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Numerical approximation of the space-time fractional diffusion problem

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Abstract: Fractional differential equations have become central tools for the accurate modeling of real-world phenomena in various fields. This work focuses on the discretization of the space-time fractional diffusion problem with Caputo derivative in time and Riesz-Caputo derivative in space. We introduce a collocation method based on a B-spline representation of the solution. This approach strategically exploits the symmetry properties of both the spline basis functions and the Riesz-Caputo operator, resulting in an efficient method for solving the given fractional differential problem. Preliminary numerical tests are presented to validate the proposed collocation method.

Keywords: Fractional Calculus, Riesz-Caputo Operator, B-Spline, Collocation Method, Greville Abscissae

1. INTRODUCTION

Nowadays, models based on fractional derivatives in time and/or space have become common in several disciplines, including biology, physics, mechanics, economics, and control theory (see, for instance, (Hilfer, 2000; Zaslavsky, 2002; Kilbas *et al.*, 2006; Magin, 2006; Mainardi, 2010; Baleanu *et al.*, 2016) and references therein). This choice is due to the unique ability of fractional derivatives, as nonlocal operators, to clearly describe memory and inheritance properties intrinsic in several physical systems.

In the field of geophysics, fractional differential equations find wide application in the modeling of anomalous diffusion in porous media. This phenomenon describes the diffusion of particles at a speed incompatible with the classical Brownian motion. In this context, the fractional Riesz derivative has been shown to be more advantageous than its left-handed counterpart because it effectively incorporates contributions from both sides of the domain (Metzler and Klafter, 2000; Zaslavsky, 2002), reflecting properties typical of diffusive processes. In particular, the Riesz derivative is a linear combination of the left and right derivatives, resulting in a fractional derivative with central symmetry over finite domains.

While the Riesz derivative, defined by the right and left Riemann–Liouville derivatives, is commonly used to model fractional diffusion, the Riesz–Caputo derivative emerges as a more suitable alternative to avoid non-physical problems, as discussed in (Pandey *et al.*, 2011). Therefore, in this paper we focus on a diffusion problem using the Riesz–Caputo derivative in space and the left–Caputo derivative in time. In particular, the paper aims to introduce a collocation method based on optimal B-spline basis functions to approximate the solution of the anomalous diffusion model we are interested in.

2. MATHEMATICAL MODEL

We consider the space-time fractional differential problem for $x \in [0, L]$, $t \in [0, T]$ together with the initial and boundary conditions (Podlubny, 1999; Chen *et al.*, 2017):

$$\begin{cases} {}^{L}D_t^{\beta} u(x,t) = {}^{RC}D_x^{\alpha} u(x,t) + f(x,t), \\ u(x,0) = u_0(x), \quad x \in [0,L] \\ u(0,t) = g_1(t), \quad t \in [0,T] \\ u(L,t) = g_2(t), \quad t \in [0,T] \end{cases} \tag{1}$$

where $0 < \beta < 1$ and $1 < \alpha < 2$.
Here ${}^{RC}D_x^{\alpha} u(x,t)$ denotes the Riesz-Caputo fractional derivative in space defined as (Podlubny, 1999; Diethelm, 2010; Agrawal, 2007)

$${}^{RC}D_x^{\alpha} u(x,t) := \frac{1}{2}({}^{L}D_x^{\alpha} + (-1)^m {}^{R}D_x^{\alpha}) u(x,t), \tag{2}$$

where the left and right Caputo derivatives are defined by:

$${}^{L}D_x^{\alpha} u(x,t) := \frac{1}{\tilde{\gamma}} \int_0^x \frac{1}{(x-\xi)^{1-\tilde{m}}} \frac{\partial^m u(\xi,t)}{\partial \xi^m} d\xi \tag{3}$$

$${}^{R}D_x^{\alpha} u(x,t) := \frac{1}{\tilde{\gamma}} \int_x^L \frac{(-1)^m}{(\xi-x)^{1-\tilde{m}}} \frac{\partial^m u(\xi,t)}{\partial \xi^m} d\xi, \tag{4}$$

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with m being the integer such that $m-1 \le \alpha < m$, $\tilde{m} = m - \alpha$, $\tilde{\gamma} = \Gamma(\tilde{m})$ and Γ the Euler gamma function. The time-fractional derivative appearing in (1) is the same as the one defined in (3) with the obvious difference in the integration variable.

