NUMERICAL METHODS FOR FRACTIONAL DIFFUSION
Lecture 3: Spectral Laplacian and Dunford-Taylor Approach

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Outline

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Space-Time Fractional PDEs

Multilevel Methods

Fractional Obstacle Problems

Spectral Fractional Laplacian: Balakrihsnan Formula

Integral Laplacian: Dunford-Taylor Formula

Conclusions

Space-Time Fractional Parabolic Problem (w. E. Otárola and A. Salgado)

- **Fractional derivatives:** Powerful tools to describe memory properties of materials (R. Gorenflo, 2002)

  R. Gorenflo and F. Mainardi, *Fractional Calculus*, Springer (1997). (1467 google scholar citations).

- **Riemann-Liouville fractional derivative:** W. McLean, V. Thomee (2013); M. Zayernouri, G. Karniadakis (2014); J.S. Hesthaven.

- **Caputo fractional derivative:** B. Jin, R. Lazarov, and Z. Zhou (2013).

Space-Time Fractional Parabolic Problem: Formulation

- **Data:** $T > 0$ total time, $f : \Omega \times (0,T) \to \mathbb{R}$ forcing, and $u_0 : \Omega \to \mathbb{R}$ initial condition.

- **PDE:** Given $\gamma \in (0,1]$ find u such that

$$\partial_t^\gamma u + (-\Delta)^s u = f \text{ in } \Omega \times (0,T] \quad u|_{t=0} = u_0 \text{ in } \Omega.$$

- **Caputo derivative:** For $\gamma < 1$, we consider the Caputo derivative

$$\partial_t^\gamma u(x,t) = \frac{1}{\Gamma(1-\gamma)} \int_0^t \frac{\partial_r u(x,r)}{(t-r)^\gamma} \,\mathrm{d}r = \left[I^{1-\gamma} \partial_r u(x,\cdot) \right](t).$$

  For $\gamma = 1$, ∂_t^γ is the usual time derivative.

- **Nonlocality:** both in space and time! We will overcome the nonlocality in space using the Caffarelli-Silvestre extension to the cylinder $\mathcal{C} = \Omega \times (0,\infty)$.

Extended Evolution Problem

- **Dynamic boundary condition:** The Caffarelli-Silvestre extension turns our problem into a quasistationary elliptic problem with dynamic boundary condition (recall d_s is a constant depending on s)

$$\begin{cases} -\mathrm{div}\ (y^\alpha \nabla \mathcal{U}) = 0, & \text{in } \mathcal{C},\ t \in (0,T), \\ \mathcal{U} = 0, & \text{on } \partial_L \mathcal{C},\ t \in (0,T), \\ d_s \partial_t^\gamma \mathcal{U} + \frac{\partial \mathcal{U}}{\partial \nu^\alpha} = d_s f, & \text{on } \Omega \times \{0\},\ t \in (0,T), \\ \mathcal{U} = \mathsf{u}_0, & \text{on } \Omega \times \{0\},\ t = 0. \end{cases}$$

- **Role of extension:** $\mathsf{u} = \mathrm{tr}_\Omega\, \mathcal{U}$, $\alpha = 1 - 2s$. Nonlocality just in time!

- **Weak formulation:** seek $\mathcal{U} \in \mathbb{V}$ such that for a.e. $t \in (0,T)$,

$$\begin{cases} \langle \mathrm{tr}_\Omega \partial_t^\gamma \mathcal{U}, \mathrm{tr}_\Omega \phi \rangle_{\mathbb{H}^{-s}(\Omega) \times \mathbb{H}^s(\Omega)} + a(w,\phi) = \langle f, \mathrm{tr}_\Omega \phi \rangle_{\mathbb{H}^{-s}(\Omega) \times \mathbb{H}^s(\Omega)}, \\ \mathrm{tr}_\Omega \mathcal{U}(0) = \mathsf{u}_0 \end{cases}$$

for all $\phi \in \mathring{H}^1_L(\mathcal{C}, y^\alpha)$, where

$$a(w,\phi) = \frac{1}{d_s} \int_{\mathcal{C}} y^\alpha \nabla w \cdot \nabla \phi.$$

- **Truncation** $\mathcal{C} \to \mathcal{C}_\mathcal{Y}$: Exponential decay as in the elliptic case.

