Stable Multi-domain Spectral Penalty Methods for Fractional Partial Differential Equation

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Abstract

We introduce stable multi-domain spectral penalty methods suitable for solving fractional partial differential equations with fractional derivatives of any order. The fractional derivative is approximated in each sub domain using orthogonal polynomials and stability of the scheme is achieved through weakly imposed boundary and interface conditions by using a penalty term. We discuss accuracy and stability of the scheme and prove that the accuracy depends on the order of the fractional derivative. The analysis is illustrated through numerical examples, including fractional advection and diffusion problems.

Keywords: fractional derivative, fractional partial differential equation, fractional differential matrix, multi-domain spectral method, penalty method

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1. Introduction

The basic ideas behind fractional calculus has a history similar to and aligned with that of more classic calculus and the topic has attracted the interests of mathematicians who contributed fundamentally to the development of classical calculus, including L'Hospital, Leibniz, Liouville, Riemann, Grünward, and Letnikov [7]. In spite of this, the development and analysis of fractional calculus and fractional differential equations is less mature than that associated with classical calculus. However, during the last decade it has become increasingly clear that fractional calculus naturally emerges as a tool for the description of a broad range of non-classical phenomena in the applied sciences and engineering [10, 17, 25]. A striking example of this is a model for anomalous transport processes and diffusion, leading to fractional partial differential equations [6, 22] but other examples

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are readily available for the modeling of frequency dependent damping behavior of many viscoelastic materials [13, 3, 4], continuum and statistical mechanics [20], solid mechanics [24], economics [5], and anomalous transport [21].

With this expanding range of applications and models based on fractional calculus comes a need for the development of robust and accurate computational methods for solving these equations. However, a fundamental difference between problems in classic calculus and fractional calculus is the global nature of the latter operators, often resulting in computational techniques that are substantially more resource intense than those associated with more classic problems. Nevertheless, methods based on finite difference methods [27] and finite element formulations [11, 12] have been developed and successfully applied. On the other hand, solutions of fractional diffusion problem are generally endowed with substantial smoothness, suggesting that higher order accurate global methods may be attractive alternatives to more traditional techniques yet there appears to be very limited work in this direction. A few notable exceptions are [19, 9, 18] in which global spectral methods are used to discretize classical space derivative to solve time fractional PDEs and confirms the possible advantages of doing so.

In this work we introduce stable spectral multi-domain methods suitable for the approximation of spatial fractional derivatives of arbitrary order. These developments are based on classic spectral methods as discussed in [16], utilizing orthogonal polynomials and introduce the notion of differentiation matrices based on the associated Gauss quadrature points. With the basics of the approximation being developed for a single element, we present a stable spectral multi-domain approach based on weakly imposed boundary conditions through a penalty term [14, 15]. The outcome is a flexible and accurate family of schemes that can be applied to the modeling of fractional partial differential equations of arbitrary order and we shall demonstrate its application to fractional advection and diffusion problems.

What remains is organized as follows. In Sec. 2 we offer some background material on fractional derivatives with a particular focus on the Caputo definition which subsequently focus on. In Sec. 3 we introduce Jacobi polynomials and apply these to express the discrete approximation of the fractional derivative through differentiation matrices and discuss the approximation properties of this formulation. This sets the stage for Sec. 4 where we propose multi-domain methods for solving fractional advection and diffusion problems and establish the stability of these penalty schemes. We also illustrate the performance of the schemes before concluding in Sec. 5 with a brief overview and outlook.

2. Fractional calculus, definitions, and basic properties

One of the complications associated with fractional derivatives is that there are several definitions of exactly what a fractional derivative means [23]. If we consider the function $f(x) \in C^n[0, b]$, then the Riemann-Liouville fractional derivative of order $\alpha \, (n-1 < \alpha \leqslant$

$n, n \in \mathbb{N}$) is of the form,

$$ {}_{0}^{RL}D_x^{\alpha} f(x) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_0^x \frac{f(\tau)}{(x-\tau)^{\alpha+1-n}} d\tau & n-1 < \alpha < n \\ f^{(n)}(x) & \alpha = n \end{cases} \tag{1} $$

An alternative definition, known as the Caputo fractional derivative, is defined as

$$ {}_{0}D_x^{\alpha} f(x) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \int_0^x \frac{f^{(n)}(\tau)}{(x-\tau)^{\alpha+1-n}} d\tau & n-1 < \alpha < n \\ f^{(n)}(x) & \alpha = n \end{cases} \tag{2} $$

These two definitions are not generally equivalent but they are related as

$$ {}_{0}D_x^{\alpha} f(x) = {}_{0}^{RL}D_x^{\alpha} f(x) - \sum_{\mu=0}^{n-1} \frac{x^{\mu-\alpha} f^{(\mu)}(0)}{\Gamma(\mu+1-\alpha)}. \tag{3} $$

One easily realizes the equivalence between the two for $f^{(\mu)}(0), \mu = 0, \ldots, n-1$. The Caputo definition is often preferred when considered in the context of differential equations since it allows for imposing initial and boundary conditions on classic derivatives. For the Riemann-Liouville definition, such conditions must be imposed on fractional derivatives which is often not available. For this reason we shall also focus on the Caputo definition in this work.

For the Caputo derivative, we have the following important properties [23],

Lemma 2.1.

$$ {}_{0}D_x^{\alpha} C = 0, \alpha > 0, C \textit{ is a constant.} \tag{4} $$

$$ {}_{0}D_x^{\alpha} (f(x) + g(x)) = {}_{0}D_x^{\alpha} f(x) + {}_{0}D_x^{\alpha} g(x) \tag{5} $$

$$ {}_{0}D_x^{\alpha} x^{\gamma} = \begin{cases} 0, \alpha > \gamma, \\ \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1-\alpha)} x^{\gamma-\alpha}, 0 < \alpha \leqslant \gamma. \end{cases} \tag{6} $$

At times, (1) and (2) are referred to as the left Riemann-Liouville derivative and left Caputo's derivative, respectively. In a similar fashion, one can likewise define the right Riemann-Liouville and Caputo's derivative as

$$ {}_{x}^{RL}D_b^{\alpha} f(x) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \left(-\frac{d}{dx}\right)^n \int_x^b \frac{f(\tau)}{(x-\tau)^{\alpha+1-n}} d\tau & n-1 < \alpha < n \\ (-1)^n f^{(n)}(x) & \alpha = n \end{cases} \tag{7} $$

$$ {}_{x}D_b^{\alpha} f(x) = \begin{cases} \frac{1}{\Gamma(n-\alpha)} \int_x^b \frac{(-1)^n f^{(n)}(\tau)}{(x-\tau)^{\alpha+1-n}} d\tau & n-1 < \alpha < n \\ (-1)^n f^{(n)}(x) & \alpha = n \end{cases} \tag{8} $$

We can verify that left fractional derivative and right fractional derivative satisfy the following lemma,

Lemma 2.2. *Suppose the fractional derivatives are defined in* $[0, L]$. *Let* $g(y) = f(L - x)$, *then*

$$ {}_{x}D_L^{\alpha} f(x) = {}_{0}D_y^{\alpha} g(y)|_{y=L-x} \tag{9} $$

3. Polynomial approximation of fractional operators

Let us in the following consider the function, $f(y)$, and assume it is represented through an expansion as

$$f(y) = \sum_{j=0}^{N} f(y_j)\phi_j(y)\,, \quad y \in [-1,1]$$

where y_j represent $N+1$ distinct points in $[-1,1]$ and $\phi_j(y)$ is a Lagrange interpolating polynomial of order N. In this work we shall use Jacobi polynomials defined via the hypergeometric function [1] as

$$J_n^{(\lambda,\nu)}(y) = \frac{(\lambda+1)_n}{n!}\,{}_2F_1(-n, 1+\lambda+\nu+n; \lambda+1; \frac{1-y}{2}) \tag{10}$$

for a polynomial of order n. Here $(\lambda+1)_n$ is Pochhammer's symbol (for the rising factorial) and have introduced the hypergeometric function ${}_2F_1(a,b;c;z)$, which can be evaluated explicitly for the cases we are concerned about, as discussed in the appendix. This yields the following equivalent expression

$$J_n^{(\lambda,\nu)}(y) = \frac{\Gamma(\lambda+n+1)}{n!\Gamma(\lambda+\nu+n+1)} \sum_{i=0}^{m} \left(\begin{array}{c} n \\ i \end{array}\right) \frac{\Gamma(\lambda+\nu+n+i+1)}{\Gamma(\lambda+i+1)} \left(\frac{y-1}{2}\right)^i, \tag{11}$$

where $\Gamma(x)$ represents the Gamma function [1]. A direct rewriting of this yields the polynomial on monomial form as

$$J_n^{(\lambda,\nu)}(y) = \frac{\Gamma(\lambda+n+1)}{n!\Gamma(\lambda+\nu+n+1)} \sum_{k=0}^{n} \left(\sum_{i=k}^{n} (-1)^{i-k} \left(\begin{array}{c} n \\ i \end{array}\right) \left(\begin{array}{c} i \\ k \end{array}\right) \frac{\Gamma(\lambda+\nu+n+i+1)}{\Gamma(\lambda+i+1)} \right) 2^{-k} y^k, \tag{12}$$

which shall be useful shortly.

