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A Lagrange Regularized Kernel Method for Solving Multi-dimensional Time-Fractional Heat Equations

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Abstract: Evolution equations containing fractional derivatives can provide suitable mathematical models for describing important physical phenomena. In this paper, we propose an accurate method for numerical solutions of multi-dimensional time-fractional heat equations. The proposed method is based on a fractional exponential integrator scheme in time and the Lagrange regularized kernel method in space. Numerical experiments show the effectiveness of the proposed approach.

Keywords: local spectral methods, Lagrange regularized kernel, time-fractional diffusion equations, exponential integrators

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1 Introduction

The use of fractional partial differential equations (FPDEs) in mathematical models has become increasingly popular in recent years. They can provide suitable mathematical models for describing anomalous diffusion and transport dynamics in complex systems that cannot be modeled accurately by normal integer order equations. Recently, researchers have found that many physical processes exhibit fractional order behavior that varies with time or space for the mathematical modeling of real-world physical problems [1–4] such as earthquake modeling, traffic flow model with fractional derivatives [5] and financial option pricing problems [6], to name these only.

In this study, we consider the time-fractional diffusion equation (TFDE) of order α, with $0 \leqslant \alpha \leqslant 1$. In recent years, various methods have been devised to find the exact and approximate solutions of FPDEs [7, 8] in order to provide more information for understanding physical phenomena arising in numerous scientific and engineering fields. Keskin and Oturanc [9] proposed a semi-analytical method known as the reduced differential transform method (RDTM) for solving fractional differential equations. Lui et al. [10] derived the solution to the time-fractional advection-dispersion equation using variable transformation, Mellin and Laplace transforms, and properties of H-functions. Lin and Xu [11] combined finite difference and spectral approximations to numerically solve time-fractional diffusion equations. Recently, Zhang et al. [12] proposed a novel implicit numerical method for the time variable fractional order mobile–immobile advection-dispersion models. They showed that the implicit difference approximation is computationally efficient. Yang et al. [13–15] studied the use of fractional derivative for nonlinear dynamics for local fractional Burgers' equation arising in fractal flow. In addition, they proposed a new numerical technique based on a certain two-dimensional extended differential transform via local fractional derivatives and derive its associated basic theorems and properties. Most recently, Bhrawy et al. proposed a family of accurate and efficient spectral methods to study a family of fractional diffusion equations and systems of fractional KdV equations [1, 2, 16–20]. Pindza and Owolabi [21] proposed a Fourier spectral method implementation of fractional-order derivatives for reaction diffusion problems.

We propose a Lagrange regularized kernel (LRK) method and exponential time integrators to numerically solve time-fractional partial differential equations. The LRK belongs to the family of local spectral methods called discrete singular convolution (DSC) methods. They were originally introduced by Hoffman et al. [22], and Hoffman and Kouri [23] as a computational tool for treating a variety of problems in physics and chemistry, with particular focus on the Schrödinger equation. Later, the DSC methods were used to solve the Fokker-Planck equation [24, 25].

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Recently, Pindza and Maré [26] proposed an accurate and efficient DSC method for numerical solutions of the fifth order Korteweg-De Vries equation.

The study of DSC methods indicates that these methods deliver spectral accuracy when used to solve Fokker-Planck equation with nonlinear drift and diffusion coefficients included. They are defined as a mapping that approximates a certain set of continuous L^2 functions onto itself [25]. Their main success in various computational practices is due to their ability to provide analytical representations of a function and its derivatives at collocation points. These approximations have different realizations depending on the problem to solve. Here we limit our study to the DSC methods of the Lagrange type. These methods are seen as local spectral methods since they produce exponential convergence of spectral methods while keeping sufficient flexibility to handle complicated boundary conditions and geometries, like finite-difference and finite-element methods. The semi-discretization of the FPDEs in space using the LRK method yield a system of fractional ordinary differential equations (FODEs) that can be solved using conventional FODE solvers.

In this work, we are concerned with exponential time integrators. Recently, Garrappa and Popolizio [27] proposed a generalization of exponential integrators to differential equations of non-integer orders and established the stability and the convergence of underlying methods. Fractional exponential time differencing (FETD) methods present a challenging problem that is the computation of the family of Mittag-Leffler functions. In the present work, we evaluate Mittag-Leffler function arguments efficiently using a Krylov subspace with the Arnoldi shift-and-invert method [28].

This paper is structured as follows; in Section 2 we describe the formulation of the DSC formalism. Section 3 describes the PDEs implementation of the LRK method. Section 4 describes fractional time integrators and their implementations. In Section 5 we perform numerical experiments to illustrate the merits of our scheme. Finally, we present a brief conclusion in Section 6.

