

# ***Numerical Solution of Fractional Diffusion Problems***

Svetozar Margenov

`marginov@parallel.bas.bg`

Institute of Information and Communication Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev Str. Bl. 25-A, 1113 Sofia, Bulgaria



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# 1. Introduction

- **Leibniz, in his correspondence with Bernoulli, L'Hospital and Wallis (1695), had several notes about the calculation of  $D^{1/2}u(x)$ . The further development of the theory of Fractional Calculus is due to the contributions of a plead of famous mathematicians such as Euler, Liouville and Riemann.**
- **The nowadays remarkable interest in fractional diffusion models is provoked by numerous applications related to Hamiltonian chaos and non-local continuum physics, discontinuities and long-range forces in elasticity, anomalous diffusion in complex systems, non-local electromagnetic fluid flows, fractional Cahn-Hilliard models of phase separation, contaminant transport in multiscale porous media, materials science, modeling of fiber enforced soft tissues and related biomedical applications, non-local epidemic models, image segmentation etc.**



# Superdiffusion



A. Einstein (1879-1955)



R. Brown (1773-1858)

- The fractional diffusion equations describe anomalous processes, that violate the Brownian motion hypothesis.
- An important subclass of such problems is defined by a fractional degree  $\alpha$  of the standard diffusion self-adjoint elliptic operator.
- The fractional operator is also self-adjoint but non-local.
- The case  $\alpha \in (0, 1)$  is referred to as sub-diffusion and corresponds to a process of superdiffusion.
- The regularity of the solution decreases for smaller  $\alpha$ .



# *Algebraic problem under consideration*

Let  $\mathcal{A}$  be a symmetric and positive definite matrix obtained from FDM or FEM approximations of a second order elliptic problem with pure Dirichlet boundary conditions.

Let  $\{\lambda_i\}_{i=1}^N$  and  $\{\Psi_i\}_{i=1}^N$  be the eigenvalues and eigenvectors of  $\mathcal{A}$ .

We consider the problem

$$\mathcal{A}^\alpha \mathbf{u} = \mathbf{f}.$$

The matrix  $\mathcal{A}^\alpha$  is defined through the spectral decomposition of  $\mathcal{A}$ , i.e.

$$\mathcal{A}^\alpha = \mathcal{W} \mathcal{D}^\alpha \mathcal{W}^T,$$

where  $\mathcal{A} = \mathcal{W} \mathcal{D} \mathcal{W}^T$ ,  $\mathcal{W} = [\Psi_1^T, \Psi_2^T, \dots, \Psi_N^T]$ ,  $\mathcal{D} = \text{diag}(\lambda_1, \dots, \lambda_N)$ , and consequently

$$\mathbf{u} = \mathcal{A}^{-\alpha} \mathbf{f} = \mathcal{W} \mathcal{D}^{-\alpha} \mathcal{W}^T \mathbf{f}.$$



## 2. The fractional diffusion problem

Consider the elliptic b.v. problem in  $\Omega \subset \mathbb{R}^d$  associated with the symmetric and positive definite bilinear form

$$A(u, v) := \int_{\Omega} (\mathbf{a}(x) \nabla u(x) \cdot \nabla v(x)) dx.$$

Let us introduce  $\mathcal{T} : L^2 := L^2(\Omega) \rightarrow V$ . For  $f \in L^2(\Omega)$ ,  $u = \mathcal{T}f \in V$  is the unique solution of  $A(u, \phi) = (f, \phi) \forall \phi \in V$ , where  $(\cdot, \cdot)$  is the inner product in  $L^2(\Omega)$ . The related operator equation is written in the form  $\mathcal{L}u = f$ ,  $\mathcal{L} = \mathcal{T}^{-1}$ .

We study the fractional diffusion equation

$$\mathcal{L}^\alpha u = f, \quad \mathcal{L}^\alpha u(x) = \sum_{i=1}^{\infty} \lambda_i^\alpha c_i \psi_i(x), \quad \text{where} \quad u(x) = \sum_{i=1}^{\infty} c_i \psi_i(x),$$

$\{\psi_i(x)\}_{i=1}^{\infty}$  are the eigenfunctions of  $\mathcal{L}$ , orthonormal in the  $L_2$ -inner product, and  $\{\lambda_i\}_{i=1}^{\infty}$  are the corresponding real and positive eigenvalues.



