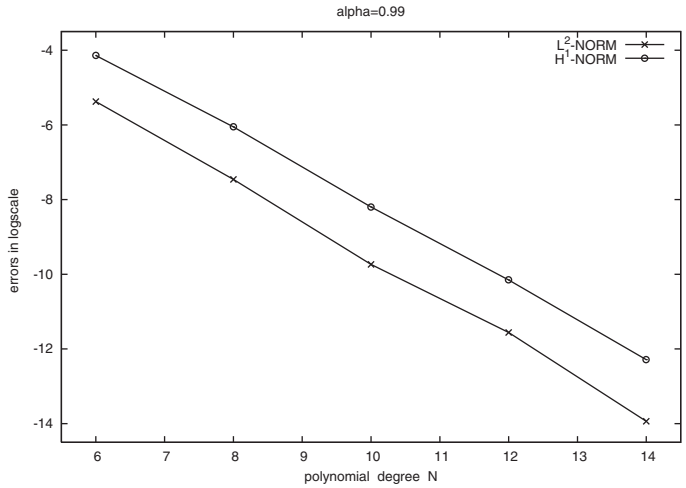

FIG. 4.4. *H^1- and L^2-errors versus N with $M = 15, \alpha = 0.99$.*

Now we investigate the temporal errors, which is more interesting to us because of the fractional derivative in time. For a similar reason mentioned above, we fix a large enough value of M, say $M = 15$, and let N vary. In Figures 4.2–4.4 we plot the errors as functions of N for three values $\alpha = 0.1, 0.5, 0.99$. It is observed that the error curves are all straight lines. This indicates that the convergence in time of the space-time spectral method is exponential. Another interesting finding of the numerical tests is that the proposed method seems to work well too for α close to 1, even though our theoretical analysis breaks down in the case $\alpha = 1$.

As for all other spectral methods, the accuracy of the present space-time spectral method depends on the regularity of the solution. In this example, we take an exact solution with limited regularity to examine the sharpness of the estimate given in (3.9). To this end, we consider the following exact solution:

$$u(x,t) = t(t-1/2)^{\gamma} \sin \pi x,$$

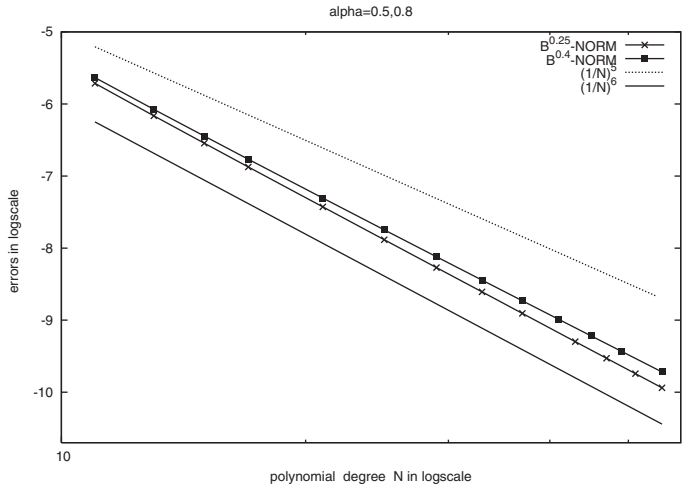

FIG. 4.5. *$B^{\alpha/2}$-errors versus N with $M = 15, \alpha = 0.5, 0.8$ for the solution of limited regularity.*