2 Discrete singular convolution

DSC is a general framework for constructing local spectral methods. It is an effective approach for the numerical realization of singular convolutions, which occur commonly in science and engineering. Consider a distribution T and $\eta(t)$ as an element of the space of test function. A *singular convolution* f can be defined as

$$f(t) = (T * \eta)(t) = \int_{-\infty}^{\infty} T(t-x)\eta(x)dx, \tag{1}$$

where $T(t-x)$ is a singular kernel. In this paper, T will designate the delta distribution δ. The basic equation associated with the Dirac delta function $\delta(x)$ is

$$\int_{-\infty}^{\infty} \delta(x)f(x)\,dx = f(0), \tag{2}$$

where f is any function that is continuous at $x = 0$. The delta function has the following properties:

$$\int_{-\infty}^{\infty} \delta(x-x')f(x)\,dx = f(x'), \tag{3}$$

$$\int_{-\infty}^{\infty} \delta'(x)f(x)\,dx = -f'(0), \tag{4}$$

$$\delta(x/a) = |a|\delta(x). \tag{5}$$

As the delta distribution does not have a value everywhere, its approximation is necessary so that it can be digitized on a computer. The discrete local spectral kernels [29] are constructed by regularizing the Shannon kernel [30]

$$\delta_{\Delta,\sigma}(x-n\Delta) = \frac{\sin\left[\frac{\pi}{\Delta}(x-n\Delta)\right]}{\frac{\pi}{\Delta}(x-n\Delta)} \exp\left[-\frac{(x-n\Delta)^2}{2\sigma^2}\right], \tag{6}$$

and the Dirichlet kernel [31]

$$\delta_{\Delta,\sigma}(x-n\Delta) = \frac{\sin\left[\frac{\pi}{\Delta}(x-n\Delta)\right]}{(2M'+1)\sin\left[\frac{\pi}{\Delta}\frac{(x-n\Delta)}{2M'+1}\right]} \exp\left[-\frac{(x-n\Delta)^2}{2\sigma^2}\right], \tag{7}$$

where M' is a parameter and Δ is the grid spacing. LRK [24] is defined by

$$\delta_{M',\sigma}(x-x_k) = \prod_{i=k-M',\, i\neq k}^{i=k+M'} \frac{x-x_i}{x_k-x_i} \exp\left[-\frac{(x-x_k)^2}{2\sigma^2}\right], \tag{8}$$

was constructed by regularizing the classic Lagrange polynomial [32]. Many other DSC kernels are given in [29, 33]. The main advantage of the LRK is its ability to accommodate the use of nonuniform grids. This is essential for efficiently solving problems with singularities in the discretization domain.

Qian et al. [34, 35] show that the error $\| f - f_{M,\sigma} \|_\infty$ of the Sinc-Gauss sampling formula decreases exponentially with respect to M for some function f. We state the convergence theorem of the LRK kernel as follows:

Theorem 2.1: *Let f be a function with $f \in L^\infty(R) \cap L^2(\mathbb{R}) \cap C^s(R)$ and bandlimited to B, $\left(B < \frac{\pi}{\Delta}\right)$, $s \in \mathbb{Z}^+$, $\sigma = r\Delta > 0$, $j!(\Delta)^{2j} \le \left(\frac{1}{r}\right)^{2j}$ for $j \ge 1$, $M > \frac{sr}{\sqrt{2}}$. Then*

$$\|f^{(s)} - f^{(s)}_{M,\sigma}\|_{L^\infty(R)} \le \beta \exp\left(-\frac{\alpha^2}{2r^2}\right), \tag{9}$$

where

$$\alpha = \min\{M, r^2(\pi - B\Delta)\}, \beta = \frac{e^\pi r(s+1)!}{\Delta^s \pi \alpha}\left(\sqrt{2B}\|f\|_{L^2(R)} + 2r\|f\|_{L^\infty(R)}\right). \tag{10}$$

The L^∞ error decays exponentially with respect to the increase of the DSC bandwidth M.

Proof: The convergence of the Lagrange-Gauss sampling formula is established by following Qian et al. [34, 35].

Definition 2.2: *For non-negative integer s and positive numbers r, Δ, we define the operators $R^{(s)}_\sigma$ and $f^{(s)}_{M,\sigma}$ approximating the s-th order derivative $f^{(s)}$ of a function f as*

$$R^{(s)}_\sigma(x) := \sum_{n=-\infty}^{\infty} f(n\Delta)\left[\left(\prod_{i=k-M', i\neq k}^{k+M'} \frac{x - x_i}{n\Delta - x_i}\right) \exp\left(-\frac{(x-n\Delta)^2}{2\sigma^2}\right)\right]^{(s)}, \tag{11}$$

$$f^{(s)}_{M,\sigma}(x) := \sum_{n=\lceil \frac{x}{\Delta}\rceil - M}^{n=\lceil \frac{x}{\Delta}\rceil + M} f(n\Delta)\left[\left(\prod_{i=k-M', i\neq k}^{k+M'} \frac{x - x_i}{n\Delta - x_i}\right) \exp\left(-\frac{(x-n\Delta)^2}{2\sigma^2}\right)\right]^{(s)}. \tag{12}$$

The error

$$E(x) = f^{(s)}(x) - f^{(s)}_{M,\sigma}(x), \tag{13}$$

breaks naturally into two components:

$$E_1(x) = f^{(s)}(x) - R^{(s)}_\sigma(x), \tag{14}$$

and

$$E_2(x) = R^{(s)}_\sigma(x) - f^{(s)}_{M,\sigma}(x). \tag{15}$$

where $E_1(x)$ and $E_2(x)$ are the regularization error and the truncation error, respectively.

