OPTIMAL FRACTIONAL INTEGRATION PRECONDITIONING AND ERROR ANALYSIS OF FRACTIONAL COLLOCATION METHOD USING NODAL GENERALIZED JACOBI FUNCTIONS*

CAN HUANG†, YUJIAN JIAO‡, LI-LIAN WANG§, AND ZHIMIN ZHANG¶

Abstract. In this paper, a nonpolynomial-based spectral collocation method and its well-conditioned variant are proposed and analyzed. First, we develop fractional differentiation matrices of nodal Jacobi polyfractonomials [M. Zayernouri and G. E. Karniadakis, *J. Comput. Phys.*, 252 (2013), pp. 495–517] and generalized Jacobi functions [S. Chen, J. Shen, and L. L. Wang, *Math. Comp.*, 85 (2016), pp. 1603–1638] on Jacobi–Gauss–Lobatto (JGL) points. We show that it suffices to compute the matrix of order $\mu \in (0,1)$ to compute that of any order $k+\mu$ with integer $k \geq 0$. With a different definition of the nodal basis, our approach also fixes a deficiency of the polyfractonomial fractional collocation method in [M. Zayernouri and G. E. Karniadakis, *SIAM J. Sci. Comput.*, 38 (2014), pp. A40–A62]. Second, we provide explicit and compact formulas for computing the inverse of direct fractional differential collocation matrices at "interior" points by virtue of fractional JGL Birkhoff interpolation. This leads to optimal integration preconditioners for direct fractional collocation schemes and results in well-conditioned collocation systems. Finally, we present a detailed analysis of the singular behavior of solutions to rather general fractional differential equations (FDEs). Based upon the result, we have the privilege to adjust an index in our nonpolynomial approximation. Furthermore, by using the result, a rigorous convergence analysis is conducted by transforming an FDE into a Volterra (or mixed Volterra–Fredholm) integral equation.

Key words. fractional differential equations, Riemann–Liouville fractional derivative, fractional Birkhoff interpolation, fractional integration preconditioners, well-conditioned collocation methods

AMS subject classifications. 65N35, 65E05, 65M70, 41A05, 41A10, 41A25

DOI. 10.1137/16M1059278

1. Introduction. With the advances in experimental technologies, more and more particle diffusions are found to be anomalous, which indicates the second moment of the random walk $x(t)$ related to the particle $\langle x(t) \rangle \sim t^\alpha, \alpha \neq 1$, as opposed to a standard diffusion with $\alpha = 1$. This naturally leads to fractional differential equations (FDEs) concerning the probability density of the stochastic process $x(t)$ [32]. Moreover, fractional derivatives, which are global in nature, become desir-

†School of Mathematical Sciences and Fujian Provincial Key Laboratory on Mathematical Modeling & High Performance Scientific Computing, Xiamen University, Fujian 361005, China (canhuang@xmu.edu.cn).

‡Department of Mathematics, Shanghai Normal University, Shanghai 200234, China, and Scientific Computing Key Laboratory of Shanghai Universities, Shanghai 200240, China (yi-jiao@shnu.edu.cn).

§Division of Mathematical Sciences, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371 (lilian@ntu.edu.sg).

¶Beijing Computational Sciences and Research Center, Beijing 100193, China, and Department of Mathematics, Wayne State University, Detroit, MI 48202 (zzhang@math.wayne.edu).

able to describe scenarios involving long-range temporal cumulative memory effects and/or long-range spatial interactions. Thence, FDEs have been widely used in modeling nonexponential relaxation patterns and viscoelastic materials, among others [12, 13, 34].

An abundance of numerical methods has been proposed for solving FDEs, mostly the finite difference method (see, e.g., [31, 28, 36, 30, 15, 16, 38, 24, 23] and the references therein). There has been growing recent interest in developing the finite element method (cf. [21, 40, 41]) and the spectral method (cf. [8, 20, 27, 39, 44, 45]). In particular, most of works related to the latter approach were polynomial-based (cf. [8, 27, 20, 39]), which led to spectrally accurate approximation if the underlying solution is sufficiently smooth (but in turn the external source term is usually singular). However, it is known that the solution of an FDE is singular even for well-behaved inputs, so it has a limited regularity in a usual Sobolev space. As a result, the polynomial approximation enjoys a very limited order of convergence. Zayernouri and Karniadakis [43] first proposed to approximate such singular solutions by Jacobi polyfractonomials (JPFs), which were defined as eigenfunctions of a fractional Sturm–Liouville problem. From a very different perspective, Chen, Shen, and Wang [9] constructed efficient GJF–Petrov–Galerkin methods for FDEs using the generalized Jacobi functions (GJFs) introduced earlier in [17] and rigorously derived the approximation results in weighted Sobolev spaces involving fractional derivatives. In fact, the JPFs turned out to be special GJFs as shown in [9].

The collocation method can be easily implemented by replacing derivative values at a set of preassigned collocation points by the differentiation matrix of the corresponding order. It has remarkable advantages in dealing with variable coefficient and nonlinear problems. In fact, for FDEs, it is more advantageous to use a collocation method than a Galerkin method, as the latter usually leads to full dense matrices as well and requires additional integration other than the involved global fractional integrals, from the inner product. However, the resulted linear system of a fractional collocation method is unpleasantly ill-conditioned. In order to circumvent this difficulty for integer order differential equations, Wang, Samson, and Zhao [42] presented a pseudospectral integration matrix method (with a similar notion in [18, 14]). The essential idea was to find a new set of basis functions based upon a suitable Birkhoff interpolation incorporating the boundary condition simultaneously, which led to optimal preconditioners for the collocation methods using polynomial basis. Such a notion was extended to polynomial-based fractional collocation schemes for Caputo and modified Riemann–Liouville (RL) FDEs in [20].

Through building the singular factor into the basis functions, the modal JPF-(GJF-) Galerkin-type methods in [43] (in [9]) demonstrated the advantages over the polynomial-based methods. It is noteworthy that Zayernouri and Karniadakis [45] also investigated a fractional spectral collocation method using nodal JPFs/GJFs, defined by (3.1) involving the Lagrange basis polynomials. In fact, we demonstrate that the collocation method therein is less efficient for solution of FDEs with a general smooth source term. This can be fixed by only involving the Lagrange basis polynomials at the "interior" Jacobi–Gauss–Lobatto (JGL) points (see (3.8)). We also remark that as illustrated in [45], the conditioning of collocation discretization of the δth-order differential operator grows like $N^{2\delta}$, so it suffers from severe round-off errors for large numbers of collocation points.

We highlight the main contributions and prominent features of our development as follows.

(i) We present a systematic way to compute the fractional differentiation matrices of nodal JPFs/GJFs at general JGL points and show that it is only necessary to compute the matrix of order $\mu \in (0,1)$ for general order $k + \mu$ with singular index ν.

(ii) The nodal basis with its singular index adapted to singular behavior of the true solution of an FDE enables the method to capture the most singular term of the true solution. Our approach also fixes the deficiency of the nodal polyfractonomial approximation proposed in [45], through an amendment of the nodal basis.

(iii) Since we provide a stable way to compute the exact inverse of fractional collocation matrix explicitly even for thousands of collocation points, our well-conditioned collocation matrix remains an identity, which enjoys the same advantage of the spectral Petrov–Galerkin method developed in [44]. Henceforth, the condition number of the method is independent of the size of collocation points, which is a significant improvement of that for either our own direct collocation matrices or polyfractonomial approximation in [45].

(iv) A detailed singular decomposition of a true solution of rather general Remann–Liouville FDEs is presented. With this at our disposal, we can choose a suitable singular index for our approximation. It also enables us to conduct a rigorous convergence analysis for our methods.

The rest of this paper is organized as follows. In section 2, we collect some preliminaries that are pertinent to our algorithms. In section 3, we propose the collocation method based upon GJF approximation. Section 4 is devoted to the well-conditioned collocation method. In section 5, singular behavior of the true solution of FDEs is studied and convergence analysis is conducted. Numerical experiments are carried out to confirm our theoretical results in this section.

2. Preliminaries.

2.1. Fractional integrals and derivatives.
Let $\mathbb{N}$ and $\mathbb{R}$ be the sets of positive integers and real numbers, respectively, and denote

$$(2.1) \qquad \mathbb{N}_0 := \{0\} \cup \mathbb{N}, \quad \mathbb{R}^+ := \{a \in \mathbb{R} : a > 0\}, \quad \mathbb{R}_0^+ := \{0\} \cup \mathbb{R}^+.$$

The fractional integrals and fractional derivatives of Caputo type and RL type are defined as in, e.g., [34, 12]. *For $\rho \in \mathbb{R}$, the left-sided and right-sided fractional integrals of order ρ are defined by*

$$(2.2) \quad (_aI_x^\rho u)(x) = \frac{1}{\Gamma(\rho)} \int_a^x \frac{u(y)}{(x-y)^{1-\rho}} dy; \quad (_xI_b^\rho u)(x) = \frac{1}{\Gamma(\rho)} \int_x^b \frac{u(y)}{(y-x)^{1-\rho}} dy,$$

for $x \in (a,b)$, respectively, where $\Gamma(\cdot)$ is the Gamma function.

Denote the ordinary derivative by $D^k = d^k/dx^k$ (with integer $k \geq 0$). In general, the fractional integral and ordinary derivative operators are not commutable, leading to two types of fractional derivatives: *For $\mu \in (k-1, k)$ with $k \in \mathbb{N}$, the left-sided and right-sided Caputo fractional derivatives of order μ are defined by*

$$(2.3) \qquad (_a^CD_x^\mu u)(x) = {}_aI_x^{k-\mu}(D^k u)(x); \quad (_x^CD_b^\mu u)(x) = (-1)^k {}_xI_b^{k-\mu}(D^k u)(x),$$

and the left-sided and right-sided RL fractional derivatives of order μ are defined by

$$(2.4) \qquad (_a^RD_x^\mu u)(x) = D^k(_aI_x^{k-\mu} u)(x); \quad (_x^RD_b^\mu u)(x) = (-1)^k D^k(_xI_b^{k-\mu} u)(x).$$

These two types of fractional derivatives are connected by the formula

$$(2.5) \qquad \left(^R_a D^\mu_x u\right)(x) = \left(^C_a D^\mu_x u\right)(x) + \sum_{j=0}^{k-1} \frac{u^{(j)}(a)}{\Gamma(1+j-\mu)}(x-a)^{j-\mu}$$

(see, e.g., [34, 12]), which implies

$$(2.6) \qquad \left(^R_a D^\mu_x u\right)(x) = \left(^C_a D^\mu_x u\right)(x) \quad \text{if} \ \ u^{(j)}(a) = 0, \quad j = 0, \ldots, k-1.$$

Hereafter, we restrict our attention to RL fractional derivatives on $\Lambda := (-1, 1)$.

2.2. Jacobi polynomials. For $\alpha, \beta \in \mathbb{R}$, the Jacobi polynomials are defined by the hypergeometric function (cf. Szegö [37, (4.21.2)]),

$$(2.7)$$
$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)} {}_2F_1\Big(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\Big), \quad x \in \Lambda, \ \ n \in \mathbb{N},$$

and $P_0^{(\alpha,\beta)}(x) \equiv 1$, where the involved hypergeometric function is defined by

$$(2.8) \qquad {}_2F_1\big(a_1, a_2; b_1; z\big) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k}{(b_1)_k} \frac{z^k}{k!}$$

with $(a)_0 = 1$ and $(a)_k = a(a+1)\cdots(a+k-1)$. Note that $P_n^{(\alpha,\beta)}(x)$ *is always a polynomial in x for all α, β, but not always of degree n* (cf. [37, p. 64] and [6]). There hold

$$(2.9) \qquad P_n^{(\alpha,\beta)}(x) = (-1)^n P_n^{(\beta,\alpha)}(-x); \quad P_n^{(\alpha,\beta)}(1) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)},$$

and

$$(2.10) \quad \partial_x^k P_n^{(\alpha,\beta)}(x) = d_{n,k}^{\alpha,\beta} P_{n-k}^{(\beta+k,\alpha+k)}(x), \quad n \geq k, \quad d_{n,k}^{\alpha,\beta} = \frac{\Gamma(n+k+\alpha+\beta+1)}{2^k \Gamma(n+\alpha+\beta+1)}.$$

For $\alpha, \beta > -1$, the classical Jacobi polynomials are orthogonal with respect to the Jacobi weight function: $\omega^{(\alpha,\beta)}(x) = (1-x)^\alpha (1+x)^\beta$, namely,

$$(2.11) \qquad \int_{-1}^{1} P_n^{(\alpha,\beta)}(x) P_{n'}^{(\alpha,\beta)}(x) \omega^{(\alpha,\beta)}(x)\, dx = \gamma_n^{(\alpha,\beta)} \delta_{nn'},$$

where $\delta_{nn'}$ is the Dirac Delta symbol, and

$$(2.12) \qquad \gamma_n^{(\alpha,\beta)} = \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)n!\,\Gamma(n+\alpha+\beta+1)}.$$

However, the orthogonality does not carry over to the general case with α or $\beta \leq -1$ (see, e.g., [25] and [22, Chap. 3]).

In particular, the case $\alpha = \beta = 0$ in formula (2.7) leads to the Legendre polynomial denoted by $P_n(x)$, and the case $\alpha = \beta = -0.5$ (up to a constant multiple) leads to the Chebyshev polynomial of the first kind denoted by $T_n(x)$.

The following formulas derived from the Bateman fractional integral formulas of Jacobi polynomials [4] (also see [2, p. 313], [37, p. 96], and [9]) are indispensable for the algorithm development.

LEMMA 2.1. *Let $s \in \mathbb{R}^+$, $n \in \mathbb{N}_0$, and $x \in \Lambda$. Then for $\alpha \in \mathbb{R}$ and $\beta > -1$, we have*

$$(2.13) \quad {}_{-1}I_x^s\big\{(1+x)^\beta P_n^{(\alpha,\beta)}(x)\big\} = \frac{\Gamma(n+\beta+1)}{\Gamma(n+\beta+s+1)}(1+x)^{\beta+s}P_n^{(\alpha-s,\beta+s)}(x), \quad n \geq 0,$$

and

$$(2.14)$$
$$\quad {}_{-1}^R D_x^s\big\{(1+x)^{\beta+s}P_n^{(\alpha-s,\beta+s)}(x)\big\} = \frac{\Gamma(n+\beta+s+1)}{\Gamma(n+\beta+1)}(1+x)^\beta P_n^{(\alpha,\beta)}(x), \quad n \geq 0.$$

In particular, for real $s > 0$ and $\alpha \in \mathbb{R}$,

$$(2.15) \quad {}_{-1}^R D_x^s\big\{(1+x)^s P_n^{(\alpha-s,s)}(x)\big\} = \frac{\Gamma(s+n+1)}{\Gamma(n+1)}P_n^{(\alpha,0)}(x), \quad n \geq 0.$$

In fact, the formula (2.14) holds in the limiting case, $\beta = -1$, which will be useful later.