# 3. Transformation to local problems

- The fractional diffusion problems are non-local, i.e. the matrix  $A^\alpha$  is dense.
- Moreover, it is not computable in general, and the spectral decomposition is not applicable to solve the system.
- The following approaches based on transformation to local problems were proposed during last 5 years:
  - **A1. Extension to  $\Omega \times \mathbb{R}_+ \subset \mathbb{R}^{d+1}$**   
[\[Chen, Nochetto, Enrique, Salgado, 2016\]](#)
  - **A2. Pseudo-parabolic problem**  
[\[Vabishchevich, 2014\]](#)
  - **A3. Integral representation**  
[\[Bonito, Pasciak 2015\]](#)
  - **A4. BURA methods**  
[\[Harizanov, Lazarov, Margenov, Marinov, Vutov 2018\]](#)



## **A1. Extension to $\Omega \times \mathbb{R}_+ \subset \mathbb{R}^{d+1}$**

**The solution of fractional Laplacian problem is obtained by  $u(x) = v(x, 0)$**

**where  $v : \Omega \times \mathbb{R}_+ \rightarrow \mathbb{R}$  is a solution of the equation**

$$-div (y^{1-2\alpha} \nabla v(x, y)) = 0, \quad (x, y) \in \Omega \times \mathbb{R}_+,$$

**where  $v(\cdot, y)$  satisfies the original boundary conditions  $\forall y \in \mathbb{R}_+$ ,**

$$\lim_{y \rightarrow \infty} v(x, y) = 0, \quad x \in \Omega, \quad \lim_{y \rightarrow 0^+} (-y^{1-2\alpha} v_y(x, y)) = f(x), \quad x \in \Omega.$$

- **The FEM approximation uses the rapid decay of the solution  $v(x, y)$  in the  $y$  direction, thus enabling truncation to a bounded domain of modest size.**
- **The proposed multilevel method is based on the Xu-Zikatanov identity.**

**[Chen, Nocketto, Enrique, Salgado, 2016]**





## A2. Pseudo-parabolic problem

Assuming the boundary condition  $a(x) \frac{\partial u}{\partial n} + \mu(x)u = 0$ ,  $x \in \partial\Omega$ , the solution of fractional power diffusion problem  $u$  is presented as

$$u(x) = w(x, 1), \quad w(x, 0) = \delta^{-\alpha} f,$$

where  $w(x, t)$ ,  $0 < t < 1$ , is the solution of pseudo-parabolic equation

$$(t\mathcal{D} + \delta\mathcal{I}) \frac{dw}{dt} + \alpha\mathcal{D}w = 0, \quad \mathcal{D} = \mathcal{L} - \delta\mathcal{I} \geq 0.$$

- Stability conditions are obtained for the fully discrete schemes.
- A further development in case of fractional order boundary conditions is studied.

[Vabishchevich, 2014], [Vabishchevich, 2015], [Lazarov, Vabishchevich, 2017]



### A3. Integral representation

The following representation of the solution of is used

$$\mathcal{L}^{-\alpha} = \frac{2 \sin(\pi\alpha)}{\pi} \int_0^{\infty} t^{2\alpha-1} (\mathcal{I} + t^2 \mathcal{L})^{-1} dt,$$

introducing an exponentially convergent quadrature scheme. Then, the approximate solution only involves evaluations of  $(\mathcal{I} + t_i \mathcal{A})^{-1} f, t_i \in (0, \infty)$ .

- The computational complexity depends on the number of quadrature nodes. For instance, approximately 40 auxiliary linear systems have to be solved to get accuracy of the quadrature scheme of order  $O(10^{-3})$  for  $\alpha \in \{0.25, 0.75\}$ .
- A further generalization of this approach provides theoretical analysis in the class of regularly accretive operators.