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for all $\phi \in \mathring{H}_L^1(\mathcal{C}, y^\alpha)$, where

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Time Discretization for $\gamma = 1$: Backward Euler

- **Uniform time step:** $\tau = T/\mathcal{K}$.
- **Backward differences:** $\partial V^{k+1} = \frac{1}{\tau}\left(V^{k+1} - V^{k}\right)$.
- **Backward Euler method:** Compute $V^{\tau} = \{V^k\}_{k=0}^{\mathcal{K}} \subset \mathring{H}_L^1(y^\alpha, \mathcal{C})$, where V^k denotes an approximation at each time step.
  - **Initialization:** Set $\mathrm{tr}_\Omega V^0 = \mathrm{u}_0$.
  - **Scheme:** For $k = 0, \dots, \mathcal{K}-1$, we find $V^{k+1} \in \mathring{H}_L^1(y^\alpha, \mathcal{C})$ solution of

    $$(\mathrm{tr}_\Omega \partial V^{k+1}, \mathrm{tr}_\Omega W)_{L^2(\Omega)} + a(V^{k+1}, W) = \langle f^{k+1}, \mathrm{tr}_\Omega W \rangle_{\mathbb{H}^{-s}(\Omega) \times \mathbb{H}^s(\Omega)},$$

    for all $W \in \mathring{H}_L^1(\mathcal{C}, y^\alpha)$, where $f^{k+1} = f(t^{k+1})$.
  - **Unconditional stability:**

    $$\|\mathrm{tr}_\Omega V^\tau\|_{\ell^\infty(L^2(\Omega))}^2 + \|V^\tau\|_{\ell^2(\mathring{H}_L^1(y^\alpha, \mathcal{C}))}^2 \lesssim \|\mathrm{u}_0\|_{L^2(\Omega)}^2 + \|f^\tau\|_{\ell^2(\mathbb{H}^{-s}(\Omega))}^2.$$

Time discretization for $\gamma \in (0,1)$: Backward Differences

- **Approximate Caputo derivative:** Replace $\partial_r u(x,r)$ by backward differences

$$\partial_t^\gamma u(x,t_{k+1}) = \frac{1}{\Gamma(1-\gamma)} \int_0^{t_{k+1}} \frac{\partial_r u(x,r)}{(t_{k+1}-r)^\gamma} \, \mathrm{d}r$$

$$\approx \frac{1}{\Gamma(2-\gamma)} \sum_{j=0}^{k} a_j \frac{u(x,t_{k+1-j}) - u(x,t_{k-j})}{\tau^\gamma} =: D^\gamma u(x)^{k+1}$$

where $a_j = (j+1)^{1-\gamma} - j^{1-\gamma}$.

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  - **Unconditional stability:** If $\mathcal{H} := L^2(\Omega)$ and $\mathcal{V} := \mathring{H}^1_L(y^\alpha, \mathcal{C})$, then we have

$$I^{1-\gamma} \|V^\tau\|^2_{\mathcal{H}}(T) + \|V^\tau\|^2_{\ell^2(\mathcal{V})} \leq I^{1-\gamma} \|v^0\|^2_{\mathcal{H}}(T) + \|f^\tau\|_{\ell^2(\mathcal{V}')}$$

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Time Discretization for $\gamma \in (0,1)$: Regularity and Consistency

- **Usual regularity:** Typical smoothness assumption of the solution is

$$u_{tt} \in L^2([0,T], \mathbb{H}^{-s}(\Omega)).$$

- **Validity:** For general data this assumption is not valid!

- **New regularity:** We show that

$$\partial_t u \in L \log L(0,T; \mathbb{H}^{-s}(\Omega))$$

and

$$\partial_{tt} u \in L^2(t^\sigma, (0,T); \mathbb{H}^{-s}(\Omega)),$$

for $\sigma > 3 - 2\gamma$.

- **Validity:** These are valid under realistic assumptions on f and u_0.

- **Consistency:** The remainder $\mathsf{r}_\gamma^\tau = \partial_t^\gamma u(x, t_{k+1}) - D^\gamma u(x)^{k+1}$ satisfies

$$\|\mathsf{r}_\gamma^\tau\|_{L^2(0,T;\mathbb{H}^{-s}(\Omega))} \lesssim \tau^\theta \left(\|\mathsf{u}_0\|_{\mathbb{H}^{2s}(\Omega)} + \|f\|_{H^2(0,T;\mathbb{H}^{-s}(\Omega))} \right) \quad \forall \theta < \frac{1}{2}.$$

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Error Estimates for Fully Discrete Schemes: $0 < \gamma < 1$

- **Lax's Theorem:** Stability plus consistency yields convergence.