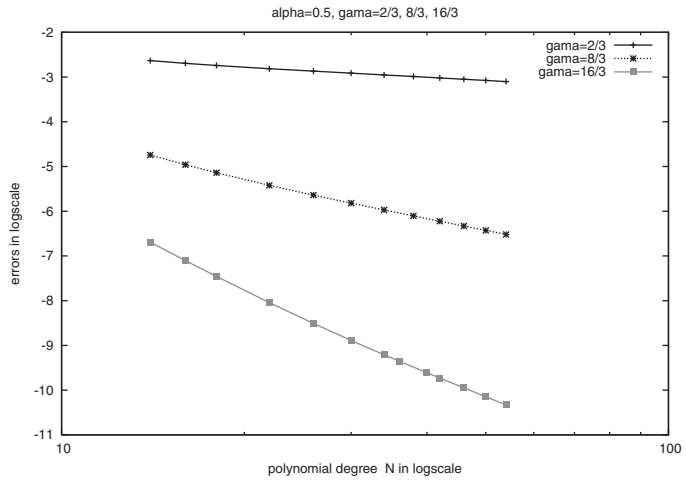

FIG. 4.6. *$B^{0.25}$-errors versus N with $M = 15$ for varying γ.*

where γ is a constant. It can be verified that this solution belongs to $H^{\gamma+1/2}$ on the time variable if γ is not an integer. We plot in Figure 4.5 the error decay rates in the $B^{\alpha/2}$-norm with respect to the polynomial degrees N with $M = 15$ and two different values of $\alpha : 0.5, 0.8$ for $\gamma = 16/3$. The N^{-5} and N^{-6} decay rates are also shown for comparison reasons. It is observed that the error curves are straight lines in this log-log representation, which indicates the algebraic convergence for the solution of limited regularity. Moreover it is seen that the errors decay with rates between N^{-5} and N^{-6}. This seems quite reasonable regarding the estimate (3.9), which predicts $N^{-5.58}$ decay rate for $\alpha = 0.5$ and $N^{-5.43}$ decay rate for $\alpha = 0.8$.

The investigation of the convergence behavior for less regular solutions can be done by decreasing γ. We plot in Figure 4.6 the errors versus N with $M = 15$ for three different values of γ: $16/3, 8/3, 2/3$. It is shown that the convergence rate slows down as γ, i.e., the regularity of the solution, decreases. These tests are in perfect agreement with what was expected for a spectral method.

5. Concluding remarks. We have presented a space-time spectral method for the time fractional diffusion equation. We established the well-posedness of this method by introducing a well-suited variational formulation. The spectral accuracy of the method is proven by providing a priori error estimate, and confirmed by a series of numerical tests. Thanks to the high accuracy of the proposed method, the storage requirement due to the time memory effect can be considerably reduced. It is worthwhile to mention that our numerical experiments show that the proposed method works also for $\alpha = 1$, for which the TFDE becomes the standard diffusion equation. In this case our method differs from (and simpler than) the existing space-time spectral methods which are based on the Petrov–Galerkin or Dual–Petrov–Galerkin formulation.

In a future work, we plan to investigate the computational complexity of the method, and look for ways to efficiently reduce the cost needed to compute the term involving the time fractional derivative. Other further work includes applying the present method to more general fractional PDEs.

Appendix A. Here we present a numerical quadrature for fast evaluations of the integrals

$$\int_0^T {}_0\partial_t^{\frac{\alpha}{2}}\phi_j(t)\ {}_t\partial_T^{\frac{\alpha}{2}}\psi_n(t)\mathrm{d}t,\ \int_0^T \phi_j(t)\ \psi_n(t)\mathrm{d}t,\ \int_0^T f(x_m,t)\psi_n(t)\mathrm{d}t$$

involved in (4.6) and (4.7).

First, in order to compute the integral

$$\int_0^T {}_0\partial_t^{\frac{\alpha}{2}}\phi_j(t)\ {}_t\partial_T^{\frac{\alpha}{2}}\psi_n(t)\mathrm{d}t,$$

we have to compute the left Riemann–Liouville derivative of $\phi_j(t)$ and right Riemann–Liouville derivative of $\psi_n(t)$. To this end, we recall here a known result from [24] (Theorem 6.4):

