On Parallel Numerical Algorithms for Fractional Diffusion Problems

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Outline

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The mean square displacement of a diffusing particle scales linearly with time:

$$\left\langle (X(t) - \langle X(t) \rangle)^2 \right\rangle \propto t$$

Anomalous Diffusion

- Numerous experimental measurements in spatially complex systems have revealed anomalous diffusion in which **the mean square displacement scales as a fractional order power law in time:**

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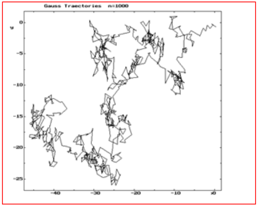
- Anomalous diffusion is "normal" in spatially disordered systems, porous media, fractal media, turbulent fluids and plasmas, biological media with traps, binding sites or macro-molecular crowding, stock price movements.

$\langle \Delta X^2 \rangle \sim t\,(\ln t)^\kappa$ $1 < \kappa < 4$	ultraslow diffusion	Sinai diffusion deterministic diffusion
$\langle \Delta X^2 \rangle \sim t^\alpha$ $0 < \alpha < 1$	subdiffusion	disordered solids biological media fractal media porous media
$\langle \Delta X^2 \rangle \sim \begin{cases} t^\alpha & t < \tau \\ t & t > \tau \end{cases}$	transient subdiffusion	biological media
$\langle \Delta X^2 \rangle \sim t$	standard diffusion	homogeneous media
$\langle \Delta X^2 \rangle \sim t^\beta$ $1 < \beta < 2$	superdiffusion	turbulent plasmas Levy flights transport in polymers
$\langle \Delta \ell^2 \rangle \sim t^3$	Richardson diffusion	atmospheric turbulence

B. I. Henry, T. A. M. Langlands, and P. Straka (2010) An Introduction to Fractional Diffusion. Complex Physical, Biophysical and Econophysical Systems: pp. 37-89.

Local vs Non-Local



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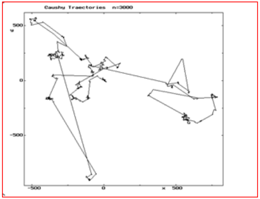

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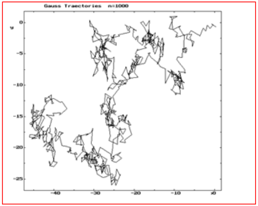

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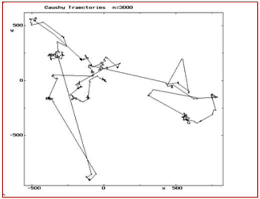

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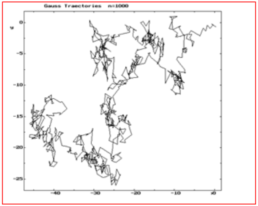

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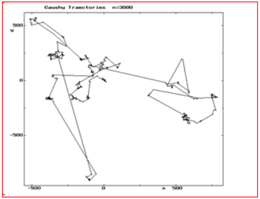

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- Macroscopically, the transport of a field of interest at a certain location is determined by an appropriate field variable. It is independent of the global structure of the transported field.

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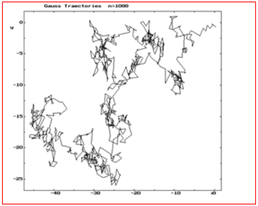

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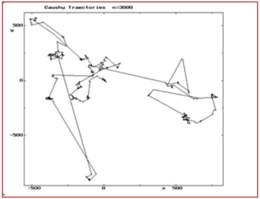

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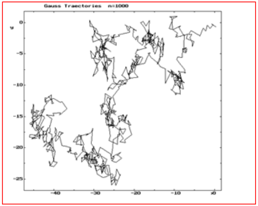

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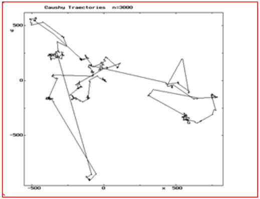

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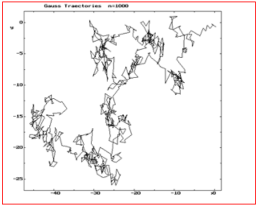

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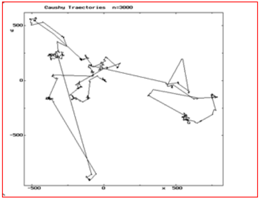

Anomalous diffusion

- In anomalous diffusion, random walkers are able to perform long jumps - Levy flights.
- Due to observed long range interactions, diffusive flux at a certain location is affected by the state of the field the entire domain.