- **Error estimates for $\mathcal{U} : \mathcal{C} \times (0,T) \to \mathbb{R}$:** If $s \in (0,1)$ and $\gamma \in (0,1)$, then

$$[I^{1-\gamma} \| \mathrm{tr}_\Omega (\mathcal{U}^\tau - V^\tau_{\mathscr{T}_\mathcal{Y}}) \|^2_{L^2(\Omega)}(T)]^{\frac{1}{2}} \lesssim \tau^\theta + |\log N|^{2s} N^{\frac{-(1+s)}{n+1}}$$

$$\| \mathcal{U}^\tau - V^\tau_{\mathscr{T}_\mathcal{Y}} \|_{\ell^2(\mathring{H}^1_L(\mathcal{C}_\mathcal{Y}, y^\alpha))} \lesssim \tau^\theta + |\log N|^s N^{\frac{-1}{n+1}},$$

for any $\theta < \frac{1}{2}$.

- **Error estimates for $u : \Omega \times (0,T) \to \mathbb{R}$:** If $s \in (0,1)$ and $\gamma \in (0,1)$, then

$$[I^{1-\gamma} \| u^\tau - U^\tau \|^2_{L^2(\Omega)}(T)]^{\frac{1}{2}} \lesssim \tau^\theta + |\log N|^{2s} N^{\frac{-(1+s)}{n+1}}$$

$$\| u^\tau - U^\tau \|_{\ell^2(\mathbb{H}^s(\Omega))} \lesssim \tau^\theta + |\log N|^s N^{\frac{-1}{n+1}},$$

for any $\theta < \frac{1}{2}$.

Outline

Multilevel Methods (w. L. Chen, E. Otárola and A. Salgado)

- **Optimal methods:** Multilevel methods have linear complexity for uniformly elliptic PDE. How do they perform for non-uniformly elliptic PDE?
- **Space decompositions:** Consider the space *macro* and *micro* decompositions

$$\mathbb{V} = \sum_{k=0}^{J} \mathbb{V}_k = \sum_{k=0}^{J} \sum_{j=1}^{\mathcal{M}_k} \mathbb{V}_{k,j}.$$

- **Smoothers:** We use line smoothers in the extended y direction.
- **Convergence of multigrid:** The contraction rate δ of the symmetric $\mathcal{V}$-cycle multigrid algorithm with line smoothers is

$$\delta \leq 1 - \frac{1}{1 + CJ},$$

where the constant C is independent of the mesh size, and it depends on y^α only through the Muckenhoupt C_{2,y^α}, and J is the number of levels.

Numerical Experiments for 2d Domains

- **Iteration count:** Start from 0 and stop when ℓ^2 relative residual is $< 10^{-7}$.

$h_{\mathscr{T}_\Omega}$	DOFs	$s = 0.3$	$s = 0.6$	$s = 0.8$
$\frac{1}{16}$	4,913	7	6	5
$\frac{1}{32}$	35,937	8	6	6
$\frac{1}{64}$	274,625	9	6	6
$\frac{1}{128}$	2,146,689	9	6	6

Table: Number of iterations for a multigrid method for the two dimensional fractional Laplacian using a line smoother in the extended direction. The mesh in Ω is uniform of size $h_{\mathscr{T}_\Omega}$. The mesh in the extended direction is geometrically graded.

- **Robustness:** Experiments show robustness with respect to $0 < s < 1$ and mesh anisotropy.

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Spectral Fractional Laplacian: Balakrihsnan Formula

Integral Laplacian: Dunford-Taylor Formula

Conclusions

Formulation: PDE Approach (N, Otárola, Salgado (2015))

- **Data:** $f \in \mathbb{H}^{-s}(\Omega)$ and an obstacle $\psi \in \mathbb{H}^s(\Omega) \cap C(\bar{\Omega})$ with $\psi \leq 0$ on $\partial\Omega$.