The total error can be written as

$$E(x) = \left(f^{(s)}(x) - R^{(s)}_\sigma(x)\right) + \left(R^{(s)}_\sigma(x) - f^{(s)}_{M,\sigma}(x)\right) = E_1(x) + E_2(x). \tag{16}$$

The corresponding error norms satisfy the triangular inequality

$$\|E\|_{L^\infty(R)} \le \|E_1\|_{L^\infty(R)} + \|E_2\|_{L^\infty(R)}. \tag{17}$$

It follows that

$$\|f^{(s)} - f^{(s)}_{M,\sigma}\|_{L^\infty(R)} \le \beta \exp\left(-\frac{\alpha^2}{2r^2}\right), \tag{18}$$

where

$$\alpha = \min\{M, r^2(\pi - B\Delta)\}, \tag{19}$$

and

$$\beta = \frac{B^s\sqrt{2B}\|f\|_{L^2(R)}}{\sqrt{2s+1}\sigma(\frac{\pi}{\Delta} - B)} + \frac{2\|f\|_{L^\infty(R)}e^\pi(s+1)!r^2}{\Delta^s \pi M} \tag{20}$$

$$\le \frac{\pi^s\sqrt{2B}\|f\|_{L^2(R)}}{\Delta^s r(\pi - B\Delta)} + \frac{2\|f\|_{L^\infty(R)}e^\pi(s+1)!r^2}{\Delta^s \pi M} \tag{21}$$

$$\le \frac{r}{\Delta^s \alpha \pi}\left(\pi^{s+1}\sqrt{2B}\|f\|_{L^2(R)} + 2\|f\|_{L^\infty(R)}e^\pi(s+1)!r\right) \tag{22}$$

$$\le \frac{e^\pi r(s+1)!}{\Delta^s \pi \alpha}\left(\sqrt{2B}\|f\|_{L^2(R)} + 2r\|f\|_{L^\infty(R)}\right). \tag{23}$$

■

The choice of M, σ and Δ are obtained from eqs (18) and (19). For instance, if the L_2-norm error is set to $10^{-\eta}$ ($\eta > 0$), i.e. $\exp\left(-\frac{\alpha^2}{2r^2}\right) = 10^{-\eta}$, then $\alpha = \sqrt{2\eta\ln(10)}$. The substitution of α in eq. (19) yields the following inequalities

$$r(\pi - Bh) > \sqrt{4.6\eta} \text{ and } \frac{M}{r} > \sqrt{4.6\eta}, \tag{24}$$

where $r = \sigma/h$ and B is the frequency bound of the underlying function f.

3 Implementation of the LRK

In this section, we propose an implementation of the LRK for numerical solutions of fractional time PDEs.

3.1 Approximation of derivatives

While solving partial differential equations, one of the most important element is an accurate representationof

differentiation operators. The success of LRK for linear and nonlinear PDEs is due to their ability to represent derivatives locally with spectral method accuracy. The s-th derivative of the LRK is analytically expressed as

$$\delta^{(s)}_{M,\sigma}(x-x_k) = \sum_{t=0}^{s} \frac{s!}{t!(s-t)!} \left(\prod_{i\neq k}^{M} \frac{x-x_i}{x^k-x_i} \right)^{(s)} \left[\exp\left(-\frac{(x-x_k)^2}{2\sigma^2} \right) \right]^{(s-t)}. \quad (25)$$

Therefore, the first two derivatives of the LRK can be written as

$$\delta^{(1)}_{M,\sigma}(x-x_k) = \left[\left(\sum_{j\neq k} \frac{1}{x-x_j} \right) - \frac{x-x_k}{\sigma^2} \right] \delta_{M,\sigma}(x-x_k) \quad (26)$$

and

$$\delta^{(2)}_{M,\sigma}(x-x_k) = \left[\left(\sum_{j_2\neq j_1,k} \sum_{j_1\neq k} \frac{1}{(x-x_{j_2})(x-x_{j_1})} \right) - \frac{2(x-x_k)}{\sigma^2} \left(\sum_{j\neq k} \frac{1}{x-x_j} \right) - \frac{1}{\sigma^4\left(\sigma^2-(x-x_k)^2\right)} \right] \delta_{M,\sigma}(x-x_k). \quad (27)$$

These two derivatives will be used in the computation of diffusion equations.

3.2 Boundary conditions

A complete numerical algorithm has to provide a scheme for handling boundaries. If the kernel, $\delta^{(s)}_{M,\sigma}$, is fixed to be symmetric (or antisymmetric) and invariant by translation, there must be cases where $f(x_k)$ are located outside of the computational domain, $[a,b]$, and their values are undefined there. In the present algorithm, such $f(x_k)$ are to be obtained by boundary conditions. In the Dirichlet boundary condition, such $f(x_k)$ are taken to be $f(a)$ or $f(b)$. In periodic boundary condition, such $f(x_k)$ are replaced by their corresponding values inside the domain $[a,b]$. For the Neumann boundary condition, the values of $f(x_k)$ are determined by $f(a)$ and $f'(a)$ or ($f(b)$ and $f'(b)$). If $f(x)$ is antisymmetric around the boundary point then values of $f(x_k)$ outside the domain $[a,b]$ are replaced by their corresponding $-f(x_k)$ inside the domain $[a,b]$. Similarly, if $f(x)$ is symmetric around the boundary point then values of $f(x_k)$ outside the domain $[a,b]$ are replaced by their corresponding $f(x_k)$ inside the domain $[a,b]$.

