A novel spectral method for the subdiffusion equation

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Abstract

In this paper, we design and analyze a novel spectral method for the subdiffusion equation. As it has been known, the solutions of this equation are usually singular near the initial time. Consequently, direct application of the traditional high-order numerical methods is inefficient. We try to overcome this difficulty in a novel approach by combining variable transformation techniques with spectral methods. The idea is to first use suitable variable transformation to re-scale the underlying equation, then construct spectral methods for the re-scaled equation. We establish a new variational framework based on the $\psi$-fractional Sobolev spaces. This allows us to prove the well-posedness of the associated variational problem. The proposed spectral method is based on the variational problem and generalized Jacobi polynomials to approximate the re-scaled fractional differential equation. Our theoretical and numerical investigation show that the proposed method is exponentially convergent for general right hand side functions, even though the exact solution has very limited regularity. Implementation details are also provided, along with a series of numerical examples to show the efficiency of the proposed method.

Keywords: Subdiffusion equation; Variable transformation; $\psi$–Sobolev spaces; Well-posedness; Spectral method; Error estimate

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1. Introduction

Fractional partial differential equations (FPDEs) appear in the investigation of transport dynamics in complex systems which are characterized by the anomalous diffusion and nonexponential relaxation patterns. Related equations of importance are the space/time fractional diffusion equations, the fractional advection-diffusion equation for anomalous diffusion with sources and sinks, and the fractional Fokker-Planck equation \cite{2,3} for anomalous diffusion in an external field, etc. In fact, it has been

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found that anomalous diffusion is ubiquitous in physical and biological systems where trapping and binding of particles can occur [5, 15]. Anomalous diffusion deviates from the standard Fickian 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 universality of anomalous diffusion phenomenon in physical and biological experiments has led to an intensive investigation on the fractional differential equations in recent years. 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 basic part in solving many other FPDEs. The TFDE and related equations have been investigated in analytical and numerical frames by a large number of authors, see, e.g., [16–30]. Spectral methods have also been applied in solving the TFDE. As is well known, any discretization including low-order approaches of a fractional derivative has to take into account its non-local structure, which results in a full linear system and a high storage requirement. Therefore it is very natural to consider a global method, such as the spectral method, since the high accuracy of spectral methods may significantly reduce the storage requirements. The first attempt in this direction was made by Li and Xu in [31, 32]. It was proven that the exponential convergence of the proposed method is attainable for smooth solutions.

A main difficulty in numerically solving the TFDE comes from the fact that the solutions of the TFDE are usually of low regularity, which lowers the accuracy of the above mentioned methods. Some efforts have been made in developing and analyzing numerical methods for solutions of low regularity. Among them, the modified time-stepping schemes are prominent, which can be roughly divided into two categories, i.e., piecewise polynomial interpolation based on a class of nonuniform grids and convolution quadrature with initial correction. Stynes et al. [33] proposed to use graded meshes in L1 scheme for a reaction-diffusion problem, and an error analysis was given taking the starting time singularity into consideration. Later on, Liao et al. [34, 35] gave a more general error analysis of L1 formula on nonuniform grids based on a discrete fractional Gronwall inequality. Some researchers [36–39] achieved optimal convergence rate by correcting the first several time steps. Several other works focused on spectral methods for non-smooth solutions of some related fractional equations, using polyfractonomials [40, 41], generalized Jacobi functions [42], Müntz Jacobi polynomials [43, 44], and log orthogonal functions/generalized log orthogonal functions [45, 46]. Numerical experiments or theoretical analysis presented therein have shown exponential convergence for non-smooth solutions having specific singularity.

Unlike these existing numerical approaches, in this paper we propose to first re-scale the time-fractional problems, then use the traditional approximations to the re-scaled problems. Li et al. [47] has tried this idea using a specific scaling function and proposed two finite difference schemes based on the linear interpolation and quadratic interpolation. The advantage of this approach is that the regularity of the re-scaled
fractional operator can be much higher than that of the original operator, which is more conducive to construct high-order schemes. Below, we describe the main contributions of the paper and how the paper is organized.

Our first contribution is the development of the \( \psi \)-fractional Sobolev spaces presented in Sect. 2 which lays the foundation for the establishment of a new variational framework in Sect. 3. In detail, we introduce the concept of \( \psi \)-fractional operators, and propose \( \psi \)-fractional Sobolev spaces on this basis and prove the equivalence of related norms of \( \psi \)-fractional Sobolev spaces.

The second contribution is to propose a new Galerkin spectral method based on the generalized Jacobi polynomials (GJPs) under the new variational framework introduced in Sect. 3. The well-posedness of the weak problem is proved in the \( \psi \)-fractional Sobolev spaces, together with error estimation established in the non-uniform Jacobi-weighted norm. Moreover, it’s shown that the new approach is as efficient as the Müntz spectral method \([43, 44]\) by using suitable scaling functions. The novel approach not only provides a theoretical support of the Müntz spectral method but also gives a guideline for the selection of the scaling parameters.

Finally, the proposed approach is applied to the time fractional subdiffusion equations in Sect. 4. A space-time Galerkin spectral method is developed based on the re-scaled weak formulation and a combination of temporal GJPs and spatial Legendre polynomials. In Sect. 5, we present some numerical tests to confirm the theoretical findings. Some concluding remarks are given in Sect. 6.

2. Functional Spaces

In order to develop the re-scaling method for fractional differential equations, we need some preparations, mainly including an introduction of the \( \psi \)-fractional Sobolev spaces and establishment of the associated variational framework. Throughout this paper, let \( c \) stand for a generic positive constant independent of any functions and of any discretization parameters. In what follows, we use the expression \( A \lesssim B \) (respectively, \( A \gtrsim B \)) to mean that \( A \leq cB \) (respectively, \( A \geq cB \)).

The first part of this section is devoted to introducing the \( \psi \)-fractional integrals, derivatives and a crucial variable transformation.

2.1. \( \psi \)-fractional operators and variable transformation

We recall some definitions of \( \psi \)-fractional integrals and \( \psi \)-fractional derivatives; see Kilbas et al. \([48, \text{Sect. 2.5}]\) or Samko et al. \([49, \text{Sect. 18.2}]\). Let \( \Gamma(\cdot) \) denote the Gamma function. For any positive integer \( n \) and real number \( \delta \), \( n - 1 \leq \delta < n \), \( v \) is an integrable function in the bounded interval \([a_\psi, b_\psi]\) with respect to the function \( \psi : [a_\psi, b_\psi] \to \mathbb{R} \) that is increasing and differentiable such that \( \psi'(t) \neq 0 \). The \( \psi \)-fractional integral, \( \psi \)-Caputo derivative, and \( \psi \)-Riemann–Liouville derivative of order \( \delta \) of \( v \) are respectively
defined as follows: $\forall t \in [a, b], \psi$

left $\psi$-fractional integral: $I_t^{\delta, \psi} v(t) := \frac{1}{\Gamma(1-\delta)} \int_{a}^{t} \psi'(z)(\psi(t) - \psi(z))^{\delta-1} v(z)dz$, \hspace{1cm} (I1)

right $\psi$-fractional integral: $I_t^{\delta, \psi} v(t) := \frac{1}{\Gamma(1-\delta)} \int_{t}^{b} \psi'(z)(\psi(z) - \psi(t))^{\delta-1} v(z)dz$, \hspace{1cm} (I2)

left $\psi$-Caputo derivative: $C_t^{\delta, \psi} v(t) := I_t^{n-\delta, \psi} \left( \frac{d}{dt} \right)^n v(t)$, \hspace{1cm} (D1)

right $\psi$-Caputo derivative: $C_t^{\delta, \psi} v(t) := I_t^{n-\delta, \psi} \left( -\frac{d}{dt} \right)^n v(t)$, \hspace{1cm} (D2)

left $\psi$-Riemann–Liouville derivative: $D_t^{\delta, \psi} v(t) = \frac{1}{\Gamma(n-\delta)} \int_{t}^{t} \psi(z)(\psi(t) - \psi(z))^{\delta-1} v(z)dz$, \hspace{1cm} (D3)

right $\psi$-Riemann–Liouville derivative: $D_t^{\delta, \psi} v(t) := \frac{1}{\Gamma(n-\delta)} \int_{t}^{b} \psi(z)(\psi(z) - \psi(t))^{\delta-1} v(z)dz$, \hspace{1cm} (D4)

When $\psi(t) = t$, the above definitions degenerate into the classical fractional integral, Caputo derivative and Riemann–Liouville derivative; see \([50, 51]\). In particular, when $\delta \in (0, 1)$, $\psi$–Caputo fractional derivative $C_t^{\delta, \psi} v(t)$ becomes $C_t^{\delta} v(t)$, where

$$C_t^{\delta} v(t) := \frac{1}{\Gamma(1-\delta)} \int_{0}^{t} (t-z)^{-\delta} v'(z)dz.$$ \hspace{1cm} (1)

On the contrary, by a change of variable $\psi(t)$, the classical Caputo fractional derivative can be turned into a class of $\psi$–Caputo fractional derivative. For example, a direct calculation gives

$$C_t^{\delta} u(s) = \frac{1}{\Gamma(1-\delta)} \int_{0}^{s} (s-x)^{-\delta} u'(x)dx, \quad s \in (0, T]$$

$$= \frac{1}{\Gamma(1-\delta)} \int_{0}^{t^{1/\gamma}} (t^{1/\gamma} - x)^{-\delta} u'(x)dx, \quad t \in (0, T^{\gamma}]$$

$$= \frac{1}{\Gamma(1-\delta)} \int_{0}^{t^{1/\gamma}} (t^{1/\gamma} - z^{1/\gamma})^{-\delta} u'(z^{1/\gamma})dz, \quad t \in (0, T^{\gamma}]$$ \hspace{1cm} (2)

Let $\psi(t) = t^{1/\gamma}, v(t) := u(\psi(t))$ for $t \in (0, T^{\gamma}]$. Then the new fractional derivative $C_t^{\delta} v(t)$, defined by

$$C_t^{\delta} v(t) := \frac{1}{\Gamma(1-\delta)} \int_{0}^{t} (t^{1/\gamma} - z^{1/\gamma})^{-\delta} v'(z)dz, \quad t \in (0, T^{\gamma}]$$ \hspace{1cm} (3)
can be regarded as a class of $\psi$–Caputo fractional derivative of $v(t)$ with $\psi(t) = t^{1/\gamma}$.