As the nodes for the Lagrange polynomials we use the Gauss quadrature points associated with the Jacobi polynomials, found as the $N+1$ roots of $J_{N+1}^{(\lambda,\nu)}(y)$. Except for special cases of (λ,μ) there are no known explicit formulas for these roots but there exists efficient and accurate ways to compute them – see [16] and references therein.

With these nodes the corresponding Lagrange polynomial is obtained on closed from as [16] as

$$\phi_j(y) = \frac{J_{N+1}^{(\lambda,\nu)}(y)}{(J_{N+1}^{(\lambda,\nu)})'(y_j)(y-y_j)}, \quad j = 0, 1, 2, \cdots, N. \tag{13}$$

One easily realizes the interpolation property since

$$\phi_i(y_j) = \left\{ \begin{array}{ll} 1, & j = i, \\ 0, & j \neq i, \end{array} \right. \quad i, j = 0, 1, \cdots, N$$

Since $\phi_j(y)$ and $J_j^{(\lambda,\nu)}(y)$ are polynomials up to order N we have

$$J_h^{(\lambda,\nu)}(y) = \sum_{i=0}^{N} J_j^{(\lambda,\nu)}(y_i)\phi_i(y) \tag{14}$$

which can be expressed as by $\boldsymbol{\phi}_N(y) = [\phi_0(y), \ldots, \phi_N(y)]^T$, $\boldsymbol{J}_N(y) = [J_0^{(\lambda,\nu)}(y), \ldots, J_N^{(\lambda,\nu)}(y)]^T$, to recover

$$\mathrm{Z}\boldsymbol{\phi}_N(y) = \boldsymbol{J}_N(y). \tag{15}$$

where

$$\mathrm{Z} = \begin{pmatrix} J_0^{(\lambda,\nu)}(y_0) & J_0^{(\lambda,\nu)}(y_1) & \cdots & J_0^{(\lambda,\nu)}(y_N) \\ J_1^{(\lambda,\nu)}(y_0) & J_1^{(\lambda,\nu)}(y_1) & \cdots & J_1^{(\lambda,\nu)}(y_N) \\ \vdots & \vdots & \ddots & \vdots \\ J_N^{(\lambda,\nu)}(y_0) & J_N^{(\lambda,\nu)}(y_1) & \cdots & J_N^{(\lambda,\nu)}(y_N) \end{pmatrix}$$

is a Vandemonde type matrix. Using this notation, we express the interpolation of $f(y)$ as

$$f_h(y) = \sum_{j=0}^{N} f(y_j)\phi_j(y) = \boldsymbol{\phi}_N^T(y)\boldsymbol{f} = (\mathrm{Z}^{-1}\boldsymbol{J}_N^{(\lambda,\nu)}(y))^T\boldsymbol{f}$$

where $\boldsymbol{f} = [f(y_0), \ldots, f(y_N)]^T$.

It is worth recalling important special cases of the general Jacobi polynomials, such as the Chebyshev polynomials

$$T_n(y) = \frac{\sqrt{\pi}n!}{\Gamma(n+\frac{1}{2})} J_n^{(-\frac{1}{2},-\frac{1}{2})}(y)$$

and the Legendre polynomials

$$P_n(y) = J_n^{(0,0)}(t) = {}_2F_1(-n, 1+n; 1; \frac{1-y}{2}),$$

both defined on $y \in [-1, 1]$.

3.1. Fractional differentiation matrix in single domain

To evaluate the Caupto derivative, defined in $x \in [0,h]$, we map $y \in [-1,1] \to x \in [0,h]$ through $y = \frac{2}{h}x - 1$. The shifted Jacobi polynomial of order $n\,(n \leqslant N)$, the fractional derivative of order $\alpha\,(\alpha < n)$ can now be recovered, through the use of (5)-(6), as

$$ {}_0D_x^\alpha\left(J_n^{(\lambda,\nu)}(x)\right) = \sum_{k=\lceil\alpha\rceil}^{n} \frac{\Gamma(\lambda+n+1)}{\Gamma(\lambda+\nu+n+1)} \left(\sum_{i=k}^{n} \frac{(-1)^{i-k}\Gamma(\lambda+\nu+i+n+1)h^{-k}}{(n-i)!(i-k)!\Gamma(k+1-\alpha)\Gamma(\lambda+i+1)}\right) x^{k-\alpha} \tag{16} $$

This allows us to directly express the fractional derivative of the Lagrangian basis as

$$ \phi_j^{(\alpha)}(x) = \sum_{i=0}^{N} \mathrm{Z}_{j,i}^{-1}(J_i^{(\lambda,\nu)}(x))^{(\alpha)}(x), $$

where $(J_n^{(\lambda,\nu)}(x))^{(\alpha)}(x) = {}_0D_x^\alpha\left(J_n^{(\lambda,\nu)}(x)\right)$. This results in an approximation to the fractional derivative on a general function on the form

$$ {}_0D_x^\alpha f(x) \quad = \quad {}_0D_x^\alpha\left(\sum_{j=0}^{N} f(x_j)\phi_j(x)\right) = \sum_{j=0}^{N} f(x_j)\,{}_0D_x^\alpha\phi_j(x) = (\boldsymbol{\phi}_N^{(\alpha)}(x))^T\boldsymbol{f}. \tag{17} $$

Here $\boldsymbol{\phi}_N^{(\alpha)}(x)$ represents the fractional derivative and it can naturally be evaluated at any point $x \in [0,h]$. In particular if we choose to evaluate these at the interpolation points x_j, we recover

$$ \boldsymbol{f}^{(\alpha)} = {}_0\mathrm{D}^{(\alpha)}\boldsymbol{f}, \;\; {}_0\mathrm{D}_{ij}^{(\alpha)} = \phi_j^{(\alpha)}(x_i), $$

where ${}_0\mathrm{D}^{(\alpha)}$ can be recognized as a generalization of the differentiation matrix [16].

3.2. Fractional differentiation matrix in multiple domains

Let us now consider the more general situation in which we need to compute the derivative of a piecewise polynomial, $f(x)$. For $x \in [0,L]$, let $0 = x_0 < x_1 < \cdots < x_K = L$, and $h_k = x_k - x_{k-1}, (k = 1,2,\cdots,K)$. Suppose $x \in [x_k, x_{k+1}]$, $n-1 < \alpha \leqslant n$ to obtain

$$ \begin{aligned} {}_0D_x^\alpha f(x) &= \frac{1}{\Gamma(n-\alpha)}\int_0^x (x-s)^{n-1-\alpha} f^{(n)}(s)\,ds \\ &= \frac{1}{\Gamma(n-\alpha)}\left(\sum_{j=1}^{k}\int_{x_{j-1}}^{x_j}(x-s)^{n-1-\alpha}f^{(n)}(s)\,ds + \int_{x_k}^{x}(x-s)^{n-1-\alpha}f^{(n)}(s)\,ds\right) \end{aligned} $$

Now consider the two part separately. Assuming $z_{i,k}, (i = 0, 1, \cdots, N, k = 1, 2, \cdots, K)$ are defined as the elementwise Gauss points in each of the K elements, and $\boldsymbol{f}_j = [f(z_{0,j}, \ldots, z_{N,j})]^T$. Then for all $s \in [x_{j-1}, x_j]$, we have $f(s) = \boldsymbol{f}_j^T \boldsymbol{\phi}_N(\mu)$ where $\mu = \frac{s - x_{j-1}}{h_j}$ and we recover

$$f^{(n)}(s) = \frac{\partial^n (\boldsymbol{f}_j^T \boldsymbol{\phi}_N(\mu))}{\partial s^n} = \boldsymbol{f}_j^T \frac{\boldsymbol{\phi}_N^{(n)}(\mu)}{h_j^n} = \frac{\boldsymbol{f}_j^T \mathrm{Z}^{-1} (\boldsymbol{J}_N^{(\lambda,\nu)})^{(n)}(\mu)}{h_j^n}$$

For the first part, we have

$$\begin{aligned}
\int_{x_{j-1}}^{x_j} (x-s)^{n-1-\alpha} f^{(n)}(s)\, ds &= \int_0^1 (x - x_{j-1} - h_j \mu)^{n-1-\alpha} \frac{\boldsymbol{f}_j^T \mathrm{Z}^{-1} \boldsymbol{J}_N^{(n)}(\mu)}{h_j^{n-1}} d\mu \\
&= h_j^{-\alpha} \boldsymbol{f}_j^T \mathrm{Z}^{-1} \int_0^1 \left(\frac{x - x_{j-1}}{h_j} - \mu \right)^{n-1-\alpha} \boldsymbol{J}_N^{(n)}(\mu) d\mu \\
&= h_j^{-\alpha} \boldsymbol{f}_j^T \mathrm{Z}^{-1} \boldsymbol{G}_j(x) \quad x \in [x_{j-1}, x_j].
\end{aligned}$$

Here $\boldsymbol{G}_j(x) = \int_0^1 \left(\frac{x - x_{j-1}}{h_j} - \mu \right)^{n-1-\alpha} \left(\boldsymbol{J}_N^{(\lambda,\nu)} \right)^{(n)} (\mu) d\mu = [G_{0,j}(x), \ldots, G_{N,j}(x)]^T$ where

$$\begin{aligned}
G_{m,j}(x) &= \int_0^1 \left(\frac{x - x_{j-1}}{h_j} - \mu \right)^{n-1-\alpha} \left(J_m^{(\lambda,\nu)} \right)^{(n)} (\mu) d\mu \\
&= \sum_{l=n}^{m} C_{l,m,n} \frac{(x - x_{j-1})^{n-1-\alpha}}{h_j^{n-1-\alpha}} {}_2F_1(\alpha + 1 - n, l + 1 - n; l - n + 2; \frac{h_j}{x - x_{j-1}}) \quad (18)
\end{aligned}$$

with

$$C_{l,m,n} = \frac{\Gamma(\lambda + m + 1)}{\Gamma(\lambda + \nu + m + 1)} \left(\sum_{i=l}^{m} \frac{(-1)^{i-l} \Gamma(\lambda + \nu + i + m + 1)}{(m-i)!(i-l)!(l-n)! \Gamma(\lambda + i + 1)} \right)$$

. As discussed in the Appendix, the hypergeometric function in Eq. (18) can be evaluated exactly.