3. MATERIALS AND METHODS

In this section, we describe the optimal B-spline basis we use to approximate the solution to the fractional differential problem (1). We also give the expression of its fractional derivatives. Finally, we introduce the collocation method used to compute the approximate solution.

3.1 The Optimal B-spline Basis

Splines are piecewise polynomials of given degree. On the real line they can be written as linear combination of the translate of cardinal B-splines, which are compactly supported piecewise polynomials having breakpoints at the integers. The cardinal B-spline N_n of integer degree $n \ge 0$ can be expressed as

$$N_n(x) = (n+1)[0, 1, \dots, n+1](y-x)_+^n, \tag{5}$$

where $x_+^n := \max(0,x)^n$ is the truncated power function and $[x_0, x_1, \dots, x_{n+1}]f$ denotes the divided difference of the function f (considered as a function of y) on the sequence of knots $\{x_0, x_1, \dots, x_{n+1}\}$.

On a finite interval splines can be represented as linear combination of the optimal basis, which have equispaced knots of multiplicity $n+1$ at the endpoints of the interval (de Boor, 1978; Schumaker, 2007).

Let L be an integer greater than n and $\mathcal{I}_0 = \{x_0, x_1, \dots, x_M\}$ be the sequence of integer knots belonging to $[0, L]$ with x_0 and x_M having multiplicity $n+1$:

$$x_0 = x_1 = \dots = x_n = 0\,,$$

$$x_j = j - n\,, \quad n+1 \le j \le M-n-1\,,$$

$$x_{M-n} = x_{M-n+1} = \dots = x_M = L\,,$$

where $M = L + 2n + 1$.
The optimal basis

$$\mathcal{N}_n(x) = \{N_{j,n}(x), 0 \le j \le L+n-1\}$$

on the interval $[0, L]$ has $L+n$ basis functions. The $2n$ functions $N_{j,n}$ and $N_{L+n-1-j,n}$, $0 \le j \le n-1$, are the left and right boundary functions, respectively. The $L-n$ functions $N_{j,n}$, $n \le j \le L-1$, are the internal functions.

The internal functions are the integer translates $N_n(x-j)$ whose support belongs to the interval $[0, L]$:

$$N_{j,n}(x) = N_n(x - j + n)\,, \qquad n \le j \le L-1\,. \tag{6}$$

The left boundary functions have expression (see (Pitolli, 2018))

$$N_{j,n}(x) = (j+1)\,\frac{|T_{j,n}(x)|}{|P_{j,n}|}\,, \qquad 0 \le j \le n-1\,, \tag{7}$$

where T_{jn} is the $(j+1)$ order collocation matrix

$$T_{j,n}(x) = M\begin{pmatrix} y^{n-j+1}, & \cdots & y^n, & (y-x)_+^n \\ 1, & \cdots & j, & j+1 \end{pmatrix},$$

and P_{jn} is the $(j+1)$ order collocation matrix

$$P_{j,n} = M\begin{pmatrix} y^{n-j+1}, & \cdots & y^n, & y^{n+1} \\ 1, & \cdots & j, & j+1 \end{pmatrix}.$$

By using the central symmetry property of the cardinal B-splines, we can obtain the right boundary functions:

$$N_{L+n-1-j,n}(x) = N_{j,n}(L-x)\,, \quad 0 \le j \le n-1\,. \tag{8}$$

We notice that by construction the optimal basis is centrally symmetric and fulfills the endpoint conditions

$$N_{j,n}(0) = \delta_{j0}\,, \quad N_{L+n-1-j,n}(L) = \delta_{j0}\,, \tag{9}$$

where δ_{j0} denotes the Kronecker symbol.