3.3 One-dimensional time-fractional heat equation

We first describe the fractional differential equation problem studied in this paper, and present some analytical solutions which will help with the numerical experiments of our methodology. Consider the time-fractional diffusion equation of the form

$$\frac{\partial^\alpha}{\partial t^\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) + f(x,t), \quad (x,t) \in (a,b)\times[0,T], \quad (28)$$

with the initial condition

$$u(x,0) = g(x), \quad x \in (a,b), \quad (29)$$

and the boundary conditions

$$u(a,t) = h_L(t) \text{ and } u(b,t) = h_R(t). \quad (30)$$

The substitution of the spatial derivative operators by the following LRK discretizations

$$\frac{\partial^2}{\partial x^2} u(x,t) = \sum_{j=1}^{N} u_j(t) \delta^{(2)}_{\sigma,M}(x-x_j), \quad \frac{\partial^\alpha}{\partial t^\alpha} u(x,t) = \sum_{j=1}^{N} u^{(\alpha)}_j(t) \delta_{\sigma,M}(x-x_j), \quad (31)$$

leads to the linear system of fractional differential equations

$$D^\alpha_0 U(t) = AU(t) + F(t), \; U(0) = U_0, \; 0 \leqslant t \leqslant T, \; 0 < \alpha < 1, \quad (32)$$

where A is a $N \times N$ matrix of entries $a_{ij} = \delta^{(2)}_{\sigma,M}(x_i - x_j)$ obtained from the semi-discretization of the underlying FPDE (28) using LRK methods, $F(t)$ is the source term which collects the function f together with the discretized boundary conditions, and $D^\alpha_0 U(t)$ is the fractional derivative of the function $U(t)$.

3.4 Two-dimensional time-fractional heat equation

Consider the two-dimensional time-fractional heat equation

$$\frac{\partial^\alpha}{\partial t^\alpha} u(x,y,t) = \nu \left(\frac{\partial^2}{\partial x^2} u(x,y,t) + \frac{\partial^2}{\partial y^2} u(x,y,t) \right), \quad (x,y) \in \mathcal{D}, \; t \in [0,T], \quad (33)$$

where v is the diffusion coefficient. We set initial condition as

$$u(x, y, 0) = h(x, y), \quad (x, y) \in \mathcal{D}, \tag{34}$$

and the boundary as

$$u(x, y, t) = p(x, y, t), \ (x, y) \in \partial\mathcal{D}, \quad t \in [0, T], \tag{35}$$

where $\mathcal{D} = \{(x, y) : a < x, y < b\}$ and $\partial\mathcal{D}$ is its boundary.

The LRK can be easily generalized to an arbitrarily high dimension by the tensorial product. For example, in 2D, one has the following spatial derivative operators

$$\frac{\partial^2}{\partial x^2}u(x, y, t) = \sum_{k_x=1}^{N_x}\sum_{k_y=1}^{N_y} u_{k_x k_y}(t)\delta^{(2)}_{\sigma_x, M_x}(x - x_{k_x})\delta_{\sigma_y, M_y}(y - y_{k_y}), \tag{36}$$

$$\frac{\partial^2}{\partial y^2}u(x, y, t) = \sum_{k_x=1}^{N_x}\sum_{k_y=1}^{N_y} u_{k_x k_y}(t)\delta^{(2)}_{\sigma_y, M_y}(y - y_{k_y})\delta_{\sigma_x, M_x}(x - x_{k_x}), \tag{37}$$

and

$$\frac{\partial^\alpha}{\partial t^\alpha}u(x, y, t) = \sum_{k_x=1}^{N_x}\sum_{k_y=1}^{N_y} u^{(\alpha)}_{k_x k_y}(t)\delta_{\sigma_y, M_y}(y - y_{k_y})\delta_{\sigma_x, M_x}(x - x_{k_x}). \tag{38}$$

We obtain a linear system of fractional differential equations of the form

$$D^\alpha_0 U(t) = AU(t) + F(t), \ U(0) = U_0, \ 0 < t \le T, \ 0 < \alpha < 1, \tag{39}$$

where $A = v(D_{xx} \otimes I_y + I_x \otimes D_{yy})$ is a $N_x^2 \times N_y^2$ matrix obtained from the semi-discretization of the underlying FPDE (33) using LRK methods, the symbol $\otimes$ is the Kronecker tensor product [36], $F(t)$ is the source term which collects the function f together with the discretized boundary conditions, and $D^\alpha_0 U(t)$ denotes the fractional derivatives.

4 Fractional exponential integrators

Before we state the definitions of fractional exponential time differencing, let us recall the definition of fractional derivative.

4.1 Basics of fractional calculus

There are several definitions of a fractional derivative of order $\alpha > 0$ (e.g. Riemann-Liouville [37] and Caputo [38] fractional derivative). Recently, Yang et al. [13] introduced a new fractional derivative without a singular kernel, with an application to the steady heat-conduction problem. However, we only consider the classical Caputo fractional derivative approach.

