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NSFDE&A'20

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NUMERICAL SOLUTION OF FRACTIONAL DIFFERENTIAL EQUATIONS AND APPLICATIONS

S. HARIZANOV, R. LAZAROV, S. MARGENOV (EDS.)

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PROCEEDINGS OF SHORT COMMUNICATIONS

S. HARIZANOV, R. LARAROV, S. MARGENOV (EDS.)

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PREFACE

The International Workshop on Numerical Solution of Fractional Differential Equations and Applications (NSFDE&A'20) is organized by the Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, in cooperation with the Bulgarian Section of SIAM and the Center of Excellence in Informatics and Information and Communication Technologies (CoE in Informatics and ICT).

The CoE in Informatics and ICT, Grant No BG05M2OP001-1.001-0003, is financed by the Science and Education for Smart Growth Operational Program (2014-2020) and co-financed by the EU through the European Structural and Investment Funds.

The workshop follows the great success of the Special Session on Fractional Diffusion Problems: Numerical Methods, Algorithms and Applications, organized within the scientific program of the 12th International Conference on Large-Scale Scientific Computations (LSSC'19), June 10–14, 2019, Sozopol, Bulgaria. The workshop is aimed to start a new chain of NSFDE&A events to be organized biannually, every even year, complementary to the well-established LSSC conferences every odd year.

The major specific topics of NSFDE&A'20 include: fractional in space diffusion problems; fractional in time problems; coupled problems; parallel algorithms and high performance computing tools; applications in science and engineering.

List of keynote speakers and lectures:

1. Raytcho Lazarov (Texas A&M University, College Station, Texas, US)

   Solution of Spectral Fractional Elliptic Problems: A Concise Overview of Methods Based on Rational Approximation

2. Virginia Kiryakova (Institute of Mathematics and Informatics, Bulgarian Academy of Sciences, Sofia, Bulgaria)

   Special Functions of Fractional Calculus in Solutions of Fractional Order Equations and Models

3. HongGuang Sun (State Key Laboratory of Hydrology-Water Resources and Hydraulic Engineering, Hohai University, Nanjing, China)

   A Survey on Fast Algorithms for Fractional Diffusion Equations and its Applications

The purpose of the workshop is to bring together scientists in the field of numerical methods working with fractional differential equations models in natural sciences and environmental and industrial applications, as well as developers of algorithms for modern high-performance computers. The keynote lectures review some of the most advanced achievements in the field of numerical solution of fractional differential equations and their

applications. The workshop talks are presented by scientists from diverse research institutions including applied mathematicians, numerical analysts, and computer experts.

Scientists from all over the world (America, Asia, and Europe) contributed to the success of the workshop, representing some of the strongest research groups in the field of the event.

This volume contains 23 short communications by authors from 13 countries.

The next International Workshop on NSFDE&A will be organized in June 2022.

April 2020

Stanislav Harizanov
Raytcho Lazarov
Svetozar Margenov

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Fast approximations of fractional powers of operators

Lidia Aceto
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Let $\mathcal{L}$ be a self-adjoint positive operator with spectrum $\sigma(\mathcal{L}) \subseteq [1, +\infty)$, acting on a Hilbert space $\mathcal{H}$ endowed with norm $\|\cdot\|_{\mathcal{H}}$ and operator norm $\|\cdot\|_{\mathcal{H}\to\mathcal{H}}$. Furthermore, suppose that $\mathcal{L}$ has a compact inverse so that $\mathcal{L}^{-\alpha}, \alpha \in (0, 1)$, can be written in terms of the spectral decomposition of $\mathcal{L}$.

By exploiting the existing representations of the function $\lambda^{-\alpha}$ in terms of contour integrals, after suitable changes of variable and quadrature rules one typically finds rational approximations of the type

$$\mathcal{L}^{-\alpha} \approx \mathcal{R}_{k-1,k}(\mathcal{L}), \quad \mathcal{R}_{k-1,k}(\lambda) = \frac{p_{k-1}(\lambda)}{q_k(\lambda)}, \quad p_{k-1} \in \Pi_{k-1}, q_k \in \Pi_k,$$

where k is an integer closely related to the number of points in the quadrature formula (see, e.g., [1, 2, 4]).

In this talk we focus on a particular integral representation that leads to the use of a double n-point Gauss-Laguerre rule which implicitly defines a $(2n-1, 2n)$-rational approximation of $\mathcal{L}^{-\alpha}$. Actually, since the functions involved are uniformly bounded with respect to $\lambda \in [1, +\infty)$, we consider a truncated approach leading to a rational approximation whose error is well estimated by

$$\left\|\mathcal{L}^{-\alpha} - \mathcal{R}_{2k_n-1,2k_n}(\mathcal{L})\right\|_{\mathcal{H}\to\mathcal{H}} \approx 8\sin(\alpha\pi)\exp(-5\alpha^{1/2}k_n^{1/2}),$$

where k_n is the number of inversions of the truncated approach. This approach is very fast and the quality of the above estimate allows us to define a-priori n and k_n in order to satisfy a given tolerance. The numerical experiments we present confirm the effectiveness of the proposed strategy.

It is worth to mention that this problem finds immediate application when solving differential mathematical models involving a fractional term like $(-\Delta)^\alpha$, where Δ denotes the standard Laplacian [3, 5, 6]. Such models are increasingly used because they provide an adequate description of many processes that exhibit an anomalous diffusion (for example, the diffusion of proteins inside the cells or the diffusion through porous media). In this case the fractional Laplacian is replaced by the product of two appropriate banded matrices. This leads to a semi-linear initial value problem in which all linear algebra tasks involve sparse matrices with a consequent decrease in computational cost.

This is joint work with Paolo Novati (University of Trieste, Italy).

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A compact difference schemes for the time-fractional diffusion equation of variable order

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Solutions of boundary value problems for a diffusion equation of variable order in differential and difference settings are studied [1]. In the paper [2] has been found a special point for the interpolation approximation of the Caputo fractional derivative and derived a numerical differentiation $L2-1_\sigma$ formula to approximate the Caputo fractional derivative at this point with the numerical accuracy of order $3-\alpha$ uniformly. In the paper [3] such scheme was constructed for a variable order Caputo derivative ($\alpha(t) \in (0,1)$ for all t).

The present talk are devoted to high-order of approximating compact difference schemes for the time-fractional diffusion equation of variable order ($\alpha(x) \in (0,1)$ for all possible x) constructed on the basis of $L2-1_\sigma$ formula. The obtained results are supported by the numerical calculations carried out for some test problems.

Consider the time - fractional diffusion equation of variable order

$$\partial_{0t}^{\alpha(x)} u(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) + f(x,t), \quad 0 < x < 1, \quad 0 < t \le T, \tag{1}$$

$$u(0,t) = 0, \quad u(1,t) = 0, \quad 0 \le t \le T, \quad u(x,0) = u_0(x) \quad 0 \le x \le 1, \tag{2}$$

where

$$\partial_{0t}^{\alpha(x)} u(x,t) = \frac{1}{\Gamma(1-\alpha(x))} \int\limits_0^t \frac{\partial u(x,\eta)}{\partial \eta} (t-\eta)^{-\alpha(x)} d\eta$$

is the Caputo derivative of the variable order $\alpha(x)$, $0 < \alpha(x) < 1$ for all $x \in (0,1)$.

In the rectangle $\overline{Q}_T = \{(x,t) : 0 \le x \le 1,\ 0 \le t \le T\}$ we introduce the grid $\overline{\omega}_{h\tau} = \overline{\omega}_h \times \overline{\omega}_\tau$, where $\overline{\omega}_h = \{x_i = ih,\ i = 0,1,\dots,N;\ hN = 1\}$, $\overline{\omega}_\tau = \{t_j = j\tau,\ j = 0,1,\dots,M;\ \tau M = T\}$. Let us assign the following difference scheme to differential problem (1)–(2)

$$\mathcal{H}_h \Delta_{0t_{j+\sigma_i}}^{\alpha_i} y_i = \sigma_i y_{\bar{x}x,i}^{j+1} + (1-\sigma_i) y_{\bar{x}x,i}^{j} + \mathcal{H}_h \varphi_i^{j+\sigma_i}, \tag{3}$$

where $\mathcal{H}_h v_i = v_i + h^2 v_{\bar{x}x,i}/12$, $\sigma_i = 1 - \frac{\alpha_i}{2}$, $\alpha_i = \alpha(x_i)$, $i = 1,2,\dots,N-1$, $v_{\bar{x},i} = (v_i - v_{i-1})/h$, $v_{x,i} = (v_{i+1} - v_i)/h$, $v_t^s = (v^{s+1} - v^s)/\tau$,

$$\Delta_{0t_{j+\sigma_i}}^{\alpha_i} v = \frac{\tau^{1-\alpha_i}}{\Gamma(1-\alpha_i)} \sum_{s=0}^{j} c_{j-s}^{(\alpha_i)} v_t^s,$$

τ	h	e	CO in $\|\cdot\|_{\mathcal{C}(\bar{\omega}_{h\tau})}$
1/4	1/16	3.60494e-3	
1/8	1/64	2.42183e-4	3.896
1/16	1/256	1.57570e-5	3.942
1/32	1/1024	9.82777e-7	4.003
1/64	1/4096	6.12760e-8	4.003
1/128	1/16384	3.81887e-9	4.004
1/256	1/65536	2.38255e-10	4.003

Table 1: Maximum norm error behavior versus grid size reduction when $\tau = h^2$

$c_0^{(\alpha_i)} = a_0^{(\alpha_i)}$, for $j = 0$; and for $j \geq 1$,

$$c_s^{(\alpha_i)} = \begin{cases} a_0^{(\alpha_i)} + b_1^{(\alpha_i)}, & s = 0, \\ a_s^{(\alpha_i)} + b_{s+1}^{(\alpha_i)} - b_s^{(\alpha_i)}, & 1 \leq s \leq j-1, \\ a_j^{(\alpha_i)} - b_j^{(\alpha_i)}, & s = j, \end{cases}$$

$$a_0^{(\alpha_i)} = \sigma_i^{1-\alpha_i}, \quad a_l^{(\alpha_i)} = (l+\sigma_i)^{1-\alpha_i} - (l-1+\sigma_i)^{1-\alpha_i}, \quad l \geq 1;$$

$$b_l^{(\alpha_i)} = \frac{1}{2-\alpha_i}\left[(l+\sigma_i)^{2-\alpha_i} - (l-1+\sigma_i)^{2-\alpha_i}\right] - \frac{1}{2}\left[(l+\sigma_i)^{1-\alpha_i} + (l-1+\sigma_i)^{1-\alpha_i}\right].$$

If $u(x,t) \in \mathcal{C}_{x,t}^{6,3}$ and $\alpha(x) \in \mathcal{C}_x^2$, then the difference scheme has the approximation order $\mathcal{O}(\tau^2 + h^4)$.

Numerical results. Numerical calculations are performed for a test problem when the function $u(x,t) = (t^4 + 2t^3 + 3t^2 + 1)\sin \pi x$ is the exact solution of the problem (1)–(2) with $\alpha(x) = \frac{4+\sin 5x}{6}$ and $T = 1$.

The errors ($e = y - u$) and convergence order (CO) in the norm $\|\cdot\|_{\mathcal{C}(\bar{\omega}_{h\tau})}$, where $\|y\|_{\mathcal{C}(\bar{\omega}_{h\tau})} = \max\limits_{(x_i,t_j)\in\bar{\omega}_{h\tau}} |y|$, are given in Table 1.

Table 1 shows that as the number of the spatial subintervals and time steps is increased keeping $h^2 = \tau$, a reduction in the maximum error takes place, as expected and the convergence order of the approximate scheme is $\mathcal{O}(h^4) = \mathcal{O}(\tau^2)$, where the convergence order is given by the formula: CO$= \log_{\frac{h_1}{h_2}} \frac{\|e_1\|}{\|e_2\|}$ (e_i is the error corresponding to h_i).

Table 2 shows that if $h = 1/1000$, then as the number of time steps of our approximate scheme is increased, a reduction in the maximum error takes place, as expected and the convergence order of time is $\mathcal{O}(\tau^2)$, where the convergence order is given by the following formula: CO$= \log_{\frac{\tau_1}{\tau_2}} \frac{\|z_1\|}{\|z_2\|}$.

Funding: The reported study was funded by RFBR and NSFC according to the research project 20-51-53007

τ	e	CO in $\|\cdot\|_{\mathcal{C}(\bar{\omega}_{h\tau})}$
1/10	3.10575e-2	
1/20	7.79443e-3	1.994
1/40	1.94974e-3	1.999
1/80	4.87052e-4	2.001
1/160	1.21604e-4	2.001
1/320	3.03576e-5	2.002
1/640	7.57888e-6	2.002

Table 2: Maximum norm error behavior versus τ-grid size reduction when $h = 1/1000$

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DOI: 10.1016/j.camwa.2020.01.003

A difference analog of a higher approximation order for the Caputo fractional derivative with generalized memory kernel and its application

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In the present work, a fractional numerical differentiation formula (L2-1$_\sigma$ formula) to approximate the Caputo fractional derivative of order $\alpha(0 < \alpha < 1)$ with generalized memory kernel $\lambda(t)$ is developed. It is established by means of the quadratic interpolation approximation using three points $(t_{s-1}, u(t_{s-1}), (t_s, u(t_s))$ and $(t_{s+1}, u(t_s))$ for the integrand $u(t)$ on each small interval $[t_{s-1}, t_s](1 \le s \le j)$, while the linear interpolation approximation is applied on the last small interval $[t_j, t_{j+\sigma}]$, where $t_{j+\sigma}$ is the special super convergence points. As a result, the formula can be formally viewed as a modification of the L1 formula, which is obtained in [1]. Both the computational efficiency and numerical accuracy of the new formula are superior to that of the L1 formula. The coefficients and truncation errors of this formula are discussed in detail. Test examples show the numerical accuracy of L2-1σ formula.

By the new formula, two improved finite difference schemes with high order accuracy in time for solving the time-fractional sub-diffusion equation with generalized memory kernel. Several numerical examples are computed. The comparison with the corresponding results of finite difference methods by the L1 formula demonstrates that the L2-1$_\sigma$ formula is much more effective and more accurate than the L1 formula when solving time-fractional differential equations with generalized memory kernel numerically.

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Quasi-Monte Carlo simulation of fractional Brownian motion for option pricing using GPUs

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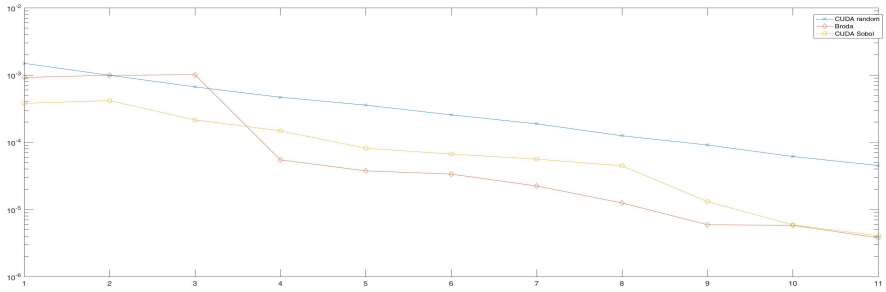
1 Introduction

The financial options are contracts that give the holder the right to purchase certain security at a given price or, in more complex cases, provide a payout based on the movements of the price of the underlying asset. The Monte Carlo method for option pricing is versatile and applicable for options with arbitrarily complex payouts. The basic procedure for obtaining the price of the financial option with payout $f(\{P_t\}_0^T)$ under the model M is to simulate multiple paths $\{P_t\}_{t=0}^T$ of the price of the underlying and evaluate the mathematical expectation of the discounted payout under the so-called risk-neutral measure, i.e., $Price = E_Q e^{-rT} f(\{P_t\}_0^T)$. The efficient use of low-discrepancy sequences instead of pseudorandom numbers gives rise of a QMC method and requires careful study of the setup of the Monte Carlo method in order achieve improvement of the accuracy. One of the basic features of the many statistical models of the price evolution is the use of one or more Brownian motions in the definition of the model. The fractional Brownian motion (fBM) is an extension that allows for incorporation of long-term memory effects. There are many relations between fBM and fractional calculus. Although the fractional Laplacian for $\alpha \in$ [] is the generator for the (radially symmetric) 2α-stable Lévy process instead, the fBM observes the following identity for $H < H\prime$: $B_H = (-\Delta)^{\frac{H\prime - H}{2}} B_{H\prime}$.
For more information about these types of relations, see, e.g., [7], while fBM and related processes are discussed in depth in [3], [4]. A Monte Carlo algorithm for simulating a fractional Brownian Motion is well known (see, e.g., [6], also available for Matlab at [2]). We investigated various ways to switch to QMC simulation when using NVIDIA CUDA GPUs for the computations and the respective numerical results.

