Parallel BURA Based Numerical Solution of Fractional Laplacian with Pure Neumann Boundary Conditions

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Abstract. The study is motivated by the increased usage of fractional Laplacian in the modeling of nonlocal problems like anomalous diffusion. We present a parallel numerical solution method for the nonlocal elliptic problem: $-\Delta^\alpha u = f$, $0 < \alpha < 1$, $-\partial u(x)/\partial n = g(x)$ on $\partial\Omega$, $\Omega \subset \mathbb{R}^d$. The Finite Element Method (FEM) is used for discretization leading to the linear system $A^\alpha \mathbf{u} = \mathbf{f}$, where A is a sparse symmetric and positive semidefinite matrix. The implemented method is based on the Best Uniform Rational Approximation (BURA) of degree k, $r_{\alpha,k}$, of the scalar function t^α, $0 \le t \le 1$. The related approximation of $A^{-\alpha}\mathbf{f}$ can be written as a linear combination of the solutions of k local problems. The latter are found using the preconditioned conjugate gradient method. The method is applicable to computational domains with general geometry. Linear finite elements on unstructured tetrahedral meshes with local refinements are used in the presented numerical tests. The behavior of the relative error, the number of Preconditioned Conjugate Gradient (PCG) iterations, and the parallel time is analyzed varying the parameter $\alpha \in \{0.25, 0.50, 0.75\}$, the BURA degree $k \in \{5, 6, \ldots, 12\}$, and the mesh size.

Keywords: BURA · fractional diffusion · Neumann boundary conditions · unstructured meshes · parallel algorithm.

1 Introduction

The recent advancement in fractional calculus and the progress towards extreme scale computing create possibilities for computer simulation and investigation of more complicated real life nonlocal phenomena. Fractional Laplacian is used to model anomalous diffusion, which appears in applications like turbulent fluid motion, material transport in fractured media, underground flow. These are just some examples of nonlocal problems, where the fractional diffusive flux at a certain location is affected by the state of the field in the entire space. An introduction to the fractional Laplacian with some emphasis on fundamental ideas and model numerical computations is given in [1]. During last years, several numerical methods for fractional diffusion problems assuming general domain were

proposed (e.g.[2–4]), following the common idea of transforming the problem to some auxiliary local differential equation in a computational domain of a higher dimension. The alternative approach proposed in [5] (see also [6]) is devoted to solution of linear systems with fractional powers of sparse SPD matrices. The developed methods are based on the best uniform rational approximations (BURA). A unified view of some numerical methods for fractional diffusion is recently published in [7], showing that the methods from [2–4] are equivalent to certain rational approximations. This means that when applicable, the BURA methods are expected to be the best. The analysis of some first parallel implementations of the methods from [2, 4, 5] (see [5, 8] and the references there in) also confirms the advantages of BURA methods. The discussed methods consider the case of fractional diffusion problems with homogeneous Dirichlet boundary conditions, where the numerical tests are mostly in domains like $\Omega = (0,1)^d$.

Our goal is to generalize the improved BURA method from [6] to the case of pure Neumann boundary conditions. The matrix A in the related linear system $A^\alpha \mathbf{u} = \mathbf{f}$ is sparse symmetric and positive semidefinite. The domain has a nontrivial geometry. Linear finite elements on unstructured tetrahedral meshes with local refinement are used in the presented numerical tests. The remainder of the paper is organized as follows. The fractional diffusion problem in terms of spectral decomposition is introduced in the next section. The main idea of the BURA method is presented briefly in Section 3. The numerical tests are presented and analyzed in Section 4. Some concluding remarks and notes on the further steps are given at the end.

2 Fractional diffusion problem

The definition of a fractional diffusion problem based on the spectral decomposition is used in this work. Let us consider the elliptic boundary value problem

$$\begin{aligned} -\Delta u(x) &= f(x), \quad x \in \Omega, \\ -\frac{\partial u(x)}{\partial \mathbf{n}} &= g(x), \quad x \in \partial\Omega \end{aligned} \tag{1}$$

in $\Omega \subset \mathbb{R}^d$ with $\mathbf{n}$ denoting the outward normal unit vector for $\partial\Omega$. The weak formulation (see [9]) of (1) is: *given* $f \in L^2(\Omega)$ *and* $g \in L^2(\partial\Omega)$ *find* $u \in H^1(\Omega)$ *such that*

$$\int_\Omega \nabla u(x) \cdot \nabla v(x) dx = \int_\Omega f(x) v(x) dx + \int_{\partial\Omega} g(\gamma) v(\gamma) d\gamma, \qquad \forall v \in H^1(\Omega),$$

where $d\gamma$ *denotes the surface measure of* $\partial\Omega$. This weak formulation is used to define the fractional power operator Δ^α, $0 < \alpha < 1$, through its spectral decomposition

$$\Delta^\alpha u = f, \; \Delta^\alpha u(x) = \sum_{i=1}^{\infty} \lambda_i^\alpha c_i \psi_i(x), \quad \text{where} \quad u(x) = \sum_{i=1}^{\infty} c_i \psi_i(x), \tag{2}$$

