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Numerical Solution of Fractional Diffusion Equation by Shifted Legendre Operational Matrix Method and Fractional Linear Multi-step Methods

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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Abstract

The paper deals with an efficient scheme to solve fractional diffusion equation including both time and spatial fractional derivative in Caputo sense. In the first time, the so-called operational matrice was obtained by

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computating fractional derivative of shifted Legendre polynomial followed by applying the spectral Tau method that convert the original equation in the system of fractionnal ordinary differential equation (FODE). The fractionnal linear multi-step metthods (FLMMS) can be used in the second time to give the approximate solution. To acces the accuracy and validity of the method, two illustratives examples are reported using Matlab code.

Keywords: Fractional diffusion equation; operational matrice; shifted legendre polynomials; tau method; fractional ordinary differential equation; linear multi-step methods.

2010 Mathematics Subject Classification: 53C25, 83C05, 57N16.

1 Introduction

To describe the density of a certain maturity in a medium, the diffusion equation is the most often used with a function of time and space, based on the mass conservation principe and Fick's law of diffusion (D. Mbainguesse, 2024; M. M. Khader, 2011; Khader, 2010). In recent years, the extension of this equation to fractional form has made it possible to introduce an improvment that take into account memory and long-term effects in fractional formulation (Ervin K. L., 2023; Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Khader, 2010; Priya and Sabarmathi, 2022, 2024b,a,c).

In this paper, we consider the problem

$$\frac{\partial^{\alpha} u}{\partial t^{\alpha}}(x,t) = \kappa \frac{\partial^{2} u}{\partial x^{2}}(x,t) + K(x,t) \tag{1.1}$$

with boundaries conditions

$$u(0,t) = p(t) \tag{1.2}$$

and

$$u(1,t) = q(t) \tag{1.3}$$

and initial condition

$$u(x,0) = g(x) \tag{1.4}$$

where $\alpha \in]0,1]$, $\sigma \in]0,2]$, $0 \leq x \leq 1$; $0 < t \leq 1$, κ is the diffusibility, K a given source function, p, q and g are known functions. The difficulty of finding analytical methods for this kind of fractional-order equations has forced research to turn to numerical methods.The most commonly used numerical methods in litterature are: homotopy perturbation method (S. Momani, 2007), Tau method (A. Saadatmandi, 2006; E. H. Doha, 2014; Saadatmandia and Dehghan, 2010), spectral method (H. Singh, 2019; D. Baleanu, 2018; H. Singh, 2020) and so on (R. Magin, 2009; M. M. Khader, 2020; H. Singh, 2018; M. M. Khader, 2011; Khader, 2010; Mbainguesse et al., 2023; Benattia and Kacem, 2017; Abdimazraeh et al., 2013; ur Rehman and Khan, 2013; Himeda and co authors, 2022). It is therefore essential to use easy and efficient methods. Our approach is to adopt a strategy similar to that used in MOL methods (Himeda and co authors, 2022). In the first step, the operational matrice (see (E. H. Doha, 2014; D. Baleanu, 2018; Saadatmandia and Dehghan, 2010)) based on shifted Legendre's fractional derivative is computed and used to convert the fractional derivative in space in vectorial form. The result is a system of fractional ordinary differential equations in time after application of Tau spectral method. Then, in the second step, the FLMM solver integrate the resulting FODE to give the approximate solution.

The paper is structured as follows: In section 2, mathematical importants tools for the paper are introduced. The operational matrice, the shifted Legendre polynomials are described in section 3. The section 4 expose the application of the method to solve fractional diffusion equation. The proposed methods are used to demonstrate his reliability and accuracy on two illustratives examples in section 5. In section 6, the concluded results are presented.

2 Mathematical Preliminaries on Fractional Calculus

Fractional calculs is a branch of mathematics that attracts a lot of research because of of its importance in capturing phenomena with memory and long effects. Litterature on the subjects is flourshing: (Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Podlubny, 1999; R. L. Bagley, 1983; Mainardi, 1997; Priya and Sabarmathi, 2022; Oldham and Spanier, 1974; Miller and Ross, 1993; Samko et al., 1993; Priya and Sabarmathi, 2024b,a,c). We recall in this section the Riemann-Liouville integral (Samko et al., 1993), the Caputo fractional derivative (Priya and Sabarmathi, 2022; Samko et al., 1993), the fractional ordinary differential equation (Xue and Bai, 2017) and the linear multi-step method for FODE (Garrappa, 2018; Lubich, 1983; Aceto et al., 2015; Sweilam et al., 2007; Wolkenfelt, 1979).