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1. Spectral (Fourier) definition.

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with some boundary conditions on $\partial\Omega$, $0 < \beta < 1$ and elliptic operator

$$Lu = -\sum_{j=1}^{n} \frac{\partial}{\partial x_j}\left(k(X)\frac{\partial u}{\partial x_j}\right).$$

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where $w_k = (u, \phi_k)$.
Note, that the direct implementation of this approach is very expensive. It requires the computation of all eigenvectors and eigenvalues of large matrices.

Definitions of fractional Laplacian

2. Singular integral (Riesz potential) definition.

$$L^{\beta} u(x) = c_{n,\beta} \text{ p.v.} \int_{\mathbb{R}^n} \frac{u(x) - u(y)}{|x - y|^{n+2\beta}} dy =$$

$$= c_{n,\beta} \lim_{\varepsilon \to 0} \int_{\mathbb{R}^n \setminus B_\varepsilon} \frac{u(x) - u(y)}{|x - y|^{n+2\beta}} dy.$$

Example. $L^{\beta} u = 1, \quad x \in \Omega = (-1, 1), \quad u(-1) = u(1) = 0.$

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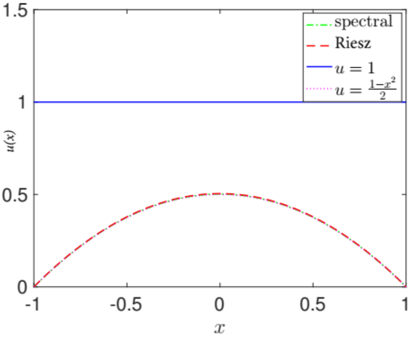
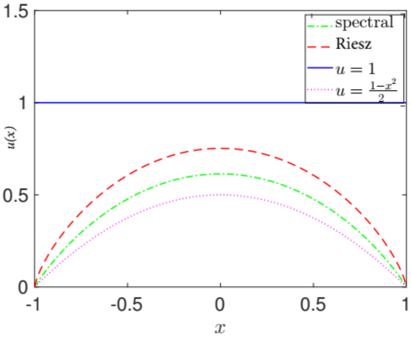


$\beta = 0.995$



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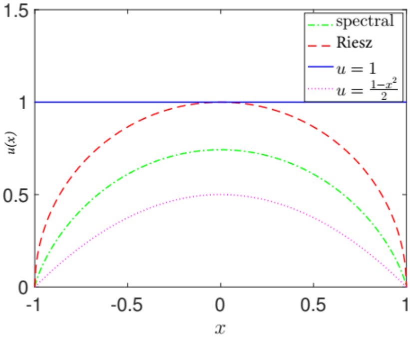
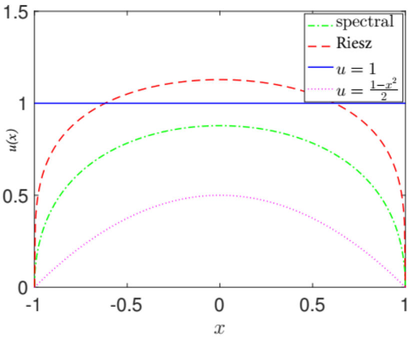


$\beta = 0.50$



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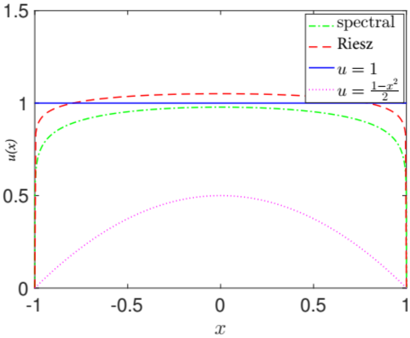