2 QMC algorithms for simulating fBM and their implementation on NVIDIA GPUs

The basic approach to obtain a QMC algorithm is to use one point of the low-discrepancy sequence in order to generate one trajectory of the price of the underlying. The algo-

Figure 1: Accuracy of computation of an Asian option



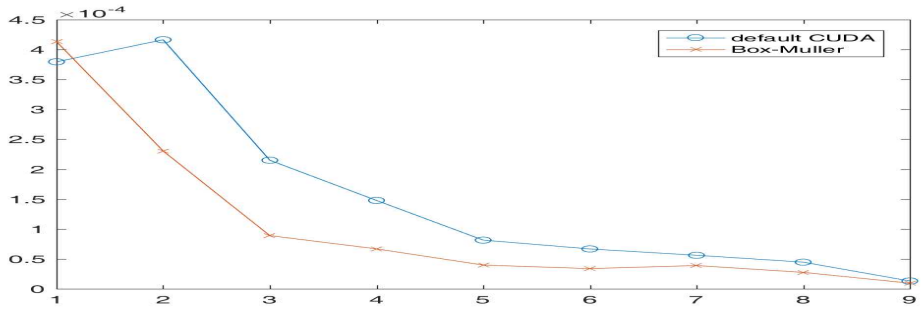
rithm mentioned above requires generation of pseudo-random or quasi-random numbers, multiplication with certain pre-computed constants and performing Fast Fourier Transform. NVIDIA CUDA provides fast generation routines with very similar interfaces for generation of both pseudo-random numbers and Sobol sequences as well as routines for FFT. We evaluated prices of both European and (arithmetic) Asian options, while the codes can be used also for exotic options. In the next figure one can see results about the accuracy obtained when computing the same option with 1024 timesteps (constructive dimensionality 4096), for number of points ranging from 2^{12} to 2^{22}. We compared the default pseudorandom generator in CUDA with the default scrambled Sobol sequence implemented in CUDA (based on the direction numbers of Joe and Kuo [5]) as well as the direction numbers provided by Sergei Kucherenko from BRODA ([9]). In all our experiments we compute the error as a root-mean-square error (RMSE) using 100 evaluations with different initial seeds for the scrambling. It is immediately obvious that the QMC algorithm greatly outperforms in terms of accuracy. The comparison between the different sets of direction numbers did not yield a definitive conclusion. In the next table one can see comparison of the computational times, which shows that the advantage of the QMC method is not negated by the slightly slower computation. When incorporating additional scrambling along the ideas of [1], additional 20% are added to the computation time. The advantage of GPU vs CPU in such types of computations is dramatic and well established, that is why we do not show such comparisons. Because of the structure of the Monte Carlo

Algorithm / N	12	14	16	18	20	22
CUDA random	0.44	1.45	2.44	4.26	10.17	42.60
CUDA Sobol	0.95	2.41	3.71	4.31	15.07	60.27

Table 1: Computational times for Asian option pricing, when using 2^N points

algorithm (pairs of normally distributed random numbers are interpreted as complex numbers) it is also interesting to replace the basic routine *curand_normal_double* / with a few lines of code using the Box-Mueller transform and *curand_uniform_double* . Giray Okten

Figure 2: Accuracy of Box-Muller transform vs curand_normal_double



advocates the use of this transform as superior, see, e.g., [8]. In the next figure one can see that the accuracy with this transform is substantially better, when using the same directional numbers (mean ratio is 1.75 when the number of points grow from 2^{12} to 2^{19}). We point out that practitioners in the field usually use only several thousand points, that is why the results for higher number of points do not have the same weight for practical applications.

Conclusions and future work

The numerical and timing results clearly show the advantages of using QMC on GPU for pricing options using fractional Brownian motion in the underlying model. Some advantage in using the Box-Muller transform is observed and is significant enough for practical purposes. Additional experiments showed advantage of reordering of the coordinates according to their importance can also provide improved accuracy.

Acknowledgments

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Meshless method for the numerical solution of space and time fractional wave equation

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1 Introduction

Fractional order differential equations have attracted many researchers because of their ability to provide extensive and detailed analysis of the model. Fundamental fractional partial differential equations are the fractional diffusion equation and the fractional wave equation. Here fractional wave equation is obtained by substituting time and space derivative with generalised Caputo fractional derivative in the classical wave equation

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^\beta u(x,t)}{\partial x^\beta} + f(x,t), \qquad 1 \leq \alpha,\ \beta \leq 2, \tag{1}$$

initial conditions and boundary conditions are

$$\begin{aligned} u(x,0) = p_1(x),\ \ u_t(x,0) = p_2(x) \\ u(a,t) = q_1(t),\ \ u(b,t) = q_2(t). \end{aligned} \tag{2}$$

Many authors studied the model in equation(1)-(2) with the perspective of numerical solution. The finite difference method based on the Hermite formula is used by Khader and Adel [1] for the solution of the wave equation. Sweilam and Nagy [2] implemented the Crank-Nicholson method to acquire the solution for the fractional wave equation. In the present study, we have proposed a novel approach of collocation with Chebyshev polynomials and radial basis functions for the numerical solution of the fractional wave equation.

2 Preliminaries

In this section, we have discussed an important definition of fractional derivatives, the notations about Chebyshev polynomials and radial basis functions (RBFs).

Definition 1 *Caputo fractional derivative of power function* $x^p,\ p \geq 0$ *is [3]*

$$D^\alpha x^p = \begin{cases} \frac{\Gamma(p+1)}{\Gamma(p+\alpha-1)} x^{p-\alpha}, & \text{for } p \geq \lceil \alpha \rceil \\ 0, & \text{for } p < \lceil \alpha \rceil \end{cases}$$

2.1 Radial basis functions

RBFs have become an effective tool for interpolating scattered data in which the univariate function $u(x)$ can be approximated as

$$u\left(x\right)=\sum_{i=1}^{N}\lambda_{i}\phi_{i}\left(r\right),$$

where λ_i are coefficients to be determined. N is the number of data points. $\phi(r)$ is any RBF and $r=\|x-x_i\|$ is the Euclidean distance. Most commonly used RBFs are the Gaussian $\phi(r)=e^{-(\epsilon r)^2}$, the multiquadric $\phi(r)=(r^2+\epsilon^2)^{\beta/2}$, $\beta=-1,\ 1,\ 3,..$, the polyharmonic splines $\phi(r)=r^n\ \log r$, $n=2,\ 4,..$ and the conical type $\phi(r)=r^n$, $n=1,\ 3,...$ In this study we have implemented the conical type RBF with $n=3$, called the cubic RBF.

2.2 Chebyshev polynomials

The analytic for of shifted Chebyshev polynomials of degree n is [3, 4]

$$T_{n}^{*}\left(x\right)=\sum_{k=0}^{n}\left(-1\right)^{n-k}2^{2k}\frac{n\left(n+k-1\right)!}{\left(2k\right)!\left(n-k\right)!}x^{k}.$$

Using definition (3), fractional derivative of shifted Chebyshev polynomial $D^{\alpha}T_{n}^{*}\left(x\right)$ is

$$D^{\alpha}T_{n}^{*}\left(x\right)=\sum_{k=\lceil\alpha\rceil}^{n}\left(-1\right)^{n-k}2^{2k}\frac{n\left(n+k-1\right)!}{\left(2k\right)!\left(n-k\right)!}\frac{\Gamma\left(k+1\right)}{\Gamma\left(k+1-\alpha\right)}\ x^{k-\alpha},\qquad n\geq\lceil\alpha\rceil$$

3 Proposed scheme

For the solution of the model in equation (1)-(2), we approximate the function $u(x,t)$ using Chebyshev polynomials and radial basis function as

$$u\left(x,t\right)\approx\sum_{i=1}^{N}\sum_{j=1}^{n}T_{j}^{*}\left(t\right)c_{ji}\Phi_{i}\left(x\right)\quad=\mathbb{T}(t)\ C\ \Phi(x)\tag{3}$$

where $\mathbb{T}(t)$, $\Phi(x)$ are Chebyshev polynomials and cubic radial basis functions respectively. n and N are the discretization parameters corresponding to time and space and c_{ji}s are unknowns.
For the discretization of time and space, m Chebyshev nodes and n uniform nodes in $[p,q]$ has been considered respectively as,

$$t_{m}=\frac{1}{2}\left(p+q\right)+\frac{1}{2}\left(q-p\right)\cos\left(\frac{2\left(n-m\right)-1}{2n}\pi\right);m=1,2,...,n,$$
$$x_{k}=x_{k-1}+\frac{q-p}{n-1};\ k=1,2,...,N,\quad x_{0}=p.$$

From equation (3) we can write

$$\begin{aligned}{}_{0}^{C}D_{t}{}^{\alpha}u\left(x,t\right)&={}_{0}^{C}D_{t}{}^{\alpha}\left(\mathbb{T}\ C\ \Phi\right)=\left[{}^{C}D_{t}{}^{\alpha}\mathbb{T}\right]C\Phi\quad&=\mathbb{T}^{\alpha}\ C\ \Phi,\\ {}_{0}^{C}D_{t}{}^{\beta}u\left(x,t\right)&={}_{0}^{C}D_{t}{}^{\beta}\left(\mathbb{T}\ C\ \Phi\right)=\mathbb{T}\ C\left[{}^{C}D_{t}{}^{\beta}\Phi\right]\quad&=\mathbb{T}\ C\ \Phi^{\beta}.\end{aligned}\tag{4}$$

Substituting equations (4), (5) in equation (1) and collocating (6) in $N-2$ uniform nodes, and $n-2$ Chebyshev nodes, it will give $(N-2)(n-2)$ equations of the form

$$\mathbb{T}^{\alpha}\ C\ \Phi - \mathbb{T}\ C\ \Phi^{\beta} = f(x,t). \tag{5}$$

Implementing equation (3) on the initial and boundary conditions given in equation (2)

$$\begin{aligned} u(x,0) = T(0)C\Phi = p_1(x), \quad u_t(x,0) = D_tT(0)C\Phi = p_2(x), \\ u(0,t) = TC\Phi(0) = q_1(t), \quad u(1,t) = TC\Phi(1) = q_2(t), \end{aligned} \tag{6}$$

For the solution of equation (5), we will convert it in a simplified form with the aid of Kronecker product (indicated by '$\otimes$')

$$\left(\Phi^t \otimes T^{\alpha} - \Phi^{\beta t} \otimes T\right) \overrightarrow{c} = \overrightarrow{f(x,t)} \Rightarrow A_1 \overrightarrow{c} = \overrightarrow{F_1}, \tag{7}$$

Initial and boundary conditions can be expressed as

$$\begin{aligned} \left(\Phi^t \otimes T(0)\right) \overrightarrow{c} = \overrightarrow{p_1(x)} \Rightarrow A_2C = \overrightarrow{F_2}, \ \left(\Phi^t \otimes T(0)\right) \overrightarrow{c} = \overrightarrow{p_2(x)} \Rightarrow A_3C = \overrightarrow{F_3}, \\ \left(\Phi(1)^t \otimes T\right) \overrightarrow{c} = \overrightarrow{q_1(t)} \Rightarrow A_4C = \overrightarrow{F_4}, \ \left(\Phi(1)^t \otimes T\right) \overrightarrow{c} = \overrightarrow{q_2(t)} \Rightarrow A_5C = \overrightarrow{F_5}, \end{aligned} \tag{8}$$

The resulted system of the equation can be illustrated by collecting equations (7) and (8)

$$A\overrightarrow{c} = \overrightarrow{F}, \tag{9}$$

where A is of size $Nn \times Nn$ and it has the form $A = [A_1, A_2, A_3, A_4, A_5]^t$. $\overrightarrow{F}$ is of the form $\overrightarrow{F} = \left[\overrightarrow{F_1}, \overrightarrow{F_2}, \overrightarrow{F_3}, \overrightarrow{F_4}, \overrightarrow{F_5}\right]^t$ with the dimension $Nn \times 1$.

Solution of the system of equation in equation (10) will give the values of unknown coefficients $\overrightarrow{c}$. Reshaping and plugging $\overrightarrow{c}$ in equation (3) will provide desired approximate solution $u(x,t)$.

4 Numerical Example

Example 1. To check the effectiveness of this new approach, we have taken the time-fractional wave equation as follows [1]:

$$\begin{aligned} u_t^{\alpha}(x,t) = u_{xx}(x,t) + \left[\frac{t^{1-\alpha}(2t+\alpha-3)}{\Gamma(3-\alpha)} + \pi^2\right]\sin(\pi x), \\ 1 < \alpha \leq 2, \quad 0 < x < 1, \quad 0 < t < 1, \end{aligned} \tag{10}$$

initial conditions and boundary conditions are

$$\begin{aligned} u(x,0) = 0, \quad u_t(x,0) = -\sin(\pi x) \quad 0 < x < 1, \\ u(0,t) = 0, \quad u(1,t) = 0 \qquad\qquad 0 < t < 1. \end{aligned} \tag{11}$$

The analytic solution of (10) is $u(x,t) = sin(\pi x)(t^2 - t)$.
The results in **table 1** are obtained using the approach in **section 3** using **MATLAB®**. Also, the obtained results have been compared with the results in [1].

Method in [1]			Proposed method		
N	n	Maximum error	N	Maximum error (n=11)	CPU Time (seconds)
6	51	0.011489	15	0.0022	0.12
11	101	0.00361	30	0.00052	0.12
21	151	0.00120	45	0.00023	0.14
31	151	0.00115	60	0.00012	0.15
31	201	0.00021	75	0.00008	0.18
41	201	0.00019	90	0.00005	0.23
41	211	0.00006	105	0.00004	0.32
46	221	0.00004	120	0.00003	0.40

Table 1: Error comparison of the equation (10) for $\alpha = 1.5$, at time t=0.2

5 Conslusion

In this study, the fractional wave equation has been solved with a novel meshless approach and the results have been compared with other methods to demonstrate the effectiveness of the approach. From the comparison, it can be concluded that the proposed approach offers improved results with fewer number points and less computational cost.

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Spatial modeling of significant wave height using deformed fractional SPDEs

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A non-stationary Gaussian random field model is developed based on a combination of the SPDE approach and the classical deformation method. With the deformation method, a stationary field is defined on a domain which is deformed so that the field is non-stationary on the new domain. We show that if the stationary field is a Matérn field defined as a solution to a fractional SPDE, the resulting non-stationary model can be represented as the solution to another fractional SPDE on the deformed domain. By defining the model in this way, the computational advantages of the rational SPDE approach can be combined with the deformation methods more intuitive parameterization of non-stationarity. In particular it allows for essentially independent control over the non-stationary practical correlation range on one hand and the variance on the other hand. This has not been possible with previously proposed non-stationary SPDE models.

Numerical methods for the model are based on rational approximations of the fractional operator in the SPDE, for which explicit convergence rates are available. The model is tested on spatial data of significant wave height, a characteristic of ocean surface conditions which is important when estimating the wear and risks associated with a planned journey of a ship. The model is fitted to data from the north Atlantic and is used to compute wave height exceedance probabilities and the distribution of accumulated fatigue damage for ships traveling a popular shipping route. The model results agree well with the data, indicating that the model could be used for route optimization in naval logistics.

Approximations for the second derivative and the Caputo fractional derivative

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The aim of the report is to propose a method for construction of approximations of the Caputo derivative whose weights have properties similar to the properties of the weights of the L1 approximation. The L1 approximation of the Caputo derivative has an order $2-\alpha$ and a second order asymptotic formula

$$\frac{1}{\Gamma(2-\alpha)h^{\alpha}}\sum_{k=0}^{n-1}\sigma_k^{(\alpha)}y_{n-k}=y_n^{(\alpha)}+\frac{\zeta(\alpha-1)}{\Gamma(2-\alpha)}y_n''h^{2-\alpha}+O\left(h^2\right), \tag{1}$$

$$\sigma_0^{(\alpha)}=1,\quad \sigma_k^{(\alpha)}=(k-1)^{1-\alpha}-2k^{1-\alpha}+(k+1)^{1-\alpha},\quad \sigma_n^{(\alpha)}=(n-1)^{1-\alpha}-n^{1-\alpha},$$

where $y^{(\alpha)}(x)$ is the Caputo derivative of order α and $h=(x-x_0)/n$, where x_0 is the lower limit of fractional differentiation. The weights of the L1 approximation have properties

$$\sigma_0^{(\alpha)}>0,\quad \sigma_1^{(\alpha)}<\sigma_2^{(\alpha)}<\cdots<\sigma_{n-1}^{(\alpha)}<0. \tag{2}$$

In [1] we construct approximations of order $2-\alpha$ of the Caputo derivative whose weights have properties (2) and we give a proof for the convergence of the numerical solutions of fractional differential equations which use the approximations. In [2] we construct approximations of the first derivative which have generating functions $A-Ae^{\frac{t-1}{A}}$ and $\frac{1}{B}\ln(B+1-Bt)$. Now we apply the method form [2] for construction of approximations of the second derivative. Let $G_1(x)=2A^2e^{-1/A}\left(e^{x/A}-\frac{e^{1/A}}{A}(x+A-1)\right)$. The generating function $G_1(x)$ and the function $H_1(x)=G_1(e^{-x})$ have Mclaurin series expansions

$$G_1(x)=2A-2A^2+2A^2e^{-1/A}+\left(2Ae^{-1/A}-2A\right)x+\sum_{k=2}^{\infty}\frac{2e^{-1/A}}{k!A^{k-2}}, \tag{3}$$

$$H_1(x)=x^2-\frac{3A+1}{3A}x^3+\frac{7A^2+6A+1}{12A^2}x^4+O\left(x^5\right). \tag{4}$$

The coefficients of the Mclaurin series of the functions $G_1(x)$ and $H_1(x)$ are the weights of an approximation of the second derivative and the coefficients of its asymptotic formula:

$$\frac{1}{h^2}\sum_{k=0}^{n} w_{1,k}y(x-kh) = y''(x) - \frac{3A+1}{3A}y'''(x)h + \frac{7A^2+6A+1}{12A^2}y^{(4)}(x)h^2 + O\left(h^3\right), \quad (5)$$

$$w_{1,0} = 2A(1-A+A)e^{-1/A},\ w_{1,1} = -2A(1-e^{-1/A}),\ w_{1,k} = \frac{2e^{-1/A}}{k!(A+1)^{k-2}}.$$

The approximation (5) requires that $y(0) = y'(0) = 0$ and it is extended to the class $C^2[x_0, x]$ by applying a modification of its weights [2]. Let $G_2(x) = \frac{2}{B^2}(B - Bx - \ln(B + 1 - Bx))$.

$$G_2(x) = \frac{2(B-\ln(B+1))}{B^2} - \frac{2x}{B+1} + \sum_{k=2}^{\infty}\frac{2B^{k-2}x^k}{k(B+1)^k},$$

$$H_2(x) = G_2(e^{-x}) = x^2 - \frac{3+2B}{3}x^3 + \frac{6B^2+12B+7}{12}x^4 + O\left(x^5\right).$$

The approximation of the second derivative with a generating function $G_2(x)$ satisfies

$$\frac{1}{h^2}\sum_{k=0}^{n} w_{2,k}y(x-kh) = y''(x) - \frac{3+2B}{3}y'''(x)h + \frac{6B^2+12B+7}{12}y^{(4)}(x)h^2 + O\left(h^3\right), \quad (6)$$

$$w_{2,0} = \frac{2(B-\ln(B+1))}{B^2},\ w_{2,1} = -\frac{2}{B+1},\ w_{2,k} = \frac{2B^{k-2}}{k(B+1)^k} \quad (k \geq 2).$$

By approximating the second derivative in (1) with (5) and (6) we obtain the second order approximations of the Caputo derivative $(i = 1, 2)$:

$$\frac{1}{\Gamma(2-\alpha)h^\alpha}\sum_{k=0}^{n-1}\delta_{i,k}^{(\alpha)}y_{n-k} = y_n^{(\alpha)} + O\left(h^2\right), \quad (7)$$

$$\delta_{1,0}^{(\alpha)} = 1 - 2A(1-A+Ae^{-1/A})\zeta(\alpha-1),\ \delta_{1,1}^{(\alpha)} = 2^{\alpha-1} - 2 + 2A(1-e^{-1/A})\zeta(\alpha-1),$$

$$\delta_{1,k}^{(\alpha)} = (k-1)^{1-\alpha} - 2k^{1-\alpha} + (k+1)^{1-\alpha} - \frac{2A^2\zeta(\alpha-1)}{e^{1/A}k!A^k}. \quad (8)$$

$$\delta_{2,0}^{(\alpha)} = 1 - \frac{2}{B^2}\zeta(\alpha-1)(B-\ln(B+1)), \quad \delta_{2,1}^{(\alpha)} = 2^{\alpha-1} - 2 + \frac{2\zeta(\alpha-1)}{B+1},$$

$$\delta_{2,k}^{(\alpha)} = (k-1)^{1-\alpha} - 2k^{1-\alpha} + (k+1)^{1-\alpha} - \frac{2\zeta(\alpha-1)B^{k-2}}{k(B+1)^k}. \quad (9)$$

When $A = 0.01, B = 10$ and $\alpha \in [0.0002, 0.96]$ the weights of approximations (8) and (9) satisfy (2). When $\alpha \in (0, 0.0002) \cup (0.96, 1)$ approximations (8) and (9) satisfy (2) for

smaller values of the parameter A and larger values of B. The two-term ordinary fractional differential equation

$$y^{(\alpha)}(x) + y(x) = F(x) = \Gamma(3-\alpha)x^2 + 2x^{2-\alpha}, \quad y(0) = 0 \tag{10}$$

has a numerical solution

$$u_n = \frac{1}{\delta_{i,0}^{(\alpha)} + \Gamma(2-\alpha)h^\alpha} \left(\Gamma(2-\alpha)h^\alpha F_n - \sum_{k=1}^{n-1} \delta_{i,k}^{(\alpha)} u_{n-k} \right), \quad u_0 = 0. \tag{NS(*)}$$

$\boldsymbol{h}$	$\boldsymbol{\alpha = 0.25,\ A = 0.01}$		$\boldsymbol{\alpha = 0.75,\ B = 5}$	
	Error	Order	Error	Order
0.003125	3.4473×10^{-6}	1.9173	9.7697×10^{-8}	1.9536
0.0015625	9.0744×10^{-7}	1.9256	2.4953×10^{-8}	1.9691
0.00078125	2.3742×10^{-7}	1.9344	6.3209×10^{-9}	1.9810

Table 1: Error and order of numerical solutions NS1(8) and NS1(9) of equation (10).