LEMMA 2.2. *Let $s \in \mathbb{R}^+$ and $x \in \Lambda$. Then for $\alpha \in \mathbb{R}$, we have*

$$\begin{aligned}
{}_{-1}^R D_x^s\big\{(1+x)^{s-1}P_n^{(\alpha-s,s-1)}(x)\big\} &= \frac{\Gamma(n+s)}{\Gamma(n)}(1+x)^{-1}P_n^{(\alpha,-1)}(x)\\
(2.16) \qquad &= \begin{cases} 0 & \text{if } n = 0,\\[2mm] \dfrac{(n+\alpha)\Gamma(n+s)}{2\,\Gamma(n+1)}\,P_{n-1}^{(\alpha,1)}(x) & \text{if } n \geq 1. \end{cases}
\end{aligned}$$

Proof. If $n = 0$, we have $P_0^{(\alpha-s,s-1)}(x) \equiv 1 \equiv P_0^{(\alpha,-1)}(x)$. Using the fractional differentiation formula (cf. [34]) yields

$$ {}_{-1}^R D_x^s\big\{(1+x)^{s-1}\big\} = \frac{\Gamma(s)}{\Gamma(0)}(1+x)^{-1}. $$

Noting that $1/\Gamma(0) = 0$ (cf. [1, (6.1.7)]), we obtain (2.2) with $n = 0$.

To derive the formula with $n \geq 1$, we proceed with two cases: (i) $s \in (0,1)$ and (ii) $s \geq 1$. If $s \in (0,1)$, recall the property (cf. [34]) ${}_{-1}^R D_x^s = D_{-1}I_x^{1-s}$, and by (2.13) (with $s \to 1-s, \alpha \to \alpha - s$ and $\beta \to s - 1$),

$$\begin{aligned}
D_{-1}I_x^{1-s}\big\{(1+x)^{s-1}P_n^{(\alpha-s,s-1)}(x)\big\} &= \frac{\Gamma(n+s)}{\Gamma(n+1)}DP_n^{(\alpha-1,0)}(x)\\
&= \frac{(n+\alpha)\Gamma(n+s)}{2\,\Gamma(n+1)}\,P_{n-1}^{(\alpha,1)}(x),
\end{aligned}$$

where in the last step, we used the derivative formula of Jacobi polynomials.

If $s \geq 1$ we use the property (cf. [34]) ${}_{-1}^R D_x^s = D\,{}_{-1}^R D_x^{s-1}$, and by (2.15) (with $s \to s - 1$ and $\alpha \to \alpha - 1$),

$$\begin{aligned}
D\,{}_{-1}^R D_x^{s-1}\big\{(1+x)^{s-1}P_n^{(\alpha-s,s-1)}(x)\big\} &= \frac{\Gamma(n+s)}{\Gamma(n+1)}DP_n^{(\alpha-1,0)}(x)\\
&= \frac{(n+\alpha)\Gamma(n+s)}{2\,\Gamma(n+1)}\,P_{n-1}^{(\alpha,1)}(x),
\end{aligned}$$

where we used the derivative formula of Jacobi polynomials again. In view of [37, (4.22.2)],

$$P_n^{(\alpha,-1)}(x) = \frac{n+\alpha}{2n}(1+x)P_{n-1}^{(\alpha,1)}(x), \quad n \geq 1,$$

we complete the proof. □

For $\alpha, \beta > -1$, let $\big\{x_j := x_{N,j}^{(\alpha,\beta)}, \omega_j := \omega_{N,j}^{(\alpha,\beta)}\big\}_{j=0}^N$ be the set of JGL quadrature nodes and weights, where the nodes are zeros of $(1-x^2)DP_N^{(\alpha,\beta)}(x)$. Hereafter, we assume that $\{x_j\}$ are arranged in ascending order so that $x_0 = -1$ and $x_N = 1$. Moreover, to alleviate the burden of heavy notation, we sometimes drop the parameters α, β in the notation whenever it is clear from the context. The JGL quadrature enjoys the exactness (see, e.g., [35, Chap. 3])

$$(2.17) \qquad \int_{-1}^1 \phi(x)\omega^{(\alpha,\beta)}(x)\,dx = \sum_{j=0}^N \phi(x_j)\omega_j \quad \forall\, \phi \in \mathbb{P}_{2N-1},$$

where $\mathbb{P}_N$ is the set of all polynomials of degree at most N.

Let $\mathcal{I}_N u$ be the Lagrange polynomial interplant of $u \in C(\bar{\Lambda})$ at JGL points defined by

$$(2.18) \qquad (\mathcal{I}_N u)(x) = \sum_{j=0}^N u(x_j)l_j(x) \in \mathbb{P}_N,$$

where the interpolating basis polynomials $\{l_j\}_{j=0}^N$ can be expressed by

$$(2.19) \quad l_j(x) = \sum_{n=0}^N t_{nj} P_n^{(\alpha,\beta)}(x), \quad 0 \leq j \leq N, \quad \text{where} \quad t_{nj} := \frac{\omega_j}{\tilde{\gamma}_n^{(\alpha,\beta)}} P_n^{(\alpha,\beta)}(x_j),$$

with

$$(2.20) \qquad \tilde{\gamma}_n^{(\alpha,\beta)} = \gamma_n^{(\alpha,\beta)}, \ \ 0 \leq n \leq N-1; \ \ \tilde{\gamma}_N^{(\alpha,\beta)} = \Big(2 + \frac{\alpha+\beta+1}{N}\Big)\gamma_N^{(\alpha,\beta)}.$$

2.3. Connection problems. In our algorithms, the transform between Jacobi expansions with different parameters will be used frequently. This defines a *connection problem* that connects the representations of polynomials between two spaces:

$$\mathbb{P}_N = \mathrm{span}\big\{P_n^{(\alpha,\beta)} : 0 \leq n \leq N\big\} = \mathrm{span}\big\{P_l^{(a,b)} : 0 \leq l \leq N\big\}, \quad \alpha, \beta, a, b > -1.$$

More precisely, *given the Jacobi expansion coefficients $\{\hat{u}_n^{(\alpha,\beta)}\}$ of $u \in \mathbb{P}_N$, find the coefficients $\{\hat{u}_l^{(a,b)}\}$ such that*

$$(2.21) \qquad u(x) = \sum_{n=0}^N \hat{u}_n^{(\alpha,\beta)} P_n^{(\alpha,\beta)}(x) = \sum_{l=0}^N \hat{u}_l^{(a,b)} P_l^{(a,b)}(x).$$

This can be resolved by the transform

$$(2.22) \qquad \hat{\boldsymbol{u}}^{(a,b)} = {}^{(\alpha,\beta)}\boldsymbol{C}^{(a,b)}\, \hat{\boldsymbol{u}}^{(\alpha,\beta)},$$

where $\hat{\boldsymbol{u}}^{(\alpha,\beta)}$ and $\hat{\boldsymbol{u}}^{(a,b)}$ are column-$(N+1)$ vectors of the coefficients, and ${}^{(\alpha,\beta)}\boldsymbol{C}^{(a,b)}$ is the connection matrix of the transform from $\big\{P_n^{(\alpha,\beta)}\big\}$ to $\big\{P_l^{(a,b)}\big\}$. One finds from

the orthogonality (2.11) and (2.21) that the entries of $^{(\alpha,\beta)}\boldsymbol{C}^{(a,b)}$, i.e., the connection coefficients, are given by

$$(2.23) \qquad {}^{(\alpha,\beta)}\boldsymbol{C}_{ln}^{(a,b)} := \frac{1}{\gamma_l^{(a,b)}} \int_{-1}^{1} P_l^{(a,b)}(x) P_n^{(\alpha,\beta)}(x)\, \omega^{(a,b)}(x) dx.$$

Note that $^{(\alpha,\beta)}\boldsymbol{C}_{ln}^{(a,b)} = 0$ if $n < l$, and the nonzero entries can be computed efficiently by using the recurrence formulas in [20, Prop. 2.1].

3. RL fractional differentiation matrices.

3.1. Fractional Lagrange interpolants in [45]. To motivate the algorithm development herein, it is necessary to recall the *nodal JPF* introduced in [45, (3.8)]. Let $-1 = x_0 < x_1 < \cdots < x_N = 1$ be a set of generic interpolation points, and define the nodal basis of fractional order $(N + \mu)$ as

$$(3.1) \qquad h_j^\mu(x) = \left(\frac{1+x}{1+x_j}\right)^\mu \prod_{k=0,k\neq j}^{N} \frac{x - x_k}{x_j - x_k} = \left(\frac{1+x}{1+x_j}\right)^\mu l_j(x), \quad 1 \leq j \leq N,$$

for $\mu \in (0,1)$, where $\{l_j\}_{j=0}^N$ are the Lagrange interpolation basis polynomials in (2.19), if $\{x_j\}_{j=0}^N$ are chosen as the JGL points. Note that $l_j(x) = \sum_{n=1}^{N+1} s_n^j P_{n-1}^{(-\nu,\nu)}(x)$, where s_n^j can be computed by (2.19) with parameters $\alpha = -\nu$ and $\beta = \nu$. The nodal version (3.1) is suggested as a counterpart of the *modal JPF* in [44], originated from fractional Sturm–Liouville problems. An important special class used in [44] is

$$(3.2) \qquad {}^{(1)}\mathcal{P}_n^\mu(x) = (1+x)^\mu P_{n-1}^{(-\mu,\mu)}(x), \quad n \geq 1, \ \mu \in (0,1).$$

To have more insight, we consider the model fractional equation of order $\nu \in (0,1)$ (cf. [45, (3.25)]):

$$(3.3) \qquad {}_{-1}^R D_x^\nu u(x) = f(x), \ x \in (-1,1); \quad u(-1) = 0,$$

where $f(x)$ is continuous in $(-1,1)$. The fractional collocation scheme using nodal JPFs is to find $u_N \in {}_0\mathcal{V}_{N+\nu} = \text{span}\{h_j^\nu : 1 \leq j \leq N\}$ such that

$$(3.4) \qquad {}_{-1}^R D_x^\nu u_N(x_j) = f(x_j), \ 1 \leq j \leq N,$$

which leads to the linear system,

$$(3.5) \qquad \boldsymbol{D}^\nu \boldsymbol{u}_N = \boldsymbol{f} \quad \text{with} \quad \boldsymbol{D}_{ij}^\nu = {}_{-1}^R D_x^\nu h_j^\nu(x_i), \ 1 \leq i, j \leq N,$$

and $\boldsymbol{u}_N = (u_N(x_1), \ldots, u_N(x_N))^t$ and $\boldsymbol{f} = (f(x_1), \ldots, f(x_N))^t$. Here, $\boldsymbol{D}^\nu$ is the fractional differentiation matrix, whose entries can be evaluated by [45, (3.14)] (thanks to (2.15))

$$(3.6) \qquad \boldsymbol{D}_{ij}^\nu = \frac{1}{(1+x_j)^\nu} \sum_{n=1}^{N+1} \frac{\Gamma(n+\nu)}{\Gamma(n)} s_n^j P_{n-1}(x_i), \quad 1 \leq i, j \leq N.$$

At this point, it is important to point out that since $l_j(-1) = 0$ for $1 \leq j \leq N$, we have

$$(3.7) \qquad h_j^\nu(x) = (1+x)^{1+\nu} \psi_j(x), \quad 1 \leq j \leq N,$$

where $\psi_j \in \mathbb{P}_{N-1}$ and $\psi_j(-1) \neq 0$. This implies $h_j^\nu(-1) = D h_j^\nu(-1) = 0$, so the scheme (3.4)–(3.5) does not lead to satisfactory approximation if the solution does not meet $u'(-1) = 0$. However, (3.3) admits the solution such that $u'(-1) \neq 0$, e.g., $C(1+x)^\nu$ if $f(x) = 1$ (cf. (2.15)).

3.2. Fractional Lagrange basis based on Gauss–Radau-type interpolation. To overcome the deficiency in (3.7), we introduce the following fractional Lagrange basis of order $(N + \mu - 1)$:

$$(3.8) \qquad \bar{h}_j^\mu(x) = \left(\frac{1+x}{1+x_j}\right)^\mu \bar{l}_j(x), \quad 1 \le j \le N, \ \mu \in (0,1),$$

where $\{\bar{l}_j\}_{j=1}^N$ are the Lagrange interpolation polynomials basis associated with the JGL points $\{x_j\}_{j=1}^N$ (exclusive of $x_0 = -1$), satisfying $\bar{l}_j \in \mathbb{P}_{N-1}$ and $\bar{l}_j(x_i) = \delta_{ij}$ for $1 \le i, j \le N$. In fact, one verifies that if $\{x_j\}_{j=0}^N$ are the JGL points (i.e., zeros of $(1-x^2)DP_N^{(\alpha,\beta)}(x)$), then we have

$$(3.9) \qquad h_j^\mu(x) = \frac{1+x}{1+x_j}\bar{h}_j^\mu(x) = \bar{h}_j^{1+\mu}(x), \quad 1 \le j \le N, \ \mu \in (0,1).$$

Indeed, we have from [35, Chap. 3] that

$$(3.10) \qquad
\begin{aligned}
l_j(x) &= \frac{(1-x^2)DP_N^{(\alpha,\beta)}(x)}{(x-x_j)D((1-x^2)DP_N^{(\alpha,\beta)}(x))|_{x=x_j}} \\
&= \frac{1+x}{1+x_j}\frac{(1-x)DP_N^{(\alpha,\beta)}(x)}{(x-x_j)D((1-x)DP_N^{(\alpha,\beta)}(x))|_{x=x_j}} \\
&= \frac{1+x}{1+x_j}\bar{l}_j(x), \quad 1 \le j \le N.
\end{aligned}$$

Thus the relation (3.9) follows from (3.1) and (3.8).

It is noteworthy that the N points $\{x_j\}_{j=1}^N$ of $(N+1)$ JGL points $\{x_j\}_{j=0}^N$ with respect to the Jacobi weight $\omega^{(\alpha,\beta)}$ are also N Jacobi–Gauss–Radau (JGR) points but with respect to the Jacobi weight $\omega^{(\alpha,\beta+1)}$ (cf. [35, Chap. 3]).

Remark 3.1. In fact, one can also choose $\{x_j\}_{j=1}^N$ to be the JGR points associated with the Jacobi weight $\omega^{\alpha,\beta}$ (i.e., zeros of $(1-x)P_{N-1}^{(\alpha+1,\beta)}(x)$), and accordingly, we have

$$(3.11) \qquad \bar{l}_j(x) = \frac{(1-x)P_{N-1}^{(\alpha+1,\beta)}(x)}{(x-x_j)D((1-x)P_{N-1}^{(\alpha+1,\beta)}(x))|_{x=x_j}}, \quad 1 \le j \le N,$$

which is different from (3.10) by noting that $DP_N^{(\alpha,\beta)}(x) = \frac{1}{2}(N+\alpha+\beta)P_{N-1}^{(\alpha+1,\beta+1)}(x)$.

Observe from the definition (3.8) that (i) $\bar{h}_j^\mu(1) = 0$ for $1 \le j \le N-1$, which allows for the imposition of boundary conditions at $x = 1$; (ii) the parameter μ in the singular factor $(1+x)^\mu$ should be chosen to fit the singularity of the underlaying solution, which might be the order ν of the equation; and (iii) in principle, the choice of JGL points (with parameters α, β) can be independent of μ and ν. In the applications, we need to compute the fractional differentiation of order ν on $\{\bar{h}_j^\mu\}_{j=1}^N$ (with $\mu \in (0,1)$ and $\nu \ge \mu$) at a set of preassigned collocation points.