For the second part,

$$\begin{aligned}
& \frac{1}{\Gamma(n-\alpha)} \int_{x_k}^{x} (x-s)^{n-1-\alpha} f^{(n)}(s)\, ds \\
= & \frac{1}{\Gamma(n-\alpha)} \int_0^{\frac{x - x_k}{h_{k+1}}} \left(\frac{x - x_k}{h_{k+1}} - \mu \right)^{n-1-\alpha} \frac{\boldsymbol{f}_k^T \mathrm{Z}^{-1} \boldsymbol{J}_N^{(n)}(\mu)}{h_{k+1}^n} d\mu \\
= & h_{k+1}^{-n} \boldsymbol{f}_k^T \mathrm{Z}^{-1} \boldsymbol{J}_N^{(\alpha)} \left(\frac{x - x_k}{h_{k+1}} \right), \quad x \in [x_k, x_{k+1}].
\end{aligned}$$

Combining these terms, we recover the an explicit formula for fractional derivative of any polynomial up to order N,

$$
{}_0D_x^\alpha f(x) = \frac{\sum_{j=0}^{k-1} h_{j+1}^{-\alpha} \boldsymbol{f}_j^T \mathrm{Z}^{-1} \boldsymbol{G}_j(x)}{\Gamma(n-\alpha)} + \frac{\boldsymbol{f}_k^T \mathrm{Z}^{-1} \boldsymbol{J}_N^{(\alpha)}\left(\frac{x-x_k}{h_{k+1}}\right)}{h_{k+1}^n} \tag{19}
$$

The latter term is recognized as the fractional derivative at the local element while the first term accounts for the global nature of the fractional derivative.

One easily realizes that the affine mapping between $y \in [-1,1]$ and $x \in [0,h]$ results in a scaling like

$$
\|{}_0D_y^\alpha\| \simeq \left(\frac{2}{h}\right)^\alpha \|{}_0D_x^\alpha\|.
$$

This shall be useful shortly.

3.3. Approximation error of the differentiation

For a polynomial $f(x)$ up to order N, the fractional derivative of $f(x)$ can be computed exactly. However, for the more general case consider ${}_0D_x^\alpha f_h(x) = {}_0D_x^\alpha\left(\sum_{j=0}^N f(x_j)\phi_j(x)\right)$ and let us seek to estimate $\|{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)\|$.

In preparation of this, let us introduce some preliminary results.

Lemma 3.1. *Assume that $y_j, (j = 0, 1\cdots, N)$ are Gauss quadrature points of order N in $[-1,1]$. Let $\pi_N(y) = \prod_{j=0}^N (y - y_j)$. Then $\forall n \leqslant N+1, n \in N$, there exist $0 < \eta_{n,1} < \cdots < \eta_{n,\lfloor\frac{N-n+1}{2}\rfloor} < 1$ and $C(N,n)$ such that,*

$$
\pi_N^{(n)}(y) = \begin{cases} C(N,n)y\prod_{j=1}^{\frac{N-n}{2}}(y^2-\eta_{n,j}^2), & if\ N-n\ even \\ \\ C(N,n)\prod_{j=1}^{\frac{N-n+1}{2}}(y^2-\eta_{n,j}^2), & if\ N-n\ odd \end{cases} \tag{20}
$$

Where $C(N,n)$ is independent of y.

Proof. We shall prove the result by induction. Let $S = \{y_0, y_1, \cdots, y_N\}$. Since y_j are chosen to be the Gauss quadrature points of order N in $[-1,1]$, the points are symmetric around $y = 0$, i.e. if $y_i \in S$, then $-y_i \in S$. We set $0 = \eta_{0,0} = y_{\frac{N}{2}} < \eta_{0,1} = y_{\frac{N}{2}+1} = -y_{\frac{N}{2}-1} < \cdots < \eta_{0,\frac{N}{2}} = y_N = -y_0 < 1$ if N is even, and $0 < \eta_{0,1} = y_{\frac{N+1}{2}} = -y_{\frac{N-1}{2}} < \cdots < \eta_{0,\frac{N+1}{2}} = x_N = -x_0 < 1$ if N is odd. In this case we have

$$
\pi_N(y) = \begin{cases} y\prod_{j=1}^{\frac{N}{2}}(y^2-\eta_{0,j}^2), & if\ N\ even \\ \prod_{j=1}^{\frac{N+1}{2}}(y^2-\eta_{0,j}^2), & if\ N\ odd \end{cases}
$$

Clearly (20) holds for $n = 0$. Now assume (20) holds for $n-1$. Then,

$$\pi_N^{(n-1)}(y) = \begin{cases} C(N, n-1)y\prod_{j=1}^{\frac{N-n+1}{2}}(y^2 - \eta_{n-1,j}^2), & if\ N-n+1\ even \\ \\ C(N, n-1)\prod_{j=1}^{\frac{N-n+2}{2}}(y^2 - \eta_{n-1,j}^2), & if\ N-n+1\ odd \end{cases}$$

Clearly, $\pi_N^{(n-1)}(y) \in C^1[-1, 1]$, and $\pi_N^{(n)}(y)$ has $N + 1 - n$ zeros.

$$\pi_N^{(n)}(y) = \begin{cases} C(N, n-1)\left(\sum_{i=1}^{\frac{N-n+1}{2}} 2y\prod_{j=1, j\neq i}^{\frac{N-n+1}{2}}(y^2 - \eta_{n-1,j}^2)\right. \\ \quad \left. + \prod_{j=1}^{\frac{N-n+1}{2}}(y^2 - \eta_{n-1,j}^2)\right), & N-n\ is\ odd, \\ C(N, n-1)\left(\sum_{i=1}^{\frac{N-n+2}{2}} 2y\prod_{j=1, j\neq i}^{\frac{N-n+2}{2}}(y^2 - \eta_{n-1,j}^2)\right), & N-n\ is\ even. \end{cases}$$

Hence, $\eta = 0$ is a zero point of $\pi_N^{(n)}(y)$ when $N - n$ is even, while $\eta = 0$ is not a zero point of $\pi_N^{(n)}(y)$ when $N - n$ is odd. It follows directly from the symmetry of the Gauss points that if $\pi_N^{(n)}(\eta_{n,j}) = 0$, then $\pi_N^{(n)}(-\eta_{n,j}) = 0$.

We denote the zeros of $\pi^{(n)}(y)$ by $\eta_{n,0} = 0, \pm\eta_{n,1}, \cdots, \pm\eta_{n,\frac{N-n}{2}}$ if $N - n$ is even, and denote the zeros of $\pi^{(n)}(y)$ by $\pm\eta_{n,1}, \cdots, \pm\eta_{n,\frac{k-n+1}{2}}$ if $N - n$ is odd. Then (20) holds for n, completing the proof. $\square$

From standard interpolation theory [26], we know $\forall f \in C^{k+1}$, there exists an $\xi \in [-1, 1]$, such that,

$$f(x) - \sum_{j=0}^{N} f(y_j)\phi_j(y) = \frac{f^{(N+1)}(\xi)}{(N+1)!}\pi_N(y) \tag{21}$$

where ξ depends on y.

Recalling Lemma 3.1, we now have the following result

Lemma 3.2. *Suppose $f(x) \in C^p[a, b], p \geqslant N + n + 1\ \forall n \leqslant N + 1, n \in \mathbb{N}$. Let $f_h(x) = \sum_{j=0}^{N} f(x_j)\phi_j(x)$. Then there exist $0 < \eta_{n,1} < \cdots < \eta_{n,\lfloor\frac{N-n+1}{2}\rfloor} < 1$ and a constant $\xi \in [a, b]$ such that,*

$$f^{(n)}(x) - f_h^{(n)}(x) = \begin{cases} C(N, n)\frac{f^{(N+1)}(\xi)}{(N+1)!}y\prod_{j=1}^{\frac{N-n}{2}}(y^2 - \eta_{n,j}^2) + O(b-a)^{N+2-n}, & if\ N-n\ even \\ \\ C(N, n)\frac{f^{(N+1)}(\xi)}{(N+1)!}\prod_{j=1}^{\frac{N-n+1}{2}}(y^2 - \eta_{n,j}^2) + O(b-a)^{N+2-n}, & if\ N-n\ odd \end{cases} \tag{22}$$

where $y = 2\frac{x-a}{b-a} - 1$.

Lemma 3.3. *$\forall m, n \in \mathbb{N}, n-1 < \alpha \leqslant n$ and $0 \leqslant \gamma \leqslant 1$, there exists a constant M, such that*

$$\frac{1}{\Gamma(n-\alpha)} \sum_{j=0}^{m-1} \int_0^1 (m+\gamma-j-\theta)^{n-1-\alpha} \left(\theta - \frac{1}{2}\right) d\theta \leqslant M, \text{ as } m \to \infty$$

This Lemma can be proved using the same method introduced in [19].