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Numerical stability and accuracy of BURA and URA solvers for fractional diffusion reaction problems

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This article is devoted to theoretical and experimental comparison analysis of Uniform Rational Approximation (URA) related numerical solvers of the algebraic problem:

$$(\mathbb{A}^{\alpha} + q\mathbb{I})\mathbf{u} = \mathbf{f}, \qquad q \geq 0, \quad \alpha \in (0,1), \tag{1}$$

where $\mathbb{A} \in \mathbb{R}^{N\times N}$, $N \in \mathbb{N}$, is an SPD matrix with eigenvalues and eigenvectors $\{(\lambda_i, \mathbf{\Psi}_i)\}_{i=1}^{N}$ and $\mathbf{f} \in \mathbb{R}^N$ is a given vector. For the matrix fractional power $\mathbb{A}^{\alpha}$ the spectral definition

$$\mathbb{A}^{\alpha} = \mathbb{W}\mathbb{D}^{\alpha}\mathbb{W}^T, \qquad \mathbb{W} = [\mathbf{\Psi}_1^T, \mathbf{\Psi}_2^T, ..., \mathbf{\Psi}_N^T], \quad \mathbb{D} = diag(\lambda_1, \ldots, \lambda_N),$$

is used. Such a problem appears for example in finite element or finite difference discretization of fractional-in-space diffusion-reaction elliptic problems.

To shorten the exposition, we assume that the spectrum of $\mathbb{A}$ is in $[1, +\infty)$, i.e., $1 \leq \lambda_1 < \lambda_2 < \cdots < \lambda_N$ (otherwise, a normalization with respect to λ_1^{-1} needs to be performed). Following [2] and denoting by $z(t) := t^{\alpha}$, we introduce the function

$$g_q(z(t)) = g_q(t;\alpha) := \frac{z}{1+qz} = \frac{t^{\alpha}}{1+qt^{\alpha}}, \qquad t \in [0,1]. \tag{2}$$

Let k be a given positive integer and α be fixed. The (k,k)-best uniform rational approximation (BURA) of $g_q(t;\alpha)$ for $t \in [0,1]$ will be denoted by $r_q(t)$, while the approximation error function – by $\varepsilon_q(t)$. In other words

$$r_q(t) = \underset{r\in\mathcal{R}(k,k)}{\operatorname{argmin}} \|r(t) - g_q(t;\alpha)\|_{C[0,1]}, \quad r_q(t) = g_q(t;\alpha) + \varepsilon_q(t), \quad E_q := \|\varepsilon_q\|_{C[0,1]}.$$

The class of functions $\{g_q\}$ possesses a nice property that motivated us to consider the (k,k)-URA elements as alternative approximations of $g_q(t;\alpha)$ (see [1, 2]). Namely,

$$g_{q_2} \circ g_{q_1} = g_{q_1+q_2} \qquad \Rightarrow \qquad \bar{r}_{q_1,q_2}(t) := g_{q_2} \circ r_{q_1} = \frac{r_{q_1}(t)}{1 + q_2 r_{q_1}(t)}, \quad q = q_1 + q_2, \ q_1, q_2 \geq 0.$$

Note that $\bar{r}_{q_1,q_2} \in \mathcal{R}(k,k)$ for every choice of (q_1,q_2). Analogously, we define the error function $\bar{\varepsilon}_{q_1,q_2}$ and its maximal absolute value $\bar{E}_{q_1,q_2}$. Assuming that [3, Lemma 2.1] holds true for every $q_1 \geq 0$, we can prove the following error estimates:

$$\begin{aligned} \|\mathbf{u} - r_q(\mathbb{A}^{-1})\mathbf{f}\|_{\ell^2} &\leq E_q \|\mathbf{f}\|_{\ell^2}, \\ \|\mathbf{u} - \bar{r}_{q_1,q_2}(\mathbb{A}^{-1})\mathbf{f}\|_{\ell^2} &\leq \frac{E_{q_1}}{\left(1+q_2 r_{q_1}(\lambda_N^{-1})\right)\left(1+q_2 g_{q_1}(\lambda_N^{-1};\alpha)\right)} \|\mathbf{f}\|_{\ell^2}, \end{aligned} \tag{3}$$

for any choice of α and $q = q_1 + q_2$. Both estimates are almost sharp and cannot be improved in general. Here, we will analyze E_q in more detail.

We have strong numerical evidence that for all choices of (k,α,q), the value $(1+q)E_q$ monotonically increases and is uniformly bounded as q increases . Thus $\lim_{q\to+\infty}(1+q)E_q = CE_0$, with constant $1 < C \leq E_0^{-1}$, independent on q. In practice, we observe $C = \mathrm{O}(1)$ for moderate values of k, meaning that

$$(1+q)E_q \sim E_0 \sim 4^{1+\alpha}|\sin(\pi\alpha)|e^{-2\pi\sqrt{\alpha k}}.$$

For the approximation of E_0 we used the result in [4]. For example, when $k=6$ and $q=400$ we have $401E_{400}/E_0 = \{5.731, 10.807, 14.804\}$ for $\alpha = \{0.25, 0.5, 0.75\}$, respectively.

Eq. (3) implies that when an a priori estimate of λ_N is available, it is sometimes better to use a (q_1,q_2)-URA solver rather than the (q_1+q_2)-BURA solver. Direct computations show that this is the case whenever

$$\lambda_N^{\alpha} < \sqrt{(1+q)(1+q_1)} + 1 \qquad \Longleftrightarrow \qquad q_1 > \frac{\left(\lambda_N^{\alpha}-1\right)^2}{1+q} - 1. \tag{4}$$

In particular, we do not need to compute BURA elements for $q > \lambda_N^{\alpha} - 2$.

To illustrate the advantages of the different URA solvers, we consider the matrix $\mathbb{A} = tridiag(-1,2,-1)/h^2$ with $h := 1/(N+1)$ that corresponds to FDM of the classical homogeneous 1D Laplace problem in $[0,1]$ on a uniform grid with mesh-size h. We have

$$\mathbf{\Psi}_i = \{\sqrt{2h}sin(ikh\pi)\}_{k=1}^{N}, \quad \lambda_i = \frac{4}{h^2}sin^2\left(\frac{i\pi h}{2}\right), \qquad i = 1,\ldots,N.$$

In what follows, we have fixed $k=6$ and $q=400$, while $\alpha = \{0.25, 0.5, 0.75\}$. The solvers we compare are generated by the pairs $(q_1,q_2) = \{(400,0),(0,400),(200,200),(100,300)\}$ and will be referred as BURA, 0-URA, 1-URA, and 2-URA, respectively since

$$\bar{r}_{400,0} = r_{400}, \quad \bar{r}_{0,400} = g_{400} \circ r_0, \quad \bar{r}_{200,200} = g_{200} \circ r_{200}, \quad \bar{r}_{100,300} = g_{200} \circ g_{100} \circ r_{100}.$$

The fractional decompositions of all the $\bar{r}_{q_1,q_2}$ elements have been taken from [1].

On Fig. 1 all the corresponding error functions $\bar{\varepsilon}_{q_1,q_2}(t)$ are plotted in logarithmic scale for $t \in [10^{-15}, 1]$. Since

$$|\bar{\varepsilon}_{q_1,q_2}(1)| = \frac{(1+q_1)^2 E_{q_1}}{(1+q)^2} \approx \frac{1+q_1}{1+q} E_q,$$

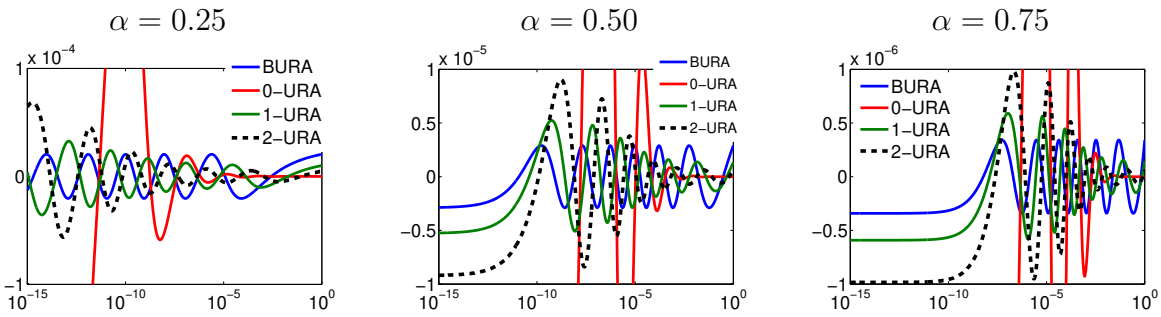

Figure 1: Logarithmic plots for the URA errors $\bar{\varepsilon}_{q_1,q_2}(t)$ for $t \in [10^{-15}, 1]$, $k = 6$, $q = 400$, $q_1 = \{400, 200, 100, 0\}$, and $\alpha = \{0.25, 0.5, 0.75\}$.

the smaller the q_1 the smaller the error function is in vicinity of 1, thus in the right end of the plots interval 0-URA behaves better than 2-URA, which is better than 1-URA, and all are better than BURA. The behavior at the other end of the interval is completely the opposite. For $\alpha = \{0.5, 0.75\}$ the BURA error function oscillations become smaller than all the URA-related ones for $t < 10^{-5}$, respectively $t < 10^{-4}$, meaning that even on very coarse meshes (e.g., $h \approx 2 \cdot 10^{-2}$) the BURA solver will outperform all the others. Indeed, since $\lambda_N \approx 4/h^2$ we have $\lambda_N^\alpha - 2 \approx 2h^{-1} - 2 = 2N$, when $\alpha = 0.5$. Hence, according to the error analysis above for $h = 2 \cdot 10^{-2}$ the BURA solver is more accurate than the URA ones for q up to approximately 798.

The most interesting case is $\alpha = 0.25$, where in the same time the BURA advantage is less obvious and the computational efforts for deriving the BURA element are more substantial, due to numerical instability and the necessity to use double-quadruple (or even higher for $k > 6$) precision in the Remez algorithm. Here, we have $\lambda_N^\alpha - 2 \approx \sqrt{2(N+1)} - 2$, so in general no higher q_1 than 43, 140, and 446 are needed for optimal accuracy of the URA solvers, when $h = 10^{-3}$, $h = 10^{-4}$ and $h = 10^{-5}$, respectively. This is experimentally confirmed in Table 1. For $h = 10^{-3}$, the BURA solver gives rise to the largest approximation error and even the 0-URA solver is a better candidate. Here the best performance is achieved by the 2-URA solver. For $h = 10^{-4}$ the 0-URA solver is the least accurate one, while the 1-URA and the 2-URA solvers are the most accurate ones. Still, due to the faster decrease in the oscillation margins of the 2-URA method, it remains the best candidate on such a mesh size. For $h = 10^{-5}$ the 0-URA and the 2-URA methods are not reliable anymore, while the BURA and the 1-URA one give rise to practically the same approximation errors in their worst-case scenarios. Again, the 1-URA method should be preferred due to the decrease in its oscillations as t increases. On finer grids, the BURA advantage will be obvious, as this is the only approximation error independent on h. However, for most of the practical applications no finer grids than $h = 10^{-5}$ are used in the uniform setting. This is not the case when adaptive refinements are performed.

h	$\max_i \bar{\varepsilon}_{400,0}(\lambda_i^{-1})$	$\max_i \bar{\varepsilon}_{0,400}(\lambda_i^{-1})$	$\max_i \bar{\varepsilon}_{200,200}(\lambda_i^{-1})$	$\max_i \bar{\varepsilon}_{100,300}(\lambda_i^{-1})$
10^{-3}	2.0456E-5	1.4238E-5	1.1289E-5	6.9056E-6
10^{-4}	2.0456E-5	5.8788E-5	1.4098E-5	1.3952E-5
10^{-5}	2.0456E-5	3.1603E-4	2.0787E-5	3.0391E-5

Table 1: Maximal error values for different mesh sizes, when $\alpha = 0.25$, $k = 6$.

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Solution of spectral fractional elliptic problems: A concise overview of methods based on rational approximations

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The purpose of the article is to present some new results in approximate solution of the problem $\mathcal{A}^\alpha u = f$. Here $\mathcal{A}$ is a self-adjoint and coercive elliptic operator defined on a dense subset of $L^2(\Omega)$, with Ω a bounded Lipschitz domain and $0 < \alpha < 1$. We discuss the discretizations $\mathcal{A}_h$ of $\mathcal{A}$ by finite difference or finite element methods on a mesh with mesh-size h and survey the existence, stability, error, and positivity of the solution of the algebraic system $\mathcal{A}_h^\alpha u_h = f_h$ for $u_h \in \mathbb{R}^N$. The fractional power of the operators $\mathcal{A}$ and $\mathcal{A}_h$ are defined through their spectra $\{\lambda_j, \psi_j\}_{j=1}^\infty$ and $\{\lambda_{j,h}, \psi_{j,h}\}_{j=1}^N$, of $\mathcal{A}$ and $\mathcal{A}_h$, respectively, so that

$$u = \sum_{j=1}^{\infty} \lambda_j^{-\alpha}(f, \psi_j)\psi_j \quad \text{and} \quad u_h = \sum_{j=1}^{N} \lambda_{j,h}^{-\alpha}(f_h, \psi_{j,h})\psi_{j,h}. \tag{1}$$

The representation (1) of the approximate solution u_h can be used for finding of the solution only in the rare case when one knows the discrete spectrum of $\mathcal{A}_h$. However, this representation could be used to find a suitable approximation using the following reasoning. Assume that $\mathcal{A}_h$ has been properly scaled so that the smallest eigenvalue $\lambda_{1,h} = 1$. Let $g(t)$ be some approximation of $t^{-\alpha}$ in $L^\infty([1, \infty))$. Then

$$w_h = \sum_{j=1}^{N} g(\lambda_{j,h}^{-1})(f_h, \psi_{j,h})\psi_{j,h} := g(\mathcal{A}_h^{-1})f_h \tag{2}$$

will be an approximation of u_h. Indeed, the L^2-norm of the error of this approximation is bounded by

$$\|u_h - w_h\| \le \max_{t\in[1,\lambda_N)} |t^{-\alpha} - g(t^{-1})|\|f_h\| \le \max_{t\in[1,\infty)} |t^{-\alpha} - g(t^{-1})|\|f_h\|. \tag{3}$$

To make this a practical algorithm one needs to find the approximation $g(t)$ and to show that evaluation of $g(\mathcal{A}_h^{-1})f_h$ is feasible and cheap. An obvious choice for $g(t)$ is the best uniform *polynomial approximation* of $t^{-\alpha}$ on $[1, \lambda_N]$. However, as discussed in [4], this will lead to an inefficient method. Here we shall explore the possibility when $g(t)$ is the *best uniform rational approximation (BURA)* of t^{α} on $(0, 1]$, which, as shown in [5], will be equivalent to the best uniform rational approximation of $t^{-\alpha}$ on $[1, \infty)$.

Now consider $g(t) = r_{\alpha,k}(t)$, where

$$r_{\alpha,k}(t) = \underset{s(t)\in\mathcal{R}_k}{\operatorname{argmin}} \|s(t) - t^{\alpha}\|_{L^{\infty}(0,1)}, \tag{4}$$

$\mathcal{R}_k = \{P_k(z)/Q_k(z)\}$, with $P_k(z)$, $Q_k(z)$ polynomials of degree k and $Q_k(0) = 1$.

The problem (4) has been extensively studied in the past, e.g. [8, 9, 12]. Moreover, [9, Theorem 1], provides an estimate of the error

$$\|r_{\alpha,k}(t) - t^{\alpha}\|_{L^{\infty}(0,1)} \leq C_{\alpha} e^{-2\pi\sqrt{k\alpha}},$$

which gives an easy estimate for the the error: $\|u_h - w_h\| \approx C_{\alpha} e^{-2\pi\sqrt{k\alpha}} \|f_h\|$.