LEMMA 3.1. *For $\alpha, \beta > -1$, let $\left\{x_j := x_{N,j}^{(\alpha,\beta)}, \omega_j := \omega_{N,j}^{(\alpha,\beta)}\right\}_{j=0}^N$ (with $x_0 = -1$) be the JGL points and corresponding quadrature weights. Then we have*

$$(3.12) \qquad \bar{l}_j(x) = \sum_{n=0}^{N-1} \bar{t}_{nj}P_n^{(\alpha,\beta)}(x) = \sum_{k=0}^{N-1}\bar{s}_{kj}P_k^{(a,b)}(x), \quad a,b > -1, \ 1 \le j \le N,$$

where

$$(3.13) \quad \bar{t}_{nj} := \bar{t}_{nj}^{(\alpha,\beta)} = \frac{1}{\gamma_n^{(\alpha,\beta)}} \left\{ -\frac{c_j}{\beta+1} \frac{P_N^{(\alpha,\beta)}(-1)}{P_N^{(\alpha,\beta)}(x_j)} P_n^{(\alpha,\beta)}(-1)\omega_0 + P_n^{(\alpha,\beta)}(x_j)\omega_j \right\},$$

with $c_j = 1$ for $1 \le j \le N-1$, and $c_N = \alpha + 1$, and

$$(3.14) \qquad \bar{s}_{kj} := \bar{s}_{kj}^{(\alpha,\beta,a,b)} = \sum_{n=k}^{N-1} \frac{\bar{t}_{nj}}{\gamma_k^{(a,b)}} \int_{-1}^{1} P_k^{(a,b)}(x) P_n^{(\alpha,\beta)}(x) \, \omega^{(a,b)}(x) dx.$$

Proof. The first expansion in (3.12) and the formula (3.13) are derived in [20, (4.14)], while the formula (3.14) follows directly from (3.12) and the orthogonality (2.11). □

In section 4, we need a similar expansion for the Lagrange interpolation involving only the interior JGL points $\{x_j\}_{j=1}^{N-1}$ (exclusive of $x_0 = -1$ and $x_N = 1$). Let $\{\hat{l}_j\}_{j=1}^{N-1}$ be the Lagrange interpolation basis satisfying $\hat{l}_j \in \mathbb{P}_{N-2}$ and $\hat{l}_j(x_i) = \delta_{ij}$ for $1 \le i, j \le N-1$. Similar to Lemma 3.1, we have following useful expressions.

LEMMA 3.2. *For $\alpha, \beta > -1$, let $\left\{ x_j := x_{N,j}^{(\alpha,\beta)}, \omega_j := \omega_{N,j}^{(\alpha,\beta)} \right\}_{j=0}^N$ (with $x_0 = -1$ and $x_N = 1$) be the JGL points and corresponding quadrature weights. Then we have*

$$(3.15) \quad \hat{l}_j(x) = \sum_{n=0}^{N-2} \hat{t}_{nj} P_n^{(\alpha,\beta)}(x) = \sum_{k=0}^{N-2} \hat{s}_{kj} P_k^{(a,b)}(x), \quad a, b > -1, \ \ 1 \le j \le N-1,$$

where

$$(3.16) \begin{aligned} \hat{t}_{nj} := \hat{t}_{nj}^{(\alpha,\beta)} = \frac{1}{\gamma_n^{(\alpha,\beta)}} &\left\{ \frac{(x_j-1)P_N^{(\alpha,\beta)}(-1)}{2(\beta+1)P_N^{(\alpha,\beta)}(x_j)} P_n^{(\alpha,\beta)}(-1)\omega_0 \right. \\ &\left. -\frac{(1+x_j)P_N^{(\alpha,\beta)}(1)}{2(\alpha+1)P_N^{(\alpha,\beta)}(x_j)} P_n^{(\alpha,\beta)}(1)\omega_N + P_n^{(\alpha,\beta)}(x_j)\omega_j \right\}, \end{aligned}$$

and

$$(3.17) \qquad \hat{s}_{kj} := \hat{s}_{kj}^{(\alpha,\beta,a,b)} = \sum_{n=k}^{N-2} \frac{\hat{t}_{nj}}{\gamma_k^{(a,b)}} \int_{-1}^{1} P_k^{(a,b)}(x) P_n^{(\alpha,\beta)}(x) \, \omega^{(a,b)}(x) dx.$$

Proof. The first expansion in (3.15) and the formula (3.16) are derived in [20, (4.17)], while the formula (3.17) follows directly from (3.15) and the orthogonality (2.11). □

3.3. Fractional differentiation matrices. Hereafter, we compute the νth-order fractional differentiation matrix:

$$(3.18) \qquad \bar{\boldsymbol{D}}_\mu^{(\nu)} \in \mathbb{R}^{N \times N} \text{ with entries } \left[\bar{\boldsymbol{D}}_\mu^{(\nu)}\right]_{ij} = {}_{-1}^R D_x^\nu \bar{h}_j^\mu(x_i), \ \ 1 \le i, j \le N,$$

for $\mu \in (0,1)$ and $0 < \nu \le 1 + \mu$, where $\{\bar{h}_j^\mu\}$ are defined in (3.8).

THEOREM 3.1. *For $\alpha, \beta > -1$, let $\left\{ x_j := x_{N,j}^{(\alpha,\beta)}, \omega_j := \omega_{N,j}^{(\alpha,\beta)} \right\}_{j=0}^N$ (with $x_0 = -1$) be the JGL points and corresponding quadrature weights. Then the entries of $\bar{\boldsymbol{D}}_\mu^{(\nu)}$ with $\mu \in (0,1)$ and $0 < \nu \le 1 + \mu$ can be computed by the following formulas:*

(i) *If $0 < \nu < 1 + \mu$, we have*

$$(3.19) \qquad [\bar{\boldsymbol{D}}_\mu^{(\nu)}]_{ij} = \frac{(1 + x_i)^{\mu - \nu}}{(1 + x_j)^\mu} \sum_{k=0}^{N-1} \tilde{s}_{kj} P_k^{(\nu - \mu, \mu - \nu)}(x_i), \;\; 1 \le i, j \le N,$$

where

$$(3.20) \qquad \tilde{s}_{kj} = \frac{\Gamma(k + \mu + 1)}{\Gamma(k + \mu - \nu + 1)} \bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)},$$

and $\bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)}$ is defined in (3.14).

(ii) *If $\nu = 1 + \mu$, we have*

$$(3.21) \qquad [\bar{\boldsymbol{D}}_\mu^{(1+\mu)}]_{ij} = \frac{1}{(1 + x_j)^\mu} \sum_{k=1}^{N-1} \tilde{s}_{kj} \, P_{k-1}^{(1,1)}(x_i), \;\; 1 \le i, j \le N,$$

where

$$(3.22) \qquad \tilde{s}_{kj} = \frac{(k+1)\Gamma(k + \mu + 1)}{2\,\Gamma(k+1)} \bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)},$$

and $\bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)}$ is defined in (3.14).

Proof. By (3.8) and (3.12),

$$(3.23) \qquad \bar{h}_j^\mu(x) = \frac{1}{(x_j + 1)^\mu} \sum_{k=0}^{N-1} \bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)} (x+1)^\mu P_k^{(-\mu, \mu)}(x).$$

Using Lemma 2.1 (with $s \to \nu, \alpha \to \nu - \mu$ and $\beta \to \mu - \nu$) leads to

$$(3.24)$$

$$\begin{aligned}
{}_{-1}^R D_x^\nu \, \bar{h}_j^\mu(x) &= \frac{1}{(x_j + 1)^\mu} \sum_{k=0}^{N-1} \bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)} \, {}_{-1}^R D_x^\nu \big\{ (x+1)^\mu P_k^{(-\mu, \mu)}(x) \big\} \\
&= \frac{1}{(x_j + 1)^\mu} \sum_{k=0}^{N-1} \bar{s}_{kj}^{(\alpha, \beta, -\mu, \mu)} \frac{\Gamma(k + \mu + 1)}{\Gamma(k + \mu - \nu + 1)} (1 + x)^{\mu - \nu} P_k^{(\nu - \mu, \mu - \nu)}(x).
\end{aligned}$$

Taking $x = x_i$ in the above yields (3.19)–(3.20).

The formula (3.21) can be derived similarly by using Lemma 2.2 in (3.24). $\qquad \square$

Remark 3.2. Observe from (3.14), (3.20), and (3.22) that if we take $(\alpha, \beta) = (-\mu, \mu)$, then $\bar{s}_{kj} = \bar{t}_{kj}$. In other words, (3.19) and (3.21) have the simplest form. Thus, it is preferable to choose these special parameters.

Remark 3.3. It is noteworthy that in [45] the algorithm (for $\nu \ne \mu$ and $\nu \ne 1 + \mu$) uses the fractional Lagrange interpolating basis $\{h_j^\mu\}$. The computation was based on (2.14), the transformation, and the inverse transformation between ${}_{-1}^R D_x^s$ and ${}_0^R D_x^s$. As shown above, we use basis $\{\bar{h}_j^\mu\}$ and the computation is based on formula (2.14) and (2.16). This leads to much concise representation and efficient, stable computation.

For notational convenience, we allow (in the following theorem and its proof) the nodal basis $\{\bar{h}_j^\mu\}$ in (3.8) to be defined for $\mu < 0$, and likewise for the differentiation matrix in (3.18). We have the following useful rules to compute higher-order fractional differentiation matrices.

THEOREM 3.2. *For $\mu \in (0,1)$ and $0 < \nu < 1 + \mu$, we have*

$$(3.25) \qquad \bar{\boldsymbol{D}}_\mu^{(k+\nu)} = \bar{\boldsymbol{D}}_{\mu-\nu}^{(k)} \, \bar{\boldsymbol{D}}_\mu^{(\nu)}, \quad k = 0, 1, \ldots,$$

and in particular, we have

$$(3.26) \qquad \bar{\boldsymbol{D}}_\mu^{(k+\mu)} = (\bar{\boldsymbol{D}})^k \, \bar{\boldsymbol{D}}_\mu^{(\mu)}, \quad k = 0, 1, \ldots,$$

where $(\bar{\boldsymbol{D}})^k$ is a product of k copies of the first-order differentiation matrix $\bar{\boldsymbol{D}}$ with entries given by $[\bar{\boldsymbol{D}}]_{ij} = \bar{l}_j'(x_i)$ for $1 \le i, j \le N$.

Proof. We find from (3.24) that $(1+x)^{\nu-\mu} {}_{-1}^R D_x^\nu \bar{h}_j^\mu \in \mathbb{P}_{N-1}$, so we can express it as

$$(3.27) \quad (1+x)^{\nu-\mu} {}_{-1}^R D_x^\nu \bar{h}_j^\mu(x) = \sum_{p=1}^N \left\{ (1+x_p)^{\nu-\mu} {}_{-1}^R D_x^\nu \bar{h}_j^\mu(x_p) \right\} \bar{l}_p(x), \quad 1 \le j \le N.$$

Thus, we have

$$(3.28)$$

$$\begin{aligned}
{}_{-1}^R D_x^{k+\nu} \bar{h}_j^\mu(x_i) &= D^k {}_{-1}^R D_x^\nu \bar{h}_j^\mu(x_i) = \sum_{p=1}^N {}_{-1}^R D_x^\nu \bar{h}_j^\mu(x_p) D^k \left\{ \frac{(1+x)^{\mu-\nu}}{(1+x_p)^{\mu-\nu}} \bar{l}_p(x) \right\}_{x=x_i} \\
&= \sum_{p=1}^N {}_{-1}^R D_x^\nu \bar{h}_j^\mu(x_p) D^k \bar{h}_p^{\mu-\nu}(x_i) = \sum_{p=1}^N [\bar{\boldsymbol{D}}_{\mu-\nu}^{(k)}]_{ip} [\bar{\boldsymbol{D}}_\mu^{(\nu)}]_{pj},
\end{aligned}$$

which yields (3.25).

As a special case of (3.25), we have $\bar{\boldsymbol{D}}_\mu^{(k+\mu)} = \bar{\boldsymbol{D}}_0^{(k)} \, \bar{\boldsymbol{D}}_\mu^{(\mu)}$, and by (3.28), $[\bar{\boldsymbol{D}}_0^{(k)}]_{ip} = \bar{l}_p^{(k)}(x_i)$. According to [35, Thm. 3.10], we have $\bar{\boldsymbol{D}}_0^{(k)} = (\bar{\boldsymbol{D}})^k$. This ends the proof. $\square$

We conclude this section by providing some numerical study of (discrete) eigenvalues of $\bar{\boldsymbol{D}}_\mu^{(\nu)}$. Remove the "boundary" row/column, and define

$$(3.29) \quad \boldsymbol{D}_{\mu,\text{in}}^{(\nu)} := \begin{cases} (\bar{\boldsymbol{D}}_\mu^{(\nu)})_{ij}, & 1 \le i, j \le N, & \text{if } \mu, \nu \in (0,1), \\ (\bar{\boldsymbol{D}}_\mu^{(\nu)})_{ij}, & 1 \le i, j \le N-1, & \text{if } \mu \in (0,1), \ 1 < \nu \le 1 + \mu, \end{cases}$$

which is invertible and allows for incorporating boundary conditions.

In Figure 1, we illustrate the condition number of $\boldsymbol{D}_{\mu,\text{in}}^{(\nu)}$ for some μ and ν under Legendre–Gauss–Lobatto points and Chebyshev–Gauss–Lobatto (CGL) points. One easily observes that in both cases, the condition number of the matrices grows dramatically as the number of collocation points N grows.

4. Inverse of RL fractional differentiation matrices. Following the spirit of [42, 20], we next compute the explicit inverse of the fractional differentiation matrix $\bar{\boldsymbol{D}}_\mu^{(\nu)}$ in Theorem 3.1 in a stable manner, through the basis functions of a suitable fractional Birkhoff interpolation problem.

Define the space

$$(4.1) \qquad \mathcal{F}_N^{(\mu)} := \left\{ (1+x)^\mu \phi(x) : \phi \in \mathbb{P}_{N-1} \right\}, \quad \mu > -1.$$
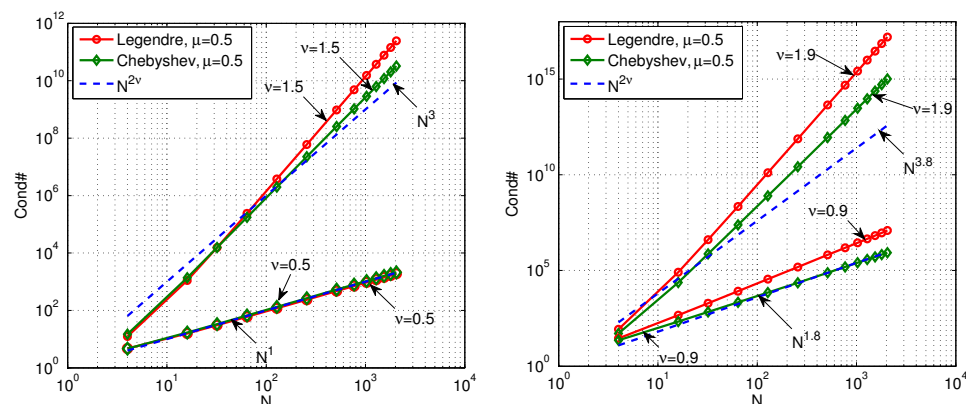
We consider the following fractional interpolation problems:

FIG. 1. *Condition number of fractional differentiation matrices $\bar{\boldsymbol{D}}_{0.5}^{0.5}, \bar{\boldsymbol{D}}_{0.5}^{1.5}$ (left) and $\bar{\boldsymbol{D}}_{0.5}^{0.9}, \bar{\boldsymbol{D}}_{0.5}^{1.9}$ (right).*

(i) For $\mu, \nu \in (0,1)$, the RL fractional Birkhoff interpolation is to find $p \in \mathcal{F}_N^{(\mu)}$ such that

$$(4.2) \qquad {}_{-1}^{R}D_x^\nu p(x_j) = {}_{-1}^{R}D_x^\nu u(x_j), \quad 1 \leq j \leq N; \quad p(-1) = u(-1),$$

for any $u \in C[-1,1]$ satisfying $u(-1) = 0$ and ${}_{-1}^{R}D_x^\nu u \in C(-1,1]$.