$\{\psi_i(x)\}_{i=1}^{\infty}$ are the L_2-orthonormal eigenfunctions of Δ, the eigenvalue $\lambda_1 = 0$ corresponds to the constant eigenfunction $\psi_1(x)$, and the rest eigenvalues $\{\lambda_i\}_{i=2}^{\infty}$ are real and positive. Similar definition of the fractional power of the related symmetric and positive semidefinite matrix is assumed.

3 Parallel BURA Based Solution Method

We generalize the method from [6] to solve in parallel the pure Neumann fractional diffusion problem (2). The essential steps are briefly presented below.

3.1 Best uniform rational approximation

The element of best uniform rational approximation (BURA) of t^α, $0 < \alpha < 1$ is a rational function $r_{\alpha,k}$ of polynomials of degree k that minimizes the error

$$\|r_{\alpha,k} - t^\alpha\|_{C[0,1]}.$$

The modified Remez algorithm is used to compute the parameters of $r_{\alpha,k}$ (see e.g. [5]). Now, the rational function $\widetilde{r}_{\alpha,k}(\xi) = r_{\alpha,k}(1/t), \xi \in [1, +\infty)$ is introduced and the coefficients $c_i > 0$ and $d_i < 0$ of the partial fraction representation

$$\widetilde{r}_{\alpha,k}(\xi) = c_0 + \sum_{i=1}^{k} \frac{c_i}{\xi - d_i}$$

are computed.

3.2 Discrete problem

The initial (local) problem (1) is discretized by linear finite elements on an unstructured (tetrahedral in the 3D case) mesh. The resulting system of linear algebraic equations (with imposed boundary conditions) can be written as

$$A\mathbf{u} = \mathbf{f}\,,$$

$A = M^{-1}S$, where S and M are the stiffness and the lumped mass matrices respectively. Following the approach in [6], the solution of the nonlocal problem (2) is approximated by

$$\mathbf{u} = A^{-\alpha}\mathbf{f} \approx \lambda_2^{-\alpha}\left(c_0\mathbf{f} + \sum_{i=1}^{k}((\lambda_2 c_i)(A - \lambda_2 d_i I)^{-1})\mathbf{f}\right) \tag{3}$$

where λ_2 is the smallest positive eigenvalue of A. A is symmetric with respect to the dot product generated by the diagonal (lumped) mass matrix M. It is important to note that A is positive definite in the subspace orthogonal to the constant vectors. The expression (3) means, that in order to find the BURA approximation of $\mathbf{u}$, one has to compute a linear combination of the solutions of k local problems with matrices $A_i = A - \lambda_2 d_i I$ scaled by $(\lambda_2 c_i)$. A parallel PCG solver is applied to these auxiliary sparse symmetric and positive definite systems.

3.3 Solution steps

The tetrahedral mesh of the Ω is distributed among processors using ParMETIS [10]. The coefficients c_i, d_i of the BURA approximation with polynomials of degree k are computed in advance and read by the program. Each of the k linear systems of algebraic equations are solved using the Preconditioned Conjugate Gradient (PCG) method (see e.g. [11] for details) with a parallel multigrid implementation BoomerAMG from the library *HYPRE* [12] as the preconditioner. The same preconditioner, constructed from the linear system with the smallest root d_1, is used for the solution of all systems. The approximation of the solution is calculated using (3). More details on the computational setting and the results of the performed numerical tests are presented in the next section.