- **Variational inequality:** Find $u \in \mathcal{K}$ such that

$$\langle (-\Delta)^s u, u - w \rangle \leq \langle f, u - w \rangle \quad \forall w \in \mathcal{K}$$

  where $\mathcal{K}$ is the convex set

$$\mathcal{K} := \{ w \in \mathbb{H}^s(\Omega) : \; w \geq \psi \text{ a.e. in } \Omega \}.$$

- **Complementarity condition:** It reads for $s \in (0,1)$

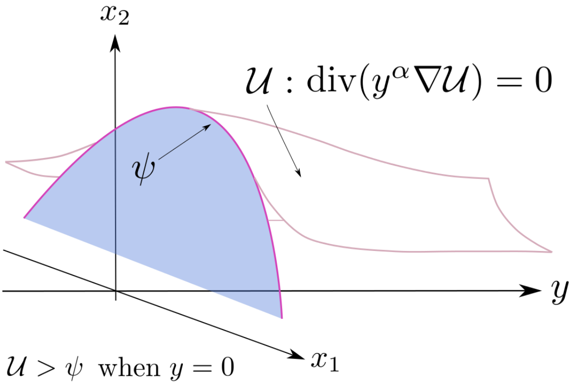
$$u \geq \psi, \qquad (-\Delta)^s u \geq 0, \qquad (-\Delta)^s u = 0 \text{ if } u > \psi,$$

- **Structure:** nonlinear and nonlocal problem, because of $(-\Delta)^s$!

- **PDE approach:** Use the Caffarelli-Silvestre extension, which in turn gives optimal regularity (L. Caffarelli, S. Salsa, and L. Silvestre).

Reformulation: Thin Obstacle Problem

- We convert the fractional obstacle problem into a thin obstacle problem over the extended domain (cylinder) $\mathcal{C} = \Omega \times (0, \infty)$.



- The restriction $\mathcal{U} \geq \psi$ only applies when $y = 0$ (thin obstacle).

FEM and Error Estimate

- **Error estimate:** If $\mathcal{U}$ is the exact solution and $V_{\mathscr{T}_{\mathcal{Y}}}$ the discrete solution, then

$$\|\mathcal{U} - V_{\mathscr{T}_{\mathcal{Y}}}\|_{\mathring{H}^1_L(y^\alpha, \mathcal{C})} \lesssim |\log(\#\mathscr{T}_{\mathcal{Y}})|^s (\#\mathscr{T}_{\mathcal{Y}})^{-1/(n+1)},$$

  where C depends on the Hölder moduli of smoothness of $\mathcal{U}$ and $\mathcal{V}$, and sobolev regularity of f and ψ.

- **Ingredients:**
  - Optimal regularity in Ω: $u \in C^{1,s}$ by Caffarelli, Salsa and Silvestre (2008).
  - This implies that $\partial_\nu^\alpha \mathcal{U}(\cdot, 0) \in C^{0,1-s}$.
  - For y "*small*" use Hölder estimates of Allen, Lindgren, and Petrosyan (2014): $s \leq \frac{1}{2} \Rightarrow \mathcal{V} \in C^{0,2s}(\mathcal{C}_{\mathcal{Y}})$ and $s > \frac{1}{2} \Rightarrow \mathcal{V} \in C^{1,2s-1}(\mathcal{C}_{\mathcal{Y}})$.
  - For y "*big*" use bounds of NOS (2014) $\mathcal{V} \in H^2(y^\beta, \mathcal{C}_{\mathcal{Y}})$ with $\beta > 1 + 2\alpha$.

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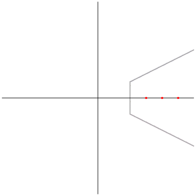
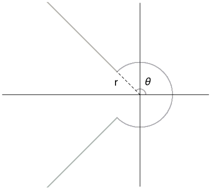
Integral Representation of Spectral Laplacian

- **Spectral Fractional Laplacian:** Recall $(-\Delta)^s w = \sum_{k=1}^{\infty} \lambda_k^s w_k \varphi_k$ with $w_k = \int_\Omega w \varphi_k$ for $s \in (0,1)$.