2.1 Definitions and properties of fractional integrals and derivatives

Definition 2.1. (Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Podlubny, 1999; R. L. Bagley, 1983; Mainardi, 1997; Samko et al., 1993): The Riemann-Liouville (RL) fractional integral of order $\alpha > 0$ and origin at a for a given function $y \in L^1[a,b]$ is defined as:

$$I_a^\alpha y(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-s)^{\alpha-1} y(s) ds. \tag{2.1}$$

Definition 2.2. (Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Podlubny, 1999; R. L. Bagley, 1983; Mainardi, 1997; Priya and Sabarmathi, 2022; Samko et al., 1993): The fractional Caputo left derivative of order $\alpha > 0$ of the function $y(t)$, $t \in [a,b]$ is given by:

$$D_a^\alpha y(t) = I_a^{n-\alpha} D^n y(t) = \frac{1}{\Gamma(n-\alpha)} \int_a^t (t-s)^{n-\alpha-1} y^{(n)}(s) ds, n-1 < \alpha \le n \tag{2.2}$$

where D^n, $y^{(n)}$ denotes the standard integer-order derivative. If $a = 0$, then $D_0^\alpha y(s) = D^\alpha y(t)$ and we have

$$D^\alpha y(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{y^{(n)}(s)}{(t-s)^{\alpha+1-n}} ds, \ n-1 < \alpha \le n, \ n \in \mathbb{N}. \tag{2.3}$$

Property 2.1. *(Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Podlubny, 1999; R. L. Bagley, 1983; Mainardi, 1997; Priya and Sabarmathi, 2022; Samko et al., 1993)*

$$D^\alpha K = 0, \ (K \text{ is a constant}), \tag{2.4}$$

$$D^\alpha t^\mu = \begin{cases} 0, & for \quad \mu \in \mathbb{N} \ and \ \mu < \lceil \alpha \rceil \\ \dfrac{\Gamma(\mu+1)}{\Gamma(\mu+1-\alpha)} t^{\mu-\alpha}, & for \quad \mu \in \mathbb{N} \ and \ \mu \ge \lceil \alpha \rceil \ or \ \mu \notin \mathbb{N} \ and \ \mu > \lfloor \alpha \rfloor, \end{cases} \tag{2.5}$$

where $\lceil \alpha \rceil$ is the smallest integer greater than or equal to α and $\lfloor \alpha \rfloor$ is the largest integer less than or equal to α

Property 2.2. *(Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Podlubny, 1999; R. L. Bagley, 1983; Mainardi, 1997; Priya and Sabarmathi, 2022; Samko et al., 1993)*

$$D^\alpha \left(\theta f(t) + \gamma g(t)\right) = \theta D^\alpha f(t) + \gamma D^\alpha g(t), with \ \ t \in [a,b], \ \theta \text{ and } \gamma \text{ constants.} \tag{2.6}$$

Property 2.3. *(Enrique C. Gabrick et al., 2023; A. A. Kilbas, 2006; Podlubny, 1999; R. L. Bagley, 1983; Mainardi, 1997; Priya and Sabarmathi, 2022; Samko et al., 1993)*

$$I_t^{n-\alpha} D_t^\alpha y(t) = y(t) - P_{n-1}[y;a](t), \tag{2.7}$$

$$where \ P_{n-1}[y;a](t) = \sum_{j=0}^{n-1} \frac{(t-a)^j}{j!} y^{(j)}(t) \tag{2.8}$$

is the Taylor polynomial.

2.2 Fractional ordinary differential equation (FODE)

We define the fractional ordinary differential equation (FODE) of the form (Garrappa, 2018; Xue and Bai, 2017; Diethelm, 2010; ur Rehman and Khan, 2013)

$$\begin{cases} D_{t_0}^{\alpha} u(t) &= g(t,u(t)),\ t \in [t_0,T] \\ u^{(j)}(t_0) &= c_j,\ \ j = 0,1,...,N-1 \end{cases} \tag{2.9}$$

where $\alpha \in]n-1,n]$, $g(t,u(t))$ is continuous and $c_0,\ \dots,\ c_{n-1}$ constants. If we apply the RL integration to both side of (2.9) and using (2.7) we can obtain the weakly singular Volterra Integration Equation (VIE) formulas: (Lubich, 1983; Wolkenfelt, 1982)

$$u(t) = P_{n-1}[u;t_0](t) + \frac{1}{\Gamma(\alpha)} \int_{t_0}^{t} (t-s)^{\alpha-1} g(s,y(s))ds. \tag{2.10}$$

2.3 Convolution quadrature rules

To solve numerically the equation (2.9), we approximate (2.10) by convolution quadrature (Lubich, 1988a,b, 2004; Schädle et al., 2006; Lubich, 1986)

$$u_n = \psi_n + \sum_{j=0}^{n} c_{n-j} g_j,\ , \tag{2.11}$$

where $g_j = g\left(t_j, y_j\right), \psi_n$ and c_n are known coefficients, $t_n = t_0 + n\Delta t$ is grid point, with a constant step-size $\Delta t > 0$ and $u_n = u(t_n)$. Two classes of convolution quadrature rules for FODE are important: the product-integration (PI) rule and Fractional linear multi-step methods.