THEOREM A.1. *If $0 < \nu < 1$, γ is an arbitrary real number, r and k are integer numbers such that $r > -1 + \gamma - \nu/2$, $k > -1 - \gamma - \nu/2$, then for $-1 < t < 1$ it holds*

$$\begin{aligned}\int_{-1}^{1}\left(sign(t-\tau)+\frac{\tan(\pi\gamma)}{\tan\frac{\pi\nu}{2}}\right)\frac{J_m^{-\gamma+\nu/2+r,\gamma+\nu/2+k}(\tau)(1-\tau)^{-\gamma+\nu/2+r}(1+\tau)^{\gamma+\nu/2+k}}{|t-\tau|^{\nu}}\mathrm{d}\tau\\ =\frac{\pi(-1)^{r+k+1}\sin\pi(\gamma-\nu/2)2^{r+k+1}\Gamma(m+\nu)}{\Gamma(m+1)\Gamma(\nu)\sin\frac{\pi\nu}{2}\cos(\gamma\pi)\sin\pi(-\gamma+\nu/2-k)}J_{m+r+k+1}^{\gamma+\nu/2-r-1,-\gamma+\nu/2-k-1}(t),\\ m+r+k+1\geq 0,\quad m=1,2,\ldots.\end{aligned}\tag{A.1}$$

By using the above theorem, we can derive the following result.

LEMMA A.1. *For any real $0 < \alpha < 1$, $0 < t < T$, and any positive integer m, we have*

$${}_0D_t^{\alpha}J_m^{-\alpha,0}\left(\frac{2t}{T}-1\right)=\frac{\Gamma(m+1)t^{-\alpha}}{\Gamma(m-\alpha+1)}J_m^{0,-\alpha}\left(\frac{2t}{T}-1\right),\tag{A.2}$$

$${}_tD_T^{\alpha}J_m^{0,-\alpha}\left(\frac{2t}{T}-1\right)=\frac{\Gamma(m+1)(T-t)^{-\alpha}}{\Gamma(m-\alpha+1)}J_m^{-\alpha,0}\left(\frac{2t}{T}-1\right).\tag{A.3}$$

Proof. The first formula (A.2) with $T = 1$ has been proved in [24], Theorem 6.10. This formula for general T can be obtained by changing the variable from interval $[0, 1]$ to $[0, T]$. To prove the second formula (A.3), we use (A.1) with $\gamma = -\nu/2$,

$$\begin{aligned}&\int_t^1 \frac{J_m^{\nu+r,k}(\tau)(1-\tau)^{\nu+r}(1+\tau)^k}{(\tau-t)^\nu}\mathrm{d}\tau\\ &= \frac{\pi(-1)^{r+k+1}2^{r+k+1}\Gamma(m+\nu)}{\Gamma(m+1)\Gamma(\nu)\sin\pi(\nu-k)}J_{m+r+k+1}^{-r-1,\nu-k-1}(t).\end{aligned} \tag{A.4}$$

Note that the condition of Theorem A.1 is now reduced to $0 < \nu < 1, r > -1-\nu$, $k > -1$. By taking $r = -1$ and $k = 0$ in (A.4), we obtain

$$\int_t^1 \frac{J_m^{\nu-1,0}(\tau)(1-\tau)^{\nu-1}}{(\tau-t)^\nu}\mathrm{d}\tau = \frac{\pi\Gamma(m+\nu)}{\Gamma(m+1)\Gamma(\nu)\sin(\pi\nu)}J_m^{0,\nu-1}(t).$$

Then applying the identity $\frac{\pi}{\sin(\pi\nu)} = \Gamma(\nu)\Gamma(1-\nu)$ to the above equality gives

$$\int_t^1 \frac{J_m^{\nu-1,0}(\tau)(1-\tau)^{\nu-1}}{(\tau-t)^\nu}\mathrm{d}\tau = \frac{\Gamma(m+\nu)\Gamma(1-\nu)}{\Gamma(m+1)}J_m^{0,\nu-1}(t). \tag{A.5}$$