(ii) For $\mu \in (0,1)$ and $1 < \nu \leq 1+\mu$, the RL fractional Birkhoff interpolation is to find $p \in \mathcal{F}_N^{(\mu)}$ such that

$$(4.3)$$
$${}_{-1}^{R}D_x^\nu p(x_j) = {}_{-1}^{R}D_x^\nu u(x_j), \quad 1 \leq j \leq N-1; \quad p(-1) = u(-1), \quad p(1) = u(1),$$

for any $u \in C[-1,1]$ satisfying $u(-1) = 0$ and ${}_{-1}^{R}D_x^\nu u \in C(-1,1)$.

Like the usual Lagrange interpolation, we represent the interpolant (for $\mu \in (0,1)$) as

$$(4.4) \qquad p(x) = \begin{cases} \displaystyle\sum_{j=1}^{N} {}_{-1}^{R}D_x^\nu u(x_j) B_{\mu,j}^{(\nu)}(x) & \text{for } \nu \in (0,1), \\ \displaystyle\sum_{j=1}^{N-1} {}_{-1}^{R}D_x^\nu u(x_j) B_{\mu,j}^{(\nu)}(x) + u(1) B_{\mu,N}^{(\nu)}(x) & \text{for } 1 < \nu \leq 1+\mu, \end{cases}$$

where $\{B_{\mu,j}^{(\nu)}\}$ are called the RL fractional Birkhoff interpolation basis in $\mathcal{F}_N^{(\mu)}$, satisfying

$$(4.5) \qquad B_{\mu,j}^{(\nu)}(x_i)(-1) = 0, \quad {}_{-1}^{R}D_x^\nu B_{\mu,j}^{(\nu)}(x_i) = \delta_{ij}, \quad 1 \leq i,j \leq N,$$

for $\nu \in (0,1)$; and for $1 < \nu \leq 1+\mu$,

$$(4.6) \qquad B_{\mu,j}^{(\nu)}(\pm 1) = 0, \quad {}_{-1}^{R}D_x^\nu B_{\mu,j}^{(\nu)}(x_i) = \delta_{ij}, \quad 1 \leq i,j \leq N-1,$$
$$B_{\mu,N}^{(\nu)}(-1) = {}_{-1}^{R}D_x^\nu B_{\mu,N}^{(\nu)}(x_i) = 0, \quad 1 \leq i \leq N-1; \quad B_{\mu,N}^{(\nu)}(1) = 1.$$

Note that as $B_{\mu,j}^{(\nu)} \in \mathcal{F}_N^{(\mu)}$, the condition $B_{\mu,j}^{(\nu)}(-1) = 0$ is automatically met if $\mu > 0$.

Remark 4.1. Different from the polynomial-based approach in [20], the above fractional Birkhoff interpolation of nodal JPFs/GJFs involves different singular indices for fractional derivatives of different orders. Also the derivation of the fractional Birkhoff interpolation basis is much more involved.

The new basis can be computed by the following explicit formulas in a stable manner.

THEOREM 4.1. *For $\alpha, \beta > -1$, let $\left\{x_j := x_{N,j}^{(\alpha,\beta)}, \omega_j := \omega_{N,j}^{(\alpha,\beta)}\right\}_{j=0}^{N}$ (with $x_0 = -1$) be the JGL points and corresponding quadrature weights.*

(i) *If $0 < \mu, \nu < 1$, we have*

$$(4.7) \qquad B_{\mu,j}^{(\nu)}(x) = \frac{(1+x)^\mu}{(1+x_j)^{\mu-\nu}} \sum_{k=0}^{N-1} \breve{s}_{kj} \, P_k^{(-\mu,\mu)}(x), \quad 1 \le j \le N,$$

where

$$(4.8) \qquad \breve{s}_{kj} = \frac{\Gamma(k+\mu-\nu+1)}{\Gamma(k+\mu+1)} \, \bar{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)},$$

and $\bar{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)}$ is defined in (3.14) with $a = \nu - \mu$ and $b = \mu - \nu$.

(ii) *If $0 < \mu < 1$ and $1 < \nu < 1 + \mu$, we have that for $1 \le j \le N - 1$,*

$$(4.9) \quad B_{\mu,j}^{(\nu)}(x) = \frac{(1+x)^\mu}{(1+x_j)^{\mu-\nu}(x_j + \tau_j)}$$
$$\times \sum_{k=0}^{N-2} \left\{ (\tau_j - 1)\breve{s}_{kj}^{(1)} \, P_k^{(-\mu,\mu)}(x) + \breve{s}_{kj}^{(2)}(1+x)P_k^{(-\mu,\mu+1)}(x) \right\},$$

where

$$\begin{aligned}
\breve{s}_{kj}^{(1)} &= \frac{\Gamma(k+\mu-\nu+1)}{\Gamma(k+\mu+1)} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)}, \\
(4.10) \qquad \breve{s}_{kj}^{(2)} &= \frac{\Gamma(k+\mu-\nu+2)}{\Gamma(k+\mu+2)} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu+1)}, \\
\tau_j - 1 &= -2 \sum_{k=0}^{N-2} \breve{s}_{kj}^{(2)} \, P_k^{(-\mu,\mu+1)}(1) \Big/ \sum_{k=0}^{N-2} \breve{s}_{kj}^{(1)} \, P_k^{(-\mu,\mu)}(1).
\end{aligned}$$

For $j = N$, we have

(4.11)
$$B_{\mu,N}^{(\nu)}(x) = \tau_N \sum_{k=0}^{N-1} \hat{s}_{kN}^{(\alpha,\beta,\nu-\mu,\mu-\nu)} \frac{\Gamma(k+\mu-\nu+1)}{\Gamma(k+\mu+1)} (1+x)^\mu P_k^{(-\mu,\mu)}(x),$$

where

$$(4.12) \qquad \frac{1}{\tau_N} = 2^\mu \sum_{k=0}^{N-1} \hat{s}_{kN}^{(\alpha,\beta,\nu-\mu,\mu-\nu)} \frac{\Gamma(k+\mu-\nu+1)}{\Gamma(k+\mu+1)} P_k^{(-\mu,\mu)}(1).$$

In the above, $\left\{\hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)}\right\}$ and $\left\{\hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu+1)}\right\}$ are defined in (3.17).

(iii) *If $0 < \mu < 1$ and $\nu = 1 + \mu$, we have that for $1 \le j \le N - 1$,*

$$(4.13) \qquad B_{\mu,j}^{(1+\mu)}(x) = 2(1+x)^{\mu} \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,1,1)}$$
$$\times \frac{(k+1)!}{(k+2+\mu)\Gamma(k+\mu)} \{ P_{k+1}^{(-\mu,\mu)}(x) - P_{k+1}^{(-\mu,\mu)}(1) \},$$

where $\{ \hat{s}_{kj}^{(\alpha,\beta,1,1)} \}$ are defined in (3.17), *and for $j = N$,*

$$(4.14) \qquad B_{\mu,N}^{(1+\mu)}(x) = \Big(\frac{1+x}{2} \Big)^{\mu}.$$

Proof. We proceed with the proof separately for two cases.

(i) For $\nu \in (0,1)$, since $B_{\mu,j}^{(\nu)} \in \mathcal{F}_N^{(\mu)}$, we can write

$$(4.15) \qquad B_{\mu,j}^{(\nu)}(x) = \sum_{k=0}^{N-1} \breve{b}_{kj} (1+x)^{\mu} P_k^{(-\mu,\mu)}(x), \quad 1 \le j \le N.$$

We next determine $\{ \breve{b}_{kj} \}$. Observe from (3.24) that $_{-1}^R D_x^\nu B_{\mu,j}^{(\nu)} \in \mathcal{F}_N^{(\mu-\nu)}$, which, together with (4.5), implies

$$(4.16) \qquad _{-1}^R D_x^\nu B_{\mu,j}^{(\nu)}(x) = \Big(\frac{1+x}{1+x_j} \Big)^{\mu-\nu} \bar{l}_j(x), \quad x \in (-1,1), \quad 1 \le j \le N,$$

where $\bar{l}_j(x)$ is defined in (3.8). Applying $_{-1}^R D_x^\nu$ to both sides of (4.15), and using (2.14) (with $s \to \nu, \alpha \to \nu - \mu$ and $\beta \to \mu - \nu$), we obtain

$$_{-1}^R D_x^\nu B_{\mu,j}^{(\nu)}(x) = \sum_{k=0}^{N-1} \breve{b}_{kj} \frac{\Gamma(k+\mu+1)}{\Gamma(k+\mu-\nu+1)} (1+x)^{\mu-\nu} P_k^{(\nu-\mu,\mu-\nu)}(x)$$
$$= \Big(\frac{1+x}{1+x_j} \Big)^{\mu-\nu} \sum_{k=0}^{N-1} \bar{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)} P_k^{(\nu-\mu,\mu-\nu)}(x),$$

where in the last step we used (4.16) and Lemma 3.1. Comparing the coefficients, we can find $\breve{s}_{kj}$ and obtain (4.7)–(4.8).

(ii) For $1 < \nu < 1 + \mu$, we first derive the formulas for $\{ B_{\mu,j}^{(\nu)} \}_{j=1}^{N-1}$. From (3.24), we find that $_{-1}^R D_x^\nu B_{\mu,j}^{(\nu)}(x) \in \mathcal{F}_N^{(\mu-\nu)}$, so by (4.6),

$$(4.17) \qquad _{-1}^R D_x^\nu B_{\mu,j}^{(\nu)}(x) = \frac{x+\tau_j}{x_j+\tau_j} \Big(\frac{1+x}{1+x_j} \Big)^{\mu-\nu} \hat{l}_j(x), \quad 1 \le j \le N-1,$$

where $\{ \hat{l}_j \}$ are the Lagrange interpolation basis polynomials associated with the interior JGL points $\{ x_j \}_{j=1}^{N-1}$ as in Lemma 3.2, and $\{ \tau_j \}$ are constants to be determined by the conditions $B_{\mu,j}^{(\nu)}(1) = 0$ later. By definition, $_{-1}^R D_x^\nu = D^2 {}_{-1} I_x^{2-\nu}$, so we have

$$(4.18) \qquad _{-1} I_x^{2-\nu} B_{\mu,j}^{(\nu)}(x) = C_j^{-1} {}_{-1} I_x^2 \{ (1+x)^{\mu-\nu+1} \hat{l}_j(x) + (\tau_j - 1)(1+x)^{\mu-\nu} \hat{l}_j(x) \}$$
$$+ A_1 + A_2(1+x),$$

where A_1 and A_2 are arbitrary constants, and $C_j = (x_j + \tau_j)(1 + x_j)^{\mu-\nu}$. Applying $_{-1}^{R}D_x^{2-\nu}$ to both sides of the above equation, and using the properties (cf. [12]) $_{-1}^{R}D_x^{2-\nu}\,_{-1}I_x^{2-\nu}v = v$ and $_{-1}^{R}D_x^{2-\nu}\,_{-1}I_x^2 = \,_{-1}I_x^{\nu}$, we obtain

$$
(4.19) \quad
\begin{aligned}
B_{\mu,j}^{(\nu)}(x) = & C_j^{-1}\,_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu+1}\hat{l}_j(x) + (\tau_j - 1)(1+x)^{\mu-\nu}\hat{l}_j(x)\big\} \\
& + \frac{A_1}{\Gamma(\nu-1)}(1+x)^{\nu-2} + \frac{A_2}{\Gamma(\nu)}(1+x)^{\nu-1},
\end{aligned}
$$

where we used the basic RL differential formula for 1 and $1 + x$. Then we infer that $A_1 = A_2 = 0$, as we require $B_{\mu,j}^{(\nu)} \in \mathcal{F}_N^{(\mu)}$. Imposing $B_{\mu,j}^{(\nu)}(1) = 0$ yields

$$
(4.20) \quad
\tau_j = 1 - \frac{_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu+1}\hat{l}_j(x)\big\}\big|_{x=1}}{_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu}\hat{l}_j(x)\big\}\big|_{x=1}}.
$$

We continue to evaluate the fractional integrals. By Lemma 3.2 and (2.13),

$$
(4.21)
$$
$$
\begin{aligned}
_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu+1}\hat{l}_j(x)\big\} &= \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu+1)}\,_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu+1}P_k^{(\nu-\mu,\mu-\nu+1)}(x)\big\} \\
&= \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu+1)} \frac{\Gamma(k+\mu-\nu+2)}{\Gamma(k+\mu+2)}(1+x)^{\mu+1}P_k^{(-\mu,\mu+1)}(x)
\end{aligned}
$$

and

$$
(4.22)
$$
$$
\begin{aligned}
_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu}\hat{l}_j(x)\big\} &= \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)}\,_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu}P_k^{(\nu-\mu,\mu-\nu)}(x)\big\} \\
&= \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)} \frac{\Gamma(k+\mu-\nu+1)}{\Gamma(k+\mu+1)}(1+x)^{\mu}P_k^{(-\mu,\mu)}(x).
\end{aligned}
$$

With these, we can obtain the formulas in (4.9)–(4.10).

We now turn to $B_{\mu,N}^{(\nu)}$. Note that by (4.6),

$$
(4.23) \quad
_{-1}^{R}D_x^{\nu} B_{\mu,N}^{(\nu)}(x) = \tau_N (1+x)^{\mu-\nu}\bar{l}_N(x),
$$

where τ_N will be determined by the boundary condition $B_{\mu,N}^{(\nu)}(1) = 1$. Following a process similar to the derivation of (4.19) and (4.22), we obtain

$$
\begin{aligned}
B_{\mu,N}^{(\nu)}(x) &= \tau_N\,_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu}\bar{l}_N(x)\big\} \\
&= \tau_N \sum_{k=0}^{N-1} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)}\,_{-1}I_x^{\nu}\big\{(1+x)^{\mu-\nu}P_k^{(\nu-\mu,\mu-\nu)}(x)\big\} \\
&= \tau_N \sum_{k=0}^{N-1} \hat{s}_{kj}^{(\alpha,\beta,\nu-\mu,\mu-\nu)} \frac{\Gamma(k+\mu-\nu+1)}{\Gamma(k+\mu+1)}(1+x)^{\mu}P_k^{(-\mu,\mu)}(x).
\end{aligned}
$$

Imposing $B_{\mu,N}^{(\nu)}(1) = 1$, we can determine τ_N and derive (4.11)–(4.12).