2.3.1 Product-Integration (PI) rules

To derive the product-integration rule ($Young$, 1954), the solution of the VIE (2.10) at t_n is first written as:

$$u(t_n) = P_{n-1}[u;t_0](t_n) + \frac{1}{\Gamma(\alpha)} \int_{t_0}^{t_n} (t_n - s)^{\alpha-1} g(s,u(s))ds, \tag{2.12}$$

If $g(s,y(s)) \simeq g\left(t_j, y_j\right)$, we have the explicit PI rectangular:

$$u_n = P_{n-1}[u;t_0](t_n) + \Delta t^{\alpha} \sum_{j=0}^{n-1} \varrho_{n-j-1}^{(\alpha)} g\left(t_j, u_j\right). \tag{2.13}$$

If $g(s,y(s)) \simeq g\left(t_{j+1}, u_{j+1}\right)$, we have the implicit PI rectangular:

$$u_n = P_{n-1}[u;t_0](t_n) + \Delta t^{\alpha} \sum_{j=1}^{n-1} \varrho_{n-j-1}^{(\alpha)} g\left(t_j, u_j\right), \tag{2.14}$$

with

$$\varrho_n^{(\alpha)} = \frac{\left((n+1)^{\alpha} - n^{\alpha}\right)}{\Gamma(\alpha+1)}$$

. If $g(s,u(s)) \simeq g\left(t_{j+1}, u_{j+1}\right) + \dfrac{s - t_{j+1}}{\Delta t^{\alpha}} \left(g\left(t_{j+1}, u_{j+1}\right)\right) + g\left(t_j, u_j\right)$, we have implicit Trapezoidal rule (Lubich, 1986; Garrappa, 2015)

$$u_n = P_{n-1}[u;t_0](t_n) + \Delta t^{\alpha} \left(\widehat{b}_n^{(\alpha)} g_0 + \sum_{j=1}^{n-1} b_{n-j}^{(\alpha)} g\left(t_j, u\left(t_j\right)\right) \right), \tag{2.15}$$

with

$$\widehat{b}_n^{(\alpha)} = \frac{(n-1)^{\alpha+1} - n^{\alpha}(n-\alpha-1)}{\Gamma(\alpha+2)},\ b_n^{(\alpha)} = \begin{cases} \dfrac{1}{\Gamma(\alpha+2)}, & for \quad n = 0, \\ \dfrac{(n-1)^{\alpha+1} - 2n^{\alpha+1} + (n+1)^{\alpha+1}}{\Gamma(\alpha+2)}, & for \quad n = 1,2,\dots. \end{cases}$$

2.3.2 Description of the fractional linear multi-step methods (FLMMs)

The FLMMs Method is a convolution quadrature well suited to approximate FODE. To begin, let us consider (see (Garrappa, 2018))

$$u'(t) = g(t),\ u(t_0) = u_0, \tag{2.16}$$

The approximation by linear multi-step method (LMM) is given by:

$$\sum_{j=0}^{p} s_j u_{n-j} = \Delta t \sum_{j=0}^{p} r_j g\left(t_{n-j}\right), \tag{2.17}$$

where $s(z) = s_0 z^p + s_1 z^{p-1} + \cdots + s_p$ and $r(z) = r_0 z^p + r_1 z^{p-1} + \cdots + r_p$ are the first and second characteric polynomials of the LMM. The equation (2.16) can be well also rewritten in the integral from:

$$u(t) = u_0 + \int_{t_0}^{t} g(s)\,ds. \tag{2.18}$$

Reformulated in terms of convolution quadrature formulas, the LMMs approximate the solution as:

$$u_n = \Delta t \sum_{j=0}^{p} \theta_{n-j} g\left(t_j\right),\ n \geq p$$

where the weights θ_n depend on $s(z)$ and $r(z)$, but not on Δt.

$$\delta\left(\eta\right) = \sum_{n=0}^{\infty} \theta_n \eta^n,\ \delta\left(\eta\right) = \frac{s\left(1/\eta\right)}{r\left(1/\eta\right)}.$$

The FLMMs permit to obtain convolution quadratures for the RL integral (2.1) and the convolution weights provided by the function:

$$F\left(\frac{\delta\left(\eta\right)}{\Delta t}\right) = \left(\frac{\delta\left(\eta\right)}{\Delta t}\right)^{-\alpha} = \Delta t^{\alpha}\left(\frac{r\left(1/\eta\right)}{s\left(1/\eta\right)}\right)^{\alpha}, \tag{2.19}$$

with $F(u) = u^{-\alpha}$ the Laplace transform of the kernel $\frac{t^{\alpha-1}}{\Gamma(\alpha)}$ in (2.1). When an LMM is generalized to Equation (2.1) in the above Lubich sense ($Lubich$, 1988a,b, 2004), the resulting FLMM reads as:

$$\Delta t I_{t_0}^{\alpha} g(t_n) = \Delta t^{\alpha} \sum_{j=0}^{n} \theta_{n-j}^{(\alpha)} g\left(t_j\right), \tag{2.20}$$

where the convolution quadratique weights $\theta_n^{(\alpha)}$ are obtained from:

$$\sum_{n=0}^{\infty} \theta_n^{(\alpha)} \eta^n = \theta^{(\alpha)}\left(\eta\right),\ \theta^{(\alpha)}\left(\eta\right) = \left(\delta\left(\eta\right)\right)^{-\alpha}.$$