4 Numerical experiments

We are solving the linear system $A^\alpha \mathbf{u} = \mathbf{f}$, where $0 < \alpha < 1$, and A and $\mathbf{f}$ correspond to FEM discretization of the following 3D Laplace problem with pure Neumann boundary conditions:

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

The computational domain consists of two cylinders (see Fig. 1), where $\partial\Omega = \Gamma_I \cup \Gamma_O \cup \Gamma_R$, Γ_I and Γ_O are the left and right bases of the larger and smaller cylinders respectively. The functions g_I and g_O satisfy the equation

$$
\int_{\Gamma_I} g_I d\gamma + \int_{\Gamma_O} g_O d\gamma = 0. \tag{4}
$$

More precisely, Γ_I and Γ_O are circles, g_O is a parabolic function vanishing at $\partial\Gamma_O$, with a value of g_O equal to 1 at the center of Γ_O, and g_I is a constant determined by (4). Using Netgen [13], the computational domain is discretized by tetrahedral elements, applying local refinement near the boundaries with nonzero boundary conditions. The resulting mesh is illustrated in Fig. 1. It consists of 109 385 nodes and 572 794 tetrahedral elements. This initial mesh $\mathcal{M}_1$ is further uniformly refined three times to get the meshes $\mathcal{M}_i$ for $i \in \{2, 3, 4\}$. Let us denote by N_i the number of nodes (number of unknowns of the FEM system) corresponding to $\mathcal{M}_i$. Then, $N_{i+1} \approx 8N_i$, and $N_4 \approx 5 \times 10^7$.

The presented numerical experiments are split in three parts. The first of them is devoted to the convergence rate of the FEM discretization with respect to the mesh size. After that, accuracy of BURA approximation on the finest

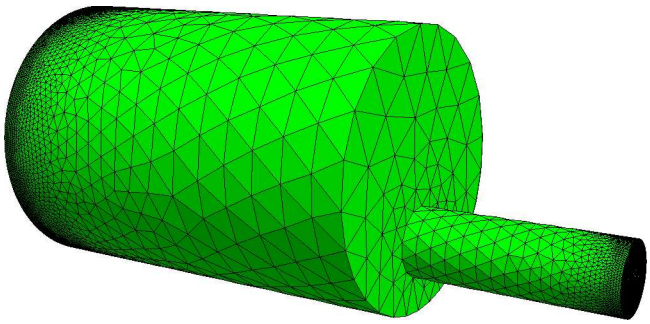

Fig. 1. Computational domain with locally refined unstructured mesh

mesh is investigated, varying the degree k. The last experiments illustrate the overall performance of the developed solver.

Further, the solution on mesh $\mathcal{M}_i$ with order of BURA k is denoted with $\mathbf{u}_i^k$. Since the exact solution of the test problem is unknown, to investigate the rate of convergence, we solve the problem on all available meshes and consider the solution, obtained on the finest mesh as a reference solution. The relative error

$$\frac{\|\hat{\mathbf{u}}_i^{12} - \hat{\mathbf{u}}_4^{12}\|_M}{\|\hat{\mathbf{u}}_4^{12}\|_M}$$

is used for that purpose, where $\hat{\mathbf{u}}_i^k$ is the restriction of the numerical solution $\mathbf{u}_i^k$ to the nodes of the mesh $\mathcal{M}_1$. For this set of experiments, PCG tolerance of $\varepsilon = 10^{-12}$ is used to make sure the PCG solver accuracy does not interfere with the analyzed results. For a similar purpose, the largest considered value of $k = 12$ is used for the BURA approximation.

Here and in what follows $\|\mathbf{u}\|_M$ stands for the energy norm $(\mathbf{u}^T M \mathbf{u})^{\frac{1}{2}}$ associated with the matrix M. Since M is the lumped mass matrix, $\mathbf{u}^T M \mathbf{u}$ is a quadrature formula for the integral $\int_\Omega u^2(x)dx$. Therefore $\|\cdot\|_M$ is approximately equal to the L_2 norm in the related FEM space.

The obtained results are presented in Fig. 2 (a). The general conclusion is that the convergence rate decreases for smaller values of α indicating some behaviour of the presented relative errors like $O(h^{2\alpha})$.

Next, we turn our attention to the BURA approximation and the influence of its degree k to the accuracy of the solution. Here, we consider only the solutions obtained on the finest mesh $\mathcal{M}_4$. Again, the PCG tolerance is set to $\varepsilon = 10^{-12}$. In this case, we consider the solution with $k = 12$ as a reference one, and compare the other solutions using a similar relative error in the form

$$\frac{\|\mathbf{u}_4^k - \mathbf{u}_4^{12}\|_M}{\|\mathbf{u}_4^{12}\|_M}.$$

The related results are plotted on Fig. 2 (b). According to the the general theory (see [6]) the BURA methods have an exponential convergence rate with respect to k, which is confirmed by the presented results.