The following results about $\psi$–fractional operators are frequently used; see [52, 53].

It is noted that the $\psi$–Riemann–Liouville fractional derivative and $\psi$–Caputo fractional derivative of $v$ have the following relationship

$$CD_t^\delta \psi v(t) = D_t^\delta \psi[v(t) - v(a_\psi)], \quad \delta \in (0, 1). \quad (4)$$

And left $\psi$–Riemann–Liouville fractional derivative and integral of order $\delta$ satisfy

$$D_t^\delta \psi I_t^\delta \psi v(t) = v(t). \quad (5)$$

With the above notations and properties, we are in a position to introduce the $\psi$-fractional Sobolev spaces.

2.2. $\psi$-fractional Sobolev spaces

We begin with some additional notations. Let $0 < \gamma \leq 1, I = (a, b)$. The function $\psi^{-1}(\cdot)$ denotes the inverse function of $\psi(\cdot)$. Let $\Lambda = (a_{\psi}, b_{\psi}) := (\psi^{-1}(a), \psi^{-1}(b))$. Thus if $s \in I$, then $t = \psi^{-1}(s) \in \Lambda$. Define the space

$$L_\psi^2(\Lambda) = \left\{ v : \Lambda \rightarrow \mathbb{R} | v \text{ is measurable and } \int_\Lambda |v(t)|^2 \psi'(t)dt < \infty \right\}.$$ 

It can be easily seen that $L_\psi^2(\Lambda)$ is a Hilbert space with respect to the scalar product

$$(v, w)_{L_\psi^2(\Lambda)} = \int_\Lambda v(t)w(t)\psi'(t)dt, \quad \forall v, w \in L_\psi^2(\Lambda). \quad (6)$$

The norm in $L_\psi^2(\Lambda)$ induced by the scalar product $(\cdot, \cdot)_{L_\psi^2(\Lambda)}$ is defined by

$$\|v\|_{L_\psi^2(\Lambda)} = \sqrt{(v, v)_{L_\psi^2(\Lambda)}} = \left(\int_\Lambda |v(t)|^2 \psi'(t)dt\right)^{1/2}, \quad \forall v \in L_\psi^2(\Lambda).$$

In particular, for $\psi(t) = t$, the space $L_\psi^2(\Lambda)$ is reduced to the classical space $L^2(\Lambda)$. Let us denote by $(\cdot, \cdot)_{L^2(\Lambda)}$ and $\|\cdot\|_{L^2(\Lambda)}$ the inner product and norm in $L^2(\Lambda)$, respectively.

We now introduce the $\psi$–fractional Sobolev spaces. Let $\mathcal{F}(v)$ denote the Fourier transform of $v$, $\tilde{v}(\cdot) := v(\psi^{-1}(\cdot))$. Define the space

$$H^{\delta, \psi}(\mathbb{R}) := \left\{ v \in L_\psi^2(\mathbb{R}) ; (1 + |\xi|^\delta)\mathcal{F}(\tilde{v})(\xi) \in L^2(\mathbb{R}) \right\}, \quad \delta \geq 0, \quad (7)$$

endowed with the semi-norm and norm

$$|v|_{H^{\delta, \psi}(\mathbb{R})} = \left\| (1 + |\xi|^\delta)\mathcal{F}(\tilde{v})(\xi) \right\|_{L^2(\mathbb{R})},$$
\[ \|v\|_{H^\delta,\psi}(\Lambda) = \left( \|v\|_{L^2(\Lambda)}^2 + |v|_{H^\delta,\psi}(\Lambda)}^2 \right)^{1/2}, \]

respectively. Note that \( F(\tilde{v}) \) rather than \( F(v) \) was used in the definition \( (7) \).

The \( \psi \)-fractional Sobolev space for the bounded domain \( \Lambda \) is defined by

\[ H^\delta,\psi(\Lambda) := \left\{ v \in L^2_\psi(\Lambda) \right| \exists v_\epsilon \in H^\delta,\psi(\mathbb{R}) \text{ such that } v_\epsilon|_{\Lambda} = v \}, \]

equipped with the norm

\[ \|v\|_{H^\delta,\psi}(\Lambda) = \inf_{v_\epsilon \in H^\delta,\psi(\mathbb{R})} \|v_\epsilon\|_{H^\delta,\psi(\mathbb{R})}. \]

It is readily seen that \( H^\delta,\psi(\Lambda) \) degenerates into the classic Sobolev space \( H^\delta(\Lambda) \) when \( \psi(t) = t \).

We define

\[ L^\delta H^\delta,\psi(\Lambda) := \left\{ v \left| \|v\|_{L^\delta H^\delta,\psi}(\Lambda) < \infty \right. \right\}, \]

where \( \| \cdot \|_{L^\delta H^\delta,\psi}(\Lambda) \) is the norm:

\[ \|v\|_{L^\delta H^\delta,\psi}(\Lambda) = \left( \|v\|_{L^2_\psi(\Lambda)}^2 + |v|_{H^\delta,\psi}(\Lambda)}^2 \right)^{1/2}, \quad \|v\|_{L^\delta H^\delta,\psi}(\Lambda) = \left\| D^\delta,\psi \right\|_{L^2(\Lambda)}^2. \]

Similarly, we define

\[ R^\delta H^\delta,\psi(\Lambda) := \left\{ v \left| \|v\|_{R^\delta H^\delta,\psi}(\Lambda) < \infty \right. \right\}, \]

with

\[ \|v\|_{R^\delta H^\delta,\psi}(\Lambda) = \left( \|v\|_{L^2_\psi(\Lambda)}^2 + |v|_{R^\delta H^\delta,\psi}(\Lambda)}^2 \right)^{1/2}, \quad \|v\|_{R^\delta H^\delta,\psi}(\Lambda) = \left\| C^\delta,\psi \right\|_{L^2(\Lambda)}^2; \]

and

\[ C^\delta H^\delta,\psi(\Lambda) := \left\{ v \left| v\|_{C^\delta H^\delta,\psi}(\Lambda) < \infty \right. \right\}, \]

with

\[ \|v\|_{C^\delta H^\delta,\psi}(\Lambda) = \left( \|v\|_{L^2_\psi(\Lambda)}^2 + |v|_{C^\delta H^\delta,\psi}(\Lambda)}^2 \right)^{1/2}, \quad \|v\|_{C^\delta H^\delta,\psi}(\Lambda) = \left\| (D^\delta,\psi v, i D^\delta,\psi v)_{L^2_\psi(\Lambda)} \right\|^{1/2}. \]

Let \( C_0^\infty(\Lambda) \) is the space of smooth functions with compact support in \( \Lambda \). Let \( L^\delta H^\delta_0(\Lambda), R^\delta H^\delta_0(\Lambda), C^\delta H^\delta_0(\Lambda), \) and \( H^\delta_0(\Lambda) \) be the closures of \( C_0^\infty(\Lambda) \) with respect to the norms \( \|v\|_{L^\delta H^\delta_0,\psi}(\Lambda) \), \( \|v\|_{R^\delta H^\delta_0,\psi}(\Lambda) \), \( \|v\|_{C^\delta H^\delta_0,\psi}(\Lambda) \), and \( \|v\|_{H^\delta_0,\psi}(\Lambda) \) respectively. Besides, let \( 0^\delta H^\delta(\Lambda) \) denote the closure of \( 0 C^\infty(\Lambda) \) with respect to \( \| \cdot \|_{H^\delta_0,\psi}(\Lambda) \), where \( 0 C^\infty(\Lambda) \) is the space of smooth functions with compact support in \( (a_\psi, b_\psi) \).

Next we give some crucial lemmas, especially the equivalence results of the related norms of the \( \psi \)-fractional Sobolev spaces. These results play a key role in the subsequent analysis, including the well-posedness analysis and error estimation of the numerical methods to be constructed.
2.3. Some useful Lemmas

Define the convolution of the functions \( h_1(t) \) and \( h_2(t) \) as follows:

\[
h_1(t) * h_2(t) := \int_{-\infty}^{+\infty} h_1(t-\tau)h_2(\tau)d\tau = \int_{-\infty}^{+\infty} h_1(\tau)h_2(t-\tau)d\tau,
\]

where \( h_1(t), h_2(t) \in (-\infty, +\infty) \).

It is known [51] that if the Fourier transform of \( h_1(t) \) and \( h_2(t) \) exists, then

\[
\mathcal{F}\{h_1(t) * h_2(t); \, \xi\} = H_1(\xi)H_2(\xi),
\]

where \( H_1(\xi) = \mathcal{F}\{h_1(t); \, \xi\}, \, H_2(\xi) = \mathcal{F}\{h_2(t); \, \xi\} \).

Then we can define Fourier transform of \( \psi \)-fractional derivatives on the above basis.

**Lemma 1.** *(Fourier transform of \( \psi \)-fractional derivatives)* Let \( v \in C^\infty_0(\mathbb{R}), \, 0 < \delta < 1 \). Assume \( \psi(\infty) = \infty \). Then

\[
\mathcal{F}\{-\infty I_{\psi}^{\delta} v(t)\} = (i\xi)^\delta \mathcal{F}(\tilde{v})(\xi), \quad \mathcal{F}\{t D_{+\infty}^{\psi} v(t)\} = (-i\xi)^\delta \mathcal{F}(\tilde{v})(\xi).
\]

**Proof.** We first evaluate the Fourier transform of the \( \psi \)-fractional integral \( -\infty I_{\psi}^{\delta} v \).