Now changing the variable $\xi = 1/t$ in $r_{\alpha,k}(t)$ we get another rational functions defined as

$$\widetilde{r}_{\alpha,k}(\xi) = r_{\alpha,k}(1/t) = \frac{t^k P_k(t^{-1})}{t^k Q_k(t^{-1})} := \frac{\widetilde{P}_k(\xi)}{\widetilde{Q}_k(\xi)}.$$

In order to claim that we have an implementable algorithm we need to show that the computation of $\mathcal{A}_h^{-\alpha} f_h$ could be done in a stable and efficient way. This is ensured by the following result [8, 9] regarding the properties of the roots $(\widetilde{\zeta}_1, \ldots, \widetilde{\zeta}_k)$ of $\widetilde{P}_k(\xi)$ and $(\widetilde{d}_1, \ldots, \widetilde{d}_k)$ of $\widetilde{Q}_k(\xi)$: all the roots are real, negative, and interlace so that

$$0 > \widetilde{d}_k > \widetilde{\zeta}_k > \widetilde{d}_{k-1} > \widetilde{\zeta}_{k-1} > \cdots > \widetilde{d}_1 > \widetilde{\zeta}_1.$$

This allows to represent $\widetilde{r}_{\alpha,k}(\xi)$ as sum of partial fractions, see e.g. [4, Remark 5.1]

$$r_{\alpha,k}(t^{-1}) = \widetilde{r}_{\alpha,k}(\xi) = \widetilde{c}_0 + \sum_{i=1}^{k} \frac{\widetilde{c}_i}{\xi - \widetilde{d}_i}, \quad \text{with } \widetilde{c}_i > 0,\ i = 0, 1, \ldots, k,$$

which will lead to the following representation of the approximation w_h:

$$w_h = \left(\widetilde{c}_0 \mathcal{I}_h + \sum_{i=1}^{k} \widetilde{c}_i (\mathcal{A}_h - \widetilde{d}_i \mathcal{I}_h)^{-1} \right) f_h, \tag{5}$$

where $\mathcal{I}_h$ is the identity matrix. This solution, called fully discrete, was introduced and studied in details in [5]. We note that to compute w_h we need to solve k systems of the type $(\mathcal{A}_h - \widetilde{d}_i \mathcal{I}_h) v_h = f_h$ with symmetric, positive definite and sparse matrices $\mathcal{A}_h - \widetilde{d}_i \mathcal{I}_h$. For more details on this algorithm and for computing BURA $r_{\alpha,k}(t)$ (its coefficients, roots and poles) for various values of α and k we refer to [4].

We note that due to the properties of the BURA coefficients, computing the approximate solution produces a stable algorithm. Moreover, since the original problem satisfies the positivity of the solution (i.e., if $f \geq 0$ then $u \geq 0$), the solution w_h has the same properties in the cases when the approximation $\mathcal{A}_h$ is done either by finite difference approximation on a rectangular mesh or by lumped mass finite element method (for details we refer to [5]).

Further, we discuss some existing methods for solving the problem (1) that are derived by using equivalent representation of the solution either by Balakrishnan integral representation formula or by embedding the problem into a relevant PDE problem in a higher dimensional space. These include the methods of Bonito and Pasciak [1, 2], Nochetto, Otárola, and Salgado, [7], (its equivalence to a rational approximation was discovered in [6]), and Vabishchevich, [10] (with improved variants in [3, 11]). We argue that all these methods directly or indirectly construct $g(t)$ as some rational approximation of $t^{-\alpha}$ on $(\lambda_{1,h}, \lambda_{N,h})$.

Further we argue and computationally show that the solution (5) based on the best uniform rational approximation (4), introduced and studied in [5], gives a new method, which is as good as the mentioned above methods and in many cases significantly outperforms them in terms of efficiency, parallelization, and robustness. We also discuss issues related to computing BURA $r_{\alpha,k}(t)$ and implementing the method. Finally, we present some numerical experiments on two computational examples involving solution of one- and two-dimensional sub-diffusion problems with smooth and non-smooth data.

Acknowledgement

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We acknowledge also the provided access to the e-infrastructure of the Centre for Advanced Computing and Data Processing, with the financial support by the Grant No. BG05M2OP001-1.001-0003, financed by the Science and Education for Smart Growth Operational Program (2014-2020) and co-financed by the European Union through the European structural and Investment funds.

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Fast and stable computation of best rational approximations with applications to fractional diffusion*

Clemens Hofreither†

Recently there has been significant activity in the development of numerical methods for solving elliptic fractional partial differential equations of the type

$$\mathcal{L}^\alpha u = f \qquad \text{in } \Omega,$$

where $\alpha \in (0,1)$, Ω is a bounded domain, $\mathcal{L}$ an elliptic diffusion operator augmented with homogeneous Dirichlet boundary conditions on $\partial\Omega$, f the right-hand side and u the sought solution. After discretization, we can take the point of view that a discrete solution $\mathbf{u} \in \mathbb{R}^n$ is given by the equation $A^\alpha \mathbf{u} = \mathbf{f}$, where $A \in \mathbb{R}^{n\times n}$ is a symmetric positive definite matrix arising from any number of popular discretization techniques, such as finite differences, finite elements, or isogeometric analysis. An attractive approach to the solution of this problem, due to its simplicity and excellent convergence properties, is to compute

$$\tilde{\mathbf{u}} = \tilde{r}(A) f$$

with a rational function $\tilde{r}(x)$ which is, or is close to, the best uniform rational approximation (BURA) to the function $x \mapsto x^{-\alpha}$ for $x \in [\lambda_1, \lambda_n]$, the interval containing the spectrum of A. This approach is particularly appealing since a recent analysis in [3] has shown that in fact most published methods for solving the fractional diffusion problem can be interpreted as such rational approximation methods of varying quality, and the use of BURAs should thus result in a method that is close to optimal. The numerical experiments in [3] confirm this assumption.

The most recent method in this class is described and analyzed in [2], where the choice

$$\tilde{r}(x) = \lambda_1^{-\alpha} r(\lambda_1 x^{-1})$$

is made with $r(x)$ being the BURA with a chosen degree of the function $x \mapsto x^\alpha$ in $[0,1]$. The method converges exponentially with the degree of r and permits a simple, fully parallel realization via the partial fraction decomposition which involves solving shifted problems with matrices of the form $A + c_j I$.

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However, until now a major obstacle to the use of these methods in practice has been the computation of the BURAs $r(x) \approx x^\alpha$. In the recent report [1], the authors provide extensive tables describing these rational approximations for $\alpha \in \{0.25, 0.5, 0.75\}$ and degrees up to $k = 8$. These results were produced using a Remez algorithm and in many cases required the use of quadruple precision floating point arithmetic and significant computing time on the order of hours.

Novel Contribution
The aim of this contribution is to describe a novel algorithm, Best Rational Approximation by Successive Interval Length Adjustment (BRASIL), which can compute the (k, k)-BURA of functions of the type $x \mapsto x^\alpha/(1 + qx^\alpha)$, $\alpha \in (0, 1)$, $q \geq 0$, $x \in [0, 1]$, in seconds on a standard workstation, using only standard double precision arithmetic, and with degrees k up to around 80.

The standard approach for computing a (k, k)-BURA, the Remez algorithm, is based on the idea of finding the $2k+2$ equioscillation points at which the absolute error assumes its local maxima, shown as stars in Figure 1, right. Between each consecutive pair of such points there lies a point (shown as dots) where the BURA interpolates the exact function. The basic idea of the BRASIL algorithm is to determine the locations $(t_j)_{j=0}^{2k}$ of these $2k+1$ interpolation nodes and compute the BURA by rational interpolation in these nodes.

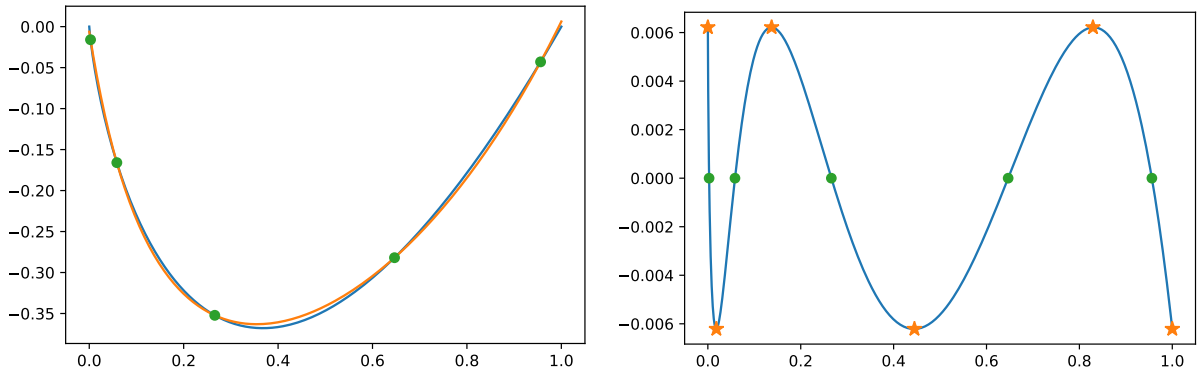

Figure 1: The function $f(x) = x \log x$, $x \in [0, 1]$, together with its $(2, 2)$-BURA (left) and the resulting error (right).

A crucial ingredient for computing these rational interpolants in a stable way is the so-called barycentric rational interpolation formula, namely,

$$r(x) = \frac{\sum_{i=0}^{k} \frac{w_i}{x - x_i} f_i}{\sum_{i=0}^{k} \frac{w_i}{x - x_i}},$$

with nodes x_i, values f_i, and weights w_i, $i = 0, \ldots, k$. This formula describes a rational function r of degree (k, k) with the interpolation property $r(x_i) = f_i$, $i = 0, \ldots, k$, as long as $w_i \neq 0$, and in fact it parametrizes all rational functions with this property by varying the weights (w_i). The barycentric formula is in a sense classical and exhibits superior

stability properties, but is still not as widely known in the numerical analysis community as it deserves to be.

The BRASIL algorithm first determines suitable initial values for the interpolation nodes $(t_j)_{j=0}^{2k}$ and then in each iteration (1) computes the rational interpolant through these nodes in barycentric representation, (2) determines the maximum error in each interval (t_j, t_{j+1}), (3) shrinks intervals where the error is too large and (4) enlarges intervals where the error is too small. These steps are repeated until the maximum errors are equilibrated to a desired tolerance. Some results obtained by this procedure are shown in Table 1.

The BRASIL algorithm exhibits exceptional numerical stability. As an example, Figure 2 shows the equioscillation property of the error $f(x) - r(x)$ for $f(x) = x^{0.25}/(1+x^{0.25})$ in $[0, 1]$ with a degree $(35, 35)$-BURA. The 71 computed interpolation nodes (t_j), shown as dots, range in order of magnitude from around 10^{-31} to 1. It is very surprising that this computation could be performed in standard double precision arithmetic. This numerical phenomenon will be further discussed during the presentation.

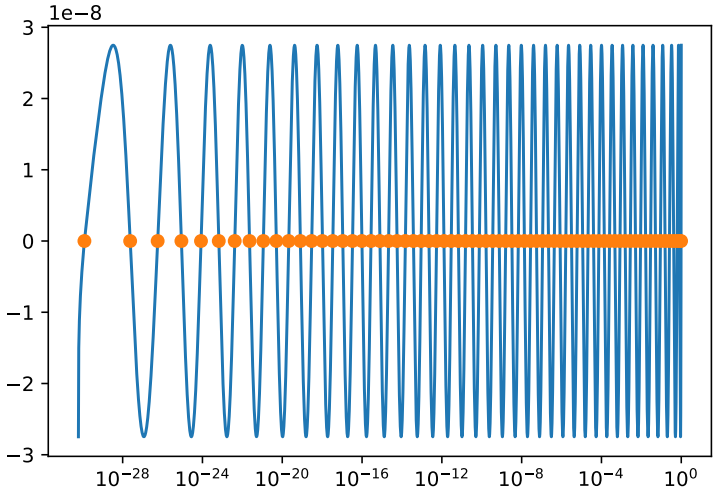

Figure 2: BURA error of degree $k = 35$ for the function $x^{0.25}/(1 + x^{0.25})$.

k	iter	error	time
5	335	2.735E-03	0.259 s
10	337	1.610E-04	0.425 s
20	327	2.777E-06	0.794 s
40	331	8.568E-09	1.83 s
60	301	1.002E-10	2.96 s
80	479	2.347E-12	7.30 s

k	iter	error	time
5	209	2.868E-05	0.152 s
10	202	2.059E-07	0.242 s
15	204	4.515E-09	0.354 s
20	201	1.783E-10	0.476 s
24	201	1.776E-11	0.572 s
28	254	2.126E-12	0.881 s

Table 1: Results for BRASIL for (k, k)-BURA of $x^{0.25}$ (left) and $x^{0.75}$ (right) in $[0, 1]$. Columns: degree, number of iterations, error of the BURA, and computation time.

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Effective diffusivity of hydrogen in bcc-Fe: Anomalous character due to quantum proton fluctuations?

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The interactions of hydrogen with crystal defects in α-Fe and their consequences are fundamentally less well understood than diffusion of hydrogen in the perfect crystal lattice, despite generally dominating the influence of hydrogen in metals. The existence of microstructural imperfections (vacancies, solute atoms, dislocations, grain boundaries, etc.) introduces trapping sites within the lattice which retard the overall diffusion rate. Intrinsic processes in H diffusion are strongly influenced by its quantum mechanical behavior. At low temperatures quantum tunneling is expected to be the dominant mechanism, while the transition is dominated by classical jumping over the barrier at high temperatures. In order to understand the process of H diffusion in Fe, it is essential to study H trapping and migration over the whole range of temperatures covering both the quantum and classical dominated regimes and the crossover between them. Theoretical approaches based on molecular dynamics (MD) have been used to study H trapping and migration in Fe [1]. The state of the art for quantum treatment of the ionic degrees of freedom involves the use of the ring-polymer MD (RPMD) method [2]. However, including quantum effects is computationally demanding compared to a simulation with classical nuclei. The kinetic Monte-Carlo (kMC) method has the advantage of being computationally less expensive because the interatomic interactions are not computed directly [3]. The fundamental transition rate constants used by kMC can be estimated without knowledge of the dynamics of the system within the framework of the classical transition state theory (TST). The application of kMC for the study of H diffusion permits simulations in larger blocks of atoms for periods of time significantly longer than one can achieve with direct MD simulation, which is essential for studying H migration and trapping in the presence of microstructural imperfections and consequent extraction of the diffusion coefficients. Unfortunately, classical energy barriers significantly deviate from the experimentally determined activation energies and kMC simulations using classical transition rates cannot account for quantum corrections arising from the low mass H atom. A quantum treatment of the hydrogen degrees of freedom is mandatory to capture such effects.

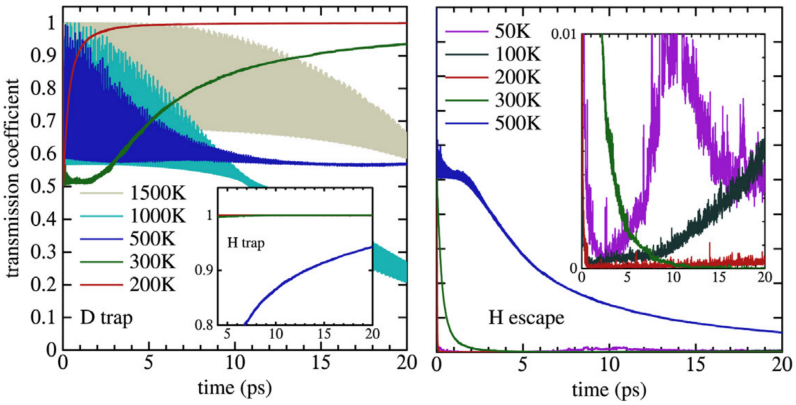

Figure 1: Trapping and escape of H and D from an α-Fe vacancy at different T.

In this work, we study the activated dynamics of hydrogen diffusion in α-Fe by employing path integral formulation of quantum transition state theory (QTST) [4] for the calculation of the corresponding activation rate constants. In the reactive flux theory, the rate coefficient $\tau^{-1}(T) = \tilde{C}^{fs}(t_p)/Z_r(T)$ can be written in terms of Kubo transformed fluxside correlation function

$$\tilde{C}^{fs}(t) = Tr(e^{-\beta H}\hat{F}e^{iHt/\hbar}\theta e^{-iHt/\hbar}), \tag{1}$$

where H and F are the Hamiltonian and flux operators, and $\theta(S)$ is a step function which is zero or one depending on whether the system is on the reactant or product sides of the dividing surface S. The ring polymer reaction rate theory is classical reaction rate theory in an extended n-bead imaginary time path integral [5] phase space. Thus, H is the classical Hamiltonian of a collection of n-bead harmonic ring polymers with an external potential of $V(q)$ acting on each bead. The ring polymer rate coefficient can be split into a product of two factors

$$\tau^{-1}(T) = \kappa(t_p)k^{QTST}(T) \tag{2}$$

The advantage of this factorization is that it allows one to split the rate calculation into two stages, the first dynamical and the second purely statistical. The transmission coefficient $\kappa(t)$, which accounts for recrossing of the dividing surface, is calculated as the canonical-ensemble average [6].

We calculate $\kappa(t)$ by means of RPMD, starting from random centroid-constrained simulation and sampling the RP momenta from the Maxwell distribution, averaging over more than 10^6 trajectories.

We use the Wang Landau Monte-Carlo algorithm (WLMC) [7] to calculate directly the partition functions participating in the QTST activation factor. The WLMC approach allows one to estimate various thermodynamic properties over a wide range of temperatures from a single simulation run.

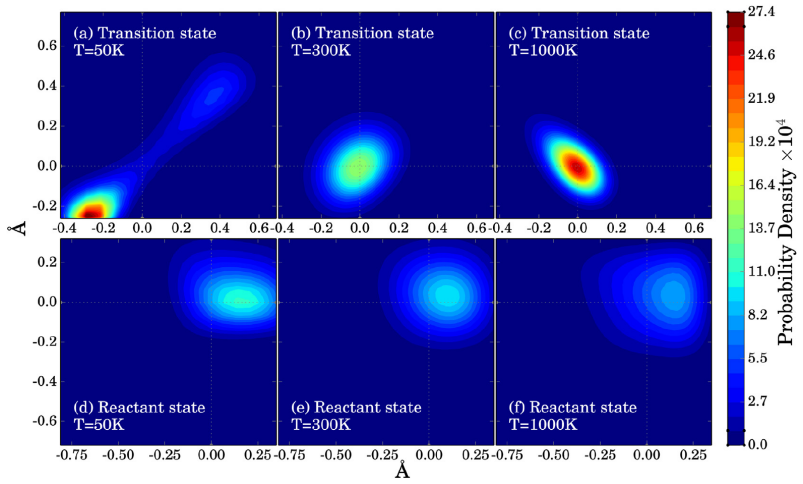

Figure 2: Particle probability density (PPD) of H trapped at an α-Fe vacancy .