For the approximate fractional derivative (19), we now recover the following approximation result

Theorem 3.4. *$\forall n-1 < \alpha \leqslant n, f(x) \in C^p[0,L], p \geqslant N+n+1$, where N is the degree of the basis. Then the error ε_N^α associated with the approximate fractional derivative (19) is bounded as*

$$\|\varepsilon_N^\alpha\|_2 = \|{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)\|_2 \leqslant \begin{cases} C, & n > N \\ Ch^{N+1-n}, & n \leqslant N, N-n \text{ odd} \\ Ch^{N+1-\alpha}, & n \leqslant N, N-n \text{ even} \end{cases} \tag{23}$$

where C is a constant independent of x and $h = \max_k h_k$.

Proof. Clearly, $\|{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)\| \leqslant C$ holds for $n > N$.

For $n \leqslant N$, and $x \in [x_k, x_{k+1}], h = x_{k+1} - x_k$, Lemma 3.2 implies

$$f^{(n)}(x) - f_h^{(n)}(x) = \begin{cases} C(N,n)\frac{f^{(N+1)}(\xi)}{(N+1)!} y \prod_{j=1}^{\frac{N-n}{2}} (y^2 - \eta_{n,j}^2) + O(h^{N+2-n}), & if\ N-n \text{ even} \\ \\ C(k,n)\frac{f^{(N+1)}(\xi)}{(N+1)!} \prod_{j=1}^{\frac{N-n+1}{2}} (y^2 - \eta_{n,j}^2) + O(h^{N+2-n}), & if\ N-n \text{ odd} \end{cases} \tag{24}$$

When $N-n$ is odd, for $x \in [x_j, x_{j+1}]$, take $\eta_{n,j,i} = x_j + \frac{(\eta_{n,i}+1)h}{2}$. There exist constants M, M', s.t.,

$$
\begin{aligned}
|\varepsilon_N^\alpha| &= |{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)| \\
&\leqslant \frac{M}{\Gamma(n-\alpha)} \sum_{j=0}^{k-1} \left| \int_{x_j}^{x_{j+1}} (x-s)^{n-1-\alpha} \prod_{i=1}^{\frac{N-n+1}{2}} (s^2 - \eta_{n,j,i}^2) ds \right| \\
&\quad + \frac{M}{\Gamma(n-\alpha)} \left| \int_{x_k}^{x} (x-s)^{n-1-\alpha} \prod_{i=1}^{\frac{N-n+1}{2}} (s^2 - \eta_{n,j,i}^2) ds \right| + M' h^{N+2-n} \\
&\leqslant \frac{M h^{n-\alpha}}{\Gamma(n-\alpha)} \sum_{j=0}^{k-1} \left| \int_0^1 (\frac{x-x_j}{h} - \theta)^{n-1-\alpha} \left(h^{N-n+1}\right) d\theta \right| \\
&\quad + \frac{M h^{n-\alpha}}{\Gamma(n-\alpha)} \left| \int_0^{\frac{x-x_k}{h}} (\frac{x-x_k}{h} - \theta)^{n-1-\alpha} \left(h^{N-n+1}\right) d\theta \right| + M' h^{N+2-n} \\
&= \frac{M h^{N+1-\alpha}}{\Gamma(n-\alpha)} \sum_{j=0}^{k-1} \left| \int_0^1 (\frac{x-x_j}{h} - \theta)^{n-1-\alpha} d\theta \right| \\
&\quad + \frac{M h^{N+1-\alpha}}{\Gamma(n-\alpha)} \left| \int_0^{\frac{x-x_k}{h}} (\frac{x-x_k}{h} - \theta)^{n-1-\alpha} d\theta \right| + M' h^{N+2-n}
\end{aligned}
$$

For the second part, let $\gamma = \frac{x-x_k}{h}$ to obtain,

$$
\begin{aligned}
|\varepsilon_N^\alpha| &\leqslant \frac{M h^{N+1-\alpha}}{\Gamma(n-\alpha)} \sum_{j=0}^{k-1} \left| \int_0^1 (k+\gamma-j-\theta)^{n-1-\alpha} d\theta \right| \\
&\quad + \frac{M h^{N+1-\alpha}}{\Gamma(n-\alpha)} \left| \int_0^{\gamma} (\gamma-\theta)^{n-1-\alpha} d\theta \right| + M' h^{N+2-n} \\
&\leqslant M h^{N+1-\alpha} (\frac{L}{h})^{n-\alpha} + M' h^{N+2-n} = O(h^{N+1-n})
\end{aligned}
$$

When $N-n$ is even, for $x \in [x_j, x_{j+1}]$, we have

$$
\begin{aligned}
|\varepsilon_N^\alpha| &= |{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)| \\
&= \frac{1}{\Gamma(n-\alpha)}\left|\int_0^x (x-s)^{n-1-\alpha}\left(f^{(n)}(x) - f_h^{(n)}(x)\right) ds\right| \\
&\leqslant \frac{M}{\Gamma(n-\alpha)}\sum_{j=0}^{k-1}\left|\int_{x_j}^{x_{j+1}} (x-s)^{n-1-\alpha}(s - x_j - \frac{h}{2})\prod_{i=1}^{\frac{N-n}{2}}(s^2 - \eta_{n,j,i}^2)ds\right| \\
&\quad + \frac{M}{\Gamma(n-\alpha)}\left|\int_{x_k}^{x} (x-s)^{n-1-\alpha}(s - x_j - \frac{h}{2})\prod_{i=1}^{\frac{N-n}{2}}(s^2 - \eta_{n,j,i}^2)ds\right| + M'h^{k+2-n} \\
&\leqslant \frac{Mh^{n+1-\alpha}}{\Gamma(n-\alpha)}\sum_{j=0}^{k-1}\left|\int_0^1 (\frac{x-x_j}{h} - \theta)^{n-1-\alpha}(\theta - \frac{1}{2})h^{N-n}d\theta\right| \\
&\quad + \frac{Mh^{n+1-\alpha}}{\Gamma(n-\alpha)}\left|\int_0^{\frac{x-x_k}{h}} (\frac{x-x_k}{h} - \theta)^{n-1-\alpha}(\theta - \frac{1}{2})h^{N-n}d\theta\right| + M'h^{N+2-n} \\
&= \frac{Mh^{N+1-\alpha}}{\Gamma(n-\alpha)}\sum_{j=0}^{k-1}\left|\int_0^1 (\frac{x-x_j}{h} - \theta)^{n-1-\alpha}\left(\theta - \frac{1}{2}\right)d\theta\right| \\
&\quad + \frac{Mh^{N+1-\alpha}}{\Gamma(n-\alpha)}\left|\int_0^{\frac{x-x_k}{h}} (\frac{x-x_k}{h} - \theta)^{n-1-\alpha}\left(\theta - \frac{1}{2}\right)d\theta\right| + M'h^{N+2-n}
\end{aligned}
$$

Set $\gamma = \frac{x-x_k}{h}$, and recall Lemma 3.3 to obtain

$$
\begin{aligned}
|\varepsilon_N^\alpha| &\leqslant \frac{Mh^{N+1-\alpha}}{\Gamma(n-\alpha)}\sum_{j=0}^{k-1}\left|\int_0^1 (k+\gamma-j-\theta)^{n-1-\alpha}\left(\theta - \frac{1}{2}\right)d\theta\right| \\
&\quad + \frac{Mh^{N+1-\alpha}}{\Gamma(n-\alpha)}\left|\int_0^{\gamma} (\gamma-\theta)^{n-1-\alpha}\left(\theta - \frac{1}{2}\right)d\theta\right| + M'h^{N+2-n} \\
&\leqslant \frac{M''h^{N+1-\alpha}}{\Gamma(n-\alpha)} + M'h^{N+2-n} = O(h^{N+1-\alpha})
\end{aligned}
$$

Combining these results, we obtain that there exists a constant M, such that

$$
\|{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)\|_2 \leqslant \begin{cases} M, & n > N \\ M\|h^{N+1-n}\|_2 \leqslant MLh^{N+1-n}, & n \leqslant N, N-n \textit{ odd} \\ M\|h^{N+1-\alpha}\|_2 \leqslant MLh^{N+1-\alpha}, & n \leqslant N, N-n \textit{ even} \end{cases} \tag{25}
$$

This completes the proof. □

To validate the analysis, let us consider the case of $f(x) = \sin_M(x) = \sum_{i=0}^{M/2} \frac{(-1)^{2i-1}}{(2i+1)!} x^{2i+1}$. Here we choose $M = 50$ so that $f(x)$ approximates $\sin(x)$ and $|f(x) - \sin(x)| < 10^{-15}\ \forall x \in [0, 1]$. We computed the approximate fractional derivative of $f(x)$ and compared the error $\varepsilon = \|{}_0D_x^\alpha f(x) - {}_0D_x^\alpha f_h(x)\|_{L_2}$ for different number of elements K. Convergence orders for $0 < \alpha < 3$ and $N = 1, 2 \cdots, 6$ (degree of basis function) are shown in Table 1.

Table 1: Convergence order, β in h^β, for different N and α. A '-' indicates no convergence.