Definition 4.1: Caputo's definition of the fractional order derivative is given as

$$D^\alpha_t f(t) = \frac{1}{\Gamma(n-\alpha)}\int_a^t \frac{f^{(n)}(\xi)}{(t-\xi)^{\alpha+1}}d\xi, \quad n-1 < \alpha \le n, \ n \in \mathbb{N}, \quad 0 < t \le T, \tag{40}$$

where the parameter α is the order of the derivative and is allowed to be real, α is the initial value of the function f. In the present work only real positive values of α are considered. For the Caputo's derivative we have

$$D^\alpha_t C = 0, \quad C \in \mathbb{R}. \tag{41}$$

$$D^\alpha_t t^\gamma = \begin{cases} 0, & (\gamma \le \alpha - 1), \\ \frac{\Gamma(\gamma+1)}{\Gamma(\gamma\,\alpha+1)}t^{\gamma-\alpha}, & (\gamma > \alpha - 1). \end{cases} \tag{42}$$

The Caputo's fractional differentiation is expressed as a linear operation

$$D^\alpha(\lambda f(x) + \omega g(x)) = \lambda D^\alpha f(x) + \omega D^\alpha g(x), \tag{43}$$

where λ and ω are constants.

Definition 4.2: *The Riemann-Liouville time-fractional derivative operator of order $\alpha > 0$ is defined as*

$$D^\alpha_t f(t) = \begin{cases} \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial\xi^n}\left(\int_a^t \frac{f(\xi)}{(t-\xi)^{\alpha+1}}d\xi\right), & n-1 < \alpha < n, \ n \in \mathbb{N}, \\ \frac{\partial^n u(x,\xi)}{\partial\xi^n}, & \alpha = n \in \mathbb{N}. \end{cases} \tag{44}$$

In order to establish fractional derivative properties, we first define the Riemann-Liouville fractional integral operator.

Definition 4.3: *The Riemann-Liouville fractional integral operator of order α is defined as*

$$J_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} f(\xi) d\xi, \ \alpha > 0, \ t > 0. \tag{45}$$

Property 4.4: *For $\alpha, \beta \geq 0$ and $\gamma \geq -1$, we have the following*

$$J_t^\alpha J_t^\beta f(t) = J_t^{\alpha+\beta} f(t), \ \ J_t^\alpha t^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+\alpha+1) t^{\gamma+\alpha}}, \tag{46}$$

$$D_t^\alpha J_t^\alpha f(t) = f(t), J_t^\alpha D_t^\alpha f(t) = f(t) - \sum_{k=0}^{m-1} f^{(k)}(0^+) \frac{t^k}{k!}, t > 0. \tag{47}$$

Definition 4.5: *The Mittag-Leffler function is defined as (Podlubny [39])*

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta + \alpha k)}, \quad \alpha, \beta > 0, \ |z| < \infty. \tag{48}$$

It is known from Kilbas et al. [40] *that the function $e_{\alpha,\beta}$ is a generalization of the Mittag-Leffler (ML) function $E_{\alpha,\beta}$ following*

$$e_{\alpha,\beta}(t;\lambda) = t^{\beta-1} E_{\alpha,\beta}(-t^\alpha \lambda), \tag{49}$$

where α and β are two (possibly complex) parameters and the function $e_{\alpha,\beta}(t;\lambda)$ is the inverse of the Laplace transform $s^{\alpha-\beta}/(s^\alpha + \lambda)$.

Definition 4.6: *The Laplace transform of $f(t)$ is denoted by $\mathcal{L}\{f(t)\}$ and is defined by the integral*

$$\mathcal{L}\{f(t)\} = F(s) = \int_0^\infty e^{-st} f(t) dt. \tag{50}$$

The inverse Laplace transform is evaluated on a contour Γ, known as the Bromwich contour, as

$$\mathcal{L}^{-1}\{F(s)\} = f(t) = \int_\Gamma e^{st} F(s) ds. \tag{51}$$

The contour Γ is chosen such that it encloses all the singularities of $F(s)$.

4.1.1 Numerical fractional exponential time differencing method

In this paper we are interested in the numerical solution of fractional differential equations (FDEs) of the type

$$D_0^\alpha U(t) = AU(t) + F(t), \ U(0) = U_0, \ 0 < t <= T, \ 0 < \alpha < 1, \tag{52}$$

where $A \in \mathbb{R}^N \times \mathbb{R}^N$ is a matrix obtained from the semi-discretization of the underlying PDEs using LRK methods, $F(t) \in \mathbb{R}^N$ is the source term which collects the discretized boundary conditions and $D_0^\alpha U(t)$ denotes the Caputo's fractional derivative defined as

$$D_0^\alpha U(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{U'(s)}{(t-s)^\alpha} ds. \tag{53}$$

In the Laplace transform domain eq. (52) can be written as

$$s^\alpha \hat{U}(s) - s^{\alpha-1} U_0 = A\hat{U}(s) + \hat{F}(s), \tag{54}$$

which is equivalent to

$$\hat{U}(s) = s^{\alpha-1}(s^\alpha I - A)^{-1} U_0 + (s^\alpha I - A)^{-1} \hat{F}(s). \tag{55}$$

The application of the inversion of the Laplace transform to eq. (55) yields the following result in the time domain

$$U(t) = e_{\alpha,1}(t; -A) U_0 + \int_0^t e_{\alpha,\alpha}(t-s; -A) F(s) ds. \tag{56}$$