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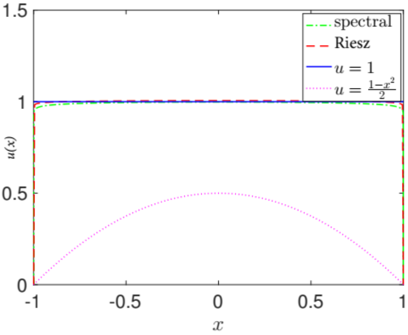

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Example. $L^{\beta}u = f(X), \;\; X \in \Omega = (0,1) \times (0,1),$

$u(X) = 0, \;\; X \in \partial\Omega,$

with $\beta = 0.25$ and f the checkerboard function:

$$f(x) = \begin{cases} 1, & \text{if } \; (x_1 - 0.5)(x_2 - 0.5) > 0; \\ -1, & \text{otherwise.} \end{cases}$$

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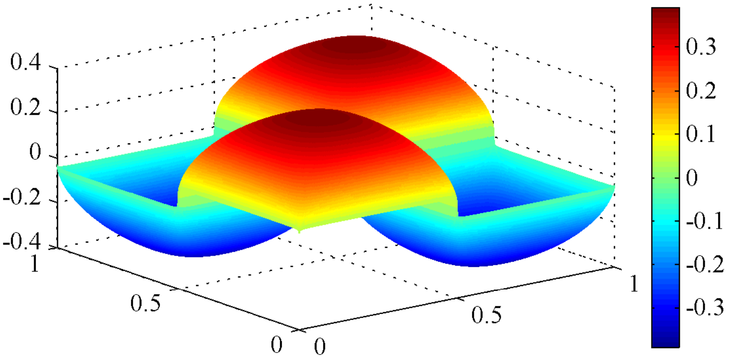

Convergence of numerical methods

Bonito A., Pasciak J.E. (2015). Numerical approximation of fractional powers of elliptic operators. *Mathematics of Computation*, **84**(295):2083-2110.

Let us assume that linear elements are used to obtain the finite element method's approximation $U_h \in V_h$, h being the mesh size and $V_h \subset H_0^1(\Omega)$ being the space of continuous piece-wise linear functions over the mesh. In the case of full regularity, the best possible convergence rate for $f \in L^2(\Omega)$ is

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$$\|u - U_h\|_{L^2(\Omega)} \leq Ch^{2\beta} |\ln h| \; \|f\|_{L^2(\Omega)}. \tag{3}$$

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This estimate illustrates how the accuracy of the numerical method is reduced, depending on power $\beta \in (0, 1)$.

Convergence of numerical methods

3D Test. $L^{\beta} u = f(X), \ X \in \Omega = (0,1) \times (0,1) \times (0,1),$
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Table : Relative error E_N^F of Fourier solution U_N^F of 3D test problem

N^3:	16^3	32^3	64^3	128^3	256^3
$\beta = 0.25$:	0.035654	0.025169	0.017792	0.012569	0.008855
$\beta = 0.75$:	0.012563	0.004399	0.001554	0.000549	0.000193

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1. Extension to the mixed boundary value problem in the semi-infinite cylinder;
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4. Method based on the best uniform rational approximations.

Extension to the mixed boundary value problem in the semi-infinite cylinder

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$$-\frac{\partial}{\partial y}\left(y^{\alpha}\frac{\partial V}{\partial y}\right) + y^{\alpha} LV = 0, \quad (X, y) \in C, \ \alpha = 1 - 2\beta, \qquad (4)$$

$$-y^{\alpha}\frac{\partial V}{\partial y} = d_{\beta} f, \quad X \in \bar{\Omega} \times \{0\},$$

$$V = 0, \quad (X, y) \in C_B = \partial C \setminus \bar{\Omega} \times \{0\}.]$$

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Then $u(X) = V(X, 0)$.