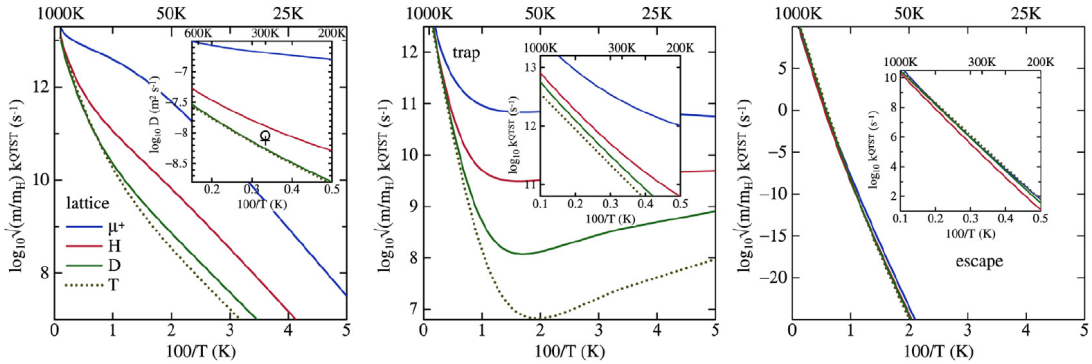

Figure 3: Rate coefficient as a function of temperature for lattice diffusion, trapping and escape from a vacancy of hydrogen and its isotopes in α-Fe.

The n-bead quantum partition function $Z_n(\beta)$ is

$$Z_n(\beta) = \left(\frac{mn}{2\pi\beta\hbar^2}\right)^{\frac{n}{2}} \int d\mathbf{x} \exp\left(-\frac{H_1(q)}{\beta} - \beta H_2(q)\right) \tag{3}$$

where $H_1(q)$ and $H_2(q)$ are temperature independent-functions

$$H_1(q) = \sum_{i=1}^{n} \frac{mn}{2\hbar^2}(q_{i+1} - q_i)^2; \qquad H_2(q) = \sum_{i=1}^{n}(n^{-1}V(q_i)) \tag{4}$$

We find large quantum effects including tunnelling at low temperature and recrossing at high temperature due to the finite extent of the PPD. In particular these serve to increase the rate of trapping and to decrease the rate of escape at low temperature. Our results also show very clear non classical isotope effects.

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Special functions of fractional calculus in solutions of fractional order equations and models

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The developments in theoretical and applied science require knowledge of the properties of the "mathematical functions", from elementary exponential and trigonometric functions to the variety of *Special Functions* (SF). These functions appear whenever natural phenomena are studied, engineering problems are formulated, and numerical simulations and algorithms are processed. They also crop up in probability theory and statistics, financial models, and economic analysis.

This talk aims to attract attention to classes of SF that were not so popular (or some of them were not introduced) until *Fractional Calculus* (FC) gained its important role, related to the boom of applications of fractional order models, as better interpretations and approximations to the real world processes. The so-called *Special Functions of Fractional Calculus* (SF of FC) are unavoidable tool in exact analytical solutions of fractional order (FO) equations, and thus also when their numerical evaluations are to be performed. Under FO equations we mean either integral equations with weak singularities, or differential equations with ordinary and partial fractional derivatives, or mixtures of these types of equations, among them: ODEs (as fractional relaxation-oscillation equations) and PDEs (as fractional wave-diffusion equations), stochastic fractional differential equations, in control systems of fractional order, quantum mechanics, etc. The SF of FC appear also as kernel-functions of the *Generalized Fractional Calculus* (GFC, [1, 9]) operators; and as pdf-, cdf- or expectations in probability, etc.

The most popular SF of FC are the *Mittag-Leffler (ML) functions*

$$E_\alpha(z)=\sum_{k=0}^{\infty}\frac{z^k}{\Gamma(\alpha k+1)}\,,\ E_{\alpha,\beta}(z)=\sum_{k=0}^{\infty}\frac{z^k}{\Gamma(\alpha k+\beta)}\,,\ \ \alpha>0,\beta\in\mathbb{C}, \tag{1}$$

as *"fractional index"* ($\alpha>0$) *extensions* of the exponential and trigonometric functions like

$$\exp(z)=\sum_{k=0}^{\infty}\frac{z^k}{\Gamma(k+1)}\,,\ \cos z=\sum_{k=0}^{\infty}\frac{(-1)^k z^{2k}}{\Gamma(2k+1)}\,,$$

satisfying ODEs of integer order $D^n y(\lambda z)=\lambda^n\, y(\lambda z)$, $n=1,2$. In the case of (1), we have *fractional order differential equations*, for example the simple one, satisfied by the so-called α-*exponential*, or *Rabotnov function*:

$$D^{\alpha} y_{\alpha}(z) = \lambda\, y_{\alpha}(z) \;\; \text{with} \;\; y_{\alpha}(z) = z^{\alpha-1}\, E_{\alpha,\alpha}(\lambda z^{\alpha}), \;\; \alpha > 0,$$

while the ML functions with arbitrary $\alpha > 0, \beta$ appear in the solutions of various more complicated equations of FO.

Although the classical ML functions incorporate a lot of widely used mathematical functions (hyperbolic functions, error functions, incomplete gamma functions, etc), in Kiryakova [3, 4, 5], etc., their extension with respect to number of indices has been studied in details, as including yet another great quantity of SF of FC. These are called *multi-index ML functions*:

$$E_{(\alpha_i),(\beta_i)}(z) = E^{(m)}_{(\alpha_i),(\beta_i)}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha_1 k + \beta_1) \ldots \Gamma(\alpha_m k + \beta_m)}\,, \tag{2}$$

with "vector indices" $(\alpha_1 > 0, ..., \alpha_m > 0)$, $(\beta_1, \ldots, \beta_m)$, $m = 1, 2, 3, \ldots$. For (2) with $m > 1$, we have provided a long list of applicable SF of FC, see [3, 4, 5], just to mention: the Wright function $\phi(\mu, \nu; z)$ known also as Bessel-Maitland function $J^{\mu}_{\nu}(z)$, Dzrbashjan's 4-parameters function $\Phi_{1/\alpha_1, 1/\alpha_2}(z; \beta_1, \beta_2)$, the Bessel, Struve, Lommel and Airy functions, the Mainardi function $M(z; \beta) = \phi(-\beta, 1-\beta; -z)$, the hyper-Bessel functions of Delerue $J^{(m)}_{\nu_1, \ldots, \nu_m}(z)$, and so on.

Going further, we note that the multi-index ML functions (2), as well as the 3-parameters ML type function (*the Prabhakar function*) $E^{\gamma}_{\alpha,\beta}(z)$ and its $3m$-parameters extensions (analogous to (2)), are special cases of the *Wright generalized hypergeometric functions* ($p < q$, $z \in \mathbb{C}$ or $p = q + 1$, $|z| < 1$):

$${}_p\Psi_q \left[\begin{array}{c} (a_1, A_1), \ldots, (a_p, A_p) \\ (b_1, B_1), \ldots, (b_q, B_q) \end{array} \middle| \, z \right] = \sum_{k=0}^{\infty} \frac{\Gamma(a_1 + kA_1) \ldots \Gamma(a_p + kA_p)}{\Gamma(b_1 + kB_1) \ldots \Gamma(b_q + kB_q)} \, \frac{z^k}{k!}\,, \tag{3}$$

namely,

$$E^{(m)}_{(\alpha_i),(\beta_i)}(z) = {}_1\Psi_m \left[\begin{array}{c} (1,1) \\ (\beta_i, \alpha_i)_1^m \end{array} \middle| \, z \right] = H^{1,1}_{1,m+1} \left[-z \middle| \begin{array}{c} (0,1) \\ (0,1), (1-\beta_i, \alpha_i)_1^m \end{array} \right].$$

For $A_1 = \cdots = A_p = 1, B_1 = \cdots = B_q = 1$, (3) are reduced to the more popular generalized hypergeometric functions ${}_pF_q$ incorporating the "classical" SF, known as "SF of Mathematical Physics". The functions ${}_p\Psi_q$ and ${}_pF_q$ on their side, are representatives of the Fox H-functions, resp. of the Meijer G-functions (details, e.g. in Appendix of [1] and recent handbooks on SF).

Recently, when referring to *SF of FC*, one has in mind the ${}_p\Psi_q$- and the Fox H-functions, which for parameters not integer and not rational, are not reduced to the classical SF, thus appearing as tools in solutions of FO differential and integral equations (in general, of multi-order $(\alpha_1, ..., \alpha_m)$).

Some of our basic results on SF of FC will be briefly discussed, as:

– full theory of operators of Generalized FC, introduced in [1] by means of integral operators with H- and G-functions as kernels, but representable as commutative compositions of classical operators of FC (Riemann-Liouville, Caputo, Erdélyi-Kober), see also [9];

– all classical SF and all SF of FC can be represented as Generalized FC operators (from [1, 9]) of basic elementary functions (among them exponential, trigonometric, the

pdf functions of some probability distributions), see [2, 4]. This can ease the perceptions, applications and numerics for the SF;

– classification and basic properties of SF of FC, see [1, 3, 4, 5], etc.;

– evaluation of FC and Generalized FC operators of these SF in the general case of (3) and of H-functions, thus covering very partial results of hundreds of other recent publications, see [6, 7, 8], etc.;

– numerous illustrative examples, see within Refs items.

For the ML function (1) and some seldom special cases of (2) and (3), *numerical algorithms and plots* have been established, by using *Maple*, *Mathematics*, etc. But in the general case of multi-index Mittag-Leffler functions this is still a *challenging Open Problem*.

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BURA methods for large scale fractional diffusion problems: efficiency of the involved iterative solvers

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The presented results concern the numerical solution of spectral fractional diffusion problems in the form $\mathcal{L}^\alpha u(x) = f(x)$, where $\mathcal{L}$ is a selfadjoint elliptic operator in the bounded domain $\Omega \subset I\!R^d$, $d \in \{1, 2, 3\}$, and $\alpha \in (0, 1]$. Two cases are considered: homogeneous pure Dirichlet, and pure Neumann boundary conditions. Let $\{\lambda_i, \phi_i(x)\}_{i=1}^\infty$ be the orthonormal spectrum of $\mathcal{L}$. Then, the fractional diffusion operator is defined by the spectral decomposition

$$\mathcal{L}^\alpha v(x) = \sum_{i=\underline{i}}^{\infty} \lambda_i^\alpha v_i \phi_i(x), \qquad v_i = \int_\Omega \phi_i(x) v(x) dx,$$

where $\underline{i} = \{1, 2\}$ in the first and second case respectively. The finite difference approximation of the problem leads to the system $A^\alpha \mathbf{u} = \mathbf{f}$, where A is a sparse, symmetric and positive (semi)definite matrix, and A^α is defined by a similar spectral decomposition. In the case of finite element approximation, A is symmetric with respect to the energy dot product associated with the mass matrix.

The fractional diffusion problems are non-local, the matrix A^α is dense, and even not computable in the case of large scale problems and general geometry of Ω. Thus, a development of special numerical methods for efficient solution of such problems is required. Independently, several different methods were proposed, see, e.g., [1, 4]. We study an alternative approach, based on best uniform rational approximations (BURA) of t^α in $[0, 1]$, denoted by $r_{\alpha,k}(x)$. By assumption, the degree k of the rational function is (relatively) small, see [5, 6] and the references there in. As was shown in [7], the rest known related methods can be interpreted as some rational approximations. In this sense (and when applicable) the BURA method has certain *a priory* advantages. In the case of Dirichlet boundary conditions, the BURA approximation of $\mathbf{u}$ is defined as $\mathbf{u} \approx \mathbf{w} = \lambda_1^{-\alpha} r_{\alpha,k}(\lambda_1 A^{-1})\mathbf{f}$. Similarly, in the case of Neumann boundary conditions $\mathbf{u} \approx \mathbf{w} = \lambda_2^{-\alpha} r_{\alpha,k}(\lambda_2 A^\dagger)\mathbf{f}$. The method is robust with respect to the condition number $\kappa(A)$. In both cases $\mathbf{w}$ is expressed in the form $\mathbf{w} = -b_0\mathbf{f} - \sum_{i=1}^k b_i(A + c_i I)^{-1}\mathbf{f}$, thus requiring solving of k auxiliary linear systems with sparse and symmetric positive definite matrices. The following estimate holds true [6]

$$||\mathbf{u} - \mathbf{w}||_{\ell^2} \leq C_\alpha \lambda_2^{-\alpha} e^{-2\pi\sqrt{k\alpha}} ||\mathbf{f}||_{\ell^2},$$

i.e., the convergence rate with respect to k is exponential.

Here, the focus is on the computational efficiency and scalability. Some related results are available in [2, 3], see also the references there in. The BURA method has almost optimal computational complexity, assuming that some optimal solution method is applied to the involved auxiliary linear algebraic systems. We have used the BoomerAMG implementation of the algebraic multigrid method in the framework of a preconditioned conjugate gradient (PCG) iterative solver.

The role of the coefficients b_i and c_i is analyzed. Larger b_i means a stronger impact of the solution of the related auxiliary system if, e.g., all $b_i > 0$. The PCG relative stopping criteria is properly scaled in order to balance the total error. In addition, larger c_i means smaller condition number $\kappa(A + c_i I)$, thus decreasing the number of PCG iterations for a fixed stopping criteria. The behaviour of (b_i, c_i) for $\alpha = 0.50$ and $k = 8$ is given in the table bellow. One can observe that the order of magnitude of the coefficients substantially vary. A rich collection of pre-computed data for BURA methods is available in [5].

i	1	2	3	4
b_i	$1.80E-11$	$4.73E-9$	$3.18E-7$	$1.08E-5$
c_i	$7.35E-8$	$3.97E-6$	$7.56E-5$	$8.70E-4$
i	5	6	7	8
b_i	$2.41E-4$	$3.9E-3$	$4.98E-2$	$6.14E-1$
c_i	$7.24E-3$	$4.78E-2$	$2.75E-1$	1.92

The performed numerical results include test problems in 3D domain with complex geometry. Linear finite elements on unstructured tetrahedral meshes with local mesh refinement are used for discretization of the diffusion operator. The large scale numerical tests are run on the supercomputer system Avitohol at IICT-BAS. The scalability analysis is made with respect to the mesh size for $\alpha \in \{0.25, 0.50, 0.75\}$.

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Robust monolithic solvers for multiphysics systems in biomechanics

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We discuss monolithic preconditioners for mathematical models of waste clearance of the brain, tissue perfusion and excitation of cardiac cells/neurons. A common characteristic of the models is a coupling between *different* physical processes posed on domains with possibly *different* topological dimension across a shared interface. This multiscale nature, however, presents a challenge for constructing efficient solution algorithms.

Here we will present monolithic preconditioners for the above applications, which lead to order optimal and parameter robust solvers. The preconditioners crucially rely on the mapping properties of the coupling operators. In particular, the operators are shown to be well-posed in suitably weighted sum and intersection spaces of fractional Sobolev spaces. In turn, the monolithic preconditioners utilize solvers for the equations $-\alpha_1\Delta^{s_1}u - \alpha_2\Delta^{s_2}u = f,\ s_1, s_2 \in (-1, 1)$ on the interface. We demonstrate that the fractional problem on the interface enables use of existing well-established multilevel techniques for the remaining components of the preconditioner and that the monolithic approach often yields superior performance to other solution methods.

Mathematical models of living tissue give rise to coupled systems of partial differential equations where the components are defined and interact on domains of different dimensionality. A simple model of an exchange between viscus flow inside a vessel, Ω_S, and the surrounding tissue is given by the Darcy-Stokes problem [8]:

$$
\begin{aligned}
-\mu\Delta\mathbf{u}_S + \nabla p_S &= \mathbf{f}_S && \text{in } \Omega_S,\\
\nabla\cdot\mathbf{u}_S &= 0,\\
K^{-1}\mathbf{u}_D + \nabla p_D &= 0 && \text{in } \Omega_D,\\
\nabla\cdot\mathbf{u}_D &= \mathbf{f}_D,\\
\mathbf{u}_D\cdot\mathbf{n} - \mathbf{u}_S\cdot\mathbf{n} &= 0 && \text{on } \Gamma,\\
-\mu\frac{\partial\mathbf{u}_S}{\partial\mathbf{n}}\cdot\mathbf{n} + p_S &= p_D,\\
-\mu\frac{\partial\mathbf{u}_S}{\partial\mathbf{n}}\cdot\tau - \alpha\mathbf{u}_S\cdot\tau &= 0,
\end{aligned}
\tag{1}
$$

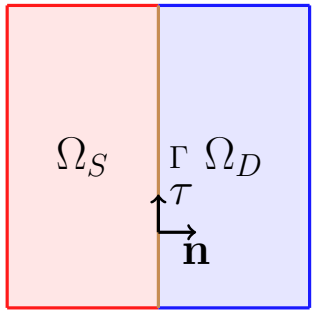

Figure 1: Darcy-Stokes domain.

with $\alpha = \alpha_{\text{BJS}}\sqrt{\frac{\mu}{K}}$. Here, the multiscale property of the system is due to the coupling con-

ditions on the interface Γ, in particular, the mass conservation condition $\mathbf{u}_D \cdot \mathbf{n} + \mathbf{u}_D \cdot \mathbf{n} = 0$. Similarly, the interface/membrane stimulation drives the dynamics of a cardiac cell Ω_i in the EMI model [9]

$$\begin{aligned} -\kappa_i \Delta u_i &= 0 && \text{in } \Omega_i, \\ -\kappa_e \Delta u_e &= 0 && \text{in } \Omega_e, \\ \kappa_i \nabla u_i \cdot \mathbf{n} - \kappa_e \nabla u_e \cdot \mathbf{n} &= 0 && \text{on } \Gamma, \\ u_i - u_e + \tfrac{\delta t}{C_m} \kappa_i \nabla u_i \cdot \mathbf{n} &= f. \end{aligned} \tag{2}$$

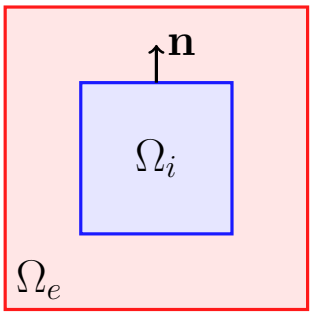

Figure 2: EMI domain.