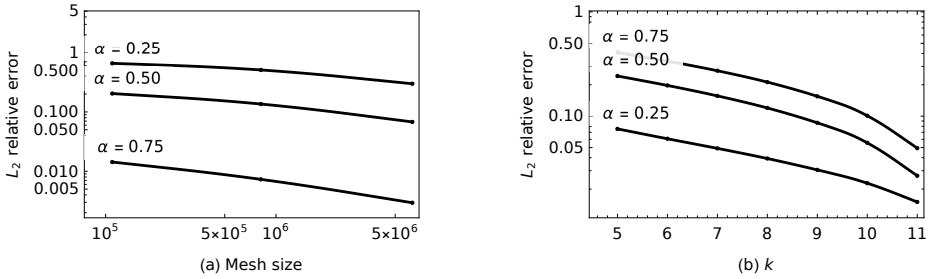

Fig. 2. Relative errors: $\frac{\|\hat{\mathbf{u}}_i^{12}-\hat{\mathbf{u}}_4^{12}\|_M}{\|\hat{\mathbf{u}}_4^{12}\|_M}$ (a) and $\frac{\|\mathbf{u}_4^{k}-\mathbf{u}_4^{12}\|_M}{\|\mathbf{u}_4^{12}\|_M}$ (b)

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Here, it is worth to remember that the introduced relative errors use reference solutions instead of the exact one. In general, the conducted 3 consecutive mesh refinements could not be enough for reliable quantitative conclusions. In this sense, the analysis of the presented results is most likely qualitative.

Lastly, we investigate the performance of the developed solver for $k = 12$. Based on the previous numerical tests and the observed behavior of the relative errors, we set $\varepsilon = 10^{-6}$ for the PCG tolerance. In this case, the approximate solution of the considered fractional diffusion problem involves solving 12 linear systems with the matrices $A_i = (A - \lambda_2 d_i I)/(\lambda_2 c_i)$, $i = 1, \ldots, 12$. One can observe that they are quite similar to matrices arising from normal time-dependent diffusion problems. This allows us to use any efficient preconditioner for such problems. In our case, we have chosen BoomerAMG – a parallel algebraic multigrid implementation from LLNL's HYPRE library [12]. The matrices A_i are differently conditioned. The first one always has the highest condition number, and in the presented numerical results, the AMG preconditioner for A_1 is used for all systems. As expected, different number of iterations are needed to converge to the set tolerance for the systems with different matrices A_i. The PCG iterations for each of the systems in the BURA approximation (3), the total number of iterations N_{tot}^{it}, the solution time T_{sol} and the total time T_{tot} are presented in Table 1, for all mesh refinements $\mathcal{M}_i$, $i = 1, 2, 3, 4$ varying also $\alpha \in \{0.25, 0.50, 0.75\}$.

The computations are performed on the Avitohol supercomputer [14] located at IICT-BAS. It consists of 16 core nodes with Intel XeonE5-2650 v2 CPU, running at 2.60GHz, interconnected with InfiniBand FDR network. All runs were performed on 64 cores using 4 nodes.

The reported total times include the solution time as well as the time for discretization of the problem.

The finer meshes require more PCG iterations for all α. This is due to the aggressive coarsening used in the BoomerAMG setting in order to get a better parallel efficiency. For all meshes $\mathcal{M}_i$, the iteration counts and the solution times decrease with the decrease of α. Let us denote by T_{tot}^i the time corresponding to

Table 1. PCG iterations and parallel times for solution of the fractional Laplacian problem with $k = 12$, $\varepsilon = 10^{-6}$, including the auxiliary linear systems with matrices $A_i = (A - \lambda_2 d_i I)/(\lambda_2 c_i)$.

α	0.25				0.50				0.75			
Mesh	$\mathcal{M}_1$	$\mathcal{M}_2$	$\mathcal{M}_3$	$\mathcal{M}_4$	$\mathcal{M}_1$	$\mathcal{M}_2$	$\mathcal{M}_3$	$\mathcal{M}_4$	$\mathcal{M}_1$	$\mathcal{M}_2$	$\mathcal{M}_3$	$\mathcal{M}_4$
A_1	11	14	17	19	13	16	19	20	15	18	20	21
A_2	7	9	12	15	8	12	14	17	10	13	16	18
A_3	5	7	9	11	6	8	11	14	7	10	13	16
A_4	3	4	6	8	5	6	8	11	6	8	10	13
A_5	2	3	4	5	3	4	6	8	4	6	8	11
A_6	3	3	2	3	2	3	4	6	3	4	6	8
A_7	3	3	3	2	3	2	3	4	2	3	4	6
A_8	2	2	2	2	2	3	3	2	3	2	3	4
A_9	2	2	2	2	3	2	2	2	3	3	2	3
A_{10}	2	2	2	2	2	2	2	2	2	3	3	2
A_{11}	2	2	2	2	2	2	2	2	2	2	2	2
A_{12}	2	2	2	2	2	2	2	2	2	2	2	2
N_{tot}^{it}	44	53	63	73	51	62	76	90	59	74	89	106
T_{sol}[s]	0.20	0.69	4.8	45	0.24	0.86	5.9	55	0.29	1.01	7.0	65
T_{tot}[s]	0.26	1.07	7.7	67	0.30	1.24	8.8	77	0.35	1.39	9.8	86