The Laplace transform \( \mathcal{L} \) of \( s^{\delta-1} \) reads

\[
\mathcal{L}\{s^{\delta-1}; \, \tau\} = \int_0^{\infty} s^{\delta-1}e^{-\tau s}ds = \Gamma(\delta)\tau^{-\delta}.
\]

Note that the above integral makes sense for all \( \delta > 0 \) by the Dirichlet theorem. Let \( h(s) \) be the function

\[
h(s) = \begin{cases} s^{\delta-1}\frac{1}{\Gamma(\delta)}, & s > 0, \\ 0, & s \leq 0. \end{cases}
\]

Then a direct calculation using (11) shows

\[
\mathcal{F}\{h(s); \xi\} = \int_{-\infty}^{\infty} h(s)e^{-i\xi s}ds = \frac{1}{\Gamma(\delta)} \int_0^{\infty} s^{\delta-1}e^{-i\xi s}ds = \frac{\mathcal{L}\{s^{\delta-1}; i\xi\}}{\Gamma(\delta)} = (i\xi)^{-\delta}.
\]

Let \( s = \psi(t) \), then the \( \psi \)-fractional integral \( -\infty I_{t}^{\psi} v \) can be expressed as a convolution of the functions \( h(\psi(t)) \) and \( \tilde{v}(\psi(t)) \), i.e.,

\[
-\infty I_{t}^{\psi} v(t) = \frac{1}{\Gamma(\delta)} \int_{-\infty}^{\psi(t)} (\psi(t) - \psi(\tau))^{\delta-1}\tilde{v}(\psi(\tau))d\psi(\tau)
\]

\[
= h(s) * \tilde{v}(s),
\]
where \( \tilde{v}(\cdot) := v(\psi^{-1}(\cdot)) \). Thus, it follows from (9) and (12):

\[
\mathcal{F}\{-\infty I_t^\delta \psi v(t); \xi\} = (i\xi)^{-\delta} \mathcal{F}(\tilde{v})(\xi).
\]

Next, we calculate the Fourier transform of the \( \psi \)-fractional derivatives. Note that

\[
-\infty D_t^\delta v(t) = -\infty I_t^{n-\delta, \psi} \left( \frac{1}{\psi'(t)} \frac{d^n}{dt^n} v(t) \right),
\]

we have

\[
\mathcal{F}\{-\infty D_t^\delta v(t)\} = (i\xi)^{\delta-n} \mathcal{F}\left\{ \left( \frac{d}{d\psi} \right)^n \tilde{v}(\psi(t)) ; \xi \right\}
= (i\xi)^{\delta-n} (i\xi)^n \mathcal{F}(\tilde{v})(\xi)
= (i\xi)^{\delta} \mathcal{F}(\tilde{v})(\xi).
\]

The second equality in (10) can be proved in a similar way.

With the help of the Fourier transform of the \( \psi \)-fractional derivatives, we can derive the following equivalence result for the \( \psi \)-fractional Sobolev spaces on the whole line \( \mathbb{R} \).

**Lemma 2.** Let \( \delta > 0, \delta \neq n - 1/2, n \in \mathbb{N} \). Then the spaces \( L^{H^\delta, \psi}(\mathbb{R}) \), \( R^{H^\delta, \psi}(\mathbb{R}) \), \( c^{H^\delta, \psi}(\mathbb{R}) \), and \( H^\delta, \psi(\mathbb{R}) \) are equal to each other with equivalent semi-norms and norms.

**Proof.** The proof will be divided into three steps.

Step 1: the equivalence of the spaces \( L^{H^\delta, \psi}(\mathbb{R}) \) and \( H^\delta, \psi(\mathbb{R}) \).

For a function \( v \in L^{H^\delta, \psi}(\mathbb{R}) \), we have \( D_t^\delta v \in L^2(\mathbb{R}) \). Using Lemma 1 and Plancherel’s theorem gives

\[
|v|_{L^{H^\delta, \psi}(\mathbb{R})}^2 = \int_{\mathbb{R}} |\mathcal{F}(\tilde{v})(\xi)|^2 d\xi
= \int_{\mathbb{R}} |D_t^\delta v(t)|^2 \psi'(t) dt.
\]

Thus,

\[
\|\xi^\delta \mathcal{F}(\tilde{v})(\xi)\|_{L^2(\mathbb{R})} = |v|_{L^{H^\delta, \psi}(\mathbb{R})}.
\]

The desired result follows immediately from the above equality and the definition of \( H^\delta, \psi(\mathbb{R}) \).

Step 2: the equivalence of the spaces \( L^{R^\delta, \psi}(\mathbb{R}) \) and \( H^\delta, \psi(\mathbb{R}) \).

Again, using the results of Lemma 1 and Plancherel’s theorem, we have

\[
|v|_{L^{R^\delta, \psi}(\mathbb{R})}^2 = \int_{\mathbb{R}} \left| (i\xi)^{\delta} \mathcal{F}(\tilde{v})(\xi) \right|^2 d\xi.
\]

Similarly,

\[
|v|_{R^{H^\delta, \psi}(\mathbb{R})}^2 = \int_{\mathbb{R}} \left| (-i\xi)^{\delta} \mathcal{F}(\tilde{v})(\xi) \right|^2 d\xi.
\]
Note that \(|(i\xi)^{\delta}| = |(-i\xi)^{\delta}|\). Thus the semi-norms \(|v|_{L^{H^{\delta,\psi}(\mathbb{R})}}\) and \(|v|_{R^{H^{\delta,\psi}(\mathbb{R})}}\), consequently the norms \(\|v\|_{L^{H^{\delta,\psi}(\mathbb{R})}}\) and \(\|v\|_{R^{H^{\delta,\psi}(\mathbb{R})}}\), are equivalent.

Step 3: the equivalence of the spaces \(c^{H^{\delta,\psi}}(\mathbb{R})\) and \(L^{H^{\delta,\psi}}(\mathbb{R})\).
Analogous to [54, Lemma 2.4], with the help of some related properties of the Fourier transform, we obtain
\[
\left( D^{\delta,\psi}_{t}v, t D^{\delta,\psi}_{t}v \right)_{L^{2}_\psi(\mathbb{R})} = \cos(\pi \delta) \left\| D^{\delta,\psi}_{t}v \right\|^{2}_{L^{2}_\psi(\mathbb{R})}.
\]
That is,
\[
|v|^{2}_{c^{H^{\delta,\psi}}(\mathbb{R})} = |\cos(\pi \delta)| |v|^{2}_{L^{H^{\delta,\psi}}(\mathbb{R})}.
\]
Thus the semi-norms of \(c^{H^{\delta,\psi}}(\mathbb{R})\) and \(L^{H^{\delta,\psi}}(\mathbb{R})\) are equivalent. So are their norms, which implies the equivalence of \(c^{H^{\delta,\psi}}(\mathbb{R})\) and \(L^{H^{\delta,\psi}}(\mathbb{R})\).

We conclude by combining Step 1–Step 3.

The equivalence of different \(\psi\)–fractional spaces on the bounded interval \(\Lambda\) are established below.

**Lemma 3.** Let \(\delta > 0, \delta \neq n - 1/2, n \in \mathbb{N}\). Then the spaces \(L^{H^{\delta,\psi}}(\Lambda)\), \(R^{H^{\delta,\psi}}(\Lambda)\), \(c^{H^{\delta,\psi}}(\Lambda)\), and \(H^{\delta,\psi}(\Lambda)\) are equal to each other with equivalent semi-norms and norms.

**Proof.** The proof is splitted into two steps.

Step 1: the equivalence of the spaces \(c^{H^{\delta,\psi}}(\Lambda)\) and \(H^{\delta,\psi}(\Lambda)\).
For \(v \in C_0^\infty(\Lambda)\), let \(v_e\) be the extension of \(v\) by zero outside of \(\Lambda\). Then
\[
supp(v_e) \subset \Lambda,
\]
\[
supp \left( D^{\delta,\psi}_{t}v_e \right) \subset (a_\psi, \infty),
\]
\[
supp \left( t D^{\delta,\psi}_{t}v_e \right) \subset (-\infty, b_\psi).
\]
Thus,
\[
supp \left( D^{\delta,\psi}_{t}v_e, t D^{\delta,\psi}_{t}v_e \right) \subset \Lambda,
\]
from which it follows
\[
|v|_{c^{H^{\delta,\psi}}(\Lambda)} = |v_e|_{H^{\delta,\psi}(\mathbb{R})}.
\]
On the other side, we have
\[
|v|_{H^{\delta,\psi}(\Lambda)} = |v_e|_{H^{\delta,\psi}(\mathbb{R})}.
\]
Then the semi-norm equivalence of \(c^{H^{\delta,\psi}}(\mathbb{R})\) and \(H^{\delta,\psi}(\mathbb{R})\), proved in Lemma 2, gives
\[
|v|_{c^{H^{\delta,\psi}}(\Lambda)} = |v|_{H^{\delta,\psi}(\Lambda)}.
\]
Thus the spaces \(c^{H^{\delta,\psi}}(\Lambda)\) and \(H^{\delta,\psi}(\Lambda)\) are equal with equivalent norms.
Step 2: the equivalence of the spaces $L^2 H_0^\delta \psi(\Lambda)$, $R^2 H_0^\delta \psi(\Lambda)$, and $H_0^\delta \psi(\Lambda)$.