[Bonito, Pasciak 2015], [Bonito, Pasciak 2016]



## 4. BURA methods

- The BURA methods are based on Best Uniform Rational Approximation of  $t^\alpha$ ,  $t \in [0, 1]$ .
- The basic concept is to construct a class of robust methods of optimal computational complexity.
- The BURA methods are developed at the level of the discrete problem, i.e. they are aimed at solving the linear system  $\mathcal{A}^\alpha \mathbf{u} = \mathbf{f}$ .
- More recently, it was explicitly shown that the approaches A1-A3 can be interpreted as some rational approximation of degree  $k$ ,  $R_k(A)$  of  $\mathcal{A}^{-\alpha}$ .  
[Hofreither 2019]

In this sense, for a fixed degree  $k$  of the related approximation, the BURA methods are the best.



## 4.1. Construction of the method

- The method is based on the best uniform rational approximation along the diagonal of the Walsh table (just BURA for simplicity)  $r_{\alpha,k}(t)$  of  $t^\alpha$  on  $[0, 1]$ , where  $k$  is a small integer. More precisely, the minimizer  $r_{\alpha,k}(t) = P_k(t)/Q_k(t) \in \mathcal{R}(k)$

$$\min_{\bar{r}_k \in \mathcal{R}(k)} \max_{t \in [0,1]} |t^\alpha - \bar{r}_k(t)|,$$

is called BURA of  $t^\alpha$ .

- Then, the approximate solution of the fractional power linear system is defined as

$$\mathbf{u} \approx \mathbf{u}_r = \lambda_2^{-\alpha} r_{\alpha,k}(\lambda_2 \mathcal{A}^{-1}) \mathbf{f},$$

where  $\lambda_2$  is the first positive eigenvalue of  $\mathcal{A}$ .

- To find the BURA of  $t^\alpha$ , we apply the modified Remez algorithm. The main difficulty in implementing the algorithm is its instability for larger  $k$ .



## 4.2. Error analysis

- Let us denote the error of BURA by

$$E_{\alpha,k} := \max_{t \in [0,1]} |t^\alpha - r_{\alpha,k}(t)|.$$

- The following estimate follows from Theorem 1 of [\[Stahl, 1993\]](#)

$$E_{\alpha,k} \leq C_\alpha e^{-2\pi\sqrt{k\alpha}}.$$

- Then the final estimate derived by a spectral decomposition of the error reads as:

$$\|\mathbf{u} - \mathbf{u}_r\| = \|\mathbf{u} - \lambda_2^{-\alpha} \mathbf{r}_{\alpha,k}(\lambda_2 \mathcal{A}^{-1}) \mathbf{f}\| \leq C_\alpha e^{-2\pi\sqrt{k\alpha}} \|\mathbf{f}\|.$$

- The convergence rate is exponential with respect to the degree  $k$ .
- The smallest positive eigenvalue  $\lambda_1 = O(1)$ , i.e. the final error estimate is robust with respect to the condition number of the (standard) diffusion matrix  $\mathcal{A}$ .
- A smaller  $\alpha$  (stronger superdiffusion) means a lower convergence rate.



# Computed values of BURA errors

- We present the computed "exact" errors of BURA  $r_{\alpha,k}(t)$  of  $t^\alpha$  using the modified Remez algorithm.
- As expected, the approximation error for large  $\alpha$  is in the very reasonable range of  $10^{-5} - 10^{-7}$  for  $k = 5 - 10$ .
- Moreover, for this range of  $k$  the Remez algorithm is stable and the coefficients of BURA function  $r_{\alpha,k}(t)$  are determined with good accuracy.