Systems (1), (2) are potentially highly relevant in computational medicine. More precisely, as the model of the so-called glymphatic system (1) can reveal insights into the Alzheimer disease [5], while personalized drugs for cardiac treatments could be developed based on studying the response of monolayers of cardiac cells [3] using the EMI model (2). However, for realistic simulations solvers for the systems, which are robust in discretization as well as (material) parameters (δt for (2) and μ, K, α_{BJS} for (1)) are needed.

Here, we discuss efficient preconditioners for monolithic formulations of (1), (2) with explicit interface variable, the Lagrange multiplier, enforcing the coupling constraint. The preconditioners for the respective problems are block diagonal operators

$$\operatorname{diag}\left(-\mu\Delta + \alpha T_\tau' T_\tau, \tfrac{1}{\mu} I, \tfrac{1}{K}\left(I - \nabla\nabla\cdot\right), KI, \tfrac{1}{\mu}(I-\Delta)^{-1/2} + K\Delta_{00}^{1/2}\right)^{-1} \tag{3}$$

and

$$\operatorname{diag}\left(-\kappa_i\Delta, -\kappa_e\Delta, (I-\Delta)^{-1/2} + \tfrac{\delta t}{C_m} I\right)^{-1}. \tag{4}$$

As such, the leading blocks of the preconditioners can be realized by standard multilevel methods, e.g. [2, 6]. On the other hand, the (small) block of the Lagrange multiplier requires non-standard preconditioners for weighted fractional Laplacian. In the talk we discuss connection between the boundary conditions taken by the fractional operators and those set on boundary of the domain and their importance for the optimality of the solver. Furthermore, efficient realization of the fractional preconditioners in terms multigrid will be addressed.

Robustness of the proposed preconditioners can be seen in Tables 1, 2. The presented results are based on works [4, 7, 1].

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μ	K \ n_h	2^3	2^4	2^5	2^6	2^7	μ	K \ n_h	2^3	2^4	2^5	2^6	2^7
10^{-6}	10^{-8}	62	62	60	59	59	10^{-2}	10^{-8}	52	50	50	50	50
	10^{-6}	67	67	66	65	65		10^{-6}	57	56	56	55	55
	10^{-4}	73	72	72	71	69		10^{-4}	62	60	60	61	61
	10^{-2}	77	76	76	76	75		10^{-2}	64	64	64	65	64
	1	75	76	74	76	77		1	58	58	56	56	57
10^{-4}	10^{-8}	57	56	56	55	55	1	10^{-8}	54	52	52	51	53
	10^{-6}	62	62	60	59	59		10^{-6}	58	58	57	57	57
	10^{-4}	67	67	66	65	65		10^{-4}	60	62	62	61	61
	10^{-2}	73	72	70	71	71		10^{-2}	56	56	56	55	55
	1	72	72	72	72	73		1	51	50	50	50	50

Table 1: Number of preconditioned MinRes iterations for solving (1) with preconditioner (3). Case $\alpha_{\text{BJS}=1}$ is shown. Uniform $2d$ mesh consisting of $2n_h$ triangle is considered.

δt \ n_h	Monolithic AMG preconditioner						Fractional preconditioner					
	2^3	2^4	2^5	2^6	2^7	2^8	2^3	2^4	2^5	2^6	2^7	2^8
10^6	8	8	8	8	8	9	10	10	10	10	10	10
10^4	8	8	8	8	8	9	15	15	15	15	15	15
10^2	7	8	8	8	8	9	18	18	18	17	17	17
1	8	8	8	9	9	9	27	27	27	26	26	26
10^{-2}	8	8	9	9	10	10	43	47	46	44	44	43
10^{-4}	28	26	19	14	11	10	49	60	62	60	57	56
10^{-6}	56	81	101	104	87	62	51	60	62	61	59	59

Table 2: Number of Krylov iterations for solving (2). (Left) Symmetric, positive- definite formulation (without the multiplier) is solved with AMG-preconditioned conjugate gradient method. The solver is sensitive to δt. (Right) Saddle point formulation with the Lagrange multiplier uses (4)-preconditioned MinRes solver. The method is robust in δt.

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Convolution operators via the Jacoby series coefficients

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In this paper we offer one method of studying some class of convolution operators. To be short we do not produce a general scheme of reasonings, but restrict our study for the case corresponding to the Riemann-Liouville operator. Now we continue studying (see [4]) the Abel equation with the right part belonging to a Lebesgue weighted space. We have improved the previously known result - the existence and uniqueness theorem formulated in terms of the Jacoby series coefficients that gives us an opportunity to find and classify a solution due to an asymptotic of some relation containing the Jacoby series coefficients of the right part. In the beginning, let us remind that the so called mapping theorems for the Riemann-Liouville operator were firstly studied by H. Hardy and Littlewood, it was proved that $I^{\alpha}_{a+} : L_p \to L_q$, $1 < p < 1/\alpha$, $q < p/(1-\alpha p)$, $\alpha \in (0,1)$. This proposition was afterwards clarified [1] and nowadays is known as the Hardy-Littlewood theorem with limit index $I^{\alpha}_{a+} : L_p \to L_q$, $q = p/(1-\alpha p)$. However there was an attempt to extend this theorem on some class of weighted Lebesgue spaces defined as functional spaces endowed with the following norm

$$\|f\|_{L_p(I,\omega)} := \left\{ \int_a^b |f(x)|^p \, \omega(x) dx \right\}^{1/p}, \ \omega(x) := (x-a)^{\beta}(b-x)^{\gamma}, \ \beta, \gamma \in \mathbb{R}, \ I := (a,b).$$

In this direction the mathematicians such as Rubin B.S. [9, 10, 11], Karapetyants N.K. [2, 3], Vakulov B.G. [15], Samko S.G. [13, 14] (the results of [2, 9, 10] are also presented in [12]) had a great success. There were formulated the analogs of Hardy-Littlewood theorem for a class of weighted Lebesgue spaces. The main disadvantage of the results presented in [12] is gaps of the parameters values in the conditions, moreover the notorious problem related to $p = 1/\alpha$ was remained completely unsolvable. All these create the prerequisite to invent another approach for studying the Riemann-Liouville operator action that was successfully applied in the paper [4] and we write out bellow some of its highlights. We confirm that the main advantage of the method, used in the paper [4] and based on the results [7, 8, 5, 6], is still relevant and allows us to obtain some interesting results. The main challenge of this paper is to improve and clarify the results of the paper [4]. In particular we need to find a simple condition, on the right part of the Abel equation, under which Theorem 2 [4] is applicable. For this purpose we have made an attempt to

study this problem having used absolute convergence of a series. The main relevance of the improvement is based on the fact that the previously used methods were determined by the relation between order α of the fractional integral and index p of a Lebesgue space (for instance the case $p = 1/\alpha$ is not considered in the monograph [12]). Here we give the highlights: The relationship between the values of the parameters and order α, by virtue of which we can provide a description of the solution smoothness, is established; The conditions providing existence and uniqueness of the solution, formulated in terms of Jacoby series coefficients, were obtained. The principal result - the independence between one of the parameters and the solution smoothness was proved.

Consider the orthonormal system of the Jacobi polynomials denoted by

$$p_n^{(\beta,\gamma)}(x) = \delta_n(\beta,\gamma)\,(x-a)^{-\beta}(b-x)^{-\gamma}\frac{d^n}{dx^n}\left[(x-a)^{\beta+n}(b-x)^{\gamma+n}\right],\ \beta,\gamma > -1,\ n \in \mathbb{N}_0,$$

where $\delta_n(\beta,\gamma)$ is the normalized multiplier. In the paper [4] we calculate the coefficients

$$(p_m, I_{a+}^{\alpha} p_n)_{L_2(I,\omega)} = (-1)^n A_{mn}^{\alpha,\beta,\gamma},\ \ (p_m, I_{b-}^{\alpha} p_n)_{L_2(I,\omega)} = (-1)^m A_{mn}^{\alpha,\gamma,\beta},$$

where the shorthand non standard notation is also used $I_{a+}^{-\alpha} = D_{a+}^{\alpha}, \alpha \in (0,1)$. In that paper the first our aim was to reformulate, in terms of the Jacoby series coefficients, the previously known theorems describing the Riemann-Liouville operator action in the weighted Lebesgue spaces. Besides the main results of the paper, we stress that there was arranged some systematization of the previously known facts of the Riemann-Liouville operator action in the weighted Lebesgue spaces, where the weighted function is represented by some kind of a power function. We managed to fill the gaps of the previously known results and formulated this result as a separate Lemma 1 [4]. The following theorem is the very mapping theorem (see [4]) formulated in terms of the Jacoby series coefficients. Here we give the modified form corresponding to the right-side case.

Theorem 1. *(Theorem 2 in [4]) Suppose*

$$\omega(x) := (x-a)^{\beta}(b-x)^{\gamma},\ \beta,\gamma \in [-1/2, 1/2],\ S_k f := \sum_{i=0}^{k} p_i^{(\beta,\gamma)} f_i,\ f_i := \int_a^b p_i^{(\beta,\gamma)}(x) f(x)\omega(x)dx,$$

the Pollard condition holds

$$4\max\left\{\frac{\beta+1}{2\beta+3}, \frac{\gamma+1}{2\gamma+3}\right\} < p < 4\min\left\{\frac{\beta+1}{2\beta+1}, \frac{\gamma+1}{2\gamma+1}\right\},$$

the right part of the Abel equation $I_{b-}^{\alpha}\varphi = f$, $\alpha \in (0,1)$ such that

$$\left\|D_{b-}^{\alpha} S_k f\right\|_{L_p(I,\omega)} \le C,\ k \in \mathbb{N}_0,\ \ \left|\sum_{n=0}^{\infty} f_n A_{mn}^{\alpha,\gamma,\beta}\right| \le C m^{-\lambda},\ m \in \mathbb{N},\ \lambda \in [0,\infty);$$

then there exists a unique solution of the Abel equation in $L_p(I,\omega)$, *the solution belongs to* $L_q(I,\omega)$, *where:* $q = p$, *if* $0 \le \lambda \le 1/2$; $q = \max\{p,t\}$, $t < (2s-1)/(s-\lambda)$, *if* $1/2 < \lambda < s$ $(s = 3/2 + \max\{\beta,\gamma\})$; q *is arbitrary large, if* $\lambda \ge s$. *Moreover if* $\lambda > 1/2$, *then the solution is represented by the convergent in* $L_q(I,\omega)$ *series*

$$\psi(x) = \sum_{m=0}^{\infty} p_m(x)(-1)^m \sum_{n=0}^{\infty} f_n A_{mn}^{-\alpha,\gamma,\beta}. \tag{1}$$

Theorem 2. *Assume that the following series is absolutely convergent*

$$\sum_{n=0}^{\infty} f_n c_n < \infty,$$

where f_n *are the Jacoby series coefficients of the right part of the Abel equation* $I_{b-}^{\alpha}\varphi = f$,

$$c_n = \frac{\delta_n' n!\Gamma(n+\beta+1)\Gamma(n+\gamma+1)}{4^n},$$

the condition $\gamma + 1 - 2\alpha > 0$ *holds, then there exists a unique solution of the Abel equation in accordance with Theorem 1, the solution is represented by series* (1), *and the value of the parameter is* $\lambda = \gamma + 3/2 - 2\alpha$.

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Reaction-ultraslow diffusion on comb structures

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Abstract

Two-dimensional (2D) comb model is proposed to characterize reaction-ultraslow diffusion of tracers both in backbones- (x direction) and sidebranches- (y direction) of the comb-like structure with two memory kernels. The memory kernels include Dirac delta, power law, logarithmic and inverse Mittag-Leffler (ML) functions, which can be also considered as the structural functions in the time structural derivative. Based on the comb model, ultraslow diffusion on a fractal comb structure is also investigated by considering spatial fractal geometry of the backbone volume. The mean squared displacement (MSD) and the corresponding concentration of the tracers, i.e., the solution of the comb model, are derived for reactive and conservative tracers. For a fractal structure of backbones, the derived MSDs and corresponding solutions depend on the backbones fractal dimension. The proposed 2D comb model with different kernel functions is feasible to describe ultraslow diffusion in both the backbone and sidebranches of the comb-like structure.

Keywords: Comb model, ultraslow diffusion, reaction, mean squared displacement, fractal.

1 Introduction

Comb-like structure, such as rock, polymer and spiny dendrite, is widely encountered in real applications. Diffusion processes of conservative and interacting diffusive particles in these comb-like structures usually deviates from Brownian motion, i.e., non-Gaussian diffusion, in which the mean squared displacement (MSD) is a nonlinear function of time [1]. The existing comb models have been an alternative tool to characterize non-Gaussian diffusion in comb-like structures [2]. It is also found that ultraslow diffusion [3], another class of non-Gaussian diffusion, exists in comb structure, such as the diffusion process in the three-dimensional (3D) cylindrical comb model with infinite sidebranches along the backbone, also in the 3D comb structure with 2D kebab lattice. Compared with anomalous diffusion, the MSD of ultraslow diffusion is not a power law function of time, but a logarithmic function of time, in which the particles diffuse more slowly than in subdiffusion. One motivation of this study is to develop new comb model by selecting simper memory kernels

with clear physical meaning for modeling ultraslow diffusion in both the backbone and sidebranches.

In this study, the comb model with new memory kernels is constructed based on the structural derivative used in the structural derivative models [3]. The structural derivative was proposed by Chen et al. [4] for modeling ultraslow diffusion using logarithmic and inverse Mittag-Leffler (ML) function as the memory kernel. Logarithmic function is a special case of inverse ML function when $\alpha = 1$. The inverse ML function is the inverse function of the famous ML function. The strategy to derive the structural derivative comb model in this study is adapted from that in [2] based on the classical 2D comb model, but to employ different memory kernels, such as the logarithmic function, the inverse ML function and their variants. In this study, the memory kernels are selected based on the patters of ultraslow diffusion both in backbones and sidebranches. The second motivation is to consider the reactive effect of the diffusive particles, in this study the first order catalytic reaction scheme of the tracer in the backbone of the comb-like structure is considered to construct the comb model. Another issue should be pointed out that for the comb-like structures with spatial fractal geometry [5], non-Gaussian diffusions can be described by generalized comb-like models. Thus, in this study ultraslow diffusion in the fractal comb structure is also investigated as the third motivation by considering the spatial fractal geometry of the backbone volume.

2 Summary

In this study ultraslow diffusion of tracers in comb-like structure is investigated by two-dimensional reaction-diffusion equation with two memory kernels for a two-dimensional comb. The first order catalytic reaction scheme is considered in the frame of the comb model, which is solved by using the inverse Laplace-Fourier transform on the general expressions of the solutions in frequency domains. The logarithmic and inverse Mittag-Leffler functions are selected as the kernels, which are frequently used in the structural derivative models. The solutions and the corresponding mean squared displacements (MSD) are derived for different memory kernels. The solutions follow a double-sided exponential distribution. Compared with the conservative cases, the reactive effect does not change the patterns of MSDs and solutions, which accelerates the ultraslow diffusion both on the two directions. Based on the proposed comb model, ultraslow diffusion on a generalized fractal comb of the backbones is also considered. The derived MSDs and solutions depend on the fractal dimension of backbones. Thus, the comb model is useful to describe the ultraslow diffusions in both the backbones and sidebranches of the comb. In further study, the comb model should be tested with real applications, and the effects of the nonlinear reaction scheme will also be discussed.

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Fractional order elliptic problems with inhomogeneous Dirichlet boundary conditions

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1 Introduction

Fractional-order elliptic problems are investigated in case of inhomogeneous Dirichlet boundary data. On a bounded domain, the incorporation of boundary conditions into a true mathematical model is by far not easy. We should use fractional order differential operators, which are non-local, at the same time, in real-life situations, we do not have any data outside of a physical domain. In other words, we are looking for functions $u : \Omega \to \mathbb{R}$ with a bounded domain Ω, whenever classical non-local operators [2] are defined for functions $u : \mathbb{R}^d \to \mathbb{R}$. This basic difficulty motivates us to find an appropriate extension of the problem, which is formulated on $\mathbb{R}^d$.

It was pointed out in [1] that the fractional order elliptic equations with inhomogeneous boundary conditions can be succesfully analyzed in the framework of boundary integral equations. Our aim is to extend this result in the following sense:

- the well-posedness is stated also in two space dimensions,
- the mapping properties of the corresponding single layer operator are generalized (boundedness also in 2D, coercivity),
- a condition is given for the existence of a classical (pointwise) solution.

An important motivation of this study is to prepare a numerical simulation in 2D, where the boundary integral form reduces the problem to compute one-dimensional integrals.

1.1 Mathematical preliminaries

The main problem in this study is the precise statement and the analysis of the elliptic boundary value problem

$$\begin{cases} -(-\Delta)^{\alpha} u(\mathbf{x}) = 0 & \mathbf{x} \in \Omega \\ u(\mathbf{x}) = g(\mathbf{x}) & \mathbf{x} \in \partial\Omega. \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz domain ($d = 2, 3$), $\alpha \in (\frac{1}{2}, 1)$ and g is a given real function. At this stage, the differential operator $(-\Delta)^\alpha$ is not yet defined.

The fractional Laplacian on $\mathbb{R}^d$ has many equivalent definitions. This operator can be defined pointwise as

$$-(-\Delta_{\mathbb{R}^d})^\alpha u(\mathbf{x}) = \lim_{r \to 0^+} \frac{2^{2\alpha}\Gamma(\frac{d}{2}+\alpha)}{\pi^{\frac{d}{2}}\Gamma(-\alpha)} \int_{B(\mathbf{0},r)^C} \frac{u(\mathbf{x}+\mathbf{z}) - u(\mathbf{x})}{|\mathbf{z}|^{d+2\alpha}} \, \mathrm{d}\mathbf{z},$$

where $B(\mathbf{x}, r)^C = \mathbb{R}^d \setminus B(\mathbf{x}, r)$. Accordingly, the weak fractional Laplacian $(-\Delta_{\mathbb{R}^d})^\alpha u$ can be given as the function for which

$$\int_{\mathbb{R}^d} v(-\Delta_{\mathbb{R}^d})^\alpha u = \int_{\mathbb{R}^d} u(-\Delta_{\mathbb{R}^d})^\alpha v$$

is satisfied for all $v \in C_0^\infty(\mathbb{R}^d)$.