It follows from (13) and the definition of $| \cdot |_{H_0^\delta \psi(\Lambda)}$:

$$\left\| D_t^\delta \psi v \right\|_{L^2_\psi(\Lambda)} = |v|_{L^2 H_0^\delta \psi(\Lambda)} \leq |v_e|_{L^2 H^\delta \psi(\mathbb{R})} = |v_e|_{L^2 H^\delta \psi(\mathbb{R})} = |v|_{H_0^\delta \psi(\Lambda)}.$$

This gives

$$H_0^\delta \psi(\Lambda) \subseteq L^2 H_0^\delta \psi(\Lambda).$$

Combining the result proved in Step 1 and Young’s inequality, we obtain

$$|v|^2_{H_0^\delta \psi(\Lambda)} \leq c |v|^2_{L^2 H_0^\delta \psi(\Lambda)} + \epsilon c |v|^2_{L^2 H_0^\delta \psi(\Lambda)}.$$

Furthermore, it follows from (13) and the definition of $| \cdot |_{H_0^\delta \psi(\Lambda)}$:

$$\left\| t D_t^\delta \psi v \right\|_{L^2_\psi(\Lambda)} = |v|_{R H_0^\delta \psi(\Lambda)} \leq |v_e|_{R H^\delta \psi(\mathbb{R})} = |v_e|_{R H^\delta \psi(\mathbb{R})} = |v|_{H_0^\delta \psi(\Lambda)}.$$

Combining the last two inequalities gives

$$|v|^2_{H_0^\delta \psi(\Lambda)} \leq \frac{c}{2\epsilon} |v|^2_{L^2 H_0^\delta \psi(\Lambda)} + \frac{c}{2} |v|^2_{H_0^\delta \psi(\Lambda)}.$$

Taking $\epsilon = 1/c$ in the above inequality yields

$$|v|^2_{H_0^\delta \psi(\Lambda)} \leq c^2 |v|^2_{L^2 H_0^\delta \psi(\Lambda)}.$$

This gives

$$L^2 H_0^\delta \psi(\Lambda) \subseteq H_0^\delta \psi(\Lambda).$$

This ends the proof of the semi-norm equivalence of the spaces $L^2 H_0^\delta \psi(\Lambda)$ and $H_0^\delta \psi(\Lambda)$, and thus the equivalence of the spaces themselves. In a similar way, we can prove the equivalence of the spaces $R^2 H_0^\delta \psi(\Lambda)$ and $H_0^\delta \psi(\Lambda)$. The proof is completed.

Now we turn to derive some Poincaré-Friedrichs-type inequalities for the functions in $\psi$–fractional spaces. The following mapping properties are useful.

**Lemma 4.** (Mapping properties) All the following mappings are bounded linear operators.

(i) $I^\delta \psi: L^2(\Lambda) \to L^2(\Lambda)$.

(ii) $I^\delta \psi: L^2(\Lambda) \to H_0^\delta \psi(\Lambda)$.
(iii) $D_t^\delta \psi : L^H(\Lambda) \to L^2(\Lambda)$.
(iv) $t^H \psi : L^2(\Lambda) \to L^2(\Lambda)$.
(v) $t^\varphi \psi : L^2(\Lambda) \to R\varphi^H(\Lambda)$.
(vi) $t\varphi D_t^\varphi \psi : R\varphi^H(\Lambda) \to L^2(\Lambda)$.

**Proof.** (i) By using [55, Lemma 2.2], we have

$$
\| I_\delta \psi t v \|_{L^2(\Lambda)} \leq \frac{1}{\Gamma(\delta)\sqrt{2\delta - 1}} \| v \|_{L^2(\Lambda)},
$$

which means $I_\delta \psi t$ is a bounded linear operator from $L^2(\Lambda)$ to $L^2(\Lambda)$.

(ii) Combining (5) and the definition of $L^H(\Lambda)$, then using (i), one obtains

$$
\| D_t^\psi v \|_{L^H(\Lambda)} = \left( \| I_\delta \psi t v \|_{L^2(\Lambda)}^2 + \| D_t^\psi I_\delta \psi t v \|_{L^2(\Lambda)}^2 \right)^{1/2} \lesssim \| v \|_{L^H(\Lambda)}.
$$

This proves that $D_t^\psi \psi$ is a bounded linear operator from $L^2(\Lambda)$ to $L^H(\Lambda)$.

(iii) It follows from the definition of the norm $\| \cdot \|_{L^H(\Lambda)}$:

$$
\| D_t^\psi v \|_{L^2(\Lambda)} \leq \left( \| v \|_{L^2(\Lambda)}^2 + \| D_t^\psi v \|_{L^2(\Lambda)}^2 \right)^{1/2} =: \| v \|_{L^H(\Lambda)}.
$$

This shows that $D_t^\psi \psi$ is a bounded linear operator from $L^H(\Lambda)$ to $L^2(\Lambda)$.

(iv)-(vi) can be proved similarly.

**Lemma 5.** ($\psi$–fractional Poincaré–Friedrichs inequalities) The following two Poincaré–Friedrichs-type inequalities hold

$$
\| v \|_{L^2(\Lambda)} \lesssim | v |_{L^H(\Lambda)}, \quad \forall v \in L^H(\Lambda).
$$

$$
\| v \|_{L^2(\Lambda)} \lesssim | v |_{R^H(\Lambda)}, \quad \forall v \in R^H(\Lambda).
$$

**Proof.** For all $v \in L^H(\Lambda)$, it follows from (5) and Lemma 2 that

$$
\| v \|_{L^2(\Lambda)} = \| I_\delta \psi t D_t^\psi v \|_{L^2(\Lambda)} \lesssim \| D_t^\psi v \|_{L^2(\Lambda)} = | v |_{L^H(\Lambda)}.
$$

This proves the first inequality. The second inequality can be derived similarly.

One of the remarkable properties of the $\psi$–Riemann–Liouville fractional derivative is given in the following lemma.
Lemma 6. For all $0 < \delta < 1$, if $v \in H^{\delta,\psi}(\Lambda)$, $w \in C^\infty_0(\Lambda)$, then
\[
\left(D_t^{\delta,\psi}v(t), \ w(t)\right)_{L^2_\psi(\Lambda)} = \left(v(t), \ tD_t^{\delta,\psi}w(t)\right)_{L^2_\psi(\Lambda)}.
\] (16)

Proof. By using integration by parts, we have
\[
\left(D_t^{\delta,\psi}v(t), \ w(t)\right)_{L^2_\psi(\Lambda)} = \frac{1}{\Gamma(1-\delta)} \int_{\Lambda} \frac{1}{\psi'(s)} dt \int_{a_\psi}^t \psi'(s)(\psi(t) - \psi(s))^{-\delta} v(s) dw(t) \psi'(t) dt
\]
\[
= \frac{1}{\Gamma(1-\delta)} \left[ w(t) \int_{a_\psi}^t \psi'(s)(\psi(t) - \psi(s))^{-\delta} v(s) ds \right]_{\partial \Lambda} - \int_{\Lambda} \int_{a_\psi}^t \psi'(s)(\psi(t) - \psi(s))^{-\delta} v(s) ds dw(t)
\]
\[
= \frac{-1}{\Gamma(1-\delta)} \int_{\Lambda} \int_{a_\psi}^t \psi'(s)(\psi(t) - \psi(s))^{-\delta} v(s) ds dw(t) dt
\]
\[
= \frac{-1}{\Gamma(1-\delta)} \int_{\Lambda} \int_{a_\psi}^{b_\psi} [\psi(t) - \psi(s)]^{-\delta} w'(t) dw(t) dt
\]
 Furthermore, a direct calculation gives
\[
\frac{d}{ds} \int_{s}^{b_\psi} \psi'(t) [\psi(t) - \psi(s)]^{-\delta} w(t) dt = \frac{d}{ds} \left[ w(t) \left[ \psi(t) - \psi(s) \right]^{1-\delta} \right]_{s}^{b_\psi} - \frac{d}{ds} \left[ \frac{\left[ \psi(t) - \psi(s) \right]^{1-\delta}}{1-\delta} \right]_{s}^{b_\psi} dw(t)
\]
\[
= - \frac{d}{ds} \int_{s}^{b_\psi} \left[ \psi(t) - \psi(s) \right]^{1-\delta} dw(t)
\]
\[
= \psi'(s) \int_{s}^{b_\psi} \left[ \psi(t) - \psi(s) \right]^{-\delta} w'(t) dt.
\]
Thus,
\[
\left( v(s), sD^{\psi} w(s) \right)_{L_\psi^2(\Lambda)} = \frac{-1}{\Gamma(1-\delta)} \int_\Lambda \frac{1}{\psi'(s)} ds \int_s^{\psi(s)} \psi'(t) [\psi(t) - \psi(s)]^{-\delta} w(t)dtv(s)\psi'(s)ds
\]
\[
= \frac{-1}{\Gamma(1-\delta)} \int_\Lambda \psi'(s) \int_s^{\psi(s)} [\psi(t) - \psi(s)]^{-\delta} w'(t)dtv(s)\psi'(s)ds
\]
\[
= \frac{-1}{\Gamma(1-\delta)} \int_\Lambda \int_s^{\psi(s)} [\psi(t) - \psi(s)]^{-\delta} w'(t)dtv(s)\psi'(s)ds
\]
\[
= \left( D^{\psi}_t v(t), w(t) \right)_{L_\psi^2(\Lambda)}.
\]

This completes the proof.