N	1	2	3	4	5	6
$\alpha = 0.01$	2.0071	1.9833	4.0025	3.9783	5.9991	6.0750
$\alpha = 0.2$	1.9946	2.0134	3.9443	4.0125	5.9321	5.9840
$\alpha = 0.5$	1.5305	2.1936	3.5250	4.2542	5.5215	6.1972
$\alpha = 0.8$	1.2041	2.1409	3.2037	4.1612	5.2040	6.1529
$\alpha = 1.0$	0.9946	1.9952	2.9959	3.9964	4.9969	5.9936
$\alpha = 1.2$	-	1.8825	2.0069	3.9284	4.0072	5.9655
$\alpha = 1.5$	-	1.5871	2.0395	3.6369	4.0572	5.6655
$\alpha = 1.8$	-	1.2396	2.0812	3.2538	4.1144	5.2601
$\alpha = 2.0$	-	0.9944	1.9951	2.9959	3.9965	4.9968
$\alpha = 2.2$	-	-	1.8584	1.9897	3.9186	3.9871
$\alpha = 2.5$	-	-	1.5277	2.0219	3.5704	4.0391
$\alpha = 2.8$	-	-	1.2060	2.0495	3.2174	4.0737
$\alpha = 3.0$	-	-	0.9953	1.9957	2.9963	3.9968

From Table 1, we observe a convergence order as predicted by Theorem 3.4. For $N = 1, 3, 5$, the order of convergence is close to $N+1$ when α is close to 0. Convergence order decreases linearly as α increases. For $N = 2, 4, 6$, convergence orders remain essentially constant for all $n-1 < \alpha < n (n = 1, 2, 3)$. In addition, if $\alpha > N$, the order of convergence is 0 as expected.

Remark: An immediate consequence of Lemma 2.2 is that similar accuracy and computational approach can be expected for the right Caputo derivative.

4. Penalty spectral method for fractional PDEs

With some understanding of the basic approximation properties of the polynomial based approximation of the fractional operators, let us now consider the use of these tools for the solution of fractional partial differential equations. As the treatment is slightly different, we split the discussion into the case of fractional advection and fractional diffusion equations.

4.1. Fractional advection problems $(0 < \alpha \leqslant 1)$

Consider the problem $(0 < \alpha \leqslant 1)$

$$\frac{\partial u(x,t)}{\partial t} + {}_0D_x^\alpha u(x,t) = f(x,t),\ x \in [0,L], t \in [0,T] \tag{26}$$

with $u(x,0) = g(x)$, and $u(0,t) = h(t)$.

Let us first consider the problem in a single domain and introduce the boundary condition into the equation using a penalty term as

$$\frac{\partial u(x,t)}{\partial t} + {}_0D_x^\alpha u(x,t) = f(x,t) - \tau\delta(x)\left[u(0,t) - h(t)\right], \tag{27}$$

where $\delta(x)$ is the classic Dirac delta function and τ a constant to be specified shortly. It is obvious that if $u(x,t)$ is a solution to the original equation it is also a solution to this modified problem. Furthermore, $\tau \to \infty$ imposes the boundary condition with increasing strength.

We seek an approximate solution expressed as

$$u_h(x,t) = \sum_{j=0}^{N} u(x_j,t)\phi_j(x) = \sum_{j=0}^{N} u_j(t)\phi_j(x)$$

where x_i represents the Gauss points of a particular orthogonal polynomial and $\phi_i(x)$ is, as usual, the Lagrange polynomial associated with these points. In what remains we choose the Chebyshev Gauss points given on the form

$$y_j = -\cos\left(\frac{2j+1}{2N+2}\pi\right),\ \ i = 0,\ldots,N,$$

shifted to $x_j = \frac{L}{2}(y_j+1)$. We emphasize that there is nothing specific about this choice.

We insert the solution into (27) and require the residual to vanish in a Galerkin sense as

$$\begin{aligned}\frac{d}{dt}\left(\sum_{j=0}^{N} u_j(t)\phi_j(x), \phi_i(x)\right) &= -\left(\sum_{j=0}^{N} u_j(t)\phi_j^{(\alpha)}(x), \phi_i(x)\right)\\ &+(\phi_i, f(x,t)) - \tau(\phi_i(x), \delta(0))[u_h(0,t) - h(t)],\ 0 \leqslant i,j \leqslant N\end{aligned} \tag{28}$$

where $(\cdot,\cdot)$ reflect the standard L_2 inner product and $\phi_j^{(\alpha)}$ reflects the left Caputo derivative of the basis. Again, it is clear that if u_h satisfies the boundary condition the penalty term vanishes and that τ reflects the strength by which the boundary condition is enforced. As we shall see shortly, this term allows us to design stable schemes

Defining the mass matrix, $\mathrm{M}_{ij} = (\phi_i, \phi_j)$, the left stiffness matrix, ${}_0\mathrm{S}^{(\alpha)}_{ij} = (\phi_i, \phi^{(\alpha)}_j(x))$, and assume the forcing is also expressed as a polynomial, $f_h(x)$, we recover the scheme

$$\mathrm{M}\frac{d\boldsymbol{u}_h}{dt} + {}_0\mathrm{S}^{(\alpha)}\boldsymbol{u}_h = \mathrm{M}\boldsymbol{f}_h - \tau\boldsymbol{\phi}(0)[\boldsymbol{\phi}(0)^T\boldsymbol{u}_h - h(t)],$$

where $\boldsymbol{u}_h = [u_h(x_0,t),\ldots,u_h(x_N,t)]^T$ and likewise for $\boldsymbol{f}_h$.

Since M is a mass matrix and, thus, positive definite and invertible, we recover the explicit scheme

$$\frac{d\boldsymbol{u}_h}{dt} + \mathrm{M}^{-1}{}_0\mathrm{S}^{(\alpha)}\boldsymbol{u}_h = \boldsymbol{f}_h - \tau\mathrm{M}^{-1}\boldsymbol{\phi}(0)[\boldsymbol{\phi}(0)^T\boldsymbol{u}_h - h(t)],$$

which can be further simplified by realizing that

$$\begin{aligned}(M_0D^{(\alpha)})_{kj} &= \sum_{i=0}^{N}(\phi_i(x),\phi_k(x))\,{}_0D^{\alpha}_x\phi_j(x_i) = \left(\left(\sum_{i=0}^{N}(\phi^{(\alpha)}_j(x_i))\phi_i(x)\right),\phi_k(x)\right)\\ &= \left(\phi^{(\alpha)}_j(x),\phi_k(x)\right) = {}_0S^{(\alpha)}_{kj},\end{aligned}$$

and

$$(\mathrm{M}^{-1}\boldsymbol{\phi}(0))_i = (-1)^N\frac{P'_{N+1}(y(x_i)) - P'_N(y(x_i))}{2}\frac{2}{L} = Q^-(x_i),$$

where $y = \frac{2}{L}x - 1, y \in [-1,1]$. The Legendre polynomials, $P_n(x)$, appear naturally as the Galerkin statement is made in the unweighted L_2-norm in which the Legendre polynomials are orthogonal. The proof of this statement is straightforward and is true for any choice of the Lagrange basis. The proof is found in [8]. We recover the semi-discrete scheme

$$\frac{d}{dt}\boldsymbol{u}_h + {}_0\mathrm{D}^{(\alpha)}\boldsymbol{u}_h = \boldsymbol{f}_h - \tau\boldsymbol{Q}^-[u_h(0) - h(t)], \tag{29}$$

where $\boldsymbol{Q}^- = [Q^-(x_0),\ldots,Q^-(x_N)]^T$. We emphasize that even though the polynomial is nodal, the equation is satisfied in a Galerkin sense and not, as one may otherwise be lead to believe, in a collocation sense.

To understand stability of this scheme, let us assume $h(t) = 0$ and $f(x,t) = 0$ without loss of generality and express the semi-discrete scheme as

$$\frac{d}{dt}\boldsymbol{u}_h = -\left[{}_0\mathrm{D}^{(\alpha)} + \tau\boldsymbol{Q}^-\boldsymbol{\phi}(0)^T\right]\boldsymbol{u}_h.$$

Let us first consider the classic case of $\alpha = 1$, in which case one recover the energy statement

$$\frac{d}{dt}\|u_h\|^2 = -u_h^2(1) - (1-2\tau)u_h^2(0),$$

by utilizing that [8]

$$\boldsymbol{u}_h^T \mathrm{M} \boldsymbol{u}_h = \|u_h\|^2, \quad \boldsymbol{u}_h^T \mathrm{S}^{(1)} \boldsymbol{u}_h = \frac{1}{2}\left(u_h^2(1) - u_h^2(0)\right).$$

Hence stability in the classic case follows provided $\tau \geq 1/2$.

The complexity of the fractional derivative does not allow a straightforward stability analysis since we loose the essential property of integration by parts. However, a computational approach reveals that the classic case is a worst case scenario. In Fig. 1 we show the maximum real parts of the eigenvalues of $-(\mathrm{D}^{(\alpha)} + \tau \boldsymbol{Q}^- \boldsymbol{\phi}(0)^T)$ for different values of α and N for $\tau = 1/2$. This clearly confirms that that stability is retained for all $\alpha < 1$ provided it is true for $\alpha = 1$.