(ii) For $\nu = 1+\mu$, one verifies readily that $B_{\mu,N}^{(1+\mu)}(x)$ must be given by (4.14), so it suffices for us to derive (4.13). We infer from Lemma 2.2 that ${}_{-1}^{R}D_x^{1+\mu}B_{\mu,j}^{(1+\mu)} \in \mathbb{P}_{N-2}$, as $B_{\mu,j}^{(1+\mu)} \in \mathcal{F}_N^{(\mu)}$. Thus, the interpolating condition (4.6) and Lemma 2.1 imply that for $1 \le j \le N - 1$,

$$D^2 {}_{-1}I_x^{1-\mu}B_{\mu,j}^{(1+\mu)}(x) = {}_{-1}^{R}D_x^{1+\mu}B_{\mu,j}^{(1+\mu)}(x) = \hat{l}_j(x) = \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,1,1)} P_k^{(1,1)}(x).$$

Similar to (4.18), one has

$$_{-1}I_x^{1-\mu}B_{\mu,j}^{(1+\mu)}(x) = A_1 + A_2(1+x) + \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,1,1)} {}_{-1}I_x^2 P_k^{(1,1)}(x).$$

Applying ${}_{-1}^{R}D_x^{1-\mu}$ to both sides of the above identity leads to

$$(4.24) \quad B_{\mu,j}^{(1+\mu)}(x) = \frac{A_1(1+x)^{\mu-1}}{\Gamma(\mu)} + \frac{A_2(1+x)^\mu}{\Gamma(1+\mu)} + \sum_{k=0}^{N-2} \hat{s}_{kj}^{(\alpha,\beta,1,1)} {}_{-1}I_x^{1+\mu} P_k^{(1,1)}(x).$$

Requiring $B_{\mu,j}^{(1+\mu)} \in \mathcal{F}_N^{(\mu)}$ leads to $A_1 = 0$. Noting that

$$P_k^{(1,1)}(x) = \frac{2}{k+2} DP_{k+1}(x), \quad k \ge 0,$$

we have from (2.13) and (4.24) that

$$\begin{aligned}
_{-1}I_x^{1+\mu}P_k^{(1,1)}(x) &= \frac{2}{k+2}{}_{-1}I_x^\mu {}_{-1}I_x^1 DP_{k+1}(x) = \frac{2}{k+2}{}_{-1}I_x^\mu\big\{P_{k+1}(x) - P_{k+1}(-1)\big\} \\
&= \frac{2(-1)^k}{(k+2)\Gamma(1+\mu)}(1+x)^\mu + \frac{2}{k+2}{}_{-1}I_x^\mu P_{k+1}(x) \\
&= \frac{2(-1)^k}{(k+2)\Gamma(1+\mu)}(1+x)^\mu + \frac{2\Gamma(k+2)}{(k+2)\Gamma(k+\mu+2)}(1+x)^\mu P_{k+1}^{(-\mu,\mu)}(x).
\end{aligned}$$

Therefore, by (4.24),

$$\begin{aligned}
B_{\mu,j}^{(1+\mu)}(x) &= \frac{A_2(1+x)^\mu}{\Gamma(1+\mu)} \\
&\quad + (1+x)^\mu \sum_{k=0}^{N-2} \frac{2\hat{s}_{kj}^{(\alpha,\beta,1,1)}}{k+2}\left\{\frac{(-1)^k}{\Gamma(1+\mu)} + \frac{\Gamma(k+2)}{\Gamma(k+\mu+2)}P_{k+1}^{(-\mu,\mu)}(x)\right\}.
\end{aligned}$$

Setting $B_{\mu,j}^{(1+\mu)}(1) = 0$, one obtains

$$\frac{A_2}{\Gamma(1+\mu)} = -\sum_{k=0}^{N-2} \frac{2\hat{s}_{kj}^{(\alpha,\beta,1,1)}}{k+2}\left\{\frac{(-1)^k}{\Gamma(1+\mu)} + \frac{\Gamma(k+2)}{\Gamma(k+\mu+2)}P_{k+1}^{(-\mu,\mu)}(1)\right\}.$$

Then, the formula for $B_{\mu,j}^{(1+\mu)}$ with $1 \le j \le N-1$ in (4.13) is derived. $\square$

Introduce the matrices

$$(4.25) \qquad \boldsymbol{B}_\mu^{(\nu)} = \begin{cases} \left(\boldsymbol{B}_\mu^{(\nu)}\right)_{lj}, & 1 \le l, j \le N, & \text{if } \mu, \nu \in (0,1), \\ \left(\boldsymbol{B}_\mu^{(\nu)}\right)_{lj}, & 1 \le l, j \le N-1, & \text{if } \mu \in (0,1), \ 1 < \nu \le 1+\mu, \end{cases}$$

where $\left(\boldsymbol{B}_\mu^{(\nu)}\right)_{lj} = B_{\mu,j}^{(\nu)}(x_l)$.

THEOREM 4.2. *For $\mu \in (0,1)$, we have*

$$(4.26) \qquad \boldsymbol{D}_{\mu,\mathrm{in}}^{(\nu)} \boldsymbol{B}_{\mu}^{(\nu)} = \boldsymbol{B}_{\mu}^{(\nu)} \boldsymbol{D}_{\mu,\mathrm{in}}^{(\nu)} = \boldsymbol{I},$$

where $\boldsymbol{I}$ is the identity matrix of order N for $\nu \in (0,1)$ and of order $N-1$ for $1 < \nu \le 1 + \mu$.

Proof. We prove only the case $\nu \in (0,1)$ because the other case is similar. Since $B_{\mu,j}^{(\nu)} \in \mathcal{F}_N^{(\mu)}$, we can write

$$B_{\mu,j}^{(\nu)}(x) = \sum_{l=1}^{N} B_{\mu,j}^{(\nu)}(x_l)\bar{h}_l^{\mu}(x), \quad 1 \le j \le N,$$

where $\{\bar{h}_l^{\mu}\}$ are the defined in (3.8). Thus,

$${}_{-1}^{R}D_x^{\nu} B_{\mu,j}^{(\nu)}(x) = \sum_{l=1}^{N} B_{\mu,j}^{(\nu)}(x_l)\,{}_{-1}^{R}D_x^{\nu}\bar{h}_l^{\mu}(x).$$

Taking $x = x_i$ for $1 \le i \le N$ in the above equation, we obtain (4.26) from (4.6) directly. □

It is noteworthy that it is more natural (than polynomials in [8, 27, 20, 39]) to consider nonpolynomial approximation for FDEs because of the singular behavior of FDE solutions for smooth input data as already mentioned in the introductory section. Interested readers are referred to [5, 33] and the forthcoming analysis for theoretical evidence.

5. Fractional collocation schemes and error analysis. In this section, we present the fractional collocation schemes for fractional initial value and fractional boundary value problems (BVPs), using the new basis derived in section 4. We also conduct rigorous error analysis of the schemes at the Chebyshev points.

5.1. Fractional initial value problems of order $\boldsymbol{\nu \in (0,1)}$. In this section, we consider the fractional initial value problem (FIVP) of order $\nu \in (0,1)$:

$$(5.1) \qquad {}_{-1}^{R}D_t^{\nu}u(t) + q(t)u(t) = f(t), \quad t \in (-1,1]; \quad u(-1) = 0,$$

where $q(t)$ and $f(t)$ are continuous functions.

The following decomposition is useful for understanding the singularity of the solution of (5.1) so as to provide a guideline for the design of the collocation scheme. Hereafter, denote $I := (-1,1)$.

THEOREM 5.1. *Let u be the solution of* (5.1).
- *Assume $q(t) = 0$ and $f(t) \in C^m(I)$. Then*
(5.2)
$$u(t) = {}_{-1}I_t^{\nu}f(t) = (t+1)^{\nu}\left\{ \sum_{i=0}^{m-1} \frac{f^{(i)}(-1)}{\Gamma(\nu+i+1)}(t+1)^i + \frac{f^{(m)}(\xi_t)}{\Gamma(\nu+m+1)}(t+1)^m \right\}$$

for some $\xi_t \in (-1,t)$.
- *Assume $q(t) \ne 0$ and $q(t), f(t) \in C^m(I)$. Then, $u(t)$ has the decomposition*

$$(5.3) \qquad u(t) = \sum_{(i,j)\in\Upsilon_m^{\nu}} \tilde{\gamma}_{ij}(\nu)(t+1)^{i+\nu(j+1)}$$
$$+ \Phi(\xi_t;\nu)(t+1)^{\nu+m}, \quad t \in (-1,1), \ \xi_t \in (-1,t),$$

where $\Upsilon_m^\nu := \{(i,j) : i + j\nu < m, \ i, j \geq 0\}$, $\Phi(\cdot;\nu) \in C^0(I)$, *and* $\{\tilde{\gamma}_{ij}(\nu)\}$ *are some constants.*

Proof. We first consider the case with $q(t) = 0$. Since we have $u(t) = {}_{-1}I_t^\nu f(t)$, using integration by parts repeatedly leads to

$$
\begin{aligned}
(\ {}_{-1}I_t^\nu f)(t) &= \frac{1}{\Gamma(\nu)} \int_{-1}^t (t-s)^{\nu-1} f(s)\, ds = \frac{f(-1)(t+1)^\nu}{\Gamma(\nu+1)} \\
&\quad + \frac{1}{\Gamma(\nu+1)} \int_{-1}^t (t-s)^\nu f'(s)\, ds \\
&= \frac{f(-1)(t+1)^\nu}{\Gamma(\nu+1)} + \frac{f'(-1)(t+1)^{\nu+1}}{\Gamma(\nu+2)} + \frac{1}{\Gamma(\nu+2)} \int_{-1}^t (t-s)^{\nu+1} f''(s)\, ds \\
&= \cdots \\
&= \sum_{i=0}^{m-1} \frac{f^{(i)}(-1)(t+1)^{\nu+i}}{\Gamma(\nu+i+1)} + \frac{1}{\Gamma(\nu+m)} \int_{-1}^t (t-s)^{\nu+m-1} f^{(m)}(s)\, ds.
\end{aligned}
\tag{5.4}
$$

Then (5.2) follows from the mean value theorem of integration immediately.

We now turn to the second case. Since ${}_{-1}I_t^\nu \ {}_{-1}^R D_t^\nu$ is an identity operator with zero initial condition [26], we introduce $z(t) = {}_{-1}^R D_t^\nu u(t)$ and transform (5.1) into

$$
z(t) + \frac{q(t)}{\Gamma(\nu)} \int_{-1}^t (t-s)^{\nu-1} z(s)\, ds = f(t), \quad t \in I,
\tag{5.5}
$$

which is a Volterra integral equation of the second type with a weakly singular kernel. As (5.1) is equivalent to (5.5), we obtain from [5, Theorem 6.1.6] that

$$
z(t) = \sum_{(i,j) \in \Upsilon_m^\nu} \gamma_{ij}(\nu)(t+1)^{i+j\nu} + Z_m(t;\nu), \quad t \in I,
\tag{5.6}
$$

where $Z_m(\cdot;\nu) \in C^m(I)$, and $\{\gamma_{ij}(\nu)\}$ are constants. By (5.2) and (5.4), we have

$$
{}_{-1}I_t^\nu Z_m(t;\nu) = \sum_{i=0}^{m-1} \frac{Z_m^{(i)}(-1;\nu)}{\Gamma(\nu+i+1)} (t+1)^{i+\nu} + \frac{Z_m^{(m)}(\xi_t;\nu)}{\Gamma(\nu+m+1)} (t+1)^{\nu+m}.
\tag{5.7}
$$

Recall that (cf. [12])

$$
{}_{-1}I_t^\nu \left\{ (t+1)^{i+j\nu} \right\} = \frac{\Gamma(i+j\nu+1)}{\Gamma(\nu+i+j\nu+1)} (t+1)^{i+(j+1)\nu}.
\tag{5.8}
$$

Therefore, by (5.6)–(5.9),

$$
u(t) = {}_{-1}I_t^\nu z(t) = \sum_{(i,j) \in \Upsilon_m^\nu} \tilde{\gamma}_{ij}(\nu)(1+t)^{i+(j+1)\nu} + \frac{Z_m^{(m)}(\xi_t;\nu)}{\Gamma(\nu+m+1)} (t+1)^{\nu+m}.
\tag{5.9}
$$

Denoting $\Phi(t;\nu) = \dfrac{Z_m^{(m)}(t;\nu)}{\Gamma(\nu+m+1)}$, we obtain (5.3). $\qquad\square$

Remark 5.1. We highlight some implications of Theorem 5.1, which can guide the selection of the basis to best fit the singular factor.

- Observe from (5.2) that if $q = 0$, $u(t) = (t+1)^\nu \Psi(t)$ (where Ψ is smooth), so the use of JPFs [45] and general Jacobi functions [9] leads to spectrally accurate approximation when $f(t)$ is sufficiently smooth.
- If $q(t) = \lambda \neq 0$, the solution of (5.1) is given by (cf. [12])

$$(5.10) \qquad u(t) = \int_{-1}^{t} e_{\nu,\nu}(t - \tau; \lambda) f(\tau) \, d\tau = \sum_{k=0}^{\infty} (-\lambda)^k \big({}_{-1}I_t^{(k+1)\nu} f \big)(t),$$

where the involved Mittag–Leffler functions of two parameters are given by
(5.11)

$$e_{\alpha,\beta}(z; \lambda) := z^{\beta-1} E_{\alpha,\beta}(-\lambda z^\alpha), \quad E_{\alpha,\beta}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}, \quad \alpha, \beta > 0.$$

We therefore derive from (5.3) and (5.10) that

$$(5.12) \qquad u(t) = \sum_{k=0}^{\infty} (-\lambda)^k (t+1)^{(k+1)\nu} \Psi_{km}(t; \nu),$$

where $\Psi_{km}(t; \nu)$ denotes the summation in the brace of (5.2). This provide a more explicit formula than (5.3), when q is a nonzero constant.

5.1.1. Collocation schemes and error estimates. Theorem 5.1 implies that an appropriate collocation scheme for (5.1) is to find $u_N \in \mathcal{F}_N^{(\nu)}$ (cf. (4.1)) such that

$$(5.13) \qquad {}_{-1}^{R}D_t^\nu u_N(t_i) + q(t_i) u_N(t_i) = f(t_i), \quad 1 \leq i \leq N; \quad u_N(-1) = 0,$$

where $\{t_i\}$ are the JGL points. Hereafter, we restrict to the CGL points.

The linear system under *fractional Lagrange interpolation basis* $\{\bar{h}_j^\nu\}$ (cf. (4.15)) reads

$$(5.14) \qquad \big(\boldsymbol{D}_{\nu,\mathrm{in}}^{(\nu)} + \boldsymbol{Q} \big) \boldsymbol{u} = \boldsymbol{f},$$

where $\boldsymbol{D}_{\nu,\mathrm{in}}^{(\nu)}$ is defined as in (3.29), $\boldsymbol{Q} = \mathrm{diag}(q(t_1), q(t_2), \ldots, q(t_N))$, and

$$\boldsymbol{u} = (u_N(t_1), u_N(t_2), \ldots, u(t_N))^T, \quad \boldsymbol{f} = (f(t_1), f(t_2), \ldots, f(t_N))^T.$$

Thanks to Theorem 4.2, we can precondition (5.14) by using $\boldsymbol{B}_\nu^{(\nu)}$ and obtain that

$$(5.15) \qquad \big(\boldsymbol{I}_N + \boldsymbol{B}_\nu^{(\nu)} \boldsymbol{Q} \big) \boldsymbol{u} = \boldsymbol{B}_\nu^{(\nu)} \boldsymbol{f}.$$

Alternatively, changing the variable $\boldsymbol{u} = \boldsymbol{B}_\nu^{(\nu)} \boldsymbol{v}$, and using Theorem 4.2, we can rewrite (5.14) as

$$(5.16) \qquad \big(\boldsymbol{I}_N + \boldsymbol{Q} \boldsymbol{B}_\nu^{(\nu)} \big) \boldsymbol{v} = \boldsymbol{f},$$

which actually is the linear system of the collocation scheme (5.13) under the Birkhoff interpolation basis $\{B_{\nu,j}^{(\nu)}\}$ in (4.7).