Based on a similar idea introduced in [32], the $\psi$–fractional derivative can be generalized as a distribution to any $L_\psi^2(\Lambda)$ functions by using the integration by parts (16). That is, for $v \in L_\psi^2(\Lambda)$, the $\psi$–fractional derivative of $v$ in the distribution sense is defined as the linear functional through
\[
\left( D^{\psi}_t v(t), w(t) \right)_{L_\psi^2(\Lambda)} = \left( D^{\psi/2}_t v(t), tD^{\psi/2}_t w(t) \right)_{L_\psi^2(\Lambda)}, \quad \forall w \in C_0^\infty(\Lambda).
\]

With this convention, we are able to derive, by following the same lines as in [32], a key result which is crucial for the proof of well-posedness of the variational problem. That is, for all $0 < \delta < 1$, if $v, w \in H^{\psi/2}_\psi(\Lambda)$, then
\[
\left( D^{\psi}_t v(t), w(t) \right)_{L_\psi^2(\Lambda)} = \left( D^{\psi/2}_t v(t), tD^{\psi/2}_t w(t) \right)_{L_\psi^2(\Lambda)}.
\]

\textbf{Remark 1.} It is worth noting that the $\psi$–fractional variational framework established in this section is valid for quite general function $\psi(t)$. The only assumption on $\psi(t)$ is its increasing differentiability and $\psi'(t) \neq 0$. In what follows we will consider a special case $\psi(t) = t^{1/\gamma}$ to demonstrate how this variational framework can be used to capture some singular solutions of fractional differential equations.

3. A spectral method for fractional ordinary differential equations

As a simple application example, we consider in this section the following initial value problem
\[
\begin{cases}
C^D_s u(s) + \lambda u(s) = g(s), \quad \lambda > 0, \quad s \in I,
\end{cases}
\]
\[u(a) = \phi.\]

(19)
Here $0 < \delta < 1$, $CD_\delta^s$ denotes the classical left-sided Caputo fractional operator defined in [1]. This model problem frequently appears in the investigation of the TFDE [56, 57]:

$$CD_\delta^su(x, s) = \Delta u(x, s) + g(x, s), \quad x \in \Omega, \quad s \in I,$$

where $\Omega$ is a spatial domain. The solution of the TFDE can be expanded in the space direction by using the eigenfunctions of the Laplacian operator $-\Delta$, resulting in the equation (19) with $\lambda$ being an eigenvalue of $-\Delta$. It is seen that the model problem (19) reflects the main difficulty of solving the TFDE, i.e., singularity feature of the solution in the time direction.

Without loss of generality, we consider the homogeneous initial condition, i.e., $\phi \equiv 0$. The case of non-homogeneous initial condition can be handled by standard homogenization. With $\phi \equiv 0$, the problem (19) can be equivalently written as [58]

$$\begin{aligned}
 \left\{ 
 D_\delta^s u(s) + \lambda u(s) = g(s), \quad \lambda > 0, \quad s \in I, \\
 I_1^{1-\delta} u(a) = 0 
\right. 
\end{aligned}$$

(20)

where the operators $D_\delta^s$ and $I_1^{1-\delta}$ are defined in (D3) and (I1) with $\psi(s) = s$.

By the change of variable $s = \psi(t)$, and denoting $v(t) = u(\psi(t)), f(t) = g(\psi(t))$, the problem (20) can be transformed into the following problem

$$\begin{aligned}
 \left\{ 
 D_t^{\delta,\psi} v(t) + \lambda v(t) = f(t), \quad t \in \Lambda, \\
 I_1^{1-\delta,\psi} v(a_\psi) = 0 
\right. 
\end{aligned}$$

(21)

We propose and analyze below a spectral Galerkin method to solve the transformed problem (21) expressed in the weak form. We first introduce the GJPs (see [59, 60]). Define the shifted GJPs

$$j_n^{\alpha,-1}(t) := (1 + x(t))J_{n-1}^{\alpha,1}(x(t)), \quad \alpha > -1, \quad t \in \Lambda, \quad n = 1, 2, \ldots,$$

(22)

where $x(t) = \frac{2t-(a_\psi+b_\psi)}{b_\psi-a_\psi}, J_n^{\alpha,\beta}(x)$ are the classical $n$-th Jacobi polynomials, i.e., orthogonal polynomials with respect to the weight function $\omega^{\alpha,\beta}(x) := (1-x)^\alpha(1+x)^\beta, \alpha, \beta > -1, \quad n = 0, 1, \ldots$.

It can be checked that

$$\frac{d}{dt}j_n^{\alpha,-1}(t) = \frac{2n}{b_\psi - a_\psi}J_n^{\alpha+1,0}(x(t)), \quad t \in \Lambda.$$  

(23)

Let $P_N$ be the standard polynomial space defined by

$$P_N := \text{span}\{1, t, t^2, \ldots, t^N\}.$$

Set the shifted polynomials space

$$V_N := \text{span}\{v \in P_N | v(0) = 0\} = \text{span}\{j_n^{\alpha,-1}(t), \quad t \in \Lambda, \quad n = 1, \ldots, N\}.$$
Define the $L^2_{\omega, \alpha, -1}$-orthogonal projection $\pi_{\alpha, -1}^N: L^2_{\omega, \alpha, -1}(\Lambda) \to V_N$, such that for all $u \in L^2_{\omega, \alpha, -1}(\Lambda)$, $\pi_{\alpha, -1}^N u \in V_N$ satisfies
\[
\left( \pi_{\alpha, -1}^N u - u, w \right)_{L^2_{\omega, \alpha, -1}(\Lambda)} = 0, \quad \forall w \in V_N.
\]

Define the non-uniform Jacobi-weighted Sobolev spaces as follows:
\[
B^m_{\omega, \alpha, -1}(\Lambda) := \left\{ v : \partial^k_t v \in L^2_{\omega, \alpha, -1+k}+m(\Lambda), 0 \leq k \leq m \right\}.
\]

An approximation result of this projection operator is given in the following lemma.

**Lemma 7.** For any $u \in B^m_{\omega, \alpha, -1}(\Lambda)$, $m \in \mathbb{N}$, $m \geq 1$, and $0 \leq \mu \leq m$, we have
\[
\left\| \pi_{\alpha, -1}^N u - u \right\|_{B^\mu_{\omega, \alpha, -1}} \lesssim N^{\mu-m} \left\| \partial^\mu_t u \right\|_{L^2_{\omega, \alpha, -1+m}(\Lambda)}.
\]  

**Proof.** This approximation result can be proved in the same way as for the projector $\pi_{N}^{1, \beta}$ given in [59]. We omit the details in order to limit the length of the paper.

The spectral approximation we propose for (21) reads: Find $v_N \in V_N$ such that
\[
\mathcal{A}(v_N, w_N) = F(w_N), \quad \forall w_N \in V_N,
\]  
where
\[
\mathcal{A}(v_N, w_N) = \left( D^\delta_{t, \psi^2} v_N, w_N \right)_{L^2_{\psi}(\Lambda)} + \lambda (v_N, w_N)_{L^2_{\psi}(\Lambda)},
\]
\[
F(w_N) = (f, w_N)_{L^2_{\psi}(\Lambda)},
\]
with $(\cdot, \cdot)_{L^2_{\psi}(\Lambda)}$ being defined in (6).

### 3.1. Well-posedness

**Theorem 1.** For any $f$ satisfying $I_{t, \psi^2}^\delta f \in L^2_{\psi^2}(\Lambda)$, $0 < \delta < 1$, the spectral approximation problem (25) is well-posed. Moreover, if $v_N$ is the solution of (25), then it holds
\[
\left\| v_N \right\|_{H^{\delta/2, \psi^2}(\Lambda)} \lesssim \left\| I_{t, \psi^2}^\delta f \right\|_{L^2_{\psi^2}(\Lambda)}.
\]  

**Proof.** The proof makes use the classical Lax-Milgram Theorem, which consists in verifying the coercivity and continuity of the bilinear form $\mathcal{A}(\cdot, \cdot)$.

Combining (18) with the definition of $\left\| \cdot \right\|_{H^{\delta/2, \psi^2}(\Lambda)}$ gives: for all $v_N \in V_N$,
\[
\mathcal{A}(v_N, v_N) = \left( D^\delta_{t, \psi^2} v_N, v_N \right)_{L^2_{\psi^2}(\Lambda)} + \lambda (v_N, v_N)_{L^2_{\psi^2}(\Lambda)}
\]
\[
= \left( D^\delta_{t, \psi^2} v_N, D^\delta_{t, \psi^2} v_N \right)_{L^2_{\psi^2}(\Lambda)} + \lambda (v_N, v_N)_{L^2_{\psi^2}(\Lambda)}
\]
\[
\gtrsim \left\| v_N \right\|^2_{H^{\delta/2, \psi^2}(\Lambda)}.
\]  

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Furthermore, the norm equivalence proved in Lemma 3 yields
\[ A(v_N, v_N) \gtrsim |v_N|^2_{H^{\delta/2, \psi}(\Lambda)}. \]

Then it follows from the fractional Poincaré-Friedrichs inequality in Lemma 5
\[ A(v_N, v_N) \gtrsim \|v_N\|^2_{H^{\delta/2, \psi}(\Lambda)}. \]

By applying (18) again, and using Cauchy-Schwarz inequality, we obtain for all \( v_N, w_N \in V_N \),
\[ |A(v_N, w_N)| \leq \left( D_t^{\delta/2} v_N, t D_t^{\delta/2} w_N \right)_{L^2(\Lambda)} + \lambda \left( v_N, w_N \right)_{L^2(\Lambda)} \]
\[ \leq |v_N|_{H^{\delta/2, \psi}(\Lambda)} |w_N|_{H^{\delta/2, \psi}(\Lambda)} + \lambda \|v_N\|_{L^2(\Lambda)} \|w_N\|_{L^2(\Lambda)}. \]

Finally, we derive from the norm equivalence and Lemma 5
\[ |A(v_N, w_N)| \lesssim |v_N|_{H^{\delta/2, \psi}(\Lambda)} |w_N|_{H^{\delta/2, \psi}(\Lambda)} \]
\[ \lesssim \|v_N\|_{H^{\delta/2, \psi}(\Lambda)} \|w_N\|_{H^{\delta/2, \psi}(\Lambda)}. \]

The well-posedness of (25) is thus proved.