Table 1: Errors  $E_{\alpha,k}$  of  $r_{\alpha,k}(t)$  for  $t \in [0, 1]$

$\alpha$	$E_{\alpha,5}$	$E_{\alpha,6}$	$E_{\alpha,7}$	$E_{\alpha,9}$	$E_{\alpha,9}$	$E_{\alpha,10}$
0.75	2.8676e-5	9.2522e-6	3.2566e-6	1.2288e-6	4.9096e-7	2.0584e-7
0.50	2.6896e-4	1.0747e-4	4.6037e-5	2.0852e-5	9.8893e-6	4.8760e-6
0.25	2.7348e-3	1.4312e-3	7.8650e-4	4.4950e-4	2.6536e-4	1.6100e-4

The first 25 correct decimal digits of the BURA error of  $t^\alpha$  for six values of  $\alpha$  are reported for degrees up to  $k = 30$  by using computer arithmetic with 200 significant digits.

[Varga, Carpenter 1992]



# Total error estimate

Let  $\Omega \subset \mathbb{R}^2$  and let BURA method is used to solve the algebraic problem arising from lumped finite element discretization of the spectral fractional diffusion problem. Then, the following total error estimate holds true

$$\begin{aligned} \|\mathcal{L}^{-\alpha} f - u_h\| &\leq C(h^{2\alpha} + h^{1+\gamma})\|f\|_{H^{1+\gamma}(\Omega)} + \lambda_1^{-\alpha} E_{\alpha,k}\|f\| \\ &\leq C(h^{2\alpha} + h^{1+\gamma})\|f\|_{H^{1+\gamma}(\Omega)} + \lambda_1^{-\alpha} e^{2\pi\sqrt{k\alpha}}\|f\|, \end{aligned}$$

$f \in H^{1+\gamma}(\Omega)$  with  $\gamma > 0$ .

- The contributions of the FEM discretization and the BURA approximation to the total error can be balanced choosing properly  $h$  and  $k$ .
- The BURA error is controlled by  $E_{\alpha,k}$  and the  $L^2$ -norm of the data  $f$ . This allows to choose  $k$  by using Table 1 once the desired accuracy is fixed.
- To choose the mesh that guarantees the same accuracy we need to use either Richardson extrapolation or any other technique for error control of the finite element method by mesh refinement.



## 4.3. Implementation and complexity

- It is proven that  $k$  zeros and poles of  $r_{\alpha,k}$  are real and negative and are interlacing.
- Then the following represented as a sum of partial fractions holds true

$$r_{\alpha,k}(t) = c_0 + \sum_{j=1}^k \frac{c_i}{t - d_i}.$$

- Therefore, the BURA methods reduce the non-local system  $\mathcal{A}^\alpha \mathbf{u} = \mathbf{f}$  to solution of  $k$  sparse systems like  $(\mathcal{A} + d\mathbf{I})\mathbf{v} = \mathbf{f}$ ,  $d > 0$ .
- The implementation of BURA methods have optimal complexity assuming that each evaluation of  $(\mathcal{A} + d\mathbf{I})^{-1}\mathbf{f}$  can be computed approximately by PCG method with optimal complexity.
- For this purpose, the BoomerAMG algebraic multigrid PCG solver is used in the numerical tests included in this presentation.





# 5. Numerical tests

Two sets of numerical tests are presented.

- A model 2D problem in the unit square  $[0, 1] \times [0, 1]$  with a uniform mesh is considered at the beginning.
  - The discretization (FDM or FEM) accuracy of order  $O(h^{2\alpha})$  is illustrated;
  - Some advantages of BURA methods in comparison with Q-methods (A3) are shown.
- The second set of numerical experiments concerns a large scale 3D problem in computational domain with complex geometry and unstructured FEM mesh.
  - Some scalability issues are discussed.
  - The computational efficiency is analyzed.



# Model problem in the unit square

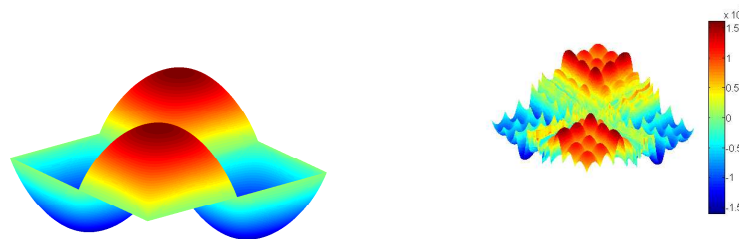


Fig. 1: Checkerboard right-hand-side: solution of fractional Laplacian and the BURA error.