By changing the variables $\tau \to \frac{2\tau}{T} - 1, t \to \frac{2t}{T} - 1$, and let $\alpha = 1-\nu$ in (A.5), we have

$$\frac{1}{\Gamma(\alpha)}\int_t^T \frac{J_m^{-\alpha,0}(\frac{2\tau}{T}-1)(T-\tau)^{-\alpha}}{(\tau-t)^{1-\alpha}}\mathrm{d}\tau = \frac{\Gamma(m+1-\alpha)}{\Gamma(m+1)}J_m^{0,-\alpha}\left(\frac{2t}{T}-1\right). \tag{A.6}$$

Now we define, as in [24], the *right* Riemann–Liouville fractional integral of order α of a function f as follows:

$${}_tD_T^{-\alpha}f(t) = \frac{1}{\Gamma(\alpha)}\int_t^T \frac{f(\tau)}{(\tau-t)^{1-\alpha}}\mathrm{d}\tau.$$

Then, (A.6) becomes

$${}_tD_T^{-\alpha}\left(J_m^{-\alpha,0}\left(\frac{2t}{T}-1\right)(T-t)^{-\alpha}\right) = \frac{\Gamma(m+1-\alpha)}{\Gamma(m+1)}J_m^{0,-\alpha}\left(\frac{2t}{T}-1\right). \tag{A.7}$$

Finally, by applying the fractional differentiation operator ${}_tD_T^{\alpha}$ to both sides of (A.7) and using the following property (see, e.g., [24]),

$${}_tD_T^{\alpha}\ {}_tD_T^{-\alpha}f(t) = f(t),\ \forall f \text{ such that LHS makes sense},$$

we obtain (A.3). The proof is complete. ∎

By virtue of Lemma A.1, we have

$$
\begin{aligned}
{}_0D_t^{\alpha/2}\phi_j(t) &= {}_0D_t^{\alpha/2}\left(J_j^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)+J_{j-1}^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)\right)\\
&= {}_0D_t^{\alpha/2}J_j^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)+{}_0D_t^{\alpha/2}J_{j-1}^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)\\
&= \left(\frac{\Gamma(j+1)}{\Gamma(j+1-\alpha/2)}J_j^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)+\frac{\Gamma(j)}{\Gamma(j-\alpha/2)}J_{j-1}^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)\right)t^{-\alpha/2}.\\
{}_tD_T^{\alpha/2}\psi_n(t) &= {}_tD_T^{\alpha/2}\left(\frac{n}{n-\alpha/2}J_n^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)+J_{n-1}^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)\right)\\
&= \frac{n}{n-\alpha/2}{}_tD_T^{\alpha/2}J_n^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)+{}_tD_T^{\alpha/2}J_{n-1}^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)\\
&= \left(\frac{\Gamma(n+1)n}{\Gamma(n+1-\alpha/2)(n-\alpha/2)}J_n^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)\right.\\
&\quad\left.+\frac{\Gamma(n)}{\Gamma(n-\alpha/2)}J_{n-1}^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)\right)(T-t)^{-\alpha/2}.
\end{aligned}
$$

Let $\tilde{\phi}_j(t)$ denote

$$
\tilde{\phi}_j(t)=\frac{\Gamma(j+1)}{\Gamma(j+1-\alpha/2)}J_j^{0,-\alpha/2}\left(\frac{2t}{T}-1\right)+\frac{\Gamma(j)}{\Gamma(j-\alpha/2)}J_{j-1}^{0,-\alpha/2}\left(\frac{2t}{T}-1\right),
$$

and $\tilde{\psi}_n(t)$ stands for

$$
\tilde{\psi}_n(t)=\frac{\Gamma(n+1)n}{\Gamma(n+1-\alpha/2)(n-\alpha/2)}J_n^{-\alpha/2,0}\left(\frac{2t}{T}-1\right)+\frac{\Gamma(n)}{\Gamma(n-\alpha/2)}J_{n-1}^{-\alpha/2,0}\left(\frac{2t}{T}-1\right).
$$