3.2. Error estimate

In this subsection we present an error estimate for a specific transformation function, i.e., \( \psi(t) = t^{1/\gamma} \). Although this is the only case for which we derive the error estimate here, we are going to see that this specific transformation can well smooth the time fractional diffusion equation, therefore is a good fit for use of the spectral method.

Before carrying out the error analysis, we recall the following definition and lemma from [61]. Define the integral operator \( (P_\delta)v(t) = \int_{-\infty}^t P_\delta(t, z)v(z)dz \), where \( P_\delta(t, z) \geq 0 \).
is not increasing in $t$ and not decreasing in $z$ in $\{(t,z) \in \mathbb{R}^2 : z < t\}$. For two nonnegative functions $\omega_1$ and $\omega_2$, we set

$$A_{\delta,p,q}(t) = \left( \int_t^{\infty} \left[ P_\delta(y,t)^{1/2} \omega_1(y) \right]^q dy \right)^{1/q} \left( \int_{-\infty}^t \left[ P_\delta(t,y)^{-1/2} \omega_2(y) \right]^{-p'} dy \right)^{1/p'}.$$  

(27)

**Lemma 9.** Let $\omega_1 \geq 0$, $\omega_2 \geq 0$, $1/p + 1/p' = 1$. If there exists a constant $C$ such that $A_{\delta,p,q}(t) \leq C, \forall t \in \mathbb{R}$. Then

$$\left( \int_{-\infty}^\infty |\omega_1(t)(P_\delta v(t))|^q dt \right)^{1/q} \leq A_1 C \left( \int_{-\infty}^\infty |\omega_2(t)v(t)|^p dt \right)^{1/p},$$

where $A_1 = ((p' + q)/q)^{1/p'}((p' + q)/p')^{1/q}$ if $1 < p \leq q < \infty$, and $A_1 = 1$ otherwise.

Next we prove two lemmas which are useful for the error estimation.

**Lemma 8.** Let $\omega_1(t) \geq 0$, $\omega_2(t) \geq 0$, $1/p + 1/p' = 1$. If there exists a constant $C$ such that $A_{\delta,p,q}(t) \leq C, \forall t \in \mathbb{R}$. Then

$$\left( \int_{-\infty}^\infty |\omega_1(t)(P_\delta v(t))|^q dt \right)^{1/q} \leq A_1 C \left( \int_{-\infty}^\infty |\omega_2(t)v(t)|^p dt \right)^{1/p},$$

where $A_1 = ((p' + q)/q)^{1/p'}((p' + q)/p')^{1/q}$ if $1 < p \leq q < \infty$, and $A_1 = 1$ otherwise.

For any differentiable function $v(t)$ defined in $\Lambda_1$, it holds

$$\int_{\Lambda_1} |\omega_1(t)(P_\delta v(t))|^2 dt \leq \int_{\Lambda_1} |\omega_2(t)v'(t)|^2 dt.$$

**Proof.** First, it is easy to check that $P_\delta(t,z) \geq 0$ is not increasing in $t$ and not decreasing in $z$. We extend $v(t)$ with zero outside of $\Lambda_1$. Taking $p = q = 2$ in (27) gives

$$A_{\delta,2,2}(t)$$

$$= \left( \int_t^1 \left[ (P_\delta(y,t))^{1/2} \omega_1(y) \right]^2 dy \right)^{1/2} \left( \int_0^t \left[ (P_\delta(t,y))^{-1/2} \omega_2(y) \right]^{-2} dy \right)^{1/2}$$

$$= \left( \int_t^1 (y^{1/\gamma} - t^{1/\gamma})^{-\delta}(1 - y)^{\alpha/2} y^{2/\gamma - 1} dy \right)^{1/2} \left( \int_0^t (t^{1/\gamma} - y^{1/\gamma})^{-\delta}(1 - y)^{\alpha/2} y^{-1} dy \right)^{1/2}.$$  

A direct calculation shows

$$\int_t^1 (y^{1/\gamma} - t^{1/\gamma})^{-\delta}(1 - y)^{\alpha/2} y^{2/\gamma - 1} dy \leq \int_t^1 (y^{1/\gamma} - t^{1/\gamma})^{-\delta} y^{2/\gamma - 1} dy$$

$$= \gamma \int_t^1 (y - t)^{-\delta} dy$$

$$\leq \frac{\gamma}{1 - \delta}.$$
Notice $1 - y^\gamma \geq \gamma (1 - y)$ for $\gamma \in (0, 1], y \in (0, 1)$, we have

$$\int_0^t \left( t^{1/\gamma} - y^{1/\gamma} \right)^{-\delta} (1 - y)^{\alpha - 1} dy \leq \gamma \int_0^t (t - y)^{-\delta} (1 - y^{\gamma})^{\alpha - 1} y^\gamma dy \leq \gamma^\alpha \int_0^t (t - y)^{-\delta} (1 - y)^{\alpha - 1} y^\gamma dy \leq \gamma^\alpha B(\alpha - \delta, \gamma)t^{\alpha - \delta + \gamma - 1}.$$ Combining the above estimates yields

$$A_{\delta, 2}(t) \leq C < \infty.$$ Then we conclude by using Lemma 8.

Lemma 10. Assume $v \in H^{1/\gamma, \psi}(\Lambda_1) \cap B^{m}_{\omega - \alpha - 1}(\Lambda_1)$, where $0 < \delta < 1$, $\psi(t) = t^{1/\gamma}$, $m \geq 1$, $\delta < \alpha < 1$. Then we have

(i) $\|v\|_{L^2_\psi(\Lambda_1)} \lesssim \|v\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)}$,

(ii) $\left( CD^\psi_t v, v \right)_{L^2_\psi(\Lambda_1)} \lesssim \|v''\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)} \|v\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)}$.

Proof. (i) Noticing $t^{1/\gamma - 1} \leq (1 - t)^{\alpha t^{-1}}$, $\forall t \in \Lambda_1$, we have

$$\|v\|_{L^2_\psi(\Lambda_1)}^2 = 1/\gamma \int_{\Lambda_1} v^2 t^{1/\gamma - 1} dt \leq \int_{\Lambda_1} v^2 (1 - t)^{-\alpha t^{-1}} dt = \|v\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)}. $$

(ii) By a direct computation, we get

$$\left( CD^\psi_t v, v \right)_{L^2_\psi(\Lambda_1)} = \frac{1}{\Gamma(1 - \delta)} \int_{\Lambda_1} \int_0^t \left( t^{1/\gamma} - z^{1/\gamma} \right)^{-\delta} v'(z) d\omega_1(t) v(t)(1 - t)^{-\alpha/2 t^{-1/2}} dt \leq \frac{1}{\gamma} \left[ \int_{\Lambda_1} \omega_1(t) (P_\delta v')(t) (1 - t)^{-\alpha/2 t^{-1/2}} dt \right]^{1/2} \|v\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)} \lesssim \left( \int_{\Lambda_1} \omega_2(t) v'(t) \right) \|v\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)} = \|v''\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)} \|v\|_{L^2_{\omega - \alpha - 1}(\Lambda_1)}.$$

Here, the Cauchy–Schwarz inequality and Lemma 8 have been used.
Finally, the desired estimate follows from combining (29), (30), and Lemma 7.

Using Lemma 10 gives

$$S_n$$ is find efficient way to form the stiffness matrix $S$.

Then, it follows from the definition of the norm fractional norms, and the relationship (4):

$$\|v - v_N\|_{H^{\delta/2},\psi}(\Lambda) \lesssim N^{1/2-m} \|\partial^m_t v\|_{L^2_{\omega-\alpha+m,-1+m}(\Lambda)} + N^{-m} \|\partial^m_t v\|_{L^2_{\omega-\alpha+m,-1+m}(\Lambda)}.$$

Proof. It follows from (21), (25), and Céa lemma that

$$\|v - v_N\|_{H^{\delta/2},\psi}(\Lambda) \leq \inf_{w_N \in \mathbb{V}} \|v - w_N\|_{H^{\delta/2},\psi}(\Lambda) \leq \|v - \pi_N^{-\alpha,-1}v\|_{H^{\delta/2},\psi}(\Lambda).$$

Furthermore it is not difficult to derive

$$\|v - \pi_N^{-\alpha,-1}v\|_{H^{\delta/2},\psi}(\Lambda) \lesssim \|v - \pi_N^{-\alpha,-1}v\|_{H^{\delta/2},\psi}(\Lambda_1).$$

Then, it follows from the definition of the norm $\| \cdot \|_{H^{\delta/2},\psi}(\Lambda)$, the equivalence of $\psi-$ fractional norms, and the relationship [4]:

\[
\|v - \pi_N^{-\alpha,-1}v\|_{H^{\delta/2},\psi}(\Lambda)
\leq \left( D_t^{\psi} (v - \pi_N^{-\alpha,-1}v), v - \pi_N^{-\alpha,-1}v \right)_{L^2_{\psi}(\Lambda_1)}^{1/2} + \|v - \pi_N^{-\alpha,-1}v\|_{L^2_{\psi}(\Lambda_1)}^{1/2}.
\]

Using Lemma 10 gives

\[
\|v - \pi_N^{-\alpha,-1}v\|_{H^{\delta/2},\psi}(\Lambda_1)
\lesssim \left\| (v - \pi_N^{-\alpha,-1}v) \right\|_{L^2_{-\alpha,0}(\Lambda_1)}^{1/2} \|v - \pi_N^{-\alpha,-1}v\|_{L^2_{-\alpha,-1}(\Lambda_1)}^{1/2} + \|v - \pi_N^{-\alpha,-1}v\|_{L^2_{-\alpha,-1}(\Lambda_1)}^{1/2}.
\]

Finally, the desired estimate follows from combining (29), (30), and Lemma 7.