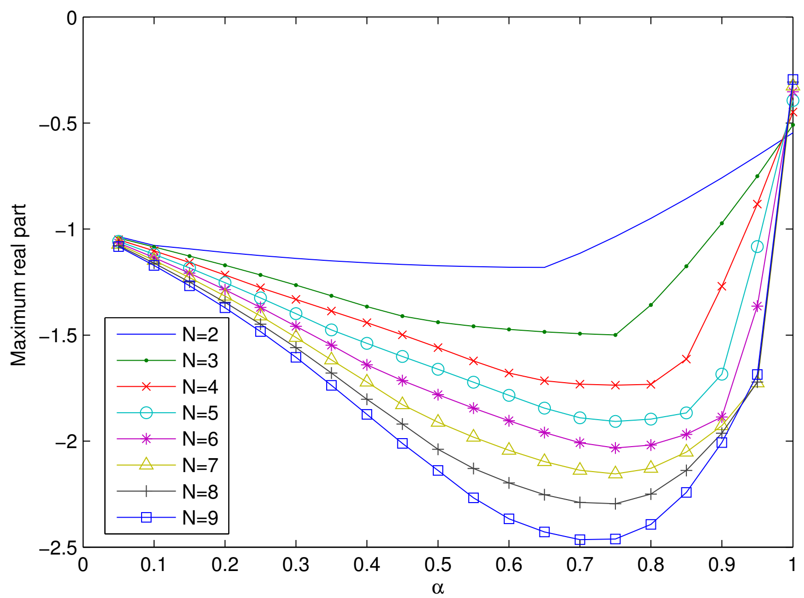

Figure 1: Maximum real part of eigenvalues of $-({}_0\mathrm{D}^{(\alpha)} + \tau \boldsymbol{Q}^- \boldsymbol{\phi}(0)^T)$ with $\tau = 1/2$ as a function of α.

Let us now consider the extension to multiple domains. We partition the domain into several subdomains $0 = x_0 < x_1 < \cdots < x_K = L,\ \Omega^k = [x_{k-1}, x_k], h_k = x_k - x_{k-1}$. In each subdomain we proceed as in the single domain case and consider the

$$\forall k: \quad \frac{d}{dt}\boldsymbol{u}_h + {}_0\mathrm{D}^{(\alpha)} \boldsymbol{u}_h = \boldsymbol{f}_h - \tau \boldsymbol{Q}^- [u_h(0) - h(t)], \quad x \in \Omega^k \tag{30}$$

with two notable exceptions. First of all the spatial fractional derivative is expressed as in (19) and $h(t)$ is obtained by unwinding, yielding an element wise scheme as

$$\frac{d}{dt}\boldsymbol{u}_h^k + {}_0\mathrm{D}_k^{(\alpha)}\boldsymbol{u}_h^k = \boldsymbol{f}_h^k - \tau_k \boldsymbol{Q}_k^-[u_h(x_0^k) - u_h^{k-1}(x_N^{k-1})], \tag{31}$$

where k reflects that all actions and representations are element wise. For this problem, only one boundary condition is needed, so we can solve the equation subdomain by subdomain. Stability follows from the single domain scheme in this case.

Let us briefly consider the reverse case of Eq.(26), defined as $(0 < \alpha \leqslant 1)$

$$\frac{\partial u(x,t)}{\partial t} + {}_xD_L^\alpha u(x,t) = f(x,t),\ \ x \in [0,L], t \in [0,T] \tag{32}$$

with $u(x,0) = g(x)$, and $u(L,t) = h(t)$.

Note that in the classic case, $\alpha = 1$, this reduced to the wave equation

$$\frac{\partial u(x,t)}{\partial t} - \frac{\partial u(x,t)}{\partial x} = f(x,t).$$

We again consider the problem in a single domain and introduce the boundary conditions using a penalty term as

$$\frac{\partial u(x,t)}{\partial t} + {}_xD_L^\alpha u(x,t) = f(x,t) - \tau\delta(x-L)\left[u(L,t) - h(t)\right]. \tag{33}$$

Using the right Caputo derivative and progressing as as above, we satisfy the equation in a Galerkin way to recover the scheme

$$\mathrm{M}\frac{d\boldsymbol{u}_h}{dt} + {}_L\mathrm{S}^{(\alpha)}\boldsymbol{u}_h = \mathrm{M}\boldsymbol{f}_h - \tau\boldsymbol{\phi}(L)[\boldsymbol{\phi}(L)^T\boldsymbol{u}_h - h(t)],$$

and we recover the explicit scheme

$$\frac{d\boldsymbol{u}_h}{dt} + \mathrm{M}^{-1}{}_L\mathrm{S}^{(\alpha)}\boldsymbol{u}_h = \boldsymbol{f}_h - \tau\mathrm{M}^{-1}\boldsymbol{\phi}(L)[\boldsymbol{\phi}(L)^T\boldsymbol{u}_h - h(t)],$$

where ${}_L\mathrm{S}^{(\alpha)}$ represents the stiffness matrix defined using the right Caputo derivative. Finally, we realize that

$$(\mathrm{M}^{-1}\boldsymbol{\phi}(L))_i = \frac{P'_{N+1}(y(x_i)) + P'_N(y(x_i))}{2}\frac{2}{L} = Q^+(x_i),$$

to recover the semi-discrete scheme

$$\frac{d}{dt}\boldsymbol{u}_h + {}_L\mathrm{D}^{(\alpha)}\boldsymbol{u}_h = \boldsymbol{f}_h - \tau\boldsymbol{Q}^+[u_h(L) - h(t)], \tag{34}$$

where $\boldsymbol{Q}^+ = [Q^+(x_0), \ldots, Q^+(x_N)]^T$ and ${}_L\mathrm{D}^{(\alpha)} = \mathrm{M}^{-1}{}_L\mathrm{S}^{(\alpha)}$ represents the differentiation matrix defined using the right Caputo derivative.

Stability of (34) follows directly from the analysis above for the left case through the connection in Lemma 2.2 and that observation that $Q^-(y) = Q^+(-y), y \in [-1,1]$.

4.1.1. Numerical results

Consider the equation ($0 < \alpha \leqslant 1$)

$$\frac{\partial u(x,t)}{\partial t} + {}_0D_x^{\alpha} u(x,t) = f(x,t), \;\; x \in [0,1], t \in [0,1] \tag{35}$$

with $u(x,0) = \sin_M(x) = \sum_{i=0}^{M/2} \frac{(-1)^{2i-1}}{(2i+1)!} x^{2i+1}$, $u(0,t) = 0$ and $f(x) = -e^{-t}(\sin_M(x) - \sin_M^{(\alpha)}(x))$. The exact solution is $u(x,t) = e^{-t}\sin_M(x)$.

Table 2: Convergence of fractional advection problem for different order of approximation, N, number of elements, K, and order of fractional derivative, α. The error is measured in the usual L_2 norm, $\|\varepsilon\|_2 = \|u - u_h\|_2$, and $h = K^{-1}$ is the element size. One clearly observed $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N+1-\alpha})$. In all cases, $\tau = K^{\alpha}$.

	$\alpha = 0.1$								
K	4	6		8		10		12	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
1	3.80E-03	1.32E-03	2.6010	6.55E-04	2.4510	3.89E-04	2.3352	2.56E-04	2.2894
2	7.07E-04	2.56E-04	2.5066	1.20E-04	2.6455	6.56E-05	2.6869	3.98E-05	2.7489
3	1.10E-05	2.01E-06	4.2038	6.14E-07	4.1160	2.48E-07	4.0687	1.19E-07	4.0369
4	7.89E-07	1.20E-07	4.6450	3.04E-08	4.7717	1.04E-08	4.8235	4.29E-09	4.8368
5	1.33E-08	1.13E-09	6.0811	1.99E-10	6.0371	5.20E-11	6.0142	1.74E-11	5.9981
6	5.44E-10	3.53E-11	6.7471	4.91E-12	6.8550	1.16E-12	6.4559	1.07E-12	-

	$\alpha = 0.5$								
K	4	6		8		10		12	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
1	2.21E-02	1.18E-02	1.5623	7.53E-03	1.5486	5.30E-03	1.5707	3.98E-03	1.5763
2	1.37E-03	4.52E-04	2.7315	2.09E-04	2.6844	1.16E-04	2.6527	7.14E-05	2.6448
3	7.16E-05	1.50E-05	3.8499	4.98E-06	3.8413	2.12E-06	3.8227	1.06E-06	3.8018
4	2.59E-06	3.58E-07	4.8790	8.84E-08	4.8619	3.00E-08	4.8355	1.25E-08	4.8044
5	8.50E-08	7.65E-09	5.9390	1.40E-09	5.9055	3.77E-10	5.8741	1.30E-10	5.8529
6	2.27E-09	1.35E-10	6.9648	1.81E-11	6.9667	3.69E-12	7.1310	1.03E-12	-

	$\alpha = 0.9$								
K	4	6		8		10		12	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
1	7.48E-02	4.68E-02	1.1592	3.39E-02	1.1166	2.64E-02	1.1248	2.16E-02	1.1030
2	4.49E-03	1.81E-03	2.2407	9.64E-04	2.1871	5.94E-04	2.1715	4.01E-04	2.1569
3	2.70E-04	7.62E-05	3.1213	3.12E-05	3.1099	1.55E-05	3.1139	8.81E-06	3.1181
4	1.03E-05	1.79E-06	4.3091	5.36E-07	4.2026	2.10E-07	4.1982	9.81E-08	4.1705
5	3.92E-07	4.95E-08	5.1035	1.13E-08	5.1514	3.59E-09	5.1172	1.41E-09	5.1176
6	1.05E-08	8.12E-10	6.3127	1.36E-10	6.2206	3.39E-11	6.2066	1.09E-11	6.2346

Based on the analysis above, we take

$$\tau \geq \frac{1}{2}\left(\frac{2}{h}\right)^{\alpha} = 2^{\alpha-1}K^{\alpha} \leq K^{\alpha},$$

where the latter scaling originates from the scaling discussed at the end of Section 3.2. It therefore suffices to take $\tau = K^{\alpha}$ in this case for any value of α.