The optimal basis $\mathcal{N}_n$ can be refined by dilation (de Boor, 1978; Schumaker, 2007). Let h be the refinement step, that is, the distance between the refined knot sequence:

$$x_{0,h} = x_{1,h} = \dots = x_{n,h} = 0\,,$$

$$x_{j,h} = jh - n\,, \quad n+1 \le j \le M-n-1\,,$$

$$x_{M_h-n,h} = x_{M_h-n+1,h} = \dots = x_{M_h,h} = L\,,$$

where $M_h = L/h + n$. The refined basis

$$\mathcal{N}_{h,n}(x) = \{N_{j,h,n}(x) = N_{j,n}(\frac{x}{h}), 0 \le j \le M_h\}\,,$$

$x \in [0, L]$, has $L/h - n$ internal functions and $2n$ boundary functions. We observe that refining the knots only corresponds to an increase of the number of the internal functions while the number of the boundary functions does not change.

An example of the optimal basis $\mathcal{N}_{h,3}$ for the cubic spline space on the interval $[0, 1]$ with refinement step $h = 1/8$ is shown in Figure 1.

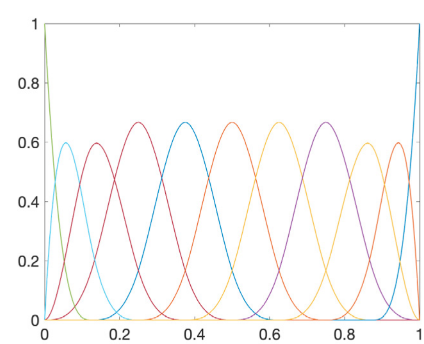

Fig. 1. The optimal cubic spline basis $\mathcal{N}_{h,3}$ on the interval $[0, 1]$ with refinement step $h = 1/8$.

3.2 Fractional Derivatives of the Optimal B-spline

The fractional derivatives of the optimal B-spline basis functions can be computed analytically using the explicit formula in (Pitolli, 2018; Pitolli et al., 2022) and exploiting the symmetry properties of the Riesz-Caputo operator and of the basis functions (see Fig. 2). In particular, the following Proposition holds (Pitolli et al., 2022):

Proposition 1. Let

$$\Phi = \{\phi_j(x), 0 \le j \le M\}$$

be a function basis centrally symmetric in the interval $[0, L]$, i.e.,

$$\phi_j(x) = \phi_{M-j}(L-x), \tag{10}$$

for $0 \le j \le M$ and $x \in [0, L]$. Then, the left and right Caputo derivatives of the basis function Φ satisfy the following symmetry properties:

$$^R D_x^\alpha \phi_j(x) = ^L D_{L-x}^\alpha \phi_j(L-x), \tag{11}$$

for $0 \le j \le M$.

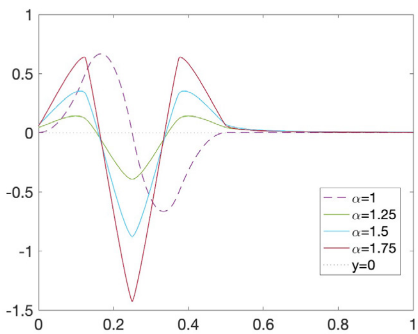

Fig. 2. The Riesz–Caputo derivative of the cubic B-spline, varying the fractional order α.