3.3. Implementation

We discuss the implementation issue of the spectral approximation [25]. The key is find efficient way to form the stiffness matrix $S$, those entries are

$$S_{mn} := \left( D_t^{\psi} j_n^{-\alpha,-1}(t), j_m^{-\alpha,-1}(t) \right)_{L^2_{\psi}(\Lambda)} = \left( C D_t^{\psi} j_n^{-\alpha,-1}(t), j_m^{-\alpha,-1}(t) \right)_{L^2_{\psi}(\Lambda)}.$$
for \( m, n = 1, 2, \ldots, N \). We compute the entries \( S_{mn} \) by using (22) and (23) as follows:

\[
\begin{align*}
\left( C D_t^\sigma, J_n^{\alpha-1}(t), J_m^{\alpha-1}(t) \right)_{L^2_\psi(\Lambda)} \\
= \left( \frac{1}{\Gamma(1-\delta)} \frac{d}{dz} J_n^{\alpha-1}(z), J_m^{\alpha-1}(s) \right)_{L^2_\psi(\Lambda)} \\
= \frac{4nT^{1-\delta}}{\gamma \Gamma(1-\delta)} \int_0^1 \int_0^1 (1-\tau)^{-\delta} \frac{\Gamma(1-\frac{r}{\gamma})}{\Gamma(1-\frac{\tau}{\gamma})} J_n^{\alpha+1,0}(2\tau s - 1) d\tau \cdot s^{(1-\delta)/\gamma+1} J_m^{\alpha+1}(2s - 1) ds \\
= \frac{4nT^{1-\delta}}{\gamma \Gamma(1-\delta)} \sum_{i=0}^N \sum_{j=0}^N \left( 1 - \eta_j^{\delta} \right)^{-\delta} J_n^{\alpha+1,0}(2\eta_i \eta_j - 1) \tilde{\omega}_j J_m^{\alpha+1}(2\eta_i - 1) \omega_i,
\end{align*}
\]

where the Gauss quadrature point sets \( \{\eta_i\}_{i=0}^N \) and \( \{\tilde{\eta}_j\}_{j=0}^N \) are zeros of the shifted Jacobi polynomials \( J_N^{\alpha+1}(x(t)), J_N^{\alpha+1,0}(x(t)) \), respectively, and \( \{\omega_i\}_{i=0}^N, \{\tilde{\omega}_j\}_{j=0}^N \) are the associated weights. Note that in our calculation, \( \gamma \) is set to be \( 1/r \), with \( r \) being the positive integers so that \( \frac{1-\tau^{1/\gamma}}{1-\tau} = \sum_{k=0}^{r-1} \tau^k \), which hasn’t singularity. The singular parts \((1-\tau)^{-\delta}\) and \(s^{(1-\delta)/\gamma+1}\) do not appear in the numerical quadrature since they are treated as the associated weights of the Jacobi polynomials. Denote

\[
f_m = (f, J_n^{\alpha-1}(x)), \quad \mathbf{f} = (f_1, \ldots, f_N)^T; \\
v_N = \sum_{n=1}^N \tilde{v}_n J_n^{\alpha-1}(x), \quad \mathbf{v} = (\tilde{v}_1, \ldots, \tilde{v}_N)^T; \\
\mathbf{M} = (M_{mn})_{1 \leq m, n \leq N} \text{ with } M_{mn} = (J_n^{\alpha-1}(t), J_m^{\alpha-1}(t))_{L^2_\psi(\Lambda)}.\]

Then the matrix form of the problem (25) reads:

\[
(S + \lambda \mathbf{M})\mathbf{v} = \mathbf{f}.
\]

**Remark 2.** In [44], the authors proposed a Müntz spectral method based on the Müntz polynomial space \( \text{span}\{1, t^\gamma, t^{2\gamma}, \ldots, t^{N\gamma}\} \) for the fractional differential equation. It can be verified that, with the particular choice of the transformation \( \psi(t) = t^{1/\gamma} \), the current method is equivalent to the one in [44] in the sense that the solution \( u_N(s) \) computed from the Müntz spectral method is linked to the solution \( v_N(t) \) of the \( \psi \)-spectral method through \( v_N(t) = u_N(\psi(t)) \). However, it is worth to note that the numerical analysis of the two methods was conducted using two quite different frameworks. The new approach in the current work not only provides an alternative tool for numerical analysis of the Müntz spectral methods proposed in [43, 44], but also provide a guideline for the selection of parameter \( \gamma \). The main goal is to choose a suitable transformation function \( \psi \) such that \( v(\cdot) = u(\psi(\cdot)) \) is as smooth as possible.
4. Application to the time fractional subdiffusion equations

Let $\Omega := (-1,1)^d$, $d = 1, 2, 3$. Consider the following time fractional diffusion equation:

$$CD^s_x u(x,s) = \Delta u(x,s) - u(x,s) + g(x,s), \ x \in \Omega, \ s \in I$$

subject to the initial and boundary conditions

$$u(x,0) = 0, \ x \in \Omega,$$

$$u(x,s) = 0, \ x \in \partial \Omega, \ s \in I.$$

We obtain the following transformed equation by applying the transformation $s = \psi(t)$ in the time direction:

$$D^\delta,\psi_t v(x,t) = \Delta v(x,t) - v(x,t) + f(x,t), \ x \in \Omega, \ t \in \Lambda.$$

For the Sobolev space $X$ with norm $\| \cdot \|_X$, let

$$H^\delta,\psi(\Lambda, X) := \{ v; \|v(\cdot, t)\|_X \in H^\delta,\psi(\Lambda) \}, \ \delta \geq 0$$

endowed with the norm

$$\|v\|_{H^\delta,\psi(\Lambda, X)} := \|\|v(\cdot, t)\|_X\|_{\delta,\Lambda}.$$

Let $O = \Lambda \times \Omega$,

$$H^\delta,\psi(O) := \mathcal{H}^\delta,\psi(\Lambda, L^2(\Omega)) \cap L^2_\delta(\Lambda, H^1_0(\Omega)),$$

$$B^{m,\alpha,\beta}_\omega(O) := B^{m,\alpha,\beta}_\omega(\Lambda, L^2(\Omega)) \cap L^2_\omega(\Lambda, H^1_0(\Omega)),$$

equipped respectively with the norms

$$\|v\|_{\mathcal{H}^\delta,\psi(O)} := \left( \|v\|^2_{H^\delta,\psi(\Lambda, L^2(\Omega))} + \|v\|^2_{L^2_\delta(\Lambda, H^1_0(\Omega))} \right)^{1/2},$$

$$\|v\|_{B^{m,\alpha,\beta}_\omega(O)} := \left( \|v\|^2_{B^{m,\alpha,\beta}_\omega(\Lambda, L^2(\Omega))} + \|v\|^2_{L^2_\omega(\Lambda, H^1_0(\Omega))} \right)^{1/2}.$$

Consider the following variational formulation of (35):

$$A(v, w) = F(w), \ \forall w \in \mathcal{H}^{\delta/2,\psi}(O),$$

where

$$A(v, w) := (D^\delta,\psi_t v, w)_\partial + (\nabla v, \nabla w)_\partial + (v, w)_\partial, \ F(w) := (f, w)_\partial.$$
with \((v, w)_O := \int_{\Lambda} \int_{\Omega} vw\psi'(t) dx dt\).

Similar to Theorem 1 we can establish the coercivity and continuity of the bilinear form \(A(v, w)\) in the space \(\mathcal{H}^{\delta/2, \psi}(\Omega) \times \mathcal{H}^{\delta/2, \psi}(\Omega)\), and therefore the well-posedness of the weak problem (36) for any \(f \in \mathcal{H}^{\delta/2, \psi}(\Omega)'\) (the dual space of \(\mathcal{H}^{\delta/2, \psi}(\Omega)\)), together with the stability estimate

\[
\|v\|_{\mathcal{H}^{\delta/2, \psi}(\Omega)} \lesssim \|f\|_{\mathcal{H}^{\delta/2, \psi}(\Omega)'}.
\]

We now propose a space-time Galerkin spectral method to discretize (36). For the time variable, we follow the approach of the previous section. For the space variable, we use standard Legendre polynomials. Let

\[
\phi_k(x) = c_k (L_k(x) - L_{k+2}(x)), \quad c_k = \frac{1}{\sqrt{4k + 6}},
\]

\[
a_{jk} = (\partial_x \phi_k(x), \partial_x \phi_j(x)), \quad b_{jk} = (\phi_k(x), \phi_j(x)),
\]

where \(L_n(x)\) is the \(n\)-th degree Legendre polynomial. Then

\[
a_{jk} = \begin{cases} 1, & k = j \\ 0, & k \neq j \end{cases}, \quad b_{jk} = b_{kj} = \begin{cases} c_k c_j (\frac{2}{2j+1} + \frac{2}{2j+3}), & k = j \\ -c_k c_j \frac{2}{2k+1}, & k = j + 2, \\ 0, & \text{otherwise} \end{cases}
\]

Set the polynomial space

\[
\mathcal{P}_M = \text{span}\{\phi_0(x), \phi_1(x), \ldots, \phi_{M-2}(x)\}.
\]

The space-time Galerkin spectral method for (36) is to seek \(v_L(x, t) \in \mathcal{P}_M \otimes V_N\) such that

\[
A(v_L, w) = F(w), \quad \forall w \in \mathcal{P}_M \otimes V_N.
\]

The error estimate is given in the following theorem without proof.