We will make use of the fundamental solution ϕ_α of $(-\Delta_{\mathbb{R}^d})^\alpha$, which is given with

$$\phi_\alpha = \mathcal{F}^{-1} \frac{1}{|\mathrm{Id}|^{2\alpha}} = 2^{\alpha - \frac{n}{2}} \frac{\Gamma\left(\frac{\alpha}{2}\right)}{\Gamma\left(\frac{n-\alpha}{2}\right)} |\mathrm{Id}|^{2\alpha - d}.$$

In the analysis, we use the notation $H^s(\Omega) \subset L_2(\Omega)$ for the classical Sobolev spaces with arbitrary positive indices. For stating the well-posedness, we also need the homogeneous Sobolev space $\dot{H}^s(\mathbb{R}^d)$ with the corresponding norm. If the underlying domain (Ω, $\partial\Omega$ or $\mathbb{R}^d$) is obvious, simply the notation $\|\cdot\|_s$ will be used for the corresponding norms.

An important tool in the analysis is the trace operator γ. For a bounded Lipschitz domain Ω,

$$\gamma : H^s(\Omega) \to H^{s-\frac{1}{2}}(\partial\Omega) \tag{2}$$

is continuous for $s \in (\frac{1}{2}, \frac{3}{2})$. We use the conventional notation $\langle \cdot, \cdot \rangle_{-\beta,\beta}$ for the duality pairing between $H^{-\beta}(\partial\Omega)$ and $H^\beta(\partial\Omega)$ with some positive exponent β.

1.2 The main objective, comparison with earlier achievements

In [1], the problem in (1) for u was transformed to a boundary integral equation and it was established, that for any bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ with $d \geq 3$ and $g \in H^{\alpha-\frac{1}{2}}(\partial\Omega)$ with $\alpha \in (\frac{1}{2}, 1)$, the problem

$$\begin{cases} -(-\Delta)^\alpha \tilde{u}(\mathbf{x}) = 0 & \mathbf{x} \in (\partial\Omega)^C \\ \gamma\tilde{u}(\mathbf{x}) = g(\mathbf{x}) & \mathbf{x} \in \partial\Omega \\ |\tilde{u}(\mathbf{x})| \lesssim |\mathbf{x}|^{2\alpha-d} & \mathbf{x} \in B(\mathbf{0}, 1)^C \end{cases} \tag{3}$$

has a unique weak solution $\tilde{u} \in \dot{H}^\alpha(\mathbb{R}^d)$.

Our aim is to sharpen this result and prove that the unique solution of (3)

(i) exists *also in case of* $d = 2$ provided that $\alpha \in (\frac{1}{2}, \frac{3}{4})$,

(ii) satisfies $-(-\Delta)^\alpha \tilde{u}(\mathbf{x}) = 0$ *also pointwise* for any $\mathbf{x} \in (\partial\Omega)^C$ under some weak condition.

2 Main results

Assume that $\alpha \in (0,1)$ for $d = 3$ or $\alpha \in (\frac{1}{2}, \frac{3}{4})$ for $d = 2$. We investigate the surface potential, which is given for any $\mathbf{x} \in \mathbb{R}^d$ with

$$S_\alpha(u)(\mathbf{x}) = \int_{\partial\Omega} \phi_\alpha(\mathbf{x}-\mathbf{y})u(\mathbf{y})\,\mathrm{d}\mathbf{y}. \tag{4}$$

In precise terms, in [3] we state the following generalization of (4.1) in [1].

For any indices s, α satisfying the assumptions above and $2\alpha - s \in (\frac{1}{2}, \frac{3}{2})$, the mapping S_α defines a continuous linear operator between $H^{s-2\alpha+\frac{1}{2}}(\partial\Omega)$ and $H^s(\Omega)$, i.e. for all $\psi \in H^{s-2\alpha+\frac{1}{2}}(\partial\Omega)$, we have

$$\|S_\alpha(\psi)\|_s \lesssim \|\psi\|_{s-2\alpha+\frac{1}{2},\partial\Omega}. \tag{5}$$

We also show that the map γS_α is a coercive operator between $H^{1/2-\alpha}(\partial\Omega)$ and $H^{\alpha-1/2}(\partial\Omega)$ in the sense that

$$\langle u, \gamma S_\alpha u\rangle_{\frac{1}{2}-\alpha,\alpha-\frac{1}{2}} = \int_{\partial\Omega} (S_\alpha u)(\mathbf{x})u(\mathbf{x})\,\mathrm{d}\mathbf{x} \gtrsim \|u\|^2_{1/2-\alpha,\partial\Omega}. \tag{6}$$

Using inequalities (5),(6) and the continuity of the trace operator γ, we can prove our main statement, that is for any $g \in H^{\alpha-\frac{1}{2}}(\partial\Omega)$, there is a unique function $G \in H^{\frac{1}{2}-\alpha}(\partial\Omega)$, that solves the equation

$$\gamma S_\alpha(G) = g$$

which yields that $\tilde{u} = S_\alpha(G) \in \dot{H}^\alpha(\mathbb{R}^d)$ solves the problem in (3).
If, we have additionally $G \in L_1(\partial\Omega)$, then the pointwise equality $-(-\Delta)^\alpha\tilde{u} = 0$ in $(\partial\Omega)^C$ is also satisfied.

Since we showed the coercivity of operator γS_α, we can formulate an appropriate form of Céa-lemma, and use a Galerkin boundary element method to simulate the problem. Let $G_h \in S_h^0(\partial\Omega)$ be the unique solution to

$$\langle v_h, \gamma S_\alpha(G - G_h)\rangle_{1/2-\alpha,\alpha-1/2} = 0 \qquad \forall v_h \in S_h^0(\partial\Omega)$$

where $S_h^0(\partial\Omega)$ is the space of piecewise constant functions defined on an appropriate triangulation $(\Gamma_j)_{j\in\{1\dots k\}}$ of $\partial\Omega$ with maximal diameter h. If we reconstruct the approximate solution $\tilde{u}_h$ from G_h, for $s \in [1/2-\alpha, 1]$ we get the a priori estimate

$$\|\tilde{u} - \tilde{u}_h\|_{\alpha,\mathbb{R}^n} \lesssim \sum_{\Gamma_j\in\partial\Omega} h^{s-(1/2-\alpha)}\|G\|_{s,\Gamma_j}.$$

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On computation of the matrix Mittag-Leffler function

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The theory of fractional differential equations is a new and important branch of differential equation theory, which has numerous applications and provides realistic models for many real-life processes and phenomena. The Mittag-Leffler function $E_{\alpha,\beta}(z)$ plays the same role in fractional differential equations that the exponential function e^z plays in ordinary differential equations.

A natural extension of the exponential function to the case of matrix arguments proved to be extremely useful in studying the linear systems of ordinary differential equations arising in engineering, mechanics, control theory etc. Similarly the matrix Mittag-Leffler function is crucial in linear systems of fractional differential equations, allowing to represent explicitly their solutions. That is why the methods for computing the matrix Mittag-Leffler function are so important.

There exists a wide range of methods for computing of the matrix exponential and many of them can be adapted for computation of the matrix Mittag-Leffler function. One of the methods is based on Jordan canonical form [8]. Here we apply this approach and propose a technique for computation the matrix Mittag-Leffler function, which is implemented with MATLAB code [7].

The numerical methods based on Jordan canonical form have major disadvantage, since the involved similarity transformation can be ill-conditioned. However the numerical experiments on the benchmark example of the Bagley–Torvik equation [1] imply that the proposed approach allows to obtain satisfactory accuracy.

The matrix Mittag-Leffler function was probably first introduced in the paper [2], where it was used in an explicit solution of a linear system of fractional order equation (FDEs)

$$D^\alpha z = Az + f,\ 0 < \alpha \leq 1. \tag{1}$$

Here $D^\alpha z$ stands for the Riemann–Liouville fractional derivative of order α [5]. In general, if g is a function having absolutely continuous derivatives up to the order $m-1$, the Riemann–Liouville derivative of fractional order α, $m-1 < \alpha \leq m$, can be defined as follows:

$$D^\alpha g(t) = \frac{1}{\Gamma(m-\alpha)} \frac{d^m}{dt^m} \int_0^t \frac{g(\tau)}{(t-\tau)^{\alpha-m+1}} d\tau.$$

Hereafter A is a fixed real $n \times n$ matrix, and $z, f : [0,\infty) \to \mathbb{R}^n$ are measurable vector-functions taking values in $\mathbb{R}^n$.

If (1) is supplied with initial condition of the form

$$\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{z(\tau)}{(t-\tau)^\alpha}d\tau\Big|_{t=0} = z^0, \tag{2}$$

then solution to the initial value problem (1), (2) can be written down in the form [3]

$$z(t) = t^{\alpha-1}E_{\alpha,\alpha}(At^\alpha)z^0 + \int_0^t (t-\tau)^{\alpha-1}E_{\alpha,\alpha}(A(t-\tau)^\alpha)f(\tau)d\tau, \tag{3}$$

where

$$E_{\alpha,\beta}(A) = \sum_{k=0}^{\infty}\frac{A^k}{\Gamma(\alpha k+\beta)},\ \alpha>0,\ \beta\in\mathbb{C}, \tag{4}$$

denotes the matrix Mittag-Leffler function of A.

The explicit expression (3) plays a key role in numerous applications related to systems with fractional dynamics [6]. That is why the methods for computing the matrix Mittag-Leffler function are so important.

Both the matrix Mittag-Leffler function and the matrix α-exponential functions are generalizations of matrix exponential function, since

$$E_{1,1}(At) = e_1^{At} = e^{At}.$$

This implies that some of numerous existing methods for computing the matrix exponential can be adapted for the matrix Mittag-Leffler functions as well. An overview and analysis of these methods can be found in the paper [8].

There exists a number of equivalent definitions of a matrix function. The following definition [4] is based on the Jordan canonical form. We will use the latter for computing the matrix Mittag-Leffler function.

Definition 1 (matrix function via Jordan canonical form). Let the function f be defined on the spectrum of A and let $A = ZJZ^{-1}$, where J is the Jordan canonical form. Then

$$f(A) = Zf(J)Z^{-1} = Z\ \mathrm{diag}\{f(J_1), f(J_2), \ldots, f(J_s)\}Z^{-1}, \tag{5}$$

where

$$f(J_k) = \begin{pmatrix} f(\lambda_k) & f'(\lambda_k) & \frac{f''(\lambda_k)}{2} & \ldots & \frac{f^{(m_k-1)}(\lambda_k)}{(m_k-1)!} \\ 0 & f(\lambda_k) & f'(\lambda_k) & \ldots & \frac{f^{(m_k-2)}(\lambda_k)}{(m_k-2)!} \\ 0 & 0 & f(\lambda_k) & \ldots & \frac{f^{(m_k-3)}(\lambda_k)}{(m_k-3)!} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & f'(\lambda_k) \\ 0 & 0 & 0 & \ldots & f(\lambda_k) \end{pmatrix}. \tag{6}$$

The generalized (scalar) Mittag-Leffler function also known as Prabhakar function is defined for complex $z, \alpha, \beta, \rho \in \mathbb{C}$, and $\Re(\alpha) > 0$ by

$$E^{\rho}_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{(\rho)_k}{\Gamma(\alpha k + \beta)} \frac{z^k}{k!},$$

where $(\rho)_k = \rho(\rho+1)\dots(\rho+k-1)$ is the Pochhammer symbol.

In particular, when $\rho = 1$, it coincides with the Mittag-Leffler function (4):

$$E^{1}_{\alpha,\beta}(z) = E_{\alpha,\beta}(z).$$

Since the expression (6) involves derivatives, the following equation [5] is important for the purpose of computing the matrix Mittag-Leffler function:

$$\left(\frac{d}{dt}\right)^m E_{\alpha,\beta}(t) = m! E^{m+1}_{\alpha,\beta+\alpha m}(t), \quad m \in \mathbb{N}. \tag{7}$$

In view of (7), the formulas (5), (6) take on the form

$$E_{\alpha,\beta}(A) = Z \operatorname{diag}\{E_{\alpha,\beta}(J_1), E_{\alpha,\beta}(J_2), \dots, E_{\alpha,\beta}(J_s)\} Z^{-1}, \tag{8}$$

$$E_{\alpha,\beta}(J_k)$$

$$= \begin{pmatrix} E_{\alpha,\beta}(\lambda_k) & E^2_{\alpha,\beta+\alpha}(\lambda_k) & \dots & E^{m_k}_{\alpha,\beta+(m_k-1)\alpha}(\lambda_k) \\ 0 & E_{\alpha,\beta}(\lambda_k) & \dots & E^{m_k-1}_{\alpha,\beta+(m_k-2)\alpha}(\lambda_k) \\ 0 & 0 & \dots & E^{m_k-2}_{\alpha,\beta+(m_k-3)\alpha}(\lambda_k) \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & E^2_{\alpha,\beta+\alpha}(\lambda_k) \\ 0 & 0 & \dots & E_{\alpha,\beta}(\lambda_k) \end{pmatrix}. \tag{9}$$

The method of computing the matrix Mittag-Leffler function based on the Jordan canonical form representation (8), (9) is implemented with MATLAB code [7].

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Implementation of fractional optimal control problems in real-world applications

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The present work intends to discuss various practical applications of fractional calculus. Specifically, we have analyzed the need of fractional-order operators in formulating various cancer-tumor models. Modelling of such systems with non-local memory preserving fractional derivatives enables us to describe the dynamics of tumor-immune interactions. The underlying motive is to review these models as fractional optimal control problems and perform suitable investigation.

Nested dissection reordering in a HSS solver for fractional diffusion problems

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1 Introduction

The *anomalous* diffusion (*fractional* diffusion) is a process where the relationship between mean square displacement and time is not linear. It has a wide range of applications in modeling transport within cells, in porous materials, ion channels in plasma membrane, atmospheric processes and others. The fractional diffusion operators and the related boundary value problems are *non-local*, thus resulting in *dense* systems of linear algebraic equations. Solving such systems with Gaussian elimination is computationally too expensive. Under certain assumptions, the Hierarchical compression methods offer better computational complexity. Initially developed for boundary element discretizations, they are also applicable to the fractional Laplacian defined through the Ritz potential. However the efficiency of the compression is highly dependent on the structure of the underlying matrix. By *good structure* we understand the existence of approximately low-rank off-diagonal blocks, which depends on the ordering of the unknowns. In this work we are interested in applying the reordering provided by the Nested Dissection algorithm when using Hierarchical Semi-Separable compression for a fractional diffusion problem. The performance of the resulting solver is analyzed.

2 Fractional diffusion

Let us consider the fractional Laplacian defined through the Ritz potential:

$$(-\Delta)^{\alpha} u(x) = C(n,\alpha)\, p.v. \int_{\mathbb{R}^n} \frac{u(x) - u(y)}{|x-y|^{n+2\alpha}} dy, \quad \alpha \in (0,1), \tag{1}$$

where $p.v.$ stands for principal value, C is the normalized constant

$$C(n,\alpha) = \frac{2^{2\alpha}\alpha\Gamma\left(\alpha + \frac{n}{2}\right)}{\pi^{n/2}\Gamma(1-\alpha)},$$

n is the dimension, Γ is the Gamma function, and Ω is a bounded domain. We consider the homogeneous Dirichlet problem associated with (1):

$$\begin{cases} (-\Delta)^{\alpha} u &= f, x \in \Omega, \\ u &= 0, x \notin \Omega. \end{cases}$$

The 2D finite element discretization presented in [1] is used in this study. The efficiency of the hierarchical solver is analyzed for test linear systems corresponding to square and circle domain Ω.

3 STRUMPACK solver

The STRUctured Matrix PACKage (STRUMPACK) is a parallel library providing computational routines for *structured* matrices – i.e. matrices that exhibit some low-rank property (sparse matrices and dense rank-deficient matrices). We are interested in the implementation of the Hierarchical Semi-Separable (HSS) compression solver [2]. Solving a system $Ax = b$ with HSS compression includes 3 steps:

1. HSS compression: A is compressed into a HSS form H using random sampling. This is done recursively by first dividing the matrix in 4 square blocks, expressing the off-diagonal blocks as a product of three matrices (U, B (small and square) and V) called generators.

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \qquad A_{ij,i \neq j} = U_i^{\text{big}} B_{ij} V_j^{\text{big}^*}.$$

   The blocks A_{ii} are recursively compressed in a similar way. The computational complexity is $O(r^2 n)$, where n is the number of unknowns and r is the calculated maximum rank of the off-diagonal blocks.

2. ULV-like factorization: Changes the variables from x to y, and solves the system in two passes. The first one solves $O(n - r)$ unknowns using the structure of H, and the second pass solves the rest $O(r)$ unknowns with Gaussian elimination. The computational complexity is $O(r^2 n)$.

3. Solution: Finds the solution x from the solution y obtained at the second step. The computational complexity is $O(rn)$.

4 Nested Dissection Reordering

The ordering of the unknowns is important for the efficiency of the hierarchical algorithm. The ordering produced by the MATLAB code in [1] results in a poor compression. In [4, 3] we have analyzed several reordering schemes. The goal of this work is to investigate the

use of the Nested Dissection (ND) algorithm for this purpose. The ND [5] is developed to reduce the fill-ins of Gaussian elimination of sparse matrices. It uses a *divide and conquer* strategy on the graph of the matrix. The selection of a set of vertices (separator) divides the matrix into a 3×3 (or more) block structure. The algorithm is applied recursively. The fractional diffusion matrix is dense, however, and ND wouldn't help solving it with Gaussian elimination. Here, the ND reordering is applied to the HSS compression solver aimed at reducing the rank of the off-diagonal blocks, and thus increasing the computational efficiency.