We consider the approximation of the integral in eq. (56) on a uniform partition of the interval $I = [0, T]$ given by

$$t_j = jh, \ \ j = 0, 1, \ldots, n, \ \ h = T/n. \tag{57}$$

We first rewrite the variation of constant formula in a piecewise way

$$U(t_n) = e_{\alpha,1}(t; -A) U_0 + \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} e_{\alpha,\alpha}(t_n - s; -A) F(s) ds. \tag{58}$$

Exponential integrators can be obtained by replacing in each subinterval $[t_j, t_{j+1}]$, the function $F(s)$ by a constant $F(t_j)$. We have

$$U_n = e_{\alpha,1}(t_n; -A) U_0 + h^\alpha \sum_{j=0}^{n-1} W_{n,j} F(t_j), \tag{59}$$

where the weights $W_{n,j}$ are the matrix functions defined as

$$W_{n,j} = e_{\alpha,\alpha+1}(n-j; -h^\alpha A) - e_{\alpha,\alpha+1}(n-(j+1); -h^\alpha A). \tag{60}$$

In real life applications, the system of ODEs (52), derived from spatial semi-discretization, is usually very large according to the number of grids. Therefore, the computation of the function $e_{\alpha,\beta}$ on a matrix argument becomes a nontrivial task. In this article, we use the Krylov projection algorithm [41] to improve the efficiency of the method. The key idea behind this method is to

approximate the product of a matrix function $e_{\alpha,\beta}(A)$ (A is a $\mathbb{R}^N \times \mathbb{R}^N$ matrix) and a vector v using projection of the matrix and the vector onto the Krylov subspace $K_m(A,v) = span\{v, Av, \ldots, A^{m-1}v\}$. The orthonormal basis $\{v_1, v_2, \ldots, v_m\}$ of $K_m(A,v)$ is constructed using the modified Arnoldi iteration [41, 42] which can be written in matrix form as

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} f_m^T, \tag{61}$$

where $h_{m+1,m}$ is an entry of the Hessenberg matrix H_m, $f_m = (0, \ldots, 0, 1, 0, \ldots, 0)^T$ is the unit vector with 1 as the m-th coordinate, $\{v_1, v_2, \ldots, v_m, v_{m+1}\}$ is an orthonormal basis of $K_m(A,b)$, $V_m = [v_1, v_2 \ldots, v_m]$ is a $N \times m$ matrix, and

$$H_m = V_m^T A V_m \tag{62}$$

is an upper Hessenberg matrix calculated as a side product of the iteration. The matrix $P = V_m V_m^T$ is a projection onto $K_m(A,v)$, thus $e_{\alpha,\beta}(A)v$ is approximated as a projection

$$e_{\alpha,\beta}(A)b \approx V_m V_m^T e_{\alpha,\beta}(A) V_m V_m^T v. \tag{63}$$

Recalling eq. (62) and observing that $v_1 = v/\|v\|_2$, we make the final approximation

$$e_{\alpha,\beta}(A)v \approx \|v\|_2 V_m e_{\alpha,\beta}(H_m) v_1. \tag{64}$$

The advantage of this formulation is that H_m is a $m \times m$ matrix of smaller size ($m \ll N$) and thus it is much cheaper to evaluate $e_{\alpha,\beta}(H_m)$ than $e_{\alpha,\beta}(A)$.

5 Numerical validations

In this section, we apply the LRK method on two different problems involving one and two dimensional heat equations. In the first example, we show efficiency of the present method by reporting the L_2- norm error

$$L_2 = ||u - \tilde{u}||_2 = \left[\Delta \sum_{i=1}^{N} (u_i - \tilde{u}_i)^2 \right]^{1/2} \tag{65}$$

and L_∞-norm error

$$L_\infty = ||u - \tilde{u}||_\infty = \max_{1 \le j \le N} |u_j - \tilde{u}_j|, \tag{66}$$

where N is the number of computational grids, u and $\tilde{u}$ represent the exact and approximate solutions, respectively. For the two-dimensional heat equation, we define the L_2-norm error by

$$L_2 = ||u - \tilde{u}||_2 = \left[\Delta_x \Delta_y \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} (u_{i,j} - \tilde{u}_{i,j})^2 \right]^{1/2} \tag{67}$$

and the L_∞-norm error by

$$L_\infty = ||u - \tilde{u}||_\infty = \max_{i \in [1,N_x], j \in [1,N_y]} |u_{i,j} - \tilde{u}_{i,j})|, \tag{68}$$

where N_x and N_y represent the number of grid points in x and y directions, respectively. For numerical flexibility, the LRK is implemented adaptively to avoid the restriction of the bandwidth when the number of grid points is very small. The LRK is implemented as a discrete convolution scheme such as the s-th order derivative of a function $u(x)$ on a given grid point x_i, and is approximated as

$$\tilde{u}^{(s)}(x_i) = \sum_{j=S_1}^{S_2} u(x_k) \left[\left(\prod_{j=S_1, j \ne k}^{S_2} \frac{x_i - x_j}{x_k - x_j} \right) \exp\left(-\frac{(x_i - x_j)^2}{2\sigma^2} \right) \right]^{(s)}. \tag{69}$$