- **Dunford Integral:** If $z^{-s} = |z|^{-s} e^{-is \arg z}$, then
$$(-\Delta)^{-s} f = \frac{1}{2\pi i} \int_{\mathcal{C}} z^{-s} (zI - \Delta)^{-1} f \, dz.$$

- **Contour $\mathcal{C}$:**





- **Balakrishnan formula:** Deform $\mathcal{C}$ upon taking $r \to 0$ and $\theta \to \pi$
$$(-\Delta)^{-s} f = \frac{\sin(\pi s)}{\pi} \int_0^{\infty} \mu^{-s} (\mu I - \Delta)^{-1} f \, d\mu.$$

Balakrishnan Formula (Bonito and Pasciak (2015))

$$u = (-\Delta)^{-s} f = \underbrace{\frac{\sin(\pi s)}{\pi}}_{=C(s)} \int_0^\infty \mu^{-s} (\mu I - \Delta)^{-1} f \, d\mu.$$

- **Sanity Check:** If $\psi \in H_0^1(\Omega)$ is an eigenfunction of $(-\Delta)$ with associated eigenvalue $\lambda > 0$ then

$$(-\Delta)^{-s}\psi = C(s)\psi \int_0^\infty \frac{\mu^{-s}}{\mu + \lambda} d\mu \overset{\mu=\lambda t}{=} \lambda^{-s} C(s)\psi \int_0^\infty \frac{t^{-s}}{t+1} dt = \lambda^{-s}\psi.$$

- **Numerical method: Game plan**
  - Step 1: use quadrature for the μ variable;
  - Step 2: use standard finite element methods on the same mesh to approximate

    $$u_\mu \in H_0^1(\Omega): \qquad \mu u_\mu - \Delta u_\mu = f \quad \text{in} \quad \Omega.$$

    This means $u_\mu = (\mu I - \Delta)^{-1} f$.
  - Step 3: Gather all contributions.

Step 1: SINC Quadrature for the μ Variable

- **Change of variable:** let $\mu = e^y$ to get

$$u = (-\Delta)^{-s} f = \frac{\sin(\pi s)}{\pi} \int_{-\infty}^{\infty} e^{(1-s)y} (e^y I - \Delta)^{-1} f \, dy.$$

- **Quadrature:** Given $N \in \mathbb{N}$, define $k = 1/\sqrt{N}$, $y_j = jk$ and the quadrature approximation

$$U^N = Q^N f = \underbrace{\frac{\sin(\pi s) k}{\pi}}_{=C(s,k)} \sum_{j=-N}^{N} e^{(1-s)y_j} (e^{y_j} I - \Delta)^{-1} f.$$

- **Exponential convergence** (Bonito, Pasciak (2015)): Let $s \in [0,1)$ and $r \in [0,1]$. If $f \in \mathbb{H}^r(\Omega)$, then

$$\|u - U^N\|_{\mathbb{H}^r(\Omega)} \leq C e^{-c\sqrt{N}} \|f\|_{\mathbb{H}^r(\Omega)}.$$

In practice $N = 20$. This uses decay when $|z| \to \infty$ and holomorphic properties of integrand $z^{-s}(zI - \Delta)^{-1}$.

Steps 2 and 3: Finite Element Method and Parallelization

- **Discrete Laplacian:** $-\Delta_{\mathscr{T}} : \mathbb{U}(\mathscr{T}) \to \mathbb{U}(\mathscr{T})$ is given by

$$\int_\Omega -\Delta_{\mathcal{T}} V\, W = \int_\Omega \nabla V \nabla W \quad \forall V, W \in \mathbb{U}(\mathcal{T}).$$

- **L^2-projection onto $\mathbb{U}(\mathcal{T})$:** $\Pi_{\mathcal{T}} : L^2(\Omega) \to \mathbb{U}(\mathcal{T})$ is given by

$$\int_\Omega \Pi_{\mathcal{T}} v W = \int_\Omega v W \quad \forall W \in \mathbb{U}(\mathcal{T}).$$

- **Semidiscrete solution:** Let $U = U_{\mathcal{T}} \in \mathbb{U}(\mathcal{T})$ be defined by

$$U_{\mathcal{T}} = \frac{\sin(s\pi)}{\pi} \int_{-\infty}^{\infty} e^{(1-s)y} (e^y I - \Delta_{\mathcal{T}})^{-1} \Pi_{\mathcal{T}} f\, dy \; (= Q^\infty \Pi_{\mathcal{T}} f).$$

- **Fully discrete solution:** Let $U = U_{\mathcal{T}}^N \in \mathbb{U}(\mathcal{T})$ satisfy

$$U = Q^N \Pi_{\mathcal{T}} f = C(s,k) \sum_{j=-N}^{N} e^{(1-s)y_j} \underbrace{(e^{y_j} I - \Delta_{\mathcal{T}})^{-1} \Pi_{\mathcal{T}} f}_{=U_j}.$$