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A survey on fast algorithms for fractional diffusion equations and its applications

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Fractional diffusion equations (FDEs), which are well known as a valid model capturing anomalous diffusion due to its memory and long range interaction, have been successfully applied to simulate the transportation process of contaminant in the underground water. The objective of our works is to provide fast algorithms and develop the meshless method (Kansa method) to dealwith the fractional diffusion equations with arbitrary angle in two dimension. For the fast algorithms on time fractional calculus, we proposed the semi-discrete method together with scale-dependent difference method, separately. Subsequently, we numerically solve the variable-order vector fractional-derivative models to simulate multi-dimensional anomalous diffusion in nonstationary media. Hence, our work can provide a fast and convenient tool to quantify complex anomalous transport in multi-dimensional and non-stationary media with continuously or abruptly changing heterogeneity, filling the knowledge gap in parsimonious non-local transport models developed in the last decades.

Contaminant transport modeling has been the prerequisite for many environmental protection applications, but efficiently predicting real-world mass transport remains a historical challenge for the geophysical and hydrological communities. The physical heterogeneity of natural geological media with intrinsic scale effects has been well recognized as the major mechanism of anomalous diffusion, but it cannot be measured exhaustively at all relevant scales. It is well-known that traditional second-order diffusion models built upon the standard Fick's law cannot efficiently capture non-Fickian features of mass transport processes. These features include apparent early-arrivals and/or heavy late-time tailing in contaminant breakthrough curves, as well as scale-dependent transport coefficients. The failure of second-order diffusion equations in capturing non-Fickian transport has motivated the application of time and space fractional-order diffusion equations (FDEs) to contaminant transport in porous media.

Although the FDE models have been successfully used to capture anomalous diffusion in the last several decades, efficient numerical solvers for the FDEs are still required for

engineering applications that involve large, geometrically complex spatial domains and long-time range predictions. The need for these solvers stems from two reasons. First, the time fractional derivative in the FDE retains a memory of its entire history. Compared with the integer-order derivative which is a local operator, the computational cost of the temporal FDE dramatically increases with the total modeling time. Second, although the global correlation defined by the space fractional derivative (especially the fractional Laplacian operator) enables the FDE to characterize the spatial non-local nature of contaminant transport, it causes a computational challenge in approximating spatial FDEs using the grid-based finite difference method (FDM) or finite element method (FEM). Because the fractional derivative is a non-local operator, the parameter matrix in the FDM (or the stiffness matrix in the FEM) for FDEs is not banded or sparse (as is the standard diffusion equation), but almost dense. This issue challenges the accuracy and efficiency of numerical approximations for high-dimensional space FDEs. Previous studies focusing on FDM and FEM methods have provided various accurate and mathematical convergent schemes for solving space FDE models, but the prohibitive computational cost challenges long-range time computation of the spatiotemporal FDEs in large spatial domains.

Vector FDEs are needed to capture real-world diffusion in multi-dimensional media. An extension of FDEs from one dimension to two or three dimensions is not as straightforward as that for the second-order diffusion equation, due to the global correlation nature of anomalous transport. Meerschaert et al. proposed a vector fractional derivative as a generalization of the Laplacian term, which satisfies the global correlation property and can efficiently describe anomalous transport in complex media with preferential flow path. Therefore, we adopt their definition and focus on the development of numerical methods for solving spatiotemporal FDEs containing the vector fractional derivative operator.

In addition, real-world anomalous diffusion can cover a large domain, challenging classical grid-based numerical solvers such as the FDM. The computational cost of the FEM on mesh generation and assembling of the asymmetric stiffness matrix also increases dramatically. The radial basis function (RBF) collocation technique, which is a global meshless method, was recognized as an efficient method to approximate the differential equations in large and irregular domains. The RBF method has also proved to be a meshless merit method with the advantages of high accuracy and ease of implementation in discretizing the space-fractional derivative.

For the fast algorithms on time fractional calculus, we proposed the semi- discrete method and scale-dependent difference method, separately. On one hand, we proposed a semi-discrete method, in which an exact solution for the ODE was obtained using the analytical technique and property of the Mittag-Leffler function, to approximate the time fractional derivative term achieving a fast and accurate solution. On the other hand, we proposed a scale-dependent finite difference method (S-FDM) to approximate the time fractional differential equations (FDEs), using Hausdroff metric to conveniently link the order of the time fractional derivative (α) and the non-uniform time intervals. Considering the complex spatial structure in geological media, we developed, evaluated, and applied variable-order, vector, spatial fractional-derivative equation (FDE) models with a Kansa solver, to capture spatiotemporal variation of super-diffusion along arbitrary angles (i.e.,

preferential pathways). Those studies aim at providing an efficient method which can solve the spatiotemporal FDE in large, two-dimensional spatial domains, and provide a long-time range prediction of anomalous pollutant transport.

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Approximate representation of the solutions of fractional elliptical BVP through the solution of parabolic IVP

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Boundary value problem for a fractional power of an elliptic operator is considered. To solve such problems we use an integral representation by means of a standard solution problem for parabolic equations.

Problem formulation. Introduce the elliptic operator as

$$Av = -\mathrm{div}(a(x)\mathrm{grad}\, v) + c(x)v, \quad x \in \Omega, \tag{1}$$

with coefficients $0 < a_1 \le a(x) \le a_2$, $c(x) \ge 0$. The operator A is defined on the set of functions $v(x)$ that satisfy on the boundary $\partial\Omega$ the following conditions:

$$v(x) = 0, \quad x \in \partial\Omega. \tag{2}$$

In the Hilbert space $H = L_2(\Omega)$, we define the scalar product and norm in the standard way:

$$(v, w) = \int_\Omega v(x)w(x)dx, \quad \|v\| = (v, v)^{1/2}.$$

In the spectral problem

$$A\varphi_k = \lambda_k\varphi_k, \quad x \in \Omega, \quad \varphi_k = 0, \quad x \in \partial\Omega,$$

we have $0 < \lambda_1 \le \lambda_2 \le ...$, and the eigenfunctions φ_k, $\|\varphi_k\| = 1$, $k = 1, 2, ...$ form a basis in H. Therefore, $v = \sum\limits_{k=1}^{\infty}(v, \varphi_k)\varphi_k$. Let the operator A be defined in the following domain:

$$D(A) = \Big\{v \mid v(x) \in L_2(\Omega),\ \sum_{k=0}^{\infty}|(v, \varphi_k)|^2\lambda_k < \infty\Big\}.$$

Under these conditions $A : H \to H$ and the operator A is self-adjoint and positive definite:

$$A = A^* \ge \nu I, \quad \nu > 0, \tag{3}$$

where I is the identity operator in H. In applications, the value of λ_1 is unknown (the spectral problem must be solved). Therefore, we suppose that $\nu \leq \lambda_1$ in (3). Let us assume for the fractional power of the operator A:

$$A^{\alpha}v = \sum_{k=0}^{\infty}(v, \varphi_k)\lambda_k^{\alpha}\varphi_k.$$

The solution $v(x)$ satisfies the equation

$$A^{\alpha}v = f \tag{4}$$

under the restriction $0 < \alpha < 1$.

Representation through parabolic IVP solutions. An approximate solution to the boundary value problem for the fractional degree of an elliptic operator (4) often based on the use of one or another integral representation. For example, in the works A. Bonito, J. E. Pasciak (2016), L. Aceto, P. Novati (2017) the Balakrishnan formula is used when

$$A^{-\alpha} = \frac{\sin(\pi\alpha)}{\pi}\int_0^{\infty}\theta^{-\alpha}(A + \theta I)^{-1}d\theta, \quad 0 < \alpha < 1. \tag{5}$$

The approximation of $A^{-\alpha}$ is based on the use of one or another quadrature formulas for the right-hand side of (5).

On this path, the possibilities of approximating both the fractional power of the operator $A^{-\alpha}$ and approximating the solution of the problem are realized.

1. Rational function approximation $A^{-\alpha}$:

$$A^{-\alpha} \approx \sum_{i=1}^{m}\gamma_i(A + \theta_i I)^{-1},$$

   where $\gamma_i > 0$ are the weights, and $\theta_i > 0$, $i = 1, 2, \ldots, m$ are the nodes of the quadrature formula for (5).

2. An approximate solution to the problem (4):

$$v \approx \sum_{i=1}^{m}\gamma_i v_i, \quad (A + \theta_i I)v_i = f, \quad i = 1, 2, \ldots, m.$$

The inverse operator of the fractional power elliptic problem is treated as a sum of inverse operators of classical elliptic operators, and required an approximate solution of the problem as the sum of the solutions of standard elliptical BVP.

The integral representation of the fractional power of the elliptic operator, which is fundamentally different from (5) used in works N. Cusimano, F. del Teso, L. Gerardo-Giorda, G. Pagnini (2018), N. Cusimano, F. del Teso, L. Gerardo-Giorda (2018). It is

based on the method of semigroups, $A^{-\alpha}$ is defined through an integral formulation as follows

$$A^{-\alpha} = \frac{1}{\Gamma(\alpha)} \int_0^\infty \theta^{\alpha-1} e^{-\theta A} d\theta, \quad 0 < \alpha < 1, \tag{6}$$

where $\Gamma(\alpha)$ is gamma function. In this case, the solution to the problem (4) is

$$v = \frac{1}{\Gamma(\alpha)} \int_0^\infty \theta^{\alpha-1} e^{-\theta A} f \, d\theta. \tag{7}$$

Function $w(t) = e^{-tA} f$ is a solution of the following Cauchy problem

$$\frac{dw}{dt} + Aw = 0, \quad 0 < t < \infty, \tag{8}$$

$$w(0) = f. \tag{9}$$

By the representation (7) we have

$$v = \frac{1}{\Gamma(\alpha)} \int_0^\infty \theta^{\alpha-1} w(\theta) d\theta. \tag{10}$$

For (1), (2) the problem (8), (9) is the standard Cauchy problem for a second-order parabolic equation. Based on (10), the fractional elliptical BVP solution is represented through the solution IVP for the parabolic equation.

We note the most important features of the approximation of the fractional power of the operator $A^{-\alpha}$ and solving the problem (4) based on the integral representation (6).

1. Using quadrature formulas for (6) we come to the approximation $A^{-\alpha}$ with operator exponentials:

   $$A^{-\alpha} \approx \sum_{i=1}^{m} \gamma_i e^{-\theta_i A}.$$

   Here, as before, $\gamma_i > 0$, $\theta_i > 0$, $i = 1, 2, \ldots, m$ there are weights and nodes corresponding quadrature formula.

2. For an approximate solution to the problem (4) from (10) we have

   $$u \approx u_m = \sum_{i=1}^{m} \gamma_i w(\theta_i), \tag{11}$$

   where $w(t)$ is the solution to the problem (8), (9).

Thus, the computational algorithm for solving the problem (4) can be built on a numerical solution of the Cauchy problem (8), (9), according to which, in accordance with the selected quadrature formula (see (11)) we have approximate solution. Approximations of the desired solution fractional elliptical BVP is based on generalized Gauss-Laguerre formula, which most fully takes into account the singularity of the integral representation.

Subdiffusion with a time-dependent coefficient: analysis and numerical approximation

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The aim of this work is to study the subdiffusion equation with a time-dependent diffusion coefficient, by using a perturbation argument [7, 8]. Let $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) be a convex polyhedral domain with a boundary $\partial\Omega$. Consider the following fractional-order parabolic problem for the function $u(x,t)$:

$$\begin{cases} \partial_t^\alpha u(x,t) - A(x,t)u(x,t) = f(x,t) & (x,t) \in \Omega \times (0,T], \\ u(x,t) = 0 & (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) = u_0(x) & x \in \Omega, \end{cases} \tag{1}$$

where $T > 0$ is a fixed final time, f and u_0 are given source term and initial data, respectively. We assume that $A(x,t)u = \nabla \cdot (a(x,t)\nabla u)$, where the diffusion coefficient matrix $a(x,t) : \Omega \times (0,T] \to \mathbb{R}^{d\times d}$ is symmetric and smooth, and satisfies the ellipticity condition. The notation $\partial_t^\alpha u(t)$ denotes the left-sided Caputo derivative of order $\alpha \in (0,1)$, defined by [9, p. 70]

$$\partial_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \partial_s u(x,s) \mathrm{d}s. \tag{2}$$

The literature on the numerical analysis of the subdiffusion problem is vast; see the overview [5] (and the references therein). However, most of these works analyzed only the case that the diffusion coefficient a is independent of the time t. These works mostly employ Laplace transform and its discrete analogue for analysis, which are not directly applicable to the case of a time-dependent coefficient.

For standard parabolic problems with a time-dependent coefficient, there are a few relevant works [10, 12, 15, 16]. Unfortunately, the fractional derivative does not satisfy the well known Leibnitz rule. Hence, some traditional techniques working for heat equation cannot be directly applied here, and the analysis of fractional diffusion with time-dependent coefficients and its numerical approximation remain fairly challenging. Very recently, Mustapha [13] analyzed the spatially semidiscrete Galerkin FEM approximation of problem (1) using a novel energy argument, and established optimal-order convergence rates for both smooth and nonsmooth initial data. However, the work [13] did not discuss the source term and the analysis is under certain regularity assumptions on the solution, which have not been rigorously established yet.

In particular, we assume that

$$v \in L^2(\Omega) \qquad \text{and} \qquad \int_0^t (t-s)^{\alpha-1} \|f_t(s)\|_{L^2(\Omega)} \, \mathrm{d}s < 0. \tag{3}$$

In general, the solution of (1) is not smooth under these conditions.

To discretize the problem, let $\mathcal{T}_h$ be a shape regular quasi-uniform triangulation of the domain Ω, with the maximal diameter h, and $S_h \subset H_0^1(\Omega)$ be the space of continuous piecewise linear functions on the triangulation $\mathcal{T}_h$. Let $A_h(t) : S_h \to S_h$ be the discrete diffusion operator defined via duality [12]. Then the spatial semidiscrete scheme reads: find $u_h(t) \in S_h$ such that

$$\partial_t^\alpha u_h(t) + A_h(t)u_h(t) = f_h(t) := P_h f(t), \quad \forall\, t \in (0, T], \tag{4}$$

with $u_h(0) = v_h := P_h v$, where P_h denotes the L^2-projection operator. Further, let $\bar{\partial}_\tau^\alpha$ be the discrete fractional time derivative by the CQ generated by the backward Euler method [11]. Then the fully discrete scheme reads: find $U_h^n \in S_h$ such that

$$\bar{\partial}_\tau^\alpha (U_h^n - u_h^0) + A_h(t_n)U_h^n = P_h f(t_n), \quad n = 1, 2, \ldots, N, \tag{5}$$

with $U_h^0 = v_h$. We shall prove the error estimate that

$$\|U_h^n - u(t_n)\|_{L^2(\Omega)} \le c(h^2 \log(1 + 1/h)t_n^{-\alpha} + \tau \log(1 + t_n/\tau)t_n^{-1}) \tag{6}$$

under the regularity assumption (3). The logarithmic factors appear due to the singularity of the solution and the application of discrete Gronwall's inequality. If the diffusion operator is independent of time, the error estimate was given in [4] via Laplace transform, which is not applicable to the time-dependent case under consideration. Our basic strategy is to combine the existing estimates in [3, 2, 4] with a novel perturbation argument.

Specifically, we can reformulate the problem for any $t_0 \in (0, T]$ as

$$\partial_t^\alpha u(t) + A(t_0)u(t) = (A(t_0) - A(t))u(t) + f(t), \quad t \in (0, T],$$

Then the solution can be expressed by

$$u(t) = E(t; t_0)v + \int_0^t \bar{E}(t - s; t_0)(f(s) + (A(t_0) - A(s))u(s))\,\mathrm{d}s, \tag{7}$$

where the solution operators $E(t; t_0)$ and $\bar{E}(t - s; t_0)$ are well understood [14]. Now the desired regularity of the solution will follow from several perturbation estimates of the diffusion operator, the smoothing property of the operators $E(t; t_0)$ and $\bar{E}(t; t_0)$, the fixed point theorem and a generalized Gronwall's inequality.

This perturbation strategy is expected to be applicable to analyze the semidiscrete scheme (4). Specifically, the solution u_h of problem (4) can be represented by (a discrete analogue to (7))

$$u_h(t) = E_h(t; t_0)P_h v + \int_0^t \bar{E}_h(t - s; t_0)\Big(P_h f(s) + (A_h(t_0) - A_h(s))u_h(s)\Big)\mathrm{d}s, \tag{8}$$

where the semidiscrete operators $E_h(t; t_0)$ and $\bar{E}_h(t; t_0)$ were thoroughly studied in [3, 2]. Let $e_h = P_h u - u_h$. Then it follows from (7) and (8) that e_h can be expressed by

$$\begin{aligned} e_h(t) =& (P_h E(t; t_0) - E_h(t; t_0)P_h v) + \int_0^t (P_h E(t - s; t_0) - E_h(t - s; t_0)P_h) f(s)\mathrm{d}s \\ &+ \int_0^t (P_h E(t - s; t_0) - E_h(t - s; t_0)P_h)(A(t_0) - A(s))u(s)\mathrm{d}s \\ &+ \int_0^t E_h(t - s; t_0)\Big((P_h A(t_0) - P_h A(s))u(s) - (A_h(t_0) - A_h(s))u_h(s)\Big)\mathrm{d}s \end{aligned}$$

The first and second terms can be bounded by the regularity estimates and existing results in [3, 2]. The third and fourth terms follow analogously with some additional perturbation properties of the semidiscrete diffusion operator $A_h(t)$ and the corresponding Ritz projection operator. These together with Gronwall's inequality imply the error estimates.

To study the fully discrete scheme (5), it is crucial to derive the temporal regularity of the solution u. In particular, for CQ generated by backward Euler method, it is sufficient to prove that $\|\partial_t u(t)\|_{L^2(\Omega)} \leq ct^{-1}$ under the assumption (3). Then the perturbation argument, together with approximation properties of fully discrete solution operators and discrete Gronwall inequality, yields the desired error estimate (6).

Finally, we shall extend the perturbation argument to high-order time stepping schemes of subdiffusion equations with time-dependent diffusion coefficients. In [8], we propose a second-order time-stepping scheme for problem (1) with nonsmooth initial data and incompatible source term. It is based on the CQ generated by the second-order backward differentiation formula (BDF2), with suitable correction at the first step. The correction is inspired by the recent works [1, 4, 6] and essential for restoring the second-order convergence. We prove the a convergence rate $O(\tau^2)$ for any fixed $t_n > 0$, of the scheme for both nonsmooth initial data and incompatible source term. The error analysis relies heavily on new temporal regularity results for the model (1) and a refined perturbation argument, which substantially extends the prior work [7].

Numerical experiments are consistent with the theoretical results.

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