Thanks to the relation between (5.1) and (5.5), we can use the analysis tools for the integral equations (cf. [19]) to conduct the L^∞-error estimate.

THEOREM 5.2. *Let u, u_N and z be defined in* (5.1), (5.13), *and* (5.5) *and $z_N = {}_{-1}D_t^\nu u_N(t)$. If $q, f \in C^m(I)$ with $I = (-1, 1)$, then we have*

$$(5.17) \quad \| {}_{-1}^R D_t^\nu u - {}_{-1}^R D_t^\nu u_N \|_\infty = \| z - z_N \|_\infty \le C(1 + \log N) \max \left\{ N^{-2\nu}, \, N^{1-m} \right\},$$

where the constant C is independent of N.

Proof. Note that $z_N(t) = {}_{-1}^R D_t^\nu u_N(t) \in \mathbb{P}_{N-1}$ is a polynomial (cf. (2.15)), which together with Lemma 2.1 leads to $u_N(t) = {}_{-1}I_t^\nu z_N(t)$. For notational simplicity, we denote

$$\mathcal{K}w(t) = \frac{q(t)}{\Gamma(\nu)} \int_{-1}^t (t - s)^{\nu-1} w(s) \, ds.$$

The scheme (5.13) is equivalent to

$$(5.18) \quad z_N(t_i) + \mathcal{K}z_N(t_i) = f(t_i), \quad 1 \le i \le N.$$

We can follow [19] (for the analysis of polynomial approximation to integral equations) to conduct the error analysis. Here, we just sketch the proof. By (5.5),

$$(5.19) \quad z(t_i) + \mathcal{K}z(t_i) = f(t_i), \quad 1 \le i \le N,$$

where $\{t_i\}_{i=0}^N$ (with $t_0 = -1$) are CGL points. Let $\mathbb{I}_{N-1}^C$ be the Chebyshev–Gauss–Radau interpolation operator at $\{t_i\}_{i=1}^N$. Then we have

$$\mathbb{I}_{N-1}^C z(t) - z_N(t) = \mathbb{I}_{N-1}^C \mathcal{K}e(t) \quad \forall \, t \in I,$$

where $e = z - z_N$. This leads to

$$e(t) = (I_1 + I_2)(t) + (\mathcal{K}e)(t), \quad \text{where} \quad I_1 := z - \mathbb{I}_{N-1}^C z, \quad I_2 := \mathbb{I}_{N-1}^C (\mathcal{K}e) - \mathcal{K}e.$$

It follows from the generalized Gronwall inequality that

$$(5.20) \quad \|e\|_\infty \le C(\|I_1\|_\infty + \|I_2\|_\infty)$$

for some constant C independent of N. It is noteworthy that the N-point Lebesgue constant of Chebyshev–Gauss–Radau interpolation is $\mathcal{O}(\log N)$[10, 29]. With some tedious calculation as in [19, Corollary 1 and Theorem 1] and using (5.6), we can show that

$$(5.21)$$
$$\|I_1\|_\infty \le C(1 + \log N) \max \left\{ N^{-2\nu}, \, N^{1-m} \right\}, \quad \|I_2\|_\infty \le C(1 + \log N)N^{-\nu} \|e\|_\infty.$$

Substituting (5.21) into (5.20), and noting that for sufficiently large N, the terms involving $\|e\|_\infty$ can be absorbed into the left-hand side, we obtain the desired estimates. □

Remark 5.2. The approximation of the leading singular factor in (5.3) leads to the error term $\mathcal{O}(N^{-2\nu})$, the approximation of the smoother function $\Phi(\xi_t; \nu)(t + 1)^{\nu+m}$ contributes the error term $\mathcal{O}(N^{1-m})$, and $\log N$ originates from the Lebesgue constant of the interpolation.

Remark 5.3. It is worth emphasizing that the approach we use to compute the approximation of $z(t)$ is essentially the iterated method recommended for integral equations in [3, p. 71] since

$$z_N^{it}(t_i) = f(t_i) - q(t_i)u_N(t_i) = f(t_i) - \mathcal{K}z_N(t_i), \quad 1 \le i \le N.$$

This simple iteration can always yield a more accurate approximation because

$$\mathbb{I}_{N-1}^{C} z_N^{it}(t) = \mathbb{I}_{N-1}^{C}[f(t) - q(t)u_N(t)] = z_N(t).$$

Note that the approximation space that $z_N^{it}(t)$ resides in is larger than the one for $z_N(t)$. Hence, the convergence rate of our numerical examples is higher than the one shown in Theorem 5.2, which is also confirmed by the numerical results below.

5.1.2. Numerical results. In order to test the efficiency and accuracy of our algorithms, we present below some numerical examples and compare the results obtained by the usual collocation scheme, preconditioned GJF approximation, and the method (Z-K method) in [45]. In the following tests, we choose $N = 8, 12, 16, 20, 24, 30, 60, 120, 240, 480$, and 960. The errors are measured in the norm $\|\cdot\|_\infty$.

Example 5.1. Consider

$$(5.22) \qquad {}_{-1}^{R}D_t^{\mu}u(t) = \sin(10t), \quad \mu \in (0,1), \ t \in (-1,1]; \quad u(-1) = 0.$$

From Theorem 5.1, we expect to obtain an exponential rate of convergence if we choose $\nu = \mu$. Here, we take $\mu = 0.8$ and use the "bicgstab" iterative solver of MATLAB to solve the final linear system. Since the true solution is unknown, we take the approximation when $N = 3840$ as the "true solution" to calculate numerical errors. Indeed, an exponential convergence rate is observed for our methods, whereas that of the Z-K method is $\mathcal{O}(N^{-1.6})$; see Figure 2. Furthermore, we can also observe that the condition number of usual collocation methods grows like $\mathcal{O}(N^{2\mu})$, while the preconditioned scheme remains a constant for all N. Indeed, the new scheme converges within 10 iterations, while the other two methods need more than 4000 iterations to converge to the expected accuracy.

Example 5.2. Consider

$$(5.23) \qquad {}_{-1}^{R}D_t^{\mu}u(t) + \sin(t)u(t) = 1, \quad \mu \in (0,1), \ t \in (-1,1]; \quad u(-1) = 0.$$

As in the previous example, we choose $\nu = \mu = 0.8$ in our algorithm and take the approximation when $N = 3840$ as the "true solution". Due to the different nature of singularity, we can only expect an algebraic decay of the errors. From Figure 3,
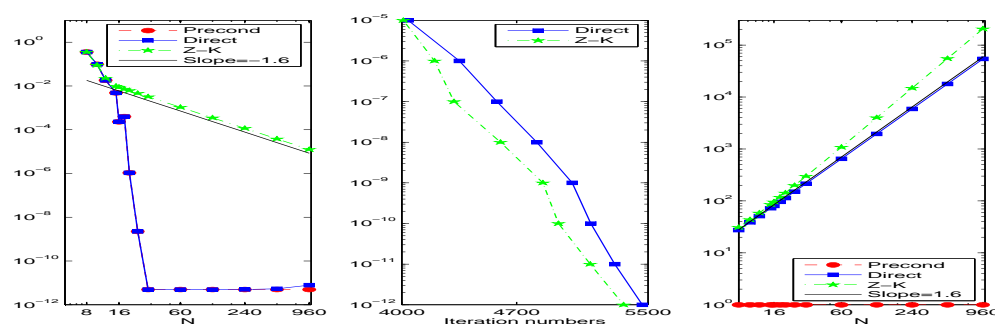

FIG. 2. *(Example* 5.1*) Left: L^∞-errors in log-log scale of the usual collocation scheme, its preconditioned collocation method, and, Z-K method [45] with respect to $\mu = \nu = 0.8$. Middle: iteration numbers of usual collocation and Z-K methods against errors for 960 collocation points (note that the preconditioned approach converges within 10 iterations). Right: plots of condition numbers of obtained linear system of these methods.*
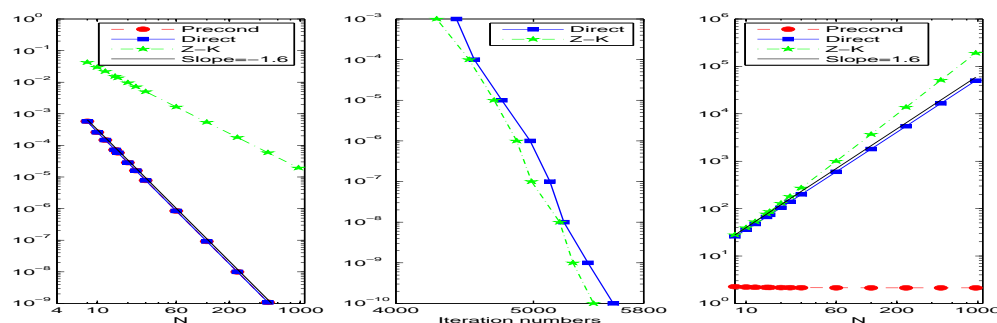
FIG. 3. *(Example* 5.2*) Left: L^∞-errors in log-log scale of the usual collocation scheme, its preconditioned collocation method, and, Z-K method [45] with respect to $\mu = \nu = 0.8$. Middle: iteration numbers of usual collocation and Z-K methods against errors for 960 collocation points (note that the preconditioned approach converges within 10 iterations). Right: plots of condition numbers of obtained linear system of these methods.*

we observe that the convergence rate of our methods is faster than that of the Z-K method, which is $\mathcal{O}(N^{-1.6})$. Moreover, as explained in Remark 5.3, the order is higher than the theoretical estimate in Theorem 5.2. On the other hand, to achieve the same numerical error, our preconditioned method only requires several iterations while others require thousands by using "bicgstab" as our linear system solver. We remark that the Z-K method should perform as well as the usual collocation method if $u'(-1) = 0$ as well.

5.2. Fractional BVPs of order $1 + \nu \in (1, 2)$. Now, we consider the BVP of order $1 + \nu \in (1, 2)$:

$$(5.24) \quad {}^{R}_{-1}D^{1+\nu}_t u(t) + q(t)u(t) = f(t), \quad t \in I = (-1, 1); \quad u(-1) = 0, \ u(1) = u_1,$$

where $q(t), f(t) \in C^m(I)$.

As with the previous study, we first examine the singular behavior of the solution based on the equivalent fractional integral formulation.

THEOREM 5.3. *Assume that $q(t), f(t) \in C^m(I)$. Then the solution $u(t)$ of (5.24) has the following decomposition:*
- *If $q(t) = 0$, then*

$$(5.25)$$
$$u(t) = \frac{(t+1)^\nu}{2^\nu}\Big\{u_1 - {}_{-1}I^{\nu+1}_t f(t)\big|_{t=1}\Big\}$$
$$+ (t+1)^{\nu+1}\Bigg\{\sum_{i=0}^{m-1} \frac{f^{(i)}(-1)}{\Gamma(\nu+i+2)}(t+1)^i + \frac{f^{(m)}(\xi_t)}{\Gamma(\nu+m+2)}(t+1)^m\Bigg\}$$

for some $\xi_t \in (-1, t)$.
- *If $q(t) \neq 0$, then*

$$(5.26) \quad u(t) = \sum_{i=0}^m \breve{\gamma}_i(\nu)(t+1)^{i+\nu} + \sum_{(i,j)\in\Upsilon^\nu_m} \tilde{\gamma}_{ij}(\nu)(1+t)^{i+1+(j+1)\nu}$$
$$+ G(\xi_t, \nu)(t+1)^{\nu+m+1},$$

where $\Upsilon_m^\nu := \{(i,j) : i+j\nu < m, \ i,j \geq 0\}$, $G(\cdot;\nu) \in C^0(I)$, *and* $\{\check{\gamma}_i(\nu), \tilde{\gamma}_{ij}(\nu)\}$ *are some constants.*

Proof. Let $z(t) = {}_{-1}^R D_t^\nu u(t)$. Since $u(-1) = 0$, we have

$$(5.27) \qquad\qquad u(t) = {}_{-1}I_t^\nu z(t).$$

Moreover, (5.24) can be transformed to

$$(5.28) \qquad \begin{aligned} z'(t) + \frac{q(t)}{\Gamma(\nu)} \int_{-1}^t (t-s)^{\nu-1} z(s) ds &= f(t), \\ \frac{1}{\Gamma(\nu)} \int_{-1}^1 (1-s)^{\nu-1} z(s) ds &= u(1) = u_1. \end{aligned}$$

If $q(t) = 0$, we have

$$(5.29) \qquad\qquad z(t) = z(-1) + \int_{-1}^t f(s)\, ds.$$

Inserting it into the second identity of (5.28), and using integration by parts, we find

$$(5.30) \qquad z(-1) = \frac{1}{2^\nu} \left(u_1 \Gamma(1+\nu) - \int_{-1}^1 (1-s)^\nu f(s) ds \right).$$

Hence, by (5.27), (5.29), and a direct calculation,

$$u(t) = {}_{-1}I_t^\nu z(t) = z(-1) \frac{(t+1)^\nu}{\Gamma(\nu+1)} + {}_{-1}I_t^{\nu+1} f(t).$$

Then (5.25) is a direct consequence of (5.2) and (5.30).

We now turn to the second case. Further let $w(t) = z'(t)$, and rewrite (5.28) as

$$(5.31) \qquad w(t) + \frac{q(t)}{\Gamma(\nu+1)} \int_{-1}^t (t-s)^\nu w(s) ds = f(t) - \frac{q(t)z(-1)}{\Gamma(\nu+1)} (t+1)^\nu,$$

where like (5.30), we have

$$(5.32) \qquad z(-1) = \frac{1}{2^\nu} \left(u_1 \Gamma(1+\nu) - \int_{-1}^1 (1-s)^\nu w(s) ds \right).$$

Note that $z(-1)$ is a well-defined constant by noting that $w(t) = {}_{-1}^R D_t^{1+\nu} u(t) = f(t) - q(t)u(t)$. Then we can derive from [7, Thm. 2.1] that

$$(5.33) \qquad w(t) = \sum_{(i,j)\in\Upsilon_m^\nu} \gamma_{ij}(\nu)(t+1)^{i+j\nu} + \phi_m(t;\nu),$$

where $\phi_m(\cdot;\nu) \in C^m(I)$, and $\{\gamma_{ij}(\nu)\}$ are constants. Therefore, $z(t)$ has the decomposition

$$(5.34) \qquad z(t) = \sum_{(i,j)\in\Upsilon_m^\nu} \hat{\gamma}_{ij}(\nu)(t+1)^{i+j\nu+1} + Z_{m+1}(t;\nu),$$

where $Z_{m+1}(\cdot; \nu) \in C^{m+1}(I)$. Like (5.7), we have

$$(5.35) \quad _{-1}I_t^\nu Z_{m+1}(t; \nu) = \sum_{i=0}^m \frac{Z_{m+1}^{(i)}(-1; \nu)}{\Gamma(\nu + i + 1)}(t+1)^{i+\nu} + \frac{Z_{m+1}^{(m+1)}(\xi_t; \nu)}{\Gamma(\nu + m + 1)}(t+1)^{\nu+m+1}.$$

Thanks to (5.27), we obtain from (5.8) and the above that we can apply the same argument for (5.3) to derive

$$
\begin{aligned}
u(t) = {}_{-1}I_t^\nu z(t) = & \sum_{(i,j)\in\Upsilon_m^\nu} \tilde{\gamma}_{ij}(\nu)(1+t)^{i+1+(j+1)\nu} \\
(5.36) \\
& + \sum_{i=0}^m \frac{Z_{m+1}^{(i)}(-1; \nu)}{\Gamma(\nu + i + 1)}(t+1)^{i+\nu} + \frac{Z_{m+1}^{(m+1)}(\xi_t; \nu)}{\Gamma(\nu + m + 1)}(t+1)^{\nu+m+1},
\end{aligned}
$$

which implies (5.26). $\qquad\square$

5.2.1. Collocation schemes and error estimates. From Theorem 5.3, one learns that the appropriate collocation scheme for (5.24) is to find $u_N \in \mathcal{F}_N^{(\nu)}$ such that

$$(5.37) \quad _{-1}^R D_t^{1+\nu} u_N(t_i) + q(t_i)u_N(t_i) = f(t_i), \quad 1 \le i \le N-1; \quad u_N(1) = u_1,$$

where $\{t_i\}$ are CGL points, and $u_N(-1) = 0$ is automatically met.