There are two ways to choose S_1 and S_2 depending on the number of grid points we want to use to approximate the derivative at discrete point x_i. For instance, if we want to approximate the derivative at discrete point x_i with $2M+1$ grid points, we choose S_1 and S_2 as

$$S_1 = \max\{\min\{i-N, N-2M\}, 1\}, S_2 = \min\{\max\{1+2M, i+M\}, N\}. \tag{70}$$

This methodology generally produces box-banded differential matrices. If it is desired to approximate the derivative at discrete points x_i with $M+1$ grid points, we select S_1 and S_2 as

$$S_1 = \max\{i - M, 1\}, \quad S_2 = \min\{i + M, N\}. \tag{71}$$

This is generally known as one side approximation. The choice of the LRK bandwidth M and the regularizer parameter σ is done according to the conditions (24). Hence, if $M = 16$, $M = 32$ and $M = 64$ then $\sigma \approx 2.5\Delta$, $\sigma \approx 3.2\Delta$ and $\sigma \approx 6.2\Delta$, respectively. Numerical experiments were obtained by choosing S_1 and S_2 as defined by eq. (71) with $M = 32$ and the Hessenberg matrix size $m = \min\{15, N\}$.

Example 5.1: *Consider the one-dimensional fractional-time heat equation of the form*

$$\frac{\partial^\alpha}{\partial t^\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t), \tag{72}$$

with the initial condition

$$u(x,0) = \sin(x), \quad 0 \le x \le \pi, \tag{73}$$

and homogenous boundary conditions

$$u(0,t) = 0, \quad u(1,t) = 0, \quad 0 \le t \le 1. \tag{74}$$

The exact solution of this problem is given by

$$u(x,t) = \sin(x) E_{\alpha,1}(-t^{\alpha}). \tag{75}$$

We first choose $\alpha \in \{0.2,\ 0.4,\ 0.6,\ 0.8\}$ and perform numerical experiments to check their agreement with the analytical solution. Clearly, Figure 1 illustrates that the LRK method solutions are very good estimates of the analytical solutions as absolute errors are of magnitude 10^{-14}.

Next, we investigate the convergence of our numerical method with respect to the number of grid points N. In Figure 2, we observe that numerical solutions of the LRK method converge towards exact soliton solutions as the number of grid points N increases. We remark that LRK method converges rapidly, in fact exponentially, as the number of mesh points increases. In the next example we investigate the convergence of the LRK method on the higher dimensional heat equation.

Example 5.2: *Consider the two-dimensional time-fractional heat equation*

$$\frac{\partial^{\alpha}}{\partial t^{\alpha}} u(x,y,t) = \frac{\partial^2}{\partial x^2} u(x,y,t) + \frac{\partial^2}{\partial y^2} u(x,y,t), \tag{76}$$

on the unit domain $\mathcal{D} = \{(x,y) : 0 < x, y < \pi\}$. *The initial condition is chosen as*

$$u(x,y,0) = \sin(x)\sin(y), \quad 0 \le x, y \le \pi, \tag{77}$$

together with homogeneous boundary conditions

$$u(0,y,t) = u(\pi,y,t) = u(x,\pi,t) = u(x,\pi,t) = 0, \quad t \in [0,T]. \tag{78}$$

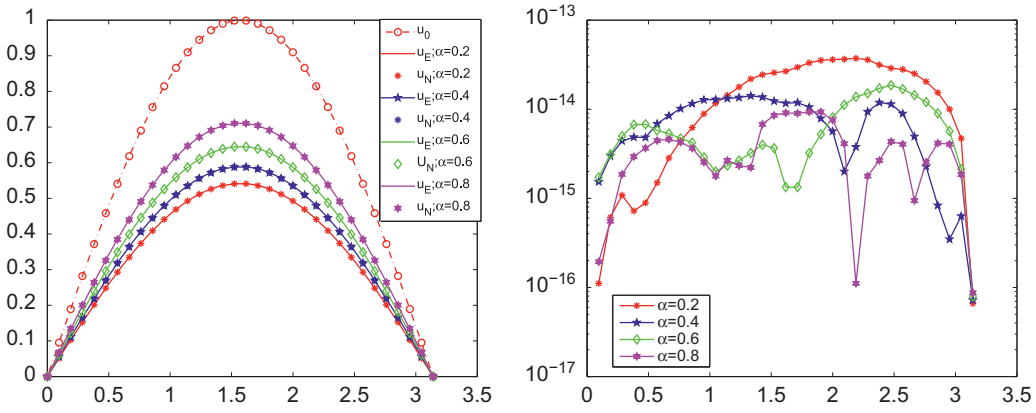

Figure 1: Comparison of numerical and exact solutions (Left) and absolute error (Right) at $t = 0.25$ for $\alpha \in \{0.2,\ 0.4,\ 0.6,\ 0.8\}$, $M = 32$, $N = 32$ and $x \in [0, \pi]$.