Table 1:  $L_\infty$  relative error of the FEM/FDM discretization:  $h = 1/(n + 1)$ ,  $\alpha = 0.25$ .

n	128	256	512	1 024	2 056
$L_\infty$	0.00946	0.00669	0.00473	0.00334	0.00236

The observed convergence rate  $O(h^{2\alpha}) = O(\sqrt{h})$  fits the theory.

Table 2:  $l_\infty$  relative error for BURA ( $k = 9$ ), Q-method ( $k = 9$ ), and  $k'$ Q-method ( $k = 120$  for  $\alpha = 0.25, 0.75$ , and  $k = 91$  for  $\alpha = 0.5$ ).

$\alpha$	$h$	BURA	Q-method	$k'$ Q-method
0.25	$2^{-12}$	7.451e-4	1.069e-2	6.413e-4
0.50	$2^{-12}$	1.909e-5	2.902e-3	1.132e-5
0.75	$2^{-12}$	4.574e-7	1.823e-3	2.079e-7

The Quadrature method needs between 10 and 13 times more systems to solve to get the same order of accuracy as BURA.



# 3D test problem on unstructured mesh

We are solving the linear system  $\mathcal{A}^\alpha \mathbf{u} = \mathbf{f}$  where  $\mathcal{A}$  and  $\mathbf{f}$  correspond to FEM discretization of the 3D Laplace problem with pure Neumann b.c.:

$$\begin{aligned} -\Delta u &= 0, \quad x \in \Omega, \\ \frac{\partial u}{\partial \mathbf{n}} &= 0, \quad x \in \Gamma_R, \\ -\frac{\partial u}{\partial \mathbf{n}} &= g_I, \text{ on } \Gamma_I, \\ -\frac{\partial u}{\partial \mathbf{n}} &= g_O, \text{ on } \Gamma_O. \end{aligned}$$

$\Omega$  consists of two cylinders, where  $\partial\Omega = \Gamma_I \cup \Gamma_O \cup \Gamma_R$ ,  $\Gamma_I$  and  $\Gamma_O$  are the left and right bases of the larger and smaller cylinders respectively. The functions  $g_I$  and  $g_O$  satisfy the equation

$$\int_{\Gamma_I} g_I dx + \int_{\Gamma_O} g_O dx = 0.$$



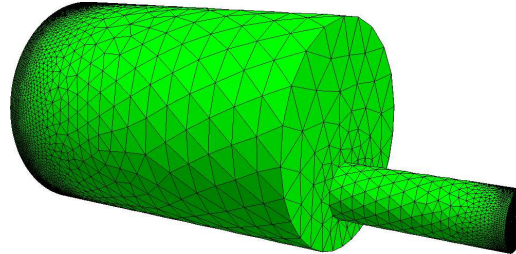


Fig. 2: Computational domain: locally refined unstructured tetrahedral mesh.

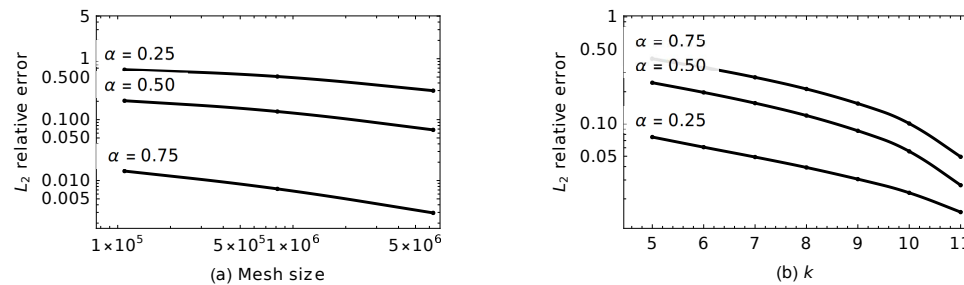


Fig. 3:  $L_2$  relative errors:  $\frac{\|\mathbf{u}_i^1 - \mathbf{u}_4^1\|_M}{\|\mathbf{u}_4^1\|_M}$  and  $\frac{\|\mathbf{u}_i - \mathbf{u}_{12}\|_M}{\|\mathbf{u}_{12}\|_M}$ .