The semi-infinite cylinder is approximated by the truncated cylinder $C_Y = \Omega \times \{0, Y\}$ with a sufficiently large Y.
A uniform mesh Ω_h is introduced in Ω and anisotropic mesh $\omega_h = \{y_j = (j/M)^\gamma Y, j = 0, \dots, M\}$ is used.

$$
\begin{aligned}
&- \left(y^\alpha_{j+1/2} \frac{V_{h,j+1} - V_{h,j}}{H_{j+1/2}} - y^\alpha_{j-1/2} \frac{V_{h,j} - V_{h,j-1}}{H_{j-1/2}} \right) \\
&\qquad + \frac{y^{\alpha+1}_{j+1/2} - y^{\alpha+1}_{j-1/2}}{\alpha+1} L_h V_h = 0, \quad (X_h, y_j) \in C_{Y_h}, \qquad (5) \\
&- y^\alpha_{1/2} \frac{V_{h,1} - V_{h,0}}{H_{1/2}} + \frac{y^{\alpha+1}_{1/2}}{\alpha+1} L_h V_h = d_\beta f_h, \\
&\qquad X_h \in \bar{\Omega}_h \times \{0\}, \\
&\quad V_h = 0, \quad (X_h, y_j) \in \partial C_{Yh} \setminus \bar{\Omega}_h \times \{0\}.
\end{aligned}
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Transformation to pseudo-parabolic problem

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The solution of nonlocal problem (1) is sought as a mapping

$$V(X,t) = \left(t(L-\delta I) + \delta I\right)^{-\beta} f,$$

where $L \geq \delta_0 I$, $\delta < \delta_0$. Thus $V(X,1) = L^{-\beta} f$.

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The function V satisfies the evolutionary pseudo-parabolic problem

$$(tG+\delta I)\frac{\partial V}{\partial t} + \beta G V = 0, \quad 0 < t \leq 1, \qquad (6)$$
$$V(0) = \delta^{-\beta} f, \quad t = 0,$$

where $G = L - \delta I$.

Transformation to pseudo-parabolic problem

We use the following finite volume scheme

$$(t^{n-1/2} G_h + \delta I_h) \frac{V_h^n - V_h^{n-1}}{\tau} + \beta G_h V_h^{n-1/2} = 0, \quad 0 < n \leq M,$$

$$V_h^0 = \delta^{-\beta} f_h,$$

where

$$G_h = L_h - \delta I_h, \quad V_h^{n-1/2} = (V_h^n + V_h^{n-1})/2, \quad t^{n-1/2} = (t^{n-1} + t^n)/2.$$

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Convergence rate of time discretization scheme with the **uniform** time-stepping depends on the smoothness of the solution. **Geometrically graded** time-stepping scheme is proposed to deal with the singular behavior of the solution for time t close to 0: Duan B., Lazarov R., Pasciak J.. *Numerical Approximation of Fractional Powers of Elliptic Operators*. 2018.

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The algorithm is based on the integral representation of the non-local operator using the classical local operators

$$L^{-\beta} = \frac{2\sin(\pi\beta)}{\pi} \int_0^\infty y^{2\beta-1}(I + y^2 L)^{-1} dy.$$

- Superior results have shown the quadrature formula with uniformly distributed quadrature points $y_j = kj$:

$$U_h^{M3} = \frac{2k\sin(\pi\beta)}{\pi} \sum_{j=-m_1}^{m_2} e^{2(\beta-1)y_j} \left(e^{-2y_j} I_h + L_h\right)^{-1} \mathbf{f}_h,$$

where $m_1 = \lceil \pi^2/(4\beta k^2) \rceil$ and $m_2 = \lceil \pi^2/(4(1-\beta)k^2) \rceil$.

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- The parameter $k > 0$ controls the accuracy of the approximation of integral, that is, the method's transformation error, and the number of discrete 3D elliptic subproblems that should to be solved: $M = m_1 + m_2 + 1$. It has been proven that this sinc quadrature converges exponentially.

Method based on the best uniform rational approximation of the function $t^{1-\beta}$

S. Harizanov, R. Lazarov, P. Marinov, S. Margenov, Y. Vutov. Optimal Solvers for Linear Systems with Fractional Powers of Sparse SPD Matrices. *arXiv*:1612.04846:1–25, 2016.