The introduction of a correction term permit to deal of non-smooth functions (see ($Garrappa$, 2018)):

$$\Delta t I_{t_0}^{\alpha} g(t_n) = \Delta t^{\alpha} \sum_{j=0}^{n} \theta_{n,j}^{(\alpha)} g\left(t_j\right) + \Delta t^{\alpha} \sum_{j=0}^{n} \theta_{n-j}^{(\alpha)} g\left(t_j\right). \tag{2.21}$$

By application of the discretized convolution quadrature rule (2.21) to integral Equation (2.10), the FLMMs for the approximate solution of FODE can be derived as:

$$u_n = P_{n-1}[u;t_0](t_n) + \Delta t^{\alpha} \sum_{j=0}^{s} \theta_{n,j}^{(\alpha)} g\left(t_j, u_j\right) + \Delta t^{\alpha} \sum_{j=0}^{n} \theta_{n-j}^{(\alpha)} g\left(t_j, u_j\right). \tag{2.22}$$

By imposing that the quadrature rule (2.21) is exact when applied to $g(t) = t^{\kappa}$, with κ assuming all the possible fractional values expected in the expansion of the true solution and by solving at each step the algebraic linear system:

$$\sum_{k=0}^{s} \theta_{n,k}^{(\alpha)} k^{\kappa} = -\sum_{k=0}^{s} \theta_{n-k}^{(\alpha)} k^{\kappa} + \frac{\Gamma(\kappa+1)}{\Gamma(1+\kappa+\alpha)} n^{\kappa+\alpha}. \tag{2.23}$$

we can properly choose $\theta_{n,j}^{(\alpha)}$. One of the simplest FLMMs is obtained from the implicit Euler method. Since the generating function is $\delta(\eta) = 1-\eta$, we see that $\theta_n^{(\alpha)}$,
$n = 0,1,2,\ldots$, are the coefficients of the generalized binomial series $(1-\eta)^{-\alpha}$, namely:

$$\theta_n^{(\alpha)} = (-1)^n \binom{-\alpha}{n} = (-1)^n \frac{\Gamma(1-\alpha)}{\Gamma(n+1)\Gamma(-\alpha-n+1)},$$

By the recurrence $\theta_n^{(\alpha)} = \left(\frac{1-(1-\alpha)}{n}\right)\theta_{n-1}^{(\alpha)}$ with $\theta_0^{(\alpha)} = 1$. This give the method:

$$u_n = P_{n-1}[u;t_0](t_n) + \Delta t^\alpha \sum_{j=0}^{n} (-1)^n \binom{-\alpha}{n-j} g\left(t_j, u_j\right),$$

referred to as the Grünwald-Letnikov scheme (Garrappa, 2018).

3 Some Important Results on Shifted Legendre Polynomials

We consider $E = L^2([0,1])$, the space of square integrable function on $[0,1]$ with scalar product

$$< f,g >= \int_0^1 f(x)g(x)dx,\ f,g \in E \tag{3.1}$$

and associate norm $\|f\| = \sqrt{\int_0^1 f^2(x)dx}$. Two vectors f,g in E are orthogonal if $< f,g >= 0$ and the family $\{e_i, i = 0,1,...\}$ of vectors in E are said orthogonal if

$$< e_i, e_j >= \delta_j^i \mu_i, \mu_i \neq 0$$

where δ_j^i is the kronecker symbol defined as

$$\delta_j^i = \begin{cases} 0 \text{ for } i \neq j \\ 1 \text{ for } i = j \end{cases}$$

The Legendre polynomial (H. Singh, 2020; Khader and Hendy, 2012; Lotfi et al., 2013) of degree i can be defined on the interval $[-1,1]$ by recurrence formulae (Saadatmandia and Dehghan, 2010; H. Singh, 2020):

$$P_{i+1}(t) = \frac{2i+1}{i+1} t P_i(t) - \frac{i}{i+1} P_{i-1}(t),\ i = 2,3,\ldots, \tag{3.2}$$

with $P_0(t) = 1$ and $P_1(t) = t$. The Legendre polynomial on $[0,1]$ is the commonly used. If $x \in [0,1]$, we can made the change of variable $t = 2x-1$ and define the so-called shifted Legendre polynomials as $P_i(2x-1)$ denoted by $G_i(x)$ (see (Saadatmandia and Dehghan, 2010)).

$$G_{i+1}(x) = \frac{(2i+1)(2x-1)}{i+1} G_i(x) - \frac{i}{i+1} G_{i-1}(x),\ i = 2,3,\ldots, \tag{3.3}$$

with $G_0(x) = 1$ and $G_1(x) = 2x-1$. The shifted Legendre polynomial $G_i(x)$ of degree i can be expressed in the analytic form as (Saadatmandia and Dehghan, 2010):

$$G_i(x) = \sum_{k=0}^{i} (-1)^{i+k} \frac{(i+k)!x^k}{(i-k)!(k!)^2}. \tag{3.4}$$

Note that $G_i(0) = (-1)^i$ and $G_i(1) = 1$.