Let $\boldsymbol{D}_{\nu,\text{in}}^{(1+\nu)}$ be defined as in (3.29), and let $\boldsymbol{d} = (d_1, \ldots, d_{N-1})^T$ be the middle $(N-1)$ elements of the last column of (3.26). Set

$$
\begin{aligned}
(5.38) \quad & \boldsymbol{Q} = \text{diag}(q(t_1), q(t_2), \ldots, q(t_{N-1})), \quad \boldsymbol{u} = (u_N(t_1), u_N(t_2), \ldots, u(t_{N-1}))^T, \\
& \boldsymbol{f} = (f(t_1) - d_1 u_1, f(t_2) - d_2 u_1, \ldots, f(t_{N-1}) - d_{N-1} u_1)^T.
\end{aligned}
$$

The linear system under the fractional Lagrange interpolation basis $\{\bar{h}_j^\nu\}$ (cf. (4.15)) reads

$$(5.39) \quad \left(\boldsymbol{D}_{\nu,\text{in}}^{(1+\nu)} + \boldsymbol{Q}\right)\boldsymbol{u} = \boldsymbol{f}.$$

Thanks to Theorem 4.2, we can precondition the above system as

$$(5.40) \quad \left(\boldsymbol{I}_{N-1} + \boldsymbol{B}_\nu^{(1+\nu)}\boldsymbol{Q}\right)\boldsymbol{u} = \boldsymbol{B}_\nu^{(1+\nu)}\boldsymbol{f}.$$

Alternatively, changing the variable, $\boldsymbol{u} = \boldsymbol{B}_\nu^{(1+\nu)}\boldsymbol{v}$, and using Theorem 4.2, we can rewrite (5.39) as

$$(5.41) \quad \left(\boldsymbol{I}_{N-1} + \boldsymbol{Q}\boldsymbol{B}_\nu^{(1+\nu)}\right)\boldsymbol{v} = \boldsymbol{f},$$

which actually is the linear system of the collocation scheme (5.37) under the Birkhoff interpolation basis $\{B_{\nu,j}^{(1+\nu)}\}$ in (4.13).

THEOREM 5.4. *Let u and u_N be the solutions of* (5.24) *and* (5.37), *respectively. If $f, q \in C^m(I)$ with $m \ge 1$, we have*

$$(5.42) \quad \|_{-1}D_t^{1+\nu}u - {}_{-1}D_t^{1+\nu}u_N\|_\infty \le C(1 + \log N)\max\{N^{-2\nu}, N^{1-m}\},$$

where u is a positive constant independent of N and any function.

Proof. Inserting (5.32) into (5.31), we can obtain the mixed Volterra–Fredholm equation:

$$(5.43) \qquad w(t) + \frac{q(t)}{\Gamma(\nu+1)} \int_{-1}^{t} (t-s)^{\nu} w(s) ds - \frac{q(t)(t+1)^{\nu}}{\Gamma(\nu+1)2^{\nu}} \int_{-1}^{1} (1-s)^{\nu} w(s) ds$$
$$= f(t) - \frac{u_1 q(t)(t+1)^{\nu}}{2^{\nu}}.$$

For notational convenience, we denote

$$(5.44) \quad \mathcal{K}_1 w := \frac{q(t)}{\Gamma(\nu+1)} \int_{-1}^{t} (t-s)^{\nu} w(s) ds, \quad \mathcal{K}_2 w := \frac{q(t)(t+1)^{\nu}}{\Gamma(\nu+1)2^{\nu}} \int_{-1}^{1} (1-s)^{\nu} w(s) ds.$$

Both are compact operators from $L^{\infty}[-1,1]$ to $L^{\infty}[-1,1]$, and so is $\mathcal{K}_2 - \mathcal{K}_1$.

Since $u_N \in \mathcal{F}_N^{(\nu)}$, we infer from Lemma 2.2 that $w_N(t) = {}_{-1}D_t^{1+\nu} u_N \in \mathbb{P}_{N-2}$. Note that

$$w_N(t_i) + \mathcal{K}_1 w_N(t_i) - \mathcal{K}_2 w_N(t_i) = f(t_i) - \frac{u_1 q(t_i)(t_i+1)^{\nu}}{2^{\nu}}, \quad 1 \le i \le N-1.$$

One also verifies

$$w_N(t) + \mathcal{I}_{N-2}^C[\mathcal{K}_1 w_N] - \mathcal{I}_{N-2}^C[\mathcal{K}_2 w_N] = \mathcal{I}_{N-2}^C f - \frac{u_1}{2^{\nu}\Gamma(1+\nu)} \mathcal{I}_{N-2}^C[q(t)(t+1)^{\nu}],$$

where $\mathcal{I}_{N-2}^C$ is the interpolation operator associated with the $(N-1)$ "interior" CGL points. Similarly, the true solution satisfies

$$\mathcal{I}_{N-2}^C w + \mathcal{I}_{N-2}^C[\mathcal{K}_1 w] - \mathcal{I}_{N-2}^C[\mathcal{K}_2 w] = \mathcal{I}_{N-2}^C f - \frac{u_1}{2^{\nu}\Gamma(1+\nu)} \mathcal{I}_{N-2}^C[q(t)(t+1)^{\nu}].$$

Hence, letting $e_N = w - w_N$, we can obtain

$$\mathcal{I}_{N-2}^C w - w_N + \mathcal{I}_{N-2}^C[\mathcal{K}_1 e_N] - \mathcal{I}_{N-2}^C[\mathcal{K}_2 e_N] = 0.$$

Therefore,

$$e_N(t) = w(t) - \mathcal{I}_{N-2}^C w(t) + \mathcal{I}_{N-2}^C w(t) - w_N(t)$$
$$= w(t) - \mathcal{I}_{N-2}^C w(t) - \mathcal{I}_{N-2}^C[\mathcal{K}_1 e_N] + \mathcal{I}_{N-2}^C[\mathcal{K}_2 e_N]$$
$$= (\mathcal{K}_2 - \mathcal{K}_1)e_N + \underbrace{w(t) - \mathcal{I}_{N-2}^C w(t)}_{I_1} - \underbrace{(\mathcal{I}_{N-2}^C \mathcal{K}_1 - \mathcal{K}_1)e_N}_{I_2} + \underbrace{(\mathcal{I}_{N-2}^C \mathcal{K}_2 - \mathcal{K}_2)e_N}_{I_3}.$$

By the Fredholm alternative, there exists a constant C independent of N and any function such that

$$(5.45) \qquad \|e_N\|_{\infty} \le C(\|I_1\|_{\infty} + \|I_2\|_{\infty} + \|I_3\|_{\infty}).$$

From [19, Thm. 2], we obtain

$$(5.46)$$
$$\|I_1\|_{\infty} \le C(1 + \log N) \max\{N^{-2\nu}, N^{1-m}\}, \quad \|I_2\|_{\infty} \le C(1 + \log N) N^{-\nu} \|e_N\|_{\infty}.$$

We now deal with I_3. We first show that $Q(t) = q(t)(t+1)^{\nu}$ is Holder continuous with index ν in the same that

$$(5.47) \qquad |Q(t_1) - Q(t_2)| \le C|t_1 - t_2|^{\nu} \quad \forall t_1, t_2 \in [-1,1].$$

To verify this, we denote $t = t_1$ and $t_2 = t + h$ and assume that $h > 0$. It is evident that

$$|Q(t + h) - Q(t)| \leq |q(t + h)[(t + 1 + h)^\nu - (t + 1)^\nu]| + |(t + 1)^\nu[q(t + h) - q(t)]|$$
$$\leq q_{max}|W(t)| + 2^\nu|q'(\xi)|h,$$

where $q_{max} := \max_{t \in [-1,1]}|q(t)|$ and $W(t) := (t+1+h)^\nu - (t+1)^\nu$. One verifies readily that $W'(t) < 0$ for $t \in [-1, 1]$ and $\nu \in (0, 1)$, so $W(t) \leq W(-1) = h^\nu$. Then we can claim (5.47). With this, the Jackson's theorem [11, Thm. 13.3.7] implies there exists a best polynomial $\pi_N Q(t)$ such that

$$\|Q - \pi_N Q\|_\infty \leq CN^{-\nu}.$$

Then using the result on the Lebesgue constant, we have

$$(5.48) \quad \|Q(t) - \mathcal{I}_{N-2}^C Q(t)]\|_\infty \leq (1 + \|\mathcal{I}_{N-2}^C\|_\infty)\|Q - \pi_N Q\|_\infty \leq C(1 + \log N)N^{-\nu}.$$

Therefore,

$$\|I_3\|_\infty = \frac{1}{2^\nu \Gamma(\nu + 1)}\|Q(t) - \mathcal{I}_{N-2}^C Q(t)]\|_\infty \left|\int_{-1}^1 (1 - s)^\nu e_N(s)ds\right|$$
$$(5.49) \qquad\qquad \leq C(1 + \log N)N^{-\nu}\|e_N\|_\infty.$$

Now, substituting (5.46) and (5.49) into (5.45), we find that for N sufficiently large, the terms involving $\|e\|_\infty$ can be absorbed into the left-hand side, so the estimate (5.42) follows.   □

5.2.2. Numerical results. We provide some numerical results and also compare with the collocation methods using nodal JPF approximation (Z-K method) in [45] in (3.1) with $\mu = \nu$. It is noteworthy that the numerical results therein were for given exact solutions with singular $f(x)$. Below, we mostly consider the fractional BVPs with smooth $f(x)$. Note that in the following figures, the samples of N are the same as for the previous FIVPs.

Example 5.3. Consider the fractional BVP:

$$_{-1}^R D_t^{1+\nu} u(t) = \cos t, \ \nu \in (0, 1), \ t \in (-1, 1); \quad u(\pm 1) = 0.$$

With understanding of the singularity of the solution in (5.25), we expect the collocation scheme (5.37) leading to spectrally accurate approximation. Indeed, we observe from Figure 4 (leftmost) (where the reference "exact" solution is computed by a large number of points as with the previous two examples) that the errors of (5.39) and (5.40) decay exponentially, though the former suffers from severe round-off errors as the conditioning of its system behaves like $O(N^{2+2\nu})$ (see Figure 4 (rightmost)). Indeed, we also observe that only a few iterations are needed for the system (5.40) to converge.

Example 5.4. Consider the fractional BVP:

$$_{-1}^R D_t^{1+\nu} u(t) + e^t u(t) = \sin t, \quad \nu \in (0, 1), \ t \in (-1, 1); \quad u(\pm 1) = 0.$$

We see from Theorems 5.3 and 5.4 that an algebraic convergence is expected for the collocation scheme, which can be clearly observed from Figure 5. Once again, the collocation scheme involving the fractional Birkhoff basis in (5.40) performs significantly better than its counterparts, so it leads to a stable computation even for large N.
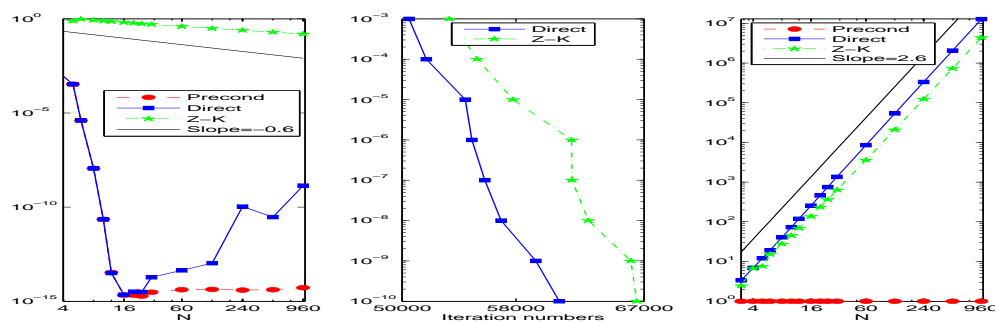
FIG. 4. *(Example 5.3) Left: L^∞-errors in log-log scale of the usual collocation method* (5.39), *its preconditioned collocation method* (5.40), *and the Z-K method* [45] *with respect to $\nu = 0.3$. Middle: iteration numbers of usual collocation and Z-K methods against errors for* 960 *collocation points (note that the preconditioned approach converges within* 10 *iterations). Right: plots of condition numbers of the linear systems of these methods.*
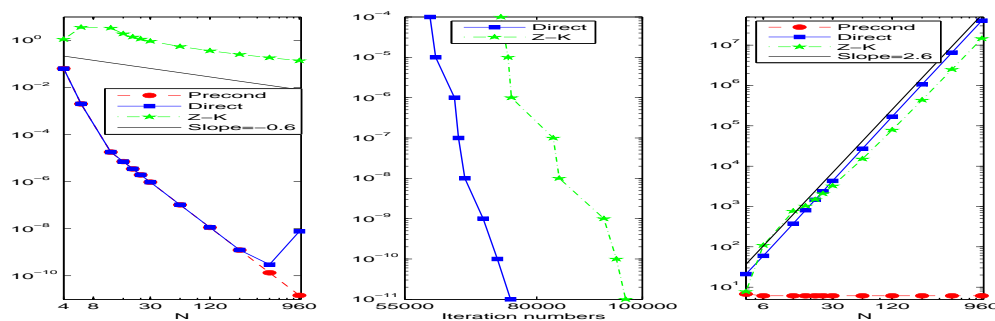

FIG. 5. *(Example 5.4) Left: L^∞-errors in log-log scale of the usual collocation method* (5.39), *its preconditioned collocation method* (5.40), *and the Z-K method* [45] *with respect to $\nu = 0.3$. Middle: iteration numbers of usual collocation and Z-K methods against errors for* 960 *collocation points (note that the preconditioned approach converges within* 10 *iterations). Right: plots of condition numbers of obtained linear system of three methods.*

5.3. Discussions and remarks. To have more insight into the proposed nonpolynomial approach, we compare the approximability of the nodal GJFs and usual polynomial basis functions in approximating typical singular solutions.

Let $\omega^a(x) = (1-x^2)^a$, and define the L^2_ω-orthogonal projection $\pi^C_N : L^2_{\omega^{-1/2}}(-1,1) \to \mathbb{P}_N$:

$$(5.50) \qquad \left(\pi^C_N u - u, v_N\right)_{\omega^{-1/2}} = 0 \quad \forall\, v_N \in \mathbb{P}_N,$$

where $(\cdot,\cdot)_{\omega^{-1/2}}$ is the inner product of $L^2_{\omega^{-1/2}}(-1,1)$. Recall the optimal estimate on Chebyshev polynomial approximation (see, e.g., [35, Thm 3.35]): *if $u^{(l)} \in L^2_{\omega^{l-1/2}}(-1,1)$ for all $0 \le l \le m$, then we have*

$$(5.51) \qquad \left\|\pi^C_N u - u\right\|_{\omega^{-1/2}} \le cN^{-m}\left\|u^{(m)}\right\|_{\omega^{m-1/2}},$$

where C is a positive constant independent of u and N.