- **Parallelization:** Each $U_j \in \mathbb{U}(\mathcal{T})$ solves $(e^{y_j} I - \Delta_{\mathcal{T}}) U_j = \Pi_{\mathcal{T}} f$, i.e.

$$\int_\Omega e^{y_j} U_j W + \nabla U_j \nabla W = \int_\Omega f W \quad \forall W \in \mathbb{U}(\mathcal{T}).$$

A Priori Error Analysis

- **Assumptions**
  - Pick-up regularity: There is $0 < \alpha \le 1$ such that for all $0 \le r \le \alpha$
    $$(-\Delta)^{-1} : \mathbb{H}^{-1+r}(\Omega) \to \mathbb{H}^{1+r}(\Omega)$$
    is an isomorphism. Note that $\alpha = 1$ when Ω is convex.
  - the L_2-projection $\Pi_{\mathcal{T}}$ onto the finite element space $\mathbb{U}(\mathcal{T})$ is bounded as an operator from $H^1(\Omega)$ to $H^1(\Omega)$ (e.g. quasi-uniform meshes).

- **Error estimate:** (Bonito and Pasciak (2015). Given $r \in [0,1]$, $r \le 2s$, set

$$\alpha_* = \frac{1}{2}(\alpha + \min(1-r,\alpha)), \quad \gamma = \max(r + 2\alpha_* - 2s, 0).$$

If $f \in \mathbb{H}^\gamma$ then

$$\|u - U\|_{\mathbb{H}^r(\Omega)} \lesssim h^{2\alpha_*}\|f\|_{\mathbb{H}^\gamma(\Omega)} + e^{-c\sqrt{N}}\|f\|_{L^2(\Omega)},$$

where the hidden constant is of the form $C|\log h|$.

  - **Proof:** it uses eigenvalue decomposition and equivalence of functional spaces.
  - **Balancing errors:** choose $N \approx |\log h|$ and use $h \approx (\mathcal{T})^{-1/d}$ for quasi-uniform meshes $\mathcal{T}$, and let $\gamma = r + 2\alpha_* - 2s = 2\alpha_* - s$, $\sigma = \max(2\alpha_* - s, 0)$, to get

$$\|u - U\|_{\mathbb{H}^s(\Omega)} \le Ch^{2\alpha_*}\|f\|_{\mathbb{H}^\sigma(\Omega)} \approx (\#\mathcal{T})^{-2\alpha_*/d}\|f\|_{\mathbb{H}^\sigma(\Omega)}.$$

Comparison with Extension Approach

- **Convex domains:** pick-up regularity $0 < \alpha \leq 1$.

- **Comparison 1:** If $r = s$ and $\alpha = 1$, then

$$2\alpha_* = 2 - s, \quad \sigma = 2 - 2s$$

  whence

$$\|u - U\|_{\mathbb{H}^s(\Omega)} \leq Ch^{2-s}\|f\|_{\mathbb{H}^{2-2s}(\Omega)}.$$

  This estimate is of optimal order $2 - s > 1$ and regularity $f \in \mathbb{H}^{2-2s}(\Omega)$; or equivalently $u \in \mathbb{H}^2(\Omega)$ which is not generic. In contrast, the Extension Approach cannot deliver orders larger than 1.

- **Comparison 2:** Extension approach requires $f \in \mathbb{H}^{1-s}(\Omega)$ to deliver order 1 accuracy. What is the regularity of f for order 1 with Dunford-Taylor?

$$f \in \mathbb{H}^{1-s}(\Omega).$$

Numerical Experiments

- **Setting:** This corresponds to $s = 1/2$ and f with checkerboard pattern

$$\Omega = (0,1)^2, \quad f(x_1, x_2) = \begin{cases} 1, & \text{if } (x_1 - 0.5)(x_2 - 0.5) > 0 \\ 0, & \text{otherwise} \end{cases}$$

The error measured in $L_2(\Omega)$ $(r = 0)$

- **Parameters:**
  - $N = 1,000,000$, $0 < \alpha \leq 1$ (pick-up regularity),
  - $f \in H^{1/2-\epsilon}(\Omega)$ because of jump discontinuity, i.e. $\gamma < 1/2$.