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The approximate solution U_h^{M4} of the discrete problem $L_h^{\beta} U_h = f_h$ is defined as

$$U_h^{M4} = c_0 A_h^{-1} \tilde{f}_h + \sum_{j=1}^{m} c_i (A_h - d_j I)^{-1} \tilde{f}_h,$$

where the matrix A_h and function $\tilde{f}_h$ on the right–hand side are scaled as $A_h = h^2/12 L_h$ and $\tilde{\mathbf{f}}_h = (h^2/12)^{\beta} f_h$.

Method based on the best uniform rational approximation of the function $t^{1-\beta}$

Coefficients c_j and d_j are obtained by solving the global optimization problem to find the best uniform rational approximation $r_m^*(t)$ of the function $t^{1-\beta}$:

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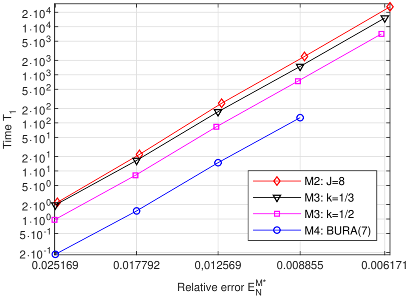
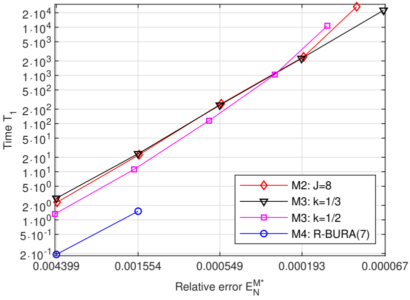
$$r_m(t) = c_0 + \sum_{j=1}^{m} \frac{c_j t}{t - d_j},$$

$$\min_{r_m} \max_{t \in [0,1]} \left| t^{1-\beta} - r_m(t) \right| = \max_{t \in [0,1]} \left| t^{1-\beta} - r_m^*(t) \right| =: \varepsilon_m(\beta).$$

Comparison: Serial solution times T_1 vs accuracy

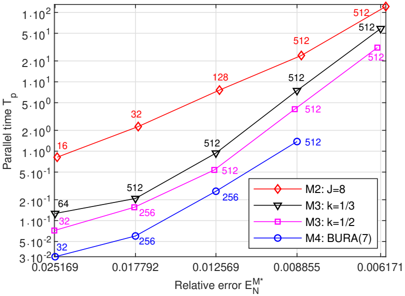


$\beta = 0.25$

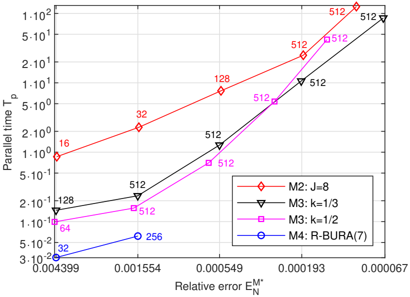


$\beta = 0.75$

Comparison: Parallel solution times T_p vs accuracy

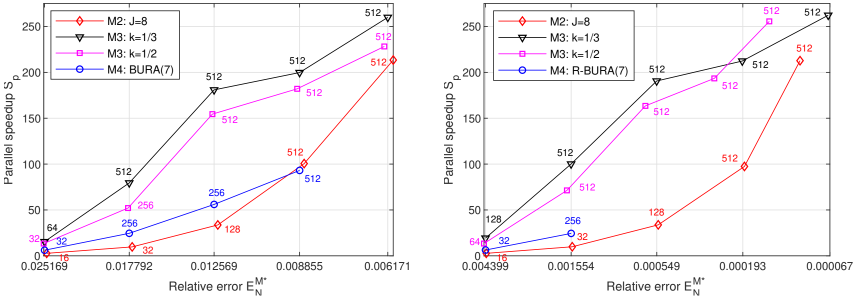


$\beta = 0.25$



$\beta = 0.75$

Comparison: Parallel speedups S_p vs accuracy



$\beta = 0.25$ $\beta = 0.75$

Conclusions

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- The software packages for their numerical solution (including parallel) are subject to a long-time development and permanent improvements.
- Computational and memory challenges are quite different for each numerical approach.
- The according parallel algorithms have very different properties. Their performance needs to be carefully studied.