Let us consider now E_n, the finite-dimensional vector subspace of E spaned by $\{G_i, i = 0,1,2,...,N\}$. We have the orthogonality condition (Saadatmandia and Dehghan, 2010)

$$< G_i, G_j >= \int_0^1 G_i(x)G_j(x) = \delta_j^i \mu_i,\ \mu_i = \frac{1}{2i+1} \tag{3.5}$$

For $z \in E$, $z \notin E_N$, there existe an unique $z_N \in E_N$ wich fufills the relation (Finlayson, 1972)

$$\|z - z_N\| = \min_{y \in E_N} \|z - y\| \tag{3.6}$$

and z_N is caractetized by the equality

$$< z - z_N, Gi >= 0 \text{ for } i = 0, 1, 2, ..., N \tag{3.7}$$

As

$$z_N(x) = \sum_{j=0}^{N} c_j G_j(x), \tag{3.8}$$

we can determie c_j using the relation

$$c_j =< z, G_j >= (2j+1) \int_0^1 z(x) G_j(x) dx, \; j = 0, 1, 2, ..., N \tag{3.9}$$

More generally, if $z \in E = L^2([0,1])$, the shifted Legendre polynomials can be used to write:

$$z(x) = \sum_{j=0}^{\infty} c_j G_j(x), \tag{3.10}$$

where c_j are given by: (3.9).

In vectorial form, (3.8) can be write for $x \in [0,1]$ as:

$$z(x) = C^T \Psi(x), \tag{3.11}$$

where the vector C and the vector $\Psi(x)$ are expressed as:

$$C^T = [c_0, c_1, \ldots, c_N],$$

$$\Psi(x) = [G_0(x), G_1(x), \ldots, G_N(x)]^T. \tag{3.12}$$

The derivative $\frac{d\Psi(x)}{dx}$ of the vector $\Psi(x)$ is

$$\frac{d\Psi(x)}{dx} = M^{(1)} \Psi(x), \tag{3.13}$$

with $M^{(1)}$ an square operational matrice of derivative with $(N+1) \times (N+1)$ given by

$$M^{(1)} = (d_{ij})_{1 \le i, j \le N}$$

where (Saadatmandia and Dehghan, 2010)

$$d_{ij} = \begin{cases} 2(2j+1), & for \quad j = i - k, \\ 0, & otherwise, \end{cases} \quad \begin{cases} k = \; 1, 3, \cdots, N, & if\ N\ odd, \\ k = \; 1, 3, \cdots, N-1, & if\ N\ even, \end{cases}$$

4 Operational Matrice of Fractional Derivative on Legendre Polynomials

The operational matrice (E. H. Doha, 2014; D. Baleanu, 2018; Saadatmandia and Dehghan, 2010) is a notion widely used in problems where the spectral method is needed to solve the equation ($Lotfi et\ al.$, 2013). If the superscript in $M^{(1)}$, denotes matrice powers, by using Eq. (3.13), we obtain for $n \in \mathbb{N}$

$$\frac{d^n \Psi(x)}{dx^n} = \left(M^{(1)}\right)^n \Psi(x), \tag{4.1}$$

and thus

$$M^{(n)} = \left(M^{(1)}\right)^n, \; n = 1, 2, 3, \ldots, \tag{4.2}$$

is the operational matrice.

Lemma 1. ($SaadatmandiaandDehghan$, 2010). *For $G_i(x)$ a shifted Legendre polynomial, we have*

$$D^{\alpha}G_i(x) = 0,\ i = 0,1,2,\ldots,\lceil\alpha\rceil - 1,\ \alpha > 0. \tag{4.3}$$

Proof. See ($SaadatmandiaandDehghan$, 2010) □

Theorem 4.1. ($SaadatmandiaandDehghan$, 2010) *Let $\Psi(x)$ be shifted Legendre vector defined in* (3.12) *and for $\alpha > 0$, we have*

$$D^{\alpha}\Psi(x) \simeq M^{(\alpha)}\Psi(x), \tag{4.4}$$

where $M^{(\alpha)}$ is the $(N+1)\times(N+1)$ operational matrice of fractional derivative of order α in the Caputo sense defined as follows:

$$M^{(\alpha)} = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & 0 \\ \sum\limits_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} m_{\lceil\alpha\rceil,0,k} & \sum\limits_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} m_{\lceil\alpha\rceil,1,k} & \cdots & \sum\limits_{k=\lceil\alpha\rceil}^{\lceil\alpha\rceil} m_{\lceil\alpha\rceil,N,k} \\ \vdots & \vdots & \cdots & \vdots \\ \sum\limits_{k=\lceil\alpha\rceil}^{i} m_{i,0,k} & \sum\limits_{k=\lceil\alpha\rceil}^{i} m_{i,1,k} & \cdots & \sum\limits_{k=\lceil\alpha\rceil}^{i} m_{i,N,k} \\ \vdots & \vdots & \cdots & \vdots \\ \sum\limits_{k=\lceil\alpha\rceil}^{N} m_{N,0,k} & \sum\limits_{k=\lceil\alpha\rceil}^{N} m_{N,1,k} & \cdots & \sum\limits_{k=\lceil\alpha\rceil}^{N} m_{N,N,k} \end{bmatrix},$$

where $m_{i,j,k}$ is given by:

$$m_{i,j,k} = (2j+1)\sum_{l=0}^{j} \frac{(-1)^{i+j+k+l}(i+k)!(j+l)!}{(i-k)!k!\Gamma(k-\alpha+1)(j-l)!(l!)^2(k+l-\alpha+1)}. \tag{4.5}$$

In $M^{(\alpha)}$, the first $\lceil\alpha\rceil$ rows, are all zero.