**Theorem 3.** Let \(v\) be the solution of problem (36), \(v_L\) is the solution of problem (39). Suppose \(v \in \mathcal{H}^{\delta/2, \psi}(\Omega) \cap B_{\alpha-1}^{m} (\Lambda, H^\sigma(\Omega))\), where \(0 < \delta < 1, \psi(t) = t^{1/\gamma}, m \geq 1, \\delta < \alpha < 1\). Then the following error estimate holds:

\[
\|v - v_N\|_{\mathcal{H}^{\delta/2, \psi}(\Omega)} \lesssim N^{1/2-m} \|\partial_t^m v\|_{L^2_{\omega-\alpha+m-1+m} (\Lambda, L^2(\Omega))} \\
+ N^{1/2-m} M^{-\sigma} \|\partial_t^m v\|_{L^2_{\omega-\alpha+m-1+m} (\Lambda, H^\sigma(\Omega))} \\
+ M^{-\sigma} \left( \|D_{\omega}^{\delta/2, \psi} v\|_{L^2_{\omega-\alpha-1} (\Lambda, H^\sigma(\Omega))} + \|v\|_{L^2_{\omega-\alpha-1} (\Lambda, H^\sigma(\Omega))} \right) \\
+ M^{1-\sigma} \|v\|_{L^2_{\omega-\alpha-1} (\Lambda, H^\sigma(\Omega))} + N^{-m} \|\partial_t^m v\|_{L^2_{\omega-\alpha+m-1+m} (\Lambda, H^\sigma_0(\Omega))}.
\]

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In the implementation, we express the solution $v_L$ of Eq. (39) using the modal basis as follows:

$$v_L(x,t) = \sum_{m=0}^{M-2} \sum_{n=1}^{N} \hat{v}_{nm} \phi_m(x) j_n^{\alpha-1}(t).$$

Substituting this expression into (39), and taking $w = \phi_p(x) j_q^{\alpha-1}(t)$, we obtain

$$\sum_{m=0}^{M-2} \sum_{n=1}^{N} \hat{v}_{nm} \left\{ (\phi_m, \phi_p)_{L^2(\Omega)} \left( D_t^{\psi} j_{n}^{\alpha-1}, j_q^{\alpha-1} \right)_{L^2(\Lambda)} + (\phi'_m, \phi'_p)_{L^2(\Omega)} \left( j_{n}^{\alpha-1}, j_q^{\alpha-1} \right)_{L^2(\Lambda)} \right\} = (f, \phi_p j_q^{\alpha-1})_\Omega.$$

Denote

\begin{align*}
B &= (b_{jk})_{0 \leq j,k \leq M-2}, \\
f_{nm} &= (f, \phi_m(x) j_n^{\alpha-1}(t))_\Omega, \quad F = (f_{nm})_{1 \leq n \leq N, 0 \leq m \leq M-2}, \\
S &= (S_{nq})_{1 \leq n,q \leq N}, \quad M = (M_{nq})_{1 \leq n,q \leq N}, \quad V = (\hat{v}_{nm})_{1 \leq n \leq N, 0 \leq m \leq M-2}.
\end{align*}

Using the above notations, (39) can be written under the following matrix form:

$$SVB + MV + MVB = F.$$ 

5. Numerical examples

In this section, we present some numerical examples to illustrate the high accuracy of the proposed method based on GJPs in solving problem (19) with smooth and nonsmooth solutions. In particular, we test the accuracy of the proposed method when the exact solution is unknown. The space-time spectral method based on GJPs and Legendre polynomials presented in Sect. 4 will also be tested for the two-dimensional time fractional subdiffusion equation. The time interval is set to $[a_\psi, b_\psi] := [0, 2^\gamma]$. Note that $\psi(t) = t^{1/\gamma}$ ($0 < \gamma \leq 1$) in the following examples.

Example 1. (Smooth solution) In this test, we choose the fabricated exact solution $u(s) = s^2$. Naturally, in this case, we take $\gamma = 1$.

The main purpose of this example is to check the high accuracy of the proposed Galerkin spectral scheme (25) for smooth solutions. The computed results are presented in Table 1, from which we observe that the numerical solutions for some different $\delta$ reach the machine accuracy with small polynomial degree $N$.

Example 2. (Nonsmooth solution) Consider problem (19) with the fabricated exact solution $u(s) = s^\sigma$ for two values of $\sigma : 3/5, \sqrt{2}/2$. 

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Table 1: (Example 1) $L^\infty$- and $L^2$-errors versus $N$ and different $\delta$.

| $\delta$ | $N$ | $\|v - v_N\|_{L^\infty}$ | $\|v - v_N\|_0$ | $\|v - v_N\|_{L^\infty}$ | $\|v - v_N\|_0$ | $\|v - v_N\|_{L^\infty}$ | $\|v - v_N\|_0$ |
|----------|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.1      | 2   | 3.3307e-16      | 4.0030e-16      | 1.1102e-16      | 1.3878e-16      | 1.4433e-15      | 1.4647e-15      |
|          | 4   | 1.3323e-15      | 1.4767e-15      | 1.5543e-15      | 1.6812e-15      | 1.1990e-14      | 1.4989e-14      |
| 0.5      | 2   | 3.3307e-16      | 4.0030e-16      | 1.1102e-16      | 1.3878e-16      | 1.4433e-15      | 1.4647e-15      |
|          | 4   | 1.3323e-15      | 1.4767e-15      | 1.5543e-15      | 1.6812e-15      | 1.1990e-14      | 1.4989e-14      |
| 0.9      | 2   | 3.3307e-16      | 4.0030e-16      | 1.1102e-16      | 1.3878e-16      | 1.4433e-15      | 1.4647e-15      |
|          | 4   | 1.3323e-15      | 1.4767e-15      | 1.5543e-15      | 1.6812e-15      | 1.1990e-14      | 1.4989e-14      |

We want to use this example to test the accuracy of the spectral method for non-smooth solutions. For the fractional $\sigma = 3/5$, we take $\gamma = 1/5$ or $1/8$. The numerical errors versus the polynomial degree $N_t$ for several $\delta$ is plotted in Figure 1. It is observed from this figure that the errors decay exponentially as the polynomial degree increases. For the irrational number $\sigma = \sqrt{2}/2$, we take $\gamma = 1/7$. The obtained result is given in Figure 2, from which we also observe the spectral convergence.

**Example 3.** *(Unknown solution)* Consider problem (19) with a given source function $f(s) = \sin(s)$. In this case the exact solution and its singularity structure are unknown.

Since the exact solution is unknown, a numerical solution computed with very fine
resolution is served as the reference solution. The solution qualities are compared for different $\delta$ by two approaches, i.e., our method and usual spectral method, by plotting the errors versus the polynomial degrees in Figure 3. We see that more accurate solutions are obtained by using $\gamma = 1/5$ or $1/6$, compared to the classical spectral method, i.e., $\gamma = 1$.

Figure 3: (Example 3) $L^\infty$- and $L^2$-errors in log scale versus the polynomial degree $N_t$ for different $\delta$ and $\gamma$.

Example 4. (2D time fractional subdiffusion equation) Consider the 2D subdiffusion equation (32)-(34) with the fabricated exact solution

$$u(x, y, s) = \sin(\pi x)\sin(\pi y)s^{3/5}.$$  

In Figure 4 we depict the exact solution, numerical solution and error at the final time computed with the polynomial degree 20 in both directions. As shown in this figure, a very accurate solution is obtained with pointwise error reaching as small as
The error history as a function of the polynomial degrees $M$ or $N$, shown in Figure 5, confirms the spectral convergence of the used method.

Figure 4: (Example 4) The exact solution $v$, numerical solution $v_L$, and error $v_L - v$ at $T = 2$ with $\gamma = 1/5$.

Figure 5: (Example 4) $L^\infty$- and $L^2$-errors in semi-log scale versus $M$ or $N$ with $\delta = 0.5$, $\gamma = 1/5$.

Remark 3. For the selection of parameter $\gamma$, our fundamental principle is to make $v(\cdot) = u((\cdot)^{1/\gamma})$ sufficiently smooth which can be made according to the following strategy:

Case I: if the solution $u$ is smooth, the optimal value is $\gamma = 1$;

Case II: if the source term $g(\cdot)$ is smooth, then (a) when $\delta$ is a rational number $p/q$, the best choice is $\gamma = 1/q$. Theoretically $\gamma = 1/nq$ ($n = 1, 2, \cdots$) works too, but larger $n$ leads to larger amount of calculation; (b) when $\delta$ is an irrational number, there is no
suitable value of $\gamma$ to make $u((\cdot)^{1/\gamma})$ smooth. In this case, we can take $\gamma = 1/q$ with a reasonably large $q$ such that $u((\cdot)^{1/\gamma})$ is smooth enough.

6. Concluding remarks

A novel spectral method has been proposed and analyzed for the subdiffusion equation. The main novelty of the proposed method is its variational framework based on fractional Sobolev spaces. The idea was to first apply suitable variable transformation to re-scale the underlying equation, then construct spectral methods for the re-scaled equation. This is particularly useful in numerical solutions of fractional differential equations, to which the solution is often singular and can be smoothed by using appropriate transformation. For this purpose, a new variational framework was established based on the fractional Sobolev spaces, which allows constructing and analyzing numerical methods following the standard Galerkin approach. Our theoretical and numerical investigation showed that the proposed method using suitable transformation is exponentially convergent for general right hand side functions, even though the exact solution has limited regularity. Implementation details was also provided, along with a series of numerical examples to demonstrate the efficiency of the proposed method.

It is worthy to mention here a number of points: First, with some specific choices of the transformation function, the new method can be proved to be equivalent to the Müntz spectral method, recently proposed in a series of papers [43, 44]. The latter was based on the Müntz polynomial approximation to the original equation; Secondly, although the error analysis was carried out only for a particular transformation, it seems extendable to some other choices; Finally, compared to the Müntz spectral method, the main benefit of the current method may be its flexibility in choosing the transformation function. This makes the new method applicable to a larger class of problems.

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