- **Convergence rate:** it is $2\alpha_*$ provided

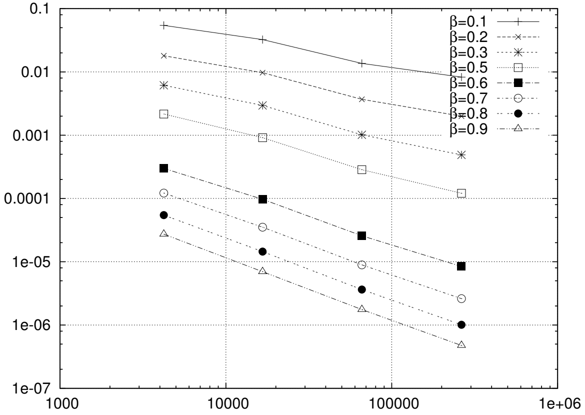
$$\gamma = \max(2\alpha_* - 2s, 0) = 2\alpha_* - 2s.$$

This implies

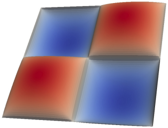
$$2\alpha_* = \begin{cases} 2 & s > \frac{3}{4} \\ 2s + \frac{1}{2} & 0 < s \leq \frac{3}{4}. \end{cases}$$

Computational L^2-Errors

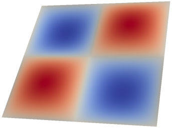
	$s=\beta\le 3/4$							$s=\beta>3/4$	
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
OBS	0.92	1.06	1.22	1.4	1.52	1.72	1.86	1.94	1.96
THM	0.7	0.9	1.1	1.3	1.5	1.7	1.9	2.0	2.0



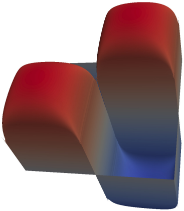
Effect of Varying s on Discontinuous Chekerboard f



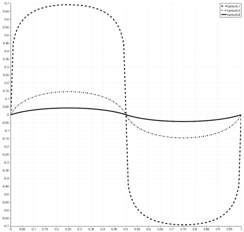
$s = 0.5$



$s = 0.8$



$s = 0.1$



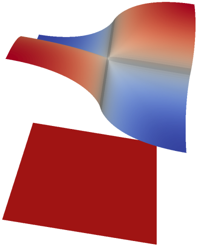
cut at $y = 0.25$

Advantages of the FEM

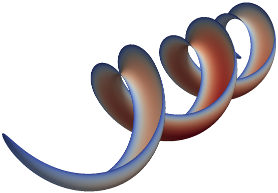
- The method is (embarrassingly) parallelizable: For each quadrature point t_*, the finite element solves are independent (tried up to $15'000$ cores).
- Minimal changes in existing codes: It relies on standard finite elements in $\mathbb{R}^d$, i.e. the quadrature component adds an additional external loop.
- Preconditionner: Standard preconditionners can be used. Moreover, the iterative solvers at each quadrature points benefits from the previous quadrature point as starting guess.

Extension I: Self-Adjoint Coercive Operators

- Pick-up regularity depends on the operator.
- Examples: diffusion with discontinuous coefficients, different boundary conditions, Laplace-Beltrami operators.



$(I - \Delta)^{1/2} u = 1$ in Ω; $\partial_\nu u = 0$ on $\partial\Omega$



$(-\Delta_\gamma)^{1/2} u = 1$

Extension II: non-Hermitian problems

- **Sectorial operator** A**:** consider sesquilinear form $a : \mathbb{V} \times \mathbb{V} \to \mathbb{R}$ satisfying

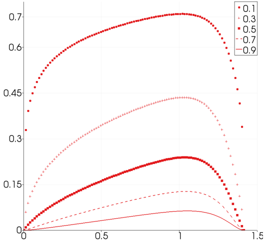
$$\mathfrak{Re}(a(v,v)) \geq c_0 \|v\|_{\mathbb{V}}^2, \quad |a(u,v)| \leq c_1 \|u\|_{\mathbb{V}} \|v\|_{\mathbb{V}} \qquad \forall u, v \in \mathbb{V}.$$

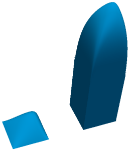
Then Balakhrisnan formula is valid

$$A^{-s} f = \frac{\sin(\pi s)}{\pi} \int_0^\infty \mu^{-s} (\mu I + A)^{-1} f \, d\mu$$