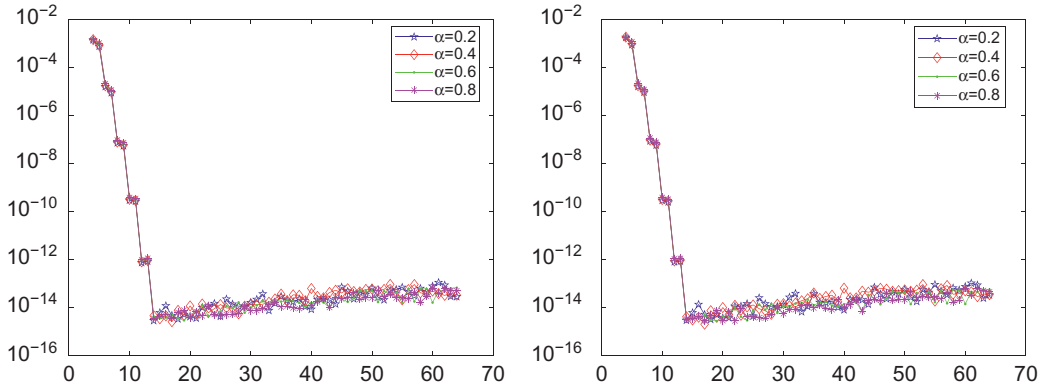

Figure 2: Errors as a function of the number of grid points N at $t = 0.25$, (Left) L_{∞} and (Right) L_2 for $\alpha \in \{0.2,\ 0.4,\ 0.6,\ 0.8\}$, $M = 32$ and $x \in [0, \pi]$.

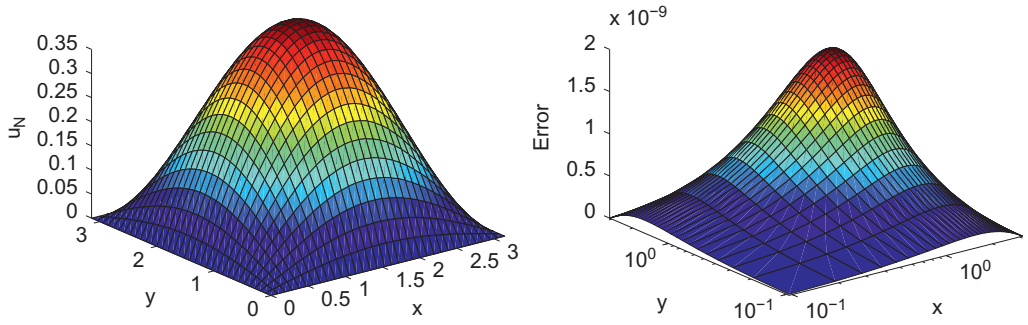

Figure 3: Numerical solution (Left) and absolute error (Right) at $t = 0.25$ for $\alpha = 0.2$, $M = 32$, $N_x = N_y = 32$ and $x, y \in [0, \pi]$.

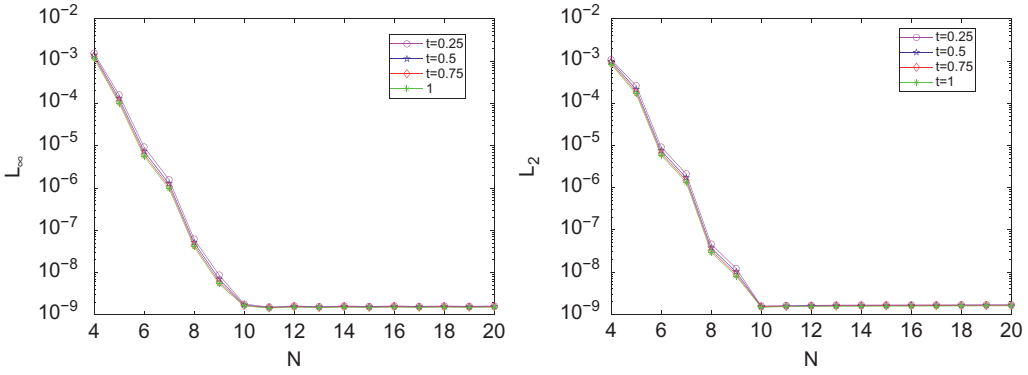

Figure 4: Errors as a function of the number of grid points $N_x = N_y$ at $t = 0.25,\ 0.5,\ 0.75,\ 1$, (Left) L_∞ and (Right) L_2, $\alpha = 0.5$, $M = 32$ and $x \in [0, \pi]$.

The analytical solution of the above problem is

$$u(x, y, t) = \sin(x)\sin(y)E_{\alpha,1}(-2t^\alpha). \tag{79}$$

When $t = 0.5$, $\alpha = 0.4$, $N_x = N_y = 32$ and the LRK bandwidth $M = 32$, we obtain very satisfactory results displayed in Figure 3. To verify the accuracy of this approximation we plot L_∞- and L_2-norm errors on the left and right part of Figure 4, respectively. The outcome turns out to be very satisfactory as the number of mesh points N increases. The error decays very rapidly with the increase of N and tends to be of the same magnitude for different time t.

Note that this method is flexible and allows numerical treatment of nonlinear PDEs since the semi-discretization of the nonlinear PDEs using the LRK method (8) yields a system of nonlinear ODEs that can be solved using fractional exponential time differencing methods [27].

6 Conclusion

A numerical technique based on the LRK method has been presented for numerical solutions of fractional-time diffusion equations. The efficiency of the method is tested against analytical solutions of fractional-time heat equations in one and two dimensions. The accuracy is examined in terms of the L_∞ and L_2 error norms. Numerical results have illustrated that our methodology is highly accurate and converges exponentially. Moreover, our results are a good representation of the theory.

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