- Fig. 3 (left) illustrates the decrease of the convergence rate for smaller  $\alpha$  like  $O(h^{2\alpha})$ .
- Fig. 3 (right) confirms the exponential convergence rate of BURA with respect to  $k$ .



## 6. Concluding remarks

- The recently introduced improved BURA methods are robust with respect to the spectral condition number  $\kappa(\mathcal{A})$ .
- The considered test problem with a Checkerboard r.h.s. confirm the advantages of BURA method.
- The presented large-scale numerical tests with up to  $O(10^7)$  DOF provide some promising proofs of concept of the proposed approach.

### Extreme size EXAMPLE:

- Standard diffusion: FEM error estimate  $O(h^2)$ ;  $h = 10^{-2}$  is needed for  $O(10^{-4})$  accuracy, leading to  $N = O(10^6)$  DOF of the 3D model problem;
- Fractional diffusion: FEM error estimate  $O(h^{2\alpha})$ ; superdiffusion case  $\alpha = 0.5$ ;  $h = 10^{-4}$  is needed for  $O(10^{-4})$  accuracy, leading to  $N = O(10^{12})$  DOF of the 3D model problem.



# *Some additional related results*

- The BURA methods provide positive approximation of the inverse of fractional powers of symmetric and positive definite M-matrices. Such results hold true for finite difference and lumped mass finite element discretization.
- The BURA methods are robust with respect to the spectral condition number  $\kappa(\mathcal{A})$ . Based on this, efficient methods and algorithms for local mesh refinement are developed. They cover for instance boundary and interior layers as well as  $\delta$ -function r.h.s.
- BURA methods for fractional diffusion-reaction problems are proposed and studied. The obtained results can be used to construct efficient solution methods for time dependent fractional-in-space problems.
- BURA methods for fractional diffusion problems with Neumann boundary conditions are proposed and analyzed. They provide approximation of the Moore-Penrose pseudo inverse of  $\mathcal{A}$ .



# ***Selected related papers***

1. S. Harizanov, S. Margenov, P. Marinov, Y. Vutov, Volume constrained 2-phase segmentation method utilizing a linear system solver based on the best uniform polynomial approximation of  $x^{1/2}$ , **J. Computational and Applied Mathematics**, 310 (2017) 115-128
2. S. Harizanov, S. Margenov, Positive approximations of the inverse of fractional powers of SPD M-matrices, **Control Systems and Mathematical Methods in Economics: Essays in Honor of Vladimir M. Veliov**, 687 (2018), 147-163
3. R. Ciegis, V. Starikovicius, S. Margenov, R. Kriauziene, Parallel solvers for fractional power diffusion problems, **Concurrency and Computation: Practice and Experience**, Vol. 29 (4) (2018), <https://doi.org/10.1002/cpe.4216>
4. R. Ciegis, V. Starikovicius, S. Margenov, R. Kriauziene, Scalability analysis of different parallel solvers for 3D fractional power diffusion problems, **Concurrency and Computation: Practice and Experience** (2019), e5163, <https://doi.org/10.1002/cpe.5163>
5. S. Harizanov, R. Lazarov, P. Marinov, S. Margenov, Numerical solution of fractional diffusion reaction problems based on BURA, **Computers and Mathematics with Applications** (2019), [tps://doi.org/10.1016/j.camwa.2019.07.002](https://doi.org/10.1016/j.camwa.2019.07.002)
6. S. Harizanov, R. Lazarov, P. Marinov, S. Margenov, J. Pasciak, Analysis of numerical methods for spectral fractional elliptic equations based on the best uniform rational approximation, **arXiv:1905.08155**, 2019



[http://parallel.bas.bg/Conferences/NSFDE&A\\_2020-Sozopol.pdf](http://parallel.bas.bg/Conferences/NSFDE&A_2020-Sozopol.pdf)

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