Proof. ($SaadatmandiaandDehghan$, 2010). □

If $\alpha = n \in \mathbb{N}$, then theorem (4.1) gives the same result as Eq. (4.2).

5 Implementing the Operational Matrice of Fractional Derivative

The operational matrice and spectral Tau method are implement in this section to convert the original problem to a system of fractional ordinary differential equation. Let us consider the equation

$$\frac{\partial^{\alpha}u}{\partial t^{\alpha}}(x,t) = a\frac{\partial^2 u}{\partial x^2}(x,t) + K(x,t) \tag{5.1}$$

with boundaries conditions

$$u(0,t) = p(t) \tag{5.2}$$

and

$$u(1,t) = q(t) \tag{5.3}$$

and initial condition

$$u(x,0) = g(x) \tag{5.4}$$

where $\alpha \in]0,1]$, $t \in [0,T]$, $x \in [0,1]$; p and q are given functions. The approximatiion of $\dfrac{\partial^2 u(x,t)}{\partial x^2}$, $K(x,t)$ and $g(x)$ using operational matrice $M^{(2)}$ give:

$$\frac{\partial^2 u(x,t)}{\partial x^2} \equiv C^T(t) M^{(2)} \Psi(x), \tag{5.5}$$

$$K(x,t) \equiv F^T(t)\Psi(x), \quad F_i(t) = (2i+1)\int_0^1 K(x,t) G_i(x)\,dx,\ i = 1,2,3,\ldots. \tag{5.6}$$

$$g(x) \equiv g^T \Psi(x), \quad g_i = (2i+1)\int_0^1 g(x) G_i(x)\,dx. \tag{5.7}$$

Then Eq. (5.1) – (5.4) become:

$$D_t^{\alpha} C^T(t)\Psi(x) = a C^T(t) M^{(2)} \Psi(x) + F^T(t)\Psi(x) \tag{5.8}$$

and boundries conditions

$$C^T(t)\Psi(0) = p(t) \tag{5.9}$$

and

$$C^T(t)\Psi(1) = q(t) \tag{5.10}$$

and initial condition

$$C^T(t)\Psi(x) = g^T \Psi(x) \tag{5.11}$$

where

$$F(t) = \begin{bmatrix} F_0(t) \\ \vdots \\ F_N(t) \end{bmatrix}, C(0) = \begin{bmatrix} c_0(0) \\ \vdots \\ c_N(0) \end{bmatrix},\ c_i(0) = g_i,\ i = 0,\ldots,N,$$

Let $R_N(x)$ be the residual defined as:

$$R_N(x,t) = \left[D_t^{\alpha} C^T(t) - a C^T(t) M^{(2)} - F(t) \right] \Psi(x) = 0,\ (x,t) \in [0,1] \times [0,T], \tag{5.12}$$

The application the spectral Tau method [($A.\ Saadatmandi$, 2006; $E.\ H.\ Doha$, 2014)], give:
$\int_0^1 R_N(x,t) G_j(x)\,dx = 0,\ j = 0,1,\ldots,m-2, t \in [0,T]$.

Using the properties of (3.5), we then have

$$D_t^{\alpha} c_i(t)\Psi(x) = a c_i(t) + F_i(t),\ i = 0,1,\ldots,N-2, t \in [0,T] \tag{5.13}$$

and boundaries conditions

$$\sum_{i=0}^{N} (-1)^i\ c_i(t) = p(t) \tag{5.14}$$

and

$$\sum_{i=0}^{N} c_i(t) = q(t) \tag{5.15}$$

and initial condition

$$c_i(0) = g_i, i = 0,1,\ldots,N \tag{5.16}$$

The problem (5.13) – (5.16) can be written in the vectorial form as:

$$D_t^{\alpha} C(t) = a\Omega C(t) + F(t) + V(t) \tag{5.17}$$

and initial condition

$$C(0) = G \tag{5.18}$$

and boundries conditions

$$\sum_{i=0}^{N} (-1)^i\ c_i(t) = p(t) \tag{5.19}$$

and

$$\sum_{i=0}^{N} c_i(t) = q(t) \tag{5.20}$$

$$\text{where} \quad \Omega = \begin{bmatrix} a & 0 & \cdots & 0 & 0 \\ 0 & a & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \quad V(t) = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ p(t) \\ q(t) \end{bmatrix}.$$

The equation (5.17) – (5.20) can be as well of the form:

$$\begin{cases} D_t^{\alpha} C(t) & = & \Theta(t, C(t)) \\ C(0) & = & G, \end{cases}$$

where $\Theta(t,C(t)) = \Omega C(t) + F(t) + V(t)$, with $\Theta_i(t,C(t)) = aC_i(t) + F_i(t) + V_i(t)$, $i = 0 \ldots N$.