Then both $\tilde{\phi}_j(t)$ and $\tilde{\psi}_n(t)$ are polynomials, and

$$
\int_0^T {}_0\partial_t^{\frac{\alpha}{2}}\phi_j(t)\ {}_t\partial_T^{\frac{\alpha}{2}}\psi_n(t)\mathrm{d}t=\int_0^T\tilde{\phi}_j(t)\tilde{\psi}_n(t)t^{-\alpha/2}(T-t)^{-\alpha/2}\mathrm{d}t. \tag{A.8}
$$

We are now led to compute the integral in the right-hand side of (A.8). We denote by $J_{N+1}^{\alpha,\beta}(\tau)$ the Jacobi polynomial of degree $N+1$ with respect to weight $w^{\alpha,\beta}(\tau)=(1-\tau)^\alpha(1+\tau)^\beta$. Let $\xi_k^{\alpha,\beta}$ be the points of the GLJ quadrature formula, defined by

$$
\xi_0^{\alpha,\beta}=-1,\ \xi_{N+1}^{\alpha,\beta}=1,\ \frac{d}{d\tau}J_{N+1}^{\alpha,\beta}\left(\xi_k^{\alpha,\beta}\right)=0,\ k=1,\ldots,N,
$$

arranged by increasing order: $\xi_0^{\alpha,\beta}<\xi_1^{\alpha,\beta}<\cdots<\xi_{N+1}^{\alpha,\beta}$. The associated weights of the GLJ quadrature formula are denoted by $\rho_k^{\alpha,\beta}$, $0\le k\le N+1$.

We define the set of GLJ quadrature points t_k in the time interval $I=[0,T]$ as follows:

$$
t_k=\frac{\left(\xi_k^{-\alpha/2,-\alpha/2}+1\right)T}{2},\ k=0,1,\ldots,N+1.
$$

The corresponding weights are then

$$
w_k=\left(\frac{2}{T}\right)^{\alpha-1}\rho_k^{-\alpha/2,-\alpha/2},\ k=0,1,\ldots,N+1.
$$

It is well known that the numerical quadrature

$$\int_0^T u(t)v(t)t^{-\alpha/2}(T-t)^{-\alpha/2}\mathrm{d}t \simeq \sum_{k=0}^{N+1} u(t_k)v(t_k)w_k$$

is exact for all functions u, v such that $uv \in P_{2N+1}(I)$. As a result, it holds

$$\int_0^T \tilde{\phi}_j(t)\tilde{\psi}_n(t)t^{-\alpha/2}(T-t)^{-\alpha/2}\mathrm{d}t = \sum_{k=1}^{N+1} \tilde{\phi}_j(t_k)\tilde{\psi}_n(t_k)w_k, \quad j,n = 1,2,\ldots,N$$

since $\tilde{\phi}_j\tilde{\psi}_n \in P_{2N}(I)$ for all $j,n = 1,2,\ldots,N$.

Now we turn to calculate $\int_0^T \phi_j(t)\ \psi_n(t)\mathrm{d}t$. We define the quadrature points $\tilde{t}_k$ and corresponding weights $\tilde{w}_k$ as follows:

$$\tilde{t}_k = \frac{\left(\xi_k^{0,0}+1\right)T}{2}, \quad \tilde{w}_k = \frac{T}{2}\rho_k^{0,0}, \quad k = 0,1,\ldots,N+1.$$

Then $\int_0^T \phi_j(t)\ \psi_n(t)\mathrm{d}t$ can be exactly evaluated by the numerical quadrature:

$$\int_0^T \phi_j(t)\ \psi_n(t)\mathrm{d}t = \sum_{k=1}^{N+1} \phi_j(\tilde{t}_k)\psi_n(\tilde{t}_k)\tilde{w}_k, \quad j,n = 1,2,\ldots,N.$$

Finally, the forcing term $\int_0^T f(x_m,t)\psi_n(t)\mathrm{d}t$ is approximated by the same quadrature as above.

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