Results are shown in Table 2 for various values of N, K and α. The computations confirm stability and shows an accuracy $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N+1-\alpha})$, consistent with the error analysis in Sec. 3.

4.2. Fractional diffusion problem$(1 < \alpha \leqslant 2)$

Let us now consider the fractional diffusion equation $(1 < \alpha \leqslant 2)$

$$\frac{\partial u(x,t)}{\partial t} = {}_0D_x^{\alpha}u(x,t) + f(x,t),\ \ x \in [0,L], t \in [0,T] \tag{36}$$

with $u(x,0) = u_0(x)$, subject to either Dirichlet boundary conditions, $u(0,t) = g_1(t), u(L,t) = g_2(t)$, Neumann boundary conditions, $u_x(0,t) = h_1(t), u_x(L,t) = h_2(t)$, or some combination thereof. It should be noted that there are alternative ways to define the fractional diffusion operator, i.e., using the right derivative or even a weighted sum of the left and right derivative to mimic the lack of preferred direction in the diffusion operator.

As in the previous case, we first consider the problem in a single domain and introduce the boundary conditions into the equation using a penalty term as

$$\begin{aligned}\frac{\partial u(x,t)}{\partial t} = \quad & {}_0D_x^{\alpha}u(x,t) + f(x,t) \\ & -\tau_D\beta_0\delta(x)\left[u(0,t) - g_1(t)\right] + \tau_N\gamma_0\delta(x)\left[u_x(0,t) - h_1(t)\right] \\ & -\tau_D\beta_L\delta(x-L)\left[u(L,t) - g_2(t)\right] - \tau_N\gamma_L\delta(x-L)\left[u_x(L,t) - h_2(t)\right],\end{aligned} \tag{37}$$

where β and γ reflects which boundary conditions are imposed to ensure wellposedness (see [14] for a discussion of this for the classic case). The constants, τ_D and τ_N reflect, as in the previous case, the strength by which the appropriate boundary conditions are imposed.

We seek an approximate solution as

$$u_h(x,t) = \sum_{j=0}^{N} u(x_j,t)\phi_j(x) = \sum_{j=0}^{N} u_j(t)\phi_j(x)$$

where x_i represents the Gauss points of a particular orthogonal polynomial and $\phi_i(x)$ is, as usual, the Lagrange polynomial associated with these points. As in the previous case, we choose the Chebyshev Gauss points shifted to $x_j = \frac{L}{2}(y_j + 1)$.

Insert the solution into (37) and proceed as in the previous case to recover the semi-discrete scheme

$$\begin{aligned}
\mathrm{M}\frac{d\boldsymbol{u}_h}{dt} = \quad & {}_0\mathrm{S}^{(\alpha)}\boldsymbol{u}_h + \mathrm{M}\boldsymbol{f}_h \\
& -\tau_D\beta_0\boldsymbol{\phi}(0)\left[\boldsymbol{\phi}(0)^T\boldsymbol{u}_h - g_1(t)\right] + \tau_N\gamma_0\boldsymbol{\phi}(0)\left[\boldsymbol{\phi}_x(0)^T\boldsymbol{u}_h - h_1(t)\right] \\
& -\tau_D\beta_L\boldsymbol{\phi}(L)\left[\boldsymbol{\phi}(L)^T\boldsymbol{u}_h - g_2(t)\right] - \tau_N\gamma_L\boldsymbol{\phi}(L)\left[\boldsymbol{\phi}_x(L)^T\boldsymbol{u}_h - h_2(t)\right],
\end{aligned} \tag{38}$$

from which we recover the explicit scheme

$$\begin{aligned}
\frac{d\boldsymbol{u}_h}{dt} = \quad & {}_0\mathrm{D}^{(\alpha)}\boldsymbol{u}_h + \boldsymbol{f}_h \\
& -\tau_D\beta_0\boldsymbol{Q}^-\left[\boldsymbol{\phi}(0)^T\boldsymbol{u}_h - g_1(t)\right] + \tau_N\gamma_0\boldsymbol{Q}^-\left[\boldsymbol{\phi}_x(0)^T\boldsymbol{u}_h - h_1(t)\right] \\
& -\tau_D\beta_L\boldsymbol{Q}^+\left[\boldsymbol{\phi}(L)^T\boldsymbol{u}_h - g_2(t)\right] - \tau_N\gamma_L\boldsymbol{Q}^+\left[\boldsymbol{\phi}_x(L)^T\boldsymbol{u}_h - h_2(t)\right],
\end{aligned}$$

where $\boldsymbol{Q}^{\pm} = [Q^{\pm}(x_0), \ldots, Q^{\pm}(x_N)]^T$.

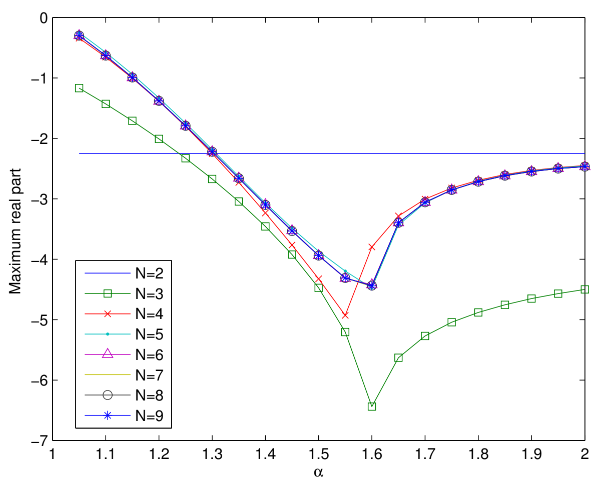

Figure 2: Maximum real part of eigenvalues of ${}_0\mathrm{D}^{(\alpha)} - \tau_D\boldsymbol{Q}^-\boldsymbol{\phi}(0)^T - \tau_D\boldsymbol{Q}^+\boldsymbol{\phi}(L)^T$ with $\tau_D = 1/2\omega$ as a function of α.

As for the fractional advection case, we shall explore the stability analysis of the classic case, $\alpha = 2$, to understand the stability of the fractional problem. BY taking into account that we are considering a Chebyshev method, the results of [14] can be adapted directly to this case as stated in the following.

Theorem 4.1. *The scheme (38) is stable for Dirichlet boundary conditions* ($\beta \neq 0$) *provided*

$$\tau_D \geq \frac{1}{2\beta\omega}, \quad \omega = \frac{2}{N(N+1)},$$

and for Neumann boundary conditions ($\gamma \neq 0$) *provided*

$$\tau_N = \frac{1}{\gamma},$$

Continuing as for the advection problem, let us evaluate the validity of this result for $1 < \alpha \leq 2$. In Fig. 2 we show the maximum real eigenvalue, confirming again that the classic limit is the upper bound. Similar results are obtained for the case of mixed boundary conditions.

The extension to the multi-domain case follows the exact same approach as that discussed for the advection case previously.

4.3. Numerical examples

Consider the diffusion equation ($1 < \alpha \leqslant 2$)

$$\frac{\partial u(x,t)}{\partial t} = {}_0D_x^\alpha u(x,t) + f(x,t), \; x \in [0,\pi], t \in [0,T] \tag{39}$$

with $u(x,0) = \sin_M(x)$, and $u(0,t) = u(\pi,t) = 0$. $f(x) = -e^{-t}(\sin_M(x) + \sin_M^{(\alpha)}(x))$. The exact solution is $u(x,t) = e^{-t}\sin_M(x)$.

Table 3: Convergence of fractional diffusion problem with Dirichlet conditions at $x = 0, \pi$ for different order of approximation, N, number of elements, K, and order of fractional derivative, α. The error is measured in the usual L_2 norm, $\|\varepsilon\|_2 = \|u - u_h\|_2$, and $h = K^{-1}$ is the element size. In all cases, τ is scaled with $\left(\frac{2}{h}\right)^{\alpha}$.