3.3 The Collocation Method

Using the optimal B-spline basis introduced in section 3.1, we can approximate the solution of the differential problem (1) as a tensor product of univariate splines of degree n and m:

$$u(x,t) \approx u_{h,k}(x,t) = \\ = \sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(x) N_{j,k,m}(t)\,, \tag{12}$$

where h and k are the space and time steps, respectively. Inserting (12) in (1), we obtain:

$$^L D_t^\beta \sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(x) N_{j,k,m}(t) \\ = ^{RC} D_x^\alpha \sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(x) N_{j,k,m}(t) + f(x,t)$$

that reads as

$$\sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(x) ^L D_t^\beta N_{j,k,m}(t) \\ = \sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{j,k,m}(t) ^{RC} D_x^\alpha N_{i,h,n}(x) + f(x,t), \tag{13}$$

so we are left with computing fractional derivative (in space and time) of the B-splines.

To compute the coefficients $\{c_{i,j}, 0 \le i \le M_h, 0 \le j \le M_k\}$ of the spline approximation (12) we use a collocation method. To this end we choose as collocation points the Greville abscissae (de Boor, 1978; Schumaker, 2007; Sablonnière, 2005) defined as:

$$\xi_{i,h} = \frac{x_{i,h} + \ldots + x_{i+n-1,h}}{n}, \quad 0 \le i \le M_h\,, \tag{14}$$

$$\tau_{i,k} = \frac{t_{i,k} + \ldots + t_{i+n-1,k}}{n}, \quad 0 \le i \le M_k\,, \tag{15}$$

see Figure 3.

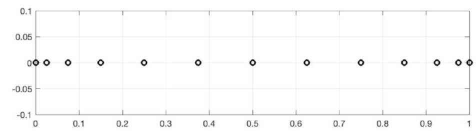

Fig. 3. The Greville Abscissae.

Collocating equation (13) in the Greville abscisse we obtain the linear system

$$\left(\mathsf{D}_{k,m} \otimes \mathsf{N}_{h,n} - \mathsf{N}_{k,m} \otimes \mathsf{D}_{h,n}\right) \mathsf{C} = \mathsf{F}, \tag{16}$$

where

$$\mathsf{C} = [c_{i,j}, 1 \le i \le M_k, 1 \le j \le M_h - 1]$$

is the unknown column vector,

$$\mathsf{D}_{k,m} = \left[D_t^\beta N_{j,k,m}(\tau_{i,k}), 1 \le i,j \le M_k\right],$$

$$\mathsf{N}_{k,m} = \left[N_{j,h,n}(\tau_{i,k}), 1 \le i,j \le M_k\right]$$

are the collocation matrices of the optimal basis and of its fractional derivative evaluated on the collocation points $\{\tau_{i,k}\}$,

$$\mathsf{D}_{h,n} = \left[^{RC} D_x^\alpha N_{i,h,n}(\xi_{i,h}), 1 \le i,j \le M_h - 1\right],$$

$$\mathsf{N}_{h,n} = \left[N_{j,h,n}(\xi_{i,h}), 1 \le i,j \le M_h - 1\right]$$

are the collocation matrices of the optimal basis and of its fractional derivative on the collocation points $\{\xi_{i,h}\}$, and

$$\mathsf{F} = [f(\tau_{i,k}, \xi_{j,k}), 1 \le i \le M_k, 1 \le j \le M_h - 1]$$

is the known term.
Here the symbol $\otimes$ denotes the Kronecker tensor product.

Finally, the initial and boundary conditions

$$\sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(\xi_{l,h}) N_{j,k,m}(0) = u_0(\xi_{l,h})\,, \tag{17}$$

$0 \le l \le M_h$, and

$$\sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(0) N_{j,k,m}(\tau_{r,k}) = g_1(\tau_{r,k})\,, \\ \sum_{i=0}^{M_h}\sum_{j=0}^{M_k} c_{i,j} N_{i,h,n}(L) N_{j,k,m}(\tau_{r,k}) = g_2(\tau_{r,k})\,, \tag{18}$$

$0 \le r \le M_k$, are added to the linear system (16).
Note that the choice of using Greville abscissae generates a square linear system, which implies no extra error due the approximation of using e.g. least squares method to solve rectangular systems.