Complex Eigenvalues $\rightarrow$ Kato property $D(A^{1/2}) = D((A^*)^{1/2}) = \mathbb{V}$

- **Example:** $A^{-s}1$, where $Au = -\Delta u + \begin{pmatrix} 1 \\ 1 \end{pmatrix} \cdot \nabla u$





$s = 0.1 \quad s = 0.9$

Outline

Definition of Integral Laplacian (Bonito, Lei, Pasciak (2017))

- **Fourier definition:**

$$[\![u,w]\!] = C\int\int_{\mathbb{R}^d\times\mathbb{R}^d} \frac{(u(x)-u(x'))(w(x)-w(x'))}{|x-x'|^{d+2s}}dxdx'$$
$$= \int_{\mathbb{R}^d} |\xi|^s \mathscr{F}(u)|\xi|^s\overline{\mathscr{F}(w)}d\xi = \int_{\mathbb{R}^d} \mathscr{F}((-\Delta)^s u)(\xi)\overline{w(\xi)}d\xi = (f,w)$$

- **Equivalent representation:**

$$[\![u,w]\!] = \frac{2\sin(s\pi)}{\pi}\int_0^\infty \mu^{1-2s}\int_{\mathbb{R}^d}\big((-\Delta)(I-\mu^2\Delta)^{-1}u\big)w\,dxd\mu.$$

- **Proof:**
  - Parseval's theorem:

$$\int_{\mathbb{R}^d}\big((-\Delta)(I-\mu^2\Delta)^{-1}u\big)w\,dx = \int_{\mathbb{R}^d}\frac{|\xi|^2}{1+\mu^2|\xi|^2}\mathscr{F}(u)(\xi)\overline{\mathscr{F}(w)(\xi)}d\xi$$

  - Change of variables: $t=\mu|\xi|$ yields

$$\int_0^\infty \frac{t^{1-2s}}{1+t^2}dt = \frac{\pi}{2\sin(\pi s)}.$$

Variational Formulation

- **Auxiliary problem:** given $\psi \in L^2(\mathbb{R}^d)$ let $v(\psi,\mu) = v(\mu) \in H^1(\mathbb{R}^d)$ satisfy

$$\int_{\mathbb{R}^d} v(\mu)\phi + \mu^2 \int_{\mathbb{R}^d} \nabla v(\mu) \cdot \nabla \phi = -\int_{\mathbb{R}^d} \psi\phi \qquad \forall \phi \in H^1(\mathbb{R}^d),$$

  which corresponds to

$$v - \mu^2 \Delta v = -\psi \quad \Rightarrow \quad v = -(I - \mu^2 \Delta)^{-1} \psi.$$

  Note that the support of $v(\psi,\mu)$ is all of $\mathbb{R}^d$ regardless of the support of ψ.

- **Equivalent expression:** Inserting back into $[\![u,w]\!]$ gives

$$[\![u,w]\!] = \frac{2\sin(s\pi)}{\pi} \int_0^\infty \mu^{-1-2s} \Big(\int_\Omega \big(u + v(u,\mu)\big) w \, \mathrm{d}x \Big) \, \mathrm{d}\mu \quad \forall u,w \in \mathbb{H}^s(\Omega).$$

- **Variational problem:** given $f \in \mathbb{H}^{-s}(\Omega)$ find $u \in \mathbb{H}^s(\Omega)$ such that

$$[\![u,w]\!] = (f,w) \quad \forall w \in \mathbb{H}^s(\Omega).$$

SINC Quadrature

- **Change of variables:** $\mu = e^{-\frac{y}{2}}$ yields

$$[\![u, w]\!] = \frac{\sin(s\pi)}{\pi} \int_{-\infty}^{\infty} e^{sy} \left(\int_{\Omega} \big(u + v(u, \mu(y))\big) w \, \mathrm{d}x \right) \mathrm{d}y$$

- **Sinc quadrature:** uniform spacing $k \approx 1/N$ and $y_j = jk$ yields

$$[\![u, w]\!]^N = \frac{\sin(s\pi)}{\pi} k \sum_{j=-N}^{N} e^{sy_j} \left(\int_{\Omega} \big(u + v(u, \mu(y_j))\big) w \, \mathrm{d}x \right) \mathrm{d}y$$

- **Quadrature consistency:** given $w \in \mathbb{H}^s(\Omega)$ and $u \in \mathbb{H}^\delta(