	$\alpha = 1.1$						
K	8	16		24		32	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	4.3e-03	1.1e-03	1.9	5.9e-04	1.6	3.9e-04	1.5
3	2.6e-04	1.5e-04	0.8	9.5e-05	1.1	6.3e-05	1.4
4	2.5e-06	2.0e-07	3.7	4.5e-08	3.6	1.7e-08	3.5
5	9.8e-08	1.3e-08	2.9	3.5e-09	3.2	1.3e-09	3.5
	$\alpha = 1.4$						
K	8	16		24		32	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	1.8e-03	8.4e-04	1.1	5.2e-04	1.2	3.6e-04	1.2
3	1.3e-04	4.6e-05	1.4	2.6e-05	1.4	1.6e-05	1.6
4	1.8e-06	1.9e-07	3.2	4.9e-08	3.3	1.9e-08	3.3
5	5.0e-08	4.8e-09	3.4	1.2e-09	3.5	4.0e-10	3.7
	$\alpha = 1.7$						
K	8	16		24		32	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	2.4e-03	3.4e-04	2.8	2.6e-04	0.6	2.3e-04	0.4
3	2.3e-04	3.5e-05	2.7	1.0e-05	3.0	4.2e-06	3.2
4	1.7e-06	6.1e-08	4.8	2.7e-08	2.1	1.3e-08	2.4
5	1.0e-07	3.8e-09	4.8	4.9e-10	5.0	1.2e-10	5.0
	$\alpha = 2.0$						
K	8	16		24		32	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	7.5e-03	2.0e-03	1.9	1.0e-03	1.7	6.6e-04	1.5
3	8.5e-04	2.2e-04	2.0	9.8e-05	2.0	5.5e-05	2.0
4	8.6e-06	5.7e-07	3.9	1.3e-07	3.7	4.6e-08	3.5
5	5.2e-07	3.4e-08	3.9	6.7e-09	4.0	2.1e-09	4.0

Results are shown in Table 3 for various values of N, K and α. The computations confirm stability. However, the picture for the error is less clear than for the fractional advection case, indicating a convergence rate with an even-odd pattern. However, the convergence is not readily concluded, i.e., for α close to 1, we observe $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N+1/2-\alpha})$ for N even and $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N-1/2-\alpha})$ for N odd. However, as α approaches the classic value of 2, we find $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N+3/2-\alpha})$ for N even and $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N+1-\alpha})$ for N odd, more in line with the previous analysis.

To further understand the source of this behavior, let is consider a slightly different scheme given as

$$\frac{d}{dt}\boldsymbol{u}_h = {}_0D^{(\alpha)}\boldsymbol{u}_h + \boldsymbol{f}_h - \tau_D \boldsymbol{Q}^{-}[\phi(0)^T \boldsymbol{u}_h(0) - g_1(t)] - \tau_N \boldsymbol{Q}^{*}[\boldsymbol{\phi}_x^T(L)\boldsymbol{u}_h - h_2(t)], \tag{40}$$

where we define the new $\boldsymbol{Q}^*(x)$ as

$$\boldsymbol{Q}^*(x) = M^{-1}\boldsymbol{\phi}_x(x).$$

Scaling for τ_D and τ_N are as above.

Table 4: Convergence of fractional diffusion problem with Dirichlet conditions at $x = 0, \pi$ for different order of approximation, N, number of elements, K, and order of fractional derivative, α. The error is measured in the usual L_2 norm, $\|\varepsilon\|_2 = \|u - u_h\|_2$, and $h = K^{-1}$ is the element size. In all cases, τ is scaled with $(\frac{2}{h})^{\alpha}$.

	$\alpha = 1.1$						
K	8	12		16		20	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	1.2e-03	3.2e-04	3.3	1.6e-04	2.5	1.1e-04	1.5
3	8.4e-05	2.3e-05	3.2	9.8e-06	3.0	5.6e-06	2.6
4	6.0e-07	1.1e-07	4.1	3.7e-08	4.0	1.5e-08	3.9
5	2.1e-08	2.6e-09	5.2	5.7e-10	5.3	1.8e-10	5.2
	$\alpha = 1.4$						
K	8	12		16		20	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	4.0e-03	1.6e-03	2.2	9.0e-04	2.1	5.8e-04	2.0
3	8.2e-05	2.7e-05	2.8	1.2e-05	2.9	6.0e-06	3.0
4	1.0e-06	1.8e-07	4.2	5.7e-08	4.1	2.3e-08	4.0
5	2.7e-08	4.2e-09	4.6	1.1e-09	4.7	3.8e-10	4.7
	$\alpha = 1.7$						
K	8	12		16		20	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	8.7e-03	4.1e-03	1.8	2.5e-03	1.7	1.7e-03	1.7
3	2.0e-04	8.3e-05	2.2	4.3e-05	2.3	2.6e-05	2.3
4	3.7e-06	8.4e-07	3.7	3.0e-07	3.6	1.3e-07	3.5
5	8.8e-08	1.6e-08	4.2	4.7e-09	4.3	1.8e-09	4.3
	$\alpha = 2.0$						
K	8	12		16		20	
N	$\|\varepsilon\|_2$	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order	$\|\varepsilon\|_2$	Order
2	1.2e-02	6.2e-03	1.6	4.1e-03	1.4	3.1e-03	1.3
3	7.2e-04	3.3e-04	1.9	1.9e-04	2.0	1.2e-04	2.0
4	7.4e-06	1.9e-06	3.3	7.8e-07	3.2	3.9e-07	3.1
5	4.1e-07	8.3e-08	4.0	2.7e-08	4.0	1.1e-08	4.0

In Table 4 we show the results for$u(x,0) = \sin_M(x)$, and $u(0,t) = u(\pi,t) = 0$. $f(x) = -e^{-t}(\sin_M(x) + \sin_M^{(\alpha)}(x))$. The exact solution is $u(x,t) = e^{-t}\sin_M(x)$.

The conclusion is, in this case, substantially easier to reach and generally reflects $\|\varepsilon\|_2 \simeq \mathcal{O}(h^{N+1-\alpha})$ in accordance with the approximation results. Unfortunately, stability of the scheme in Eq. (40) remains an open questions as it does not appear it can be resolved using the techniques leading to the results in Theorem 4.1. Nevertheless, we observe no stability problems and conjecture that this scheme is stable while having optimal convergence rates.

5. Conclusion

We have introduced a high order accurate approximation for fractional derivative in single and multi domain and discussed the accuracy of the approximation. The stability of the numerical scheme is ensured by imposing boundary conditions through a penalty term and we have shown that this approach is applicable for both single and multi-domain formulations. The schemes have been developed and demonstrated for both fractional advection and diffusion equation. For the advection equation, the convergence rate is consistent with the analysis. However, the examples showed that a more careful analysis is required to fully understand the behavior of the scheme for the fractional diffusion case.

As one of the few papers dealing with high-order accurate schemes for the modeling and solution of fractional differential equations, it leaves many questions open. While the extension to deal with nonlinear terms appears straightforward, the associated analysis is far from trivial. Furthermore, the development of related schemes for problems in complex geometries, requiring unstructured multi-dimensional grids, if far from obvious and we hope to be able to report on progress along these lines in the future

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Appendix A. Special case of Gaussian hypergeometric functions

When expressing the fractional derivative, we only consider the special case of the Gaussian hypergeometric function- ${}_2F_1(\beta, n; n+1; \frac{1}{z})$. For this special case, the hypergeometric functions can be computed exactly for any $z > 1$, as follows

$$\begin{aligned}
{}_2F_1(\beta,0;1;\frac{1}{z}) &= \frac{z^{\beta}(z-1)^{1-\beta}-z}{\beta-1} \\
{}_2F_1(\beta,1;2;\frac{1}{z}) &= \frac{2z^2+2z^{\beta}(z-1)^{1-\beta}(\beta-z-1)}{(1-\beta)(2-\beta)} \\
{}_2F_1(\beta,n;n+1;\frac{1}{z}) &= \frac{(n+1)\Gamma(1-\beta)z^{\beta}(z-1)^{-\beta}H_n(z,\beta)}{\Gamma(n+2-\beta)}
\end{aligned}$$

where $H_n(z,\beta)$ is defined as,

$$\begin{aligned}
H_2(z,\beta) &= -2\,(z-1)^{\beta}\,z^{-\beta+3}-\beta^2+z\beta^2-2-\beta\,z-2\,z^2\beta+3\,\beta+2\,z^3 \\
H_3(z,\beta) &= 6\,(z-1)^{\beta}\,z^{-\beta+4}-\beta^3+6-3z\beta^2+6\beta^2+3z^2\beta+2\beta z-11\beta+z\beta^3-3z^2\beta^2 \\
&\quad -6z^4+6z^3\beta \\
H_4(z,\beta) &= 24\,(z-1)^{\beta}\,z^{5-\beta}+24-z\beta^4+6\beta z+8z^2\beta+6z\beta^3+12z^3\beta+24z^4\beta+4z^2\beta^3 \\
&\quad -11z\beta^2-12\,z^2\beta^2-12\,z^3\beta^2+\beta^4-10\,\beta^3-50\,\beta+35\,\beta^2-24\,z^5 \\
H_5(z,\beta) &= 120(z-1)^{\beta}z^{6-\beta}-\beta^5+15\beta^4+225\beta^2-85\beta^3-274\beta-120z^6+120-60z^3\beta^2 \\
&\quad -10z\beta^4-50z\beta^2+60z^4\beta+35z\beta^3+30z^2\beta+30z^2\beta^3+24\beta z-55z^2\beta^2+40z^3\beta \\
&\quad +z\beta^5-60z^4\beta^2-5z^2\beta^4+120z^5\beta+20z^3\beta^3 \\
H_6(z,\beta) &= -720-6z^2\beta^5-720z^6\beta+360z^5\beta^2-120z^4\beta^3+30z^3\beta^4+1764\beta+274z\beta^2 \\
&\quad +720z^7-210z^2\beta^3+330z^3\beta^2-240z^4\beta+85z\beta^4+\beta^6z-720\,(z-1)^{\beta}\,z^{-\beta+7} \\
&\quad -175\beta^4-15z\beta^5+360z^4\beta^2+60z^2\beta^4-360z^5\beta-180z^3\beta^3+21\beta^5-1624\beta^2 \\
&\quad -\beta^6+735\beta^3-225z\beta^3-180z^3\beta-120\beta z+300z^2\beta^2-144z^2\beta
\end{aligned}$$

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