the mesh $\mathcal{M}_i$. Let us consider the efficiency ratio $E_i = 8\, T_{tot}^{i-1}/T_{tot}^{i}$ to illustrate the total time scalability. Then $E_4 \approx 91\%$ for all α.

5 Concluding remarks

The recently introduced improved BURA method [6] is generalized to the case of fractional diffusion problems with pure Neumann boundary conditions. The considered test problem concerns FEM discretization on unstructured tetrahedral meshes in realistic computational domain with general geometry. The presented large-scale (up to $O(10^7)$ degrees of freedom) numerical results provide some promising proofs of concept of the proposed approach. The following open questions are derived.

The theoretical error estimates of the FEM numerical solutions of fractional diffusion problems with pure Neumann boundary conditions are beyond the scope of this study. However, they are strongly required for future development of the discussed solution methods. Then, a more accurate reference solution will be needed to get some reliable quantitative results analyzing the experimental data. The accuracy (when applicable) of the gradient of BURA computed approximation is the next important question, taking into account the lower regularity of the solution for smaller values of α.

In many of the currently available papers, when comparing some methods for numerical solution of fractional diffusion problems, the number of auxiliary local systems needed to get a certain accuracy is accepted as a measure of the

related computational complexity. However, the results presented in Table 1 show rather different numbers of iterations to solve the systems with different matrices A_i. The conclusion is that some more involved study at this point is required, including the reasonable stopping criteria for the PCG iterations.

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References

1. Pozrikidis, C.: The Fractional Laplacian, CRC Press, Taylor&Francis Group (2016)
2. Bonito, A., Pasciak, J.: Numerical approximation of fractional powers of elliptic operators. Mathematics of Computation, **84**(295), 2083–2110 (2015)
3. Chen, L., Nochetto, R., Enrique, O., Salgado, A.J.: Multilevel methods for nonuniformly elliptic operators and fractional diffusion. Mathematics of Computation, **85**, 2583–2607 (2016)
4. Vabishchevich, P.N.: Numerically Solving an Equation for Fractional Powers of Elliptic Operators. Journal of Computational Physics. 282, 289–302 (2015)
5. Harizanov, S., Lazarov, R., Margenov, S., Marinov, P., Vutov, Y.: Optimal solvers for linear systems with fractional powers of sparse SPD matrices. Numer Linear Algebra Appl. **25**(5), e2167. https://doi.org/10.1002/nla.2167 (2018)
6. Harizanov, S., Lazarov, R., Marinov, P., Margenov, S., Pasciak, J.: Analysis of numerical methods for spectral fractional elliptic equations based on the best uniform rational approximation. arXiv preprint arXiv:1905.08155 (https://arxiv.org/abs/1905.08155) (2019)
7. Hofreither, C.: A unified view of some numerical methods for fractional diffusion. Computers & Mathematics with Applications. https://doi.org/10.1016/j.camwa.2019.07.025 (2019)
8. Čiegis, R., Starikovičius, V., Margenov, S., Kriauzienė, R.: Scalability analysis of different parallel solvers for 3D fractional power diffusion problems. Concurrency Computat Pract Exper. e5163. https://doi.org/10.1002/cpe.5163 (2019)
9. Quarteroni, A., Valli, A.: Numerical Approximation of Partial Differential Equations. Springer Series in Computational Mathematics v. 23. (1997)
10. ParMETIS: http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview (2019)
11. Axelsson, O.: Iterative Solution Methods. Cambridge University Press, New York (1996)
12. HYPRE library: https://computation.llnl.gov/projects/hypre-scalable-linear-solvers-multigrid-methods (2019)
13. Netgen mesher: https://ngsolve.org/ (2019)
14. Supercomputer System Avitohol: http://iict.bas.bg/avitohol/ (2019)