5.1 Linear fractional diffusion differential equation with fractional order

Consider the linear fractional diffusion equation

$$\frac{\partial^{\alpha} u}{\partial t^{\alpha}}(x,t) = a \frac{\partial^{\sigma} u}{\partial x^{\sigma}}(x,t) + k(x,t) \tag{5.21}$$

with boundaries conditions

$$u(0,t) = r(t) \tag{5.22}$$

and

$$u(1,t) = s(t) \tag{5.23}$$

and initial condition

$$u(x,0) = h(x) \tag{5.24}$$

where $\alpha \in]0,1]$, $\sigma \in]1,2], t \in [0,T]$, $x \in [0,1]$; r and s are two given functions. We approximate $h(x)$ and $k(x,t)$ as follows:

$$k(x,t) \equiv K^T(t)\Psi(x), \quad k_i(t) = (2i+1)\int_0^1 k(x,t)G_i(x)dx. \tag{5.25}$$

$$h(x) \equiv H^T \Psi(x), \quad H_i = (2i+1)\int_0^1 h(x)G_i(x)dx. \tag{5.26}$$

The Eq. (5.21) – (5.24) become:

$$D_t^{\alpha} C^T(t)\Psi(x) = aC^T(t)M^{(\sigma)}\Psi(x) + K^T(t)\Psi(x) \tag{5.27}$$

and boundries conditions

$$C^T(t)\Psi(0) = r(t) \tag{5.28}$$

and

$$C^T(t)\Psi(1) = s(t) \tag{5.29}$$

and initial condition

$$C^T(t)\Psi(x) = H^T \Psi(x) \tag{5.30}$$

Where $C_i(0) = H_i$, $i = 0, \ldots, m$. Define the residual $R_N(x,t)$ as:

$$R_N(x,t) = \left[D_t^{\alpha} C^T(t) - aC^T(t)M^{(\sigma)} - K(t)\right]\Psi(x) = 0, \ (x,t) \in [0,1] \times [0,T]. \tag{5.31}$$

The application of the Galerkin-Tau method give

$$\int_0^1 R_N(x,t)G_j(x)dx = 0, \quad j = 0,1,\ldots,m-2, \ t \in [0,T]. \tag{5.32}$$

6 Numerical Experiment

We present numerical test using shifted Legendre operational method followed by multi-step method described in the previous section.

Example 6.1. *Let us consider the following fractional equation:*

$$\frac{\partial^{\frac{1}{2}} u}{\partial t^{\frac{1}{2}}}(x,t) - \frac{\partial^2 u}{\partial x^2}(x,t) = \frac{2t^{\frac{3}{2}}\sin(2\pi x)}{\Gamma\left(\frac{3}{2}\right)} + 4\pi^2 \sin(2\pi x)$$

with boundaries conditions

$$u(0,t) = 0$$

and

$$u(1,t) = 0$$

and initial condition

$$u(x,0) = 0$$

The function $u(x,t) = 2t^2 \sin(2\pi x)$ is the exact solution. We consider the approximate solution for $N = 3$ as

$$u_{app}(x,t) = c_0(t)G_0(x) + c_1(t)G_1(x) + c_2(t)G_2(x) + c_3(t)G_3(x) = C^T \Psi(x),$$

where c_0, c_1, c_2, c_3 are found from:

$$\begin{cases} D_t^{\alpha} c_0(t) = 0 \\ D_t^{\alpha} c_1(t) = \frac{12}{\pi}\left(\frac{t^{\frac{3}{2}}}{\sqrt{\pi}} + \pi^2 t^2\right) \\ c_0(0) = 0 \\ c_1(0) = 0 \end{cases}$$

and the boundary condition are

$$c_0(t) - c_1(t) + c_2(t) - c_3(t) = 0$$

and

$$c_0(t) + c_1(t) + c_2(t) + c_3(t) = 0$$

using the operational matrice

$$M^{(2)} = 2\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 \\ 0 & 30 & 0 & 0 \end{bmatrix}, \quad F(t) = \begin{bmatrix} 0 \\ -\frac{12}{\pi}\left(\frac{t^{\frac{3}{2}}}{\sqrt{\pi}} + \pi^2 t^2\right) \\ 0 \\ 28\left(\frac{t^{\frac{3}{2}}}{\sqrt{\pi}} + \pi^2 t^2\right)\left(\frac{19}{\pi} - \frac{15}{\pi^3}\right) \end{bmatrix}.$$

Setting $N = 101$ in space and $\Delta t = \frac{1}{2^5}$ for step time, Figure 1 displays the profil of exact and approximate solution and show the profil of error $E = u - u_{app}$.