4. NUMERICAL EXPERIMENTS

In order to test the proposed numerical method, we compare the numerical approximation with the analytical solution of (1) given by

$$u(x,t) = t^\mu + \sin(\omega x), \tag{19}$$

in the interval $[0, 1] \times [0, 1]$, $f(x,t)$ is computed accordingly and

n/j	3	4	5
3	1.7e-03	2.9e-04	5.1e-05
4	9.9e-06	5.8e-07	2.9e-08
5	5.4e-06	2.3e-07	1.0e-08

Table 1. Error computed as in (21) for the parameters $\omega = \pi,\ \beta = 0.5,\ \gamma = 1.5,\ \mu = 2.8$.

n/j	3	4	5
3	7.8e-03	1.8e-03	4.3e-04
4	4.1e-05	2.9e-06	1.9e-07
5	2.0e-05	1.2e-06	7.2e-08

Table 2. Error computed as in (21) for the parameters $\omega = \pi,\ \beta = 0.1,\ \gamma = 1.9,\ \mu = 4$.

n/j	3	4	5
3	2.1e-01	4.7e-02	8.9e-03
4	1.2e-01	5.1e-03	2.2e-04
5	5.4e-02	1.9e-03	6-4e-05

Table 3. Error computed as in (21) for the parameters $\omega = 6\pi,\ \beta = 0.5,\ \gamma = 1.5,\ \mu = 2.8$.

$$\begin{cases} u(x,0) = \sin(\omega x), \quad x \in [0,1], \\ u(0,t) = t^{\mu} \quad t \in [0,1,] \\ u(L,t) = t^{\mu} + \sin(\omega L), \quad t \in [0,1]. \end{cases} \tag{20}$$

The error is computed as:

$$e_{h,k} = \max_{x\in[0,1],t\in[0,1]} |u(x,t) - u_{h,k}(x,t)|. \tag{21}$$

We test the method for different values of the time fractional derivative β, the space fractional derivative γ, the regularity of the solution μ, the wave number ω and the degree of the B-splines. In Figure 4 we show the approximated solution for the parameter selection $\omega = 6\pi, \beta = 0.5, \gamma = 1.5$ and $\mu = 2.8$. Tables 1–3 report the error for different choices of the above mentioned parameters, showing the good performance of the proposed method.

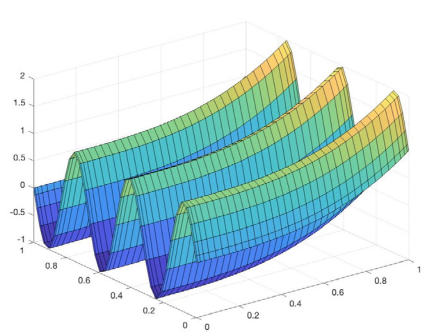

Fig. 4. Approximated solution of the numerical experiment (19) for the parameter selection $\omega = 6\pi, \beta = 0.5, \gamma = 1.5$ and $\mu = 2.8$, see also Table 3.

5. CONCLUSION AND FUTURE WORK

In this study we present a spline collocation method to solve the space-time fractional diffusion problem, where the fractional derivative in time is represented by the left Caputo operator and the fractional derivative in space is given by the Riesz–Caputo derivative. We exploit the symmetry properties of both the spline basis functions and of the Riesz-Caputo operator to provide an efficient numerical method.

Numerical tests varying the fractional order in space and time show the good performance of the numerical method for different degrees of the splines used to represent the approximated solution.

In the next future we plan to extend the present work to analyze the convergence of the method and better understand its dependence on the different quantities involved (fractional order in space and time, degree of the splines, regularity of the solution, etc).

We also plan to work on a weak formulation to solve the space-time fractional diffusion problem; in this context analytical expression of the refinable functions used (see Pellegrino et al. (2023)) will provide an efficient and accurate evaluation of the integrals required for the computation of the connection coefficients in the Galerkin method.

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