We now consider approximation by nonpolynomial basis functions of $\mathcal{F}_N^{(\nu)}$ defined in (4.1). Note that

$$\hat{\pi}_N^\nu u = (1+x)^\nu \pi_{N-1}^C \big((1+x)^{-\nu} u \big) \in \mathcal{F}_N^{(\nu)}. \tag{5.52}$$

One verifies readily that it is an orthogonal projection in the sense

$$\big(\hat{\pi}_N^\nu u - u, w_N \big)_{\omega^{-1/2}} = 0, \quad \forall\, w_N \in \mathcal{F}_N^{(\nu)}, \tag{5.53}$$

since $(1+x)^{-\nu} w_N \in \mathbb{P}_{N-1}$ and by (5.50)–(5.52),

$$\big(\hat{\pi}_N^\nu u - u, w_N \big)_{\omega^{-1/2}} = \big(\pi_{N-1}^C \big((1+x)^{-\nu} u \big) - (1+x)^{-\nu} u, (1+x)^{-\nu} w_N \big)_{\omega^{-1/2}} = 0.$$

Thus, by (5.51)–(5.52), we derive that for $\nu > 0$,

$$\begin{aligned} \big\| \hat{\pi}_N^\nu u - u \big\|_{\omega^{-1/2}} &\le \big\| (1+x)^{-\nu} (\hat{\pi}_N^\nu u - u) \big\|_{\omega^{-1/2}} \\ &= \big\| \pi_{N-1}^C \big((1+x)^{-\nu} u \big) - (1+x)^{-\nu} u \big\|_{\omega^{-1/2}} \\ &\le c N^{-m} \big\| ((1+x)^{-\nu} u)^{(m)} \big\|_{\omega^{m-1/2}}. \end{aligned} \tag{5.54}$$

We see that the convergence rate of the nonpolynomial approximation of u turns out to be the same as the polynomial approximation of $(1+x)^{-\nu} u$.

As an example, we examine the convergence rates of two approaches in approximating the one-sided singular function:

$$u(x) = (1+x)^\nu g_1(x) + (1+x)^{\nu+\varrho} g_2(x) + (1+x) g_3(x), \quad 0 < \nu < 1, \ \varrho > 0, \tag{5.55}$$

where $\{g_i\}_{i=1}^3$ are smooth functions. We add the factor $(1+x)$ before g_3 so that u meets the homogeneous initial condition. A direct calculation shows that

- if $m < 2\nu + 1/2$, then $\|u^{(m)}\|_{\omega^{m-1/2}} < \infty$;
- If $m < 2\min\{\varrho, 1-\nu\} + 1/2$, then $\|((1+x)^{-\nu} u)^{(m)}\|_{\omega^{m-1/2}} < \infty$.

Thus, it is expected that if $\varrho > \nu$ (when $g_2 \ne 0$) and $\nu < 1/2$ (when $g_3 \ne 0$), the nonpolynomial approximation leads to a higher convergence rate. In other words, the nonpolynomial approach outperforms its counterpart for small ν. Note that if $g_2 = g_3 = 0$, then $(1+x)^{-\nu} u = g_1(x)$, so the nonpolynomial approximation can achieve spectral accuracy if g_1 is sufficiently smooth.

We next compare the convergence of two approaches for two FIVPs of small-order ν with (i) a singular exact solution and a singular source term, and (ii) a smooth source term (so the solution is singular), respectively.

Example 5.5. Consider the FIVP

$$_{-1}^R D_t^\nu u(t) + e^t u(t) = f(t), \quad t \in (-1, 1]; \quad u(-1) = 0, \tag{5.56}$$

where $f(t)$ is chosen so that the exact solution $u(t) = (1+t)^\nu \cos(\pi t) + (1+t)^{3.8} + (1+t)$ with $\nu = 0.1$.

In Figure 6 (left), we plot the L^∞-errors against various $N = 20, 24, 30, 60, 120, 240, 480, 960$ in log-log scale for both the polynomial and nodal GJF approximations. We observe that for small ν, the proposed GJF spectral method has a much faster convergence rate than the usual polynomial-based spectral scheme.

Example 5.6. Consider the FIVP

$$_{-1}^R D_t^\nu u(t) + \sin(\pi t) u(t) = 1, \quad t \in (-1, 1]; \quad u(-1) = 0, \tag{5.57}$$
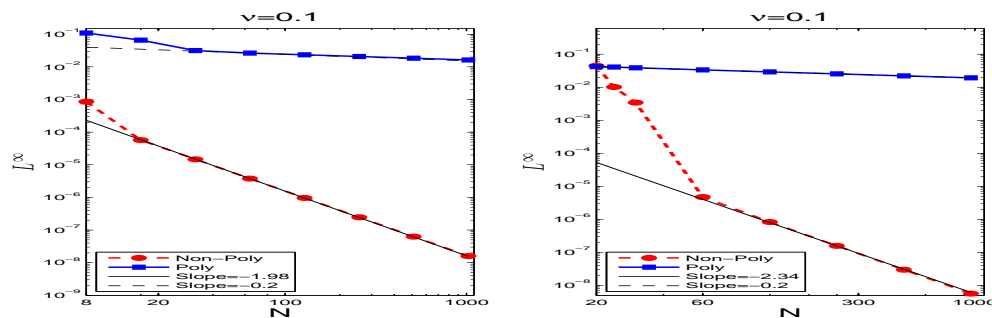
with $\nu = 0.1$.

FIG. 6. *Left: Example* 5.5 *and Right: Example* 5.6. L^∞*-errors against* N *in* log-log *scale obtained by the proposed nodal GJF-collocation scheme, and the polynomial approximation.*

As before, we consider the numerical solution obtained by the preconditioned method with $N = 3840$ as the "true" solution. In Figure 6 (right), we depict the errors for various N as in the previous example. Once again, we observe a much faster convergence rate for the new approach.

To conclude the paper, we reiterate some advantages of using global spectral methods over the local low-order methods. Compared with finite difference and finite element approximations, the spectral grids are denser and basis functions oscillate more near the boundaries, so the spectral approximation can better resolve singular solutions. From the theoretical point of view, it is known that the approximation results on piecewise polynomials are in nonweighted spaces, so the singular functions have much lower regularity in such spaces, which should be in contrast to the weighted bounds in (5.50) and (5.54).

On the other hand, there exist useful fractional calculus formulas for orthogonal polynomials and GJFs (see, e.g., Lemma 2.1), which significantly facilitate the implementation of spectral methods.

REFERENCES

[1] M. ABRAMOWITZ AND I. A. STEGUN, *Handbook of Mathematical Functions*, Dover, New York, 1972.

[2] G. E. ANDREWS, R. ASKEY, AND R. ROY, *Special Functions*, Encyclopedia Math. its Appl. 71, Cambridge University Press, Cambridge, UK, 1999.

[3] K. ATKINSON, *The Numerical Solution of Integral Equation of the Second Kind*, Cambridge University Press, Cambridge, UK, 1997.

[4] H. BATEMAN, *The solution of linear differential equations by means of definite integrals*, Trans. Camb. Phil. Soc., 21 (1909), pp. 171–196.

[5] H. BRUNNER, *Collocation Methods for Volterra and Related Functional Differential Equations*, Cambridge University Press, Cambridge, UK, 2004.

[6] L. CAGLIERO AND T. H. KOORNWINDER, *Explicit matrix inverses for lower triangular matrices with entries involving Jacobi polynomials*, J. Approx. Theory, 193 (2015), pp. 20–38.

[7] Y. CAO, T. HERDMAN, AND Y. XU, *A hybrid collocation method for Volterra integral equations with weakly singular kernels*, SIAM J. Numer. Anal., 41 (2003), pp. 364–381.

[8] F. CHEN, Q. XU, AND J. HESTHAVEN, *A multi-domain spectral method for time-fractional differential equations*, J. Comput. Phys., 293 (2015), pp. 157–172.

[9] S. CHEN, J. SHEN, AND L. L. WANG, *Generalized Jacobi functions and their applications to fractional differential equations*, Math. Comp., 85 (2016), pp. 1603–1638.

[10] Y. P. CHEN AND T. TANG, *Convergence analysis of the Jacobi spectral-collocation methods for Volterra integral equations with a weakly singular kernel*, Math. Comp., 79 (2010), pp. 147–167.

[11] P. J. DAVIS, *Interpolation and Approximation*, Dover, New York, 1975.

[12] K. DIETHELM, *The Analysis of Fractional Differential Equations*, Lecture Notes in Math., 2004, Springer, Berlin, 2010.

[13] Q. DU, M. GUNZBURGER, R. B. LEHOUCQ, AND K. ZHOU, *Analysis and approximation of nonlocal diffusion problems with volume constraints*, SIAM Rev., 54 (2012), pp. 667–696.

[14] M. E. ELBARBARY, *Integration preconditioning matrix for ultraspherical pseudospectral operators*, SIAM J. Sci. Comput., 28 (2006), pp. 1186–1201.

[15] V. J. ERVIN, N. HEUER, AND J. P. ROOP, *Numerical approximation of a time dependent, nonlinear, space-fractional diffusion equation*, SIAM J. Numer. Anal., 45 (2007), pp. 572–591.

[16] V. J. ERVIN AND J. P. ROOP, *Variational solution of fractional advection dispersion equations on bounded domains in $\mathbb{R}^d$*, Numer. Methods Partial Differential Equations, 23 (2007), pp. 256–281.

[17] B. Y. GUO, J. SHEN, AND L. L. WANG, *Generalized Jacobi polynomials/functions and their applications*, Appl. Numer. Math., 59 (2009), pp. 1011–1028.

[18] J. HESTHAVEN, *Integration preconditioning of pseudospectral operators. I. Basic linear operators*, SIAM J. Numer. Anal., 35 (1998), pp. 1571–1593.

[19] C. HUANG AND M. STYNES, *A spectral collocation method for a weakly singular Volterra integral equation of the second kind*, Adv. Comput. Math. (2016), doi:10.1007/s10444-016-9451-6.

[20] Y. JIAO, L. L. WANG, AND C. HUANG, *Well-conditioned fractional collocation methods using fractional Birkhoff interpolation basis*, J. Comput. Phys., 305 (2016), pp. 1–28.

[21] B. T. JIN, R. LAZAROV, AND Z. ZHOU, *Error estimates for a semidiscrete finite element method for fractional order parabolic equations*, SIAM J. Numer. Anal., 51 (2013), pp. 445–466.

[22] R. KOEKOEK, P. LESKY, AND R. SWARTTOUW, *Hypergeometric Orthogonal Polynomials and Their q-Analogues*, Springer, New York, 2010.

[23] N. KOPTEVA AND M. STYNES, *Analysis and numerical solution of a Riemann-Liouville fractional derivative two-point boundary value problem*, Adv. Comput. Math. (2016), doi:10.1007/s10444-016-9476-x.

[24] N. KOPTEVA AND M. STYNES, *An efficient collocation method for a Caputo two-point boundary value problem*, BIT, 55 (2015), pp. 1105–1123.

[25] A. KUIJLAARS, A. MARTINEZ-FINKELSHTEIN, AND R. ORIVE, *Orthogonality of Jacobi polynomials with general parameters*, Electron. Trans. Numer. Anal., 19 (2005), pp. 1–17.

[26] C. LI AND W. DENG, *Remarks on fractional derivatives*, Appl. Math. Comput., 187 (2007), pp. 777–784.

[27] X. LI AND C. XU, *A space-time spectral method for the time fractional diffusion equation*, SIAM J. Numer. Anal., 47 (2009), pp. 2108–2131.

[28] F. LIU, V. ANH, AND I. TURNER, *Numerical solution of the space fractional Fokker-Planck equation*, J. Comput. Appl. Math., 166 (2004), pp. 209–219.

[29] G. MASTROIANNI AND D. OCCORSIO, *Optimal systems of nodes for Lagrange interpolation on bounded intervals. A survey*, J. Comput. Appl. Math., 134 (2001), pp. 325–341.

[30] M. M. MEERSCHAERT, H. P. SCHEFFLER, AND C. TADJERAN, *Finite difference methods for two-dimensional fractional dispersion equation*, J. Comput. Phys., 211 (2006), pp. 249–261.

[31] M. M. MEERSCHAERT AND C. TADJERAN, *Finite difference approximations for fractional advection-dispersion flow equations*, J. Comput. Appl. Math., 172 (2004), pp. 65–77.

[32] R. METZLER AND J. KLAFTER, *The random walk's guide to anomalous diffusion: A fractional dynamics approach*, Phys. Reports, 339 (2000), pp. 1–77.

[33] A. PEDAS AND E. TAMME, *Piecewise polynomial collocation for linear boundary value problems of fractional differential equations*, J. Comput. Appl. Math., 236 (2012), pp. 3349–3359.

[34] I. PODLUBNY, *Fractional Differential Equations*, Math. Sci. Engrg. 198, Academic Press, San Diego, CA, 1999.

[35] J. SHEN, T. TANG, AND L. L. WANG, *Spectral Methods: Algorithms, Analysis and Applications*, Ser. Comput. Math. 41, Springer-Verlag, Berlin, 2011.

[36] Z. Z. SUN AND X. N. WU, *A fully discrete difference scheme for a diffusion-wave system*, Appl. Numer. Math., 56 (2006), pp. 193–209.

[37] G. SZEGÖ, *Orthogonal Polynomials*, 4th ed., AMS, Providence, RI, 1975.

[38] C. Tadjeran and M. M. Meerschaert, *A second-order accurate numerical method for the two-dimensional fractional diffusion equation*, J. Comput. Phys., 220 (2007), pp. 813–823.

[39] W. Tian, W. Deng, and Y. Wu, *Polynomial spectral collocation method for space fractional advection-diffusion equation*, Numer. Methods Partial Differential Equations, 30 (2014), pp. 514–535.

[40] H. Wang and D. Yang, *Well posedness of variable coefficient conservative fractional elliptic differential equations*, SIAM J. Numer. Anal., 51 (2013), pp. 1088–1107.

[41] H. Wang, D. Yang, and S. Zhu, *Inhomogeneous Dirichlet boundary-value problems of space-fractional diffusion equations and their finite element approximations*, SIAM J. Numer. Anal., 52 (2014), pp. 1292–1310.

[42] L. L. Wang, M. D. Samson, and X. D. Zhao, *A well-conditioned collocation method using a pseudospectral integration matrix*, SIAM J. Sci. Comput., 36 (2014), pp. A907–A929.

[43] M. Zayernouri and G. E. Karniadakis, *Fractional Sturm–Liouville eigen-problems: Theory and numerical approximation*, J. Comput. Phys., 252 (2013), pp. 495–517.

[44] M. Zayernouri and G. E. Karniadakis, *Exponentially accurate spectral and spectral element methods for fractional ODEs*, J. Comput. Phys., 257 (2014), pp. 460–480.

[45] M. Zayernouri and G. E. Karniadakis, *Fractional spectral collocation method*, SIAM J. Sci. Comput., 38 (2014), pp. A40–A62.