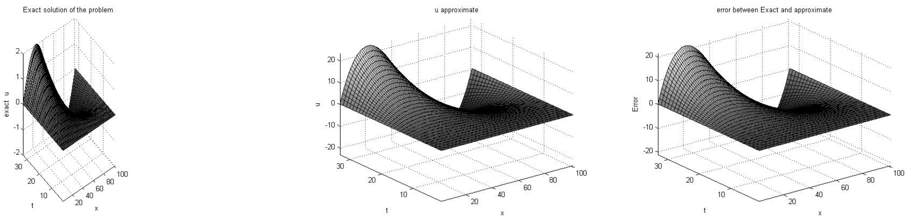

Fig. 1. Left: (a) Exact solution, Center: (b) Approximate solution, Right: (c) Error

In Fig. 1, the comparison between the plot of exact solution in profil (a) and the numerical solution in profil (b) show an excellent agreement and demonstrate the accuracy of the scheme.

Example 6.2. *Let us consider the following fractional équation in time and in space:*

$$\frac{\partial^\alpha u}{\partial t^\alpha}(x,t)+\frac{\partial^\sigma u}{\partial x^\sigma}(x,t)=f(x,t) \tag{6.1}$$

with boudaries conditions

$$u(0,t)=t^2+1$$

and

$$u(1,t)=2(t^2+1)$$

and initial condition

$$u(x,0)=x^2+1$$

where

$$(x,t)\in[0,1]\times[0,1],\alpha\in]0,1],\sigma\in]0,2],f(x,t)=\frac{2\Gamma(3)x^{2-\alpha}\left(t^2+1\right)}{\Gamma(3-\alpha)}+\frac{2\Gamma(3)t^{2-\sigma}\left(x^2+1\right)}{\Gamma(3-\sigma)}$$

and $\alpha=\sigma=\frac{1}{2}$. *As exact solution of the problem* (6.1), *we have* $u(x,t)=\left(x^2+1\right)\left(t^2+1\right)$. *Taking* $m=2$ *and using the numerical method described in section* 5.1 *the approximate solution can be written as*

$$u_{app}(x,t)=c_0(t)G_0(x)+c_1(t)G_1(x)+c_2(t)G_2(x)=C^T\Psi(x).$$

where c_0,c_1,c_2 *are found by solving*

$$\begin{cases} D_t^{\frac{1}{2}}c_0(t) &= \frac{8}{\sqrt{\pi}}\left(\frac{4}{15}\left(t^2+1\right)+\frac{1}{9}t^{\frac{3}{2}}\right) \\ c_0(0) &= \frac{4}{3}\end{cases}$$

and the boundary conditon

$$c_0(t)-c_1(t)+c_2(t)=t^2+1$$

and

$$c_0(t)+c_1(t)+c_2(t)=2\left(t^2+1\right)$$

using the operational matrice

$$M^{\left(\frac{1}{2}\right)}=\frac{8}{\sqrt{\pi}}\begin{bmatrix}0&0&0\\ \frac{1}{3}&\frac{1}{5}&\frac{-1}{21}\\ \frac{3}{5}&\frac{3}{7}&\frac{1}{3}\end{bmatrix},\quad F(t)=\frac{8}{\sqrt{\pi}}\begin{bmatrix}\frac{4}{15}\left(t^2+1\right)+\frac{1}{9}t^{\frac{3}{2}}\\ \frac{12}{35}\left(t^2+1\right)+\frac{1}{3}t^{\frac{3}{2}}\\ \frac{4}{63}\left(t^2+1\right)+\frac{1}{9}t^{\frac{3}{2}}\end{bmatrix}.$$

As in the previous problem, by setting $N = 101$ *and* $\Delta t = \dfrac{1}{2^5}$ *the Fig. 2 displays the profil exact and approximate solution and show the error* $E = u - u_{app}$.

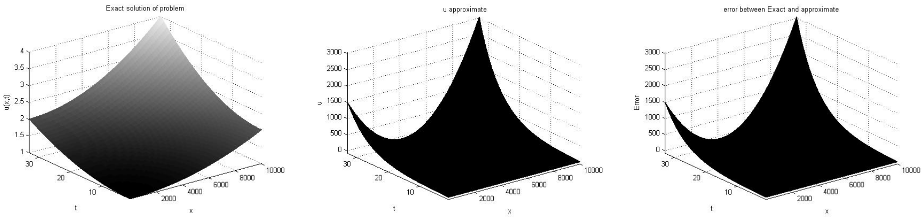

Fig. 2. Left: (a) Exact solution, Center: (b) Approximate solution, Right: (c) Error.

In Fig. 2, the comparison between the plot of exact solution in profil (a) and the numerical solution in profil (b) show an excellent agreement and demonstrate the accuracy of the scheme.

7 Conclusions

In this paper, we have presented a numerical scheme for solving fractional-order diffusion equations in time and in space. Inspired by the MOL methods, the operational matrix of fractional-order derivative in Cauto's sense on the shifted Legendre polynomial was computed and used to handle the spatial part of equation. Application of the Tau spectral method transform the original problem into a system of fractional ordinary differentials equations. The approximate solutions computed by our numerical scheme compared with the exact solutions of two test problems have shown their efficiecy and accuraty.

Disclaimer (Artificial Intelligence)

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc) and text-to-image generators have been used during writing or editing of this manuscript.

Competing Interests

Authors have declared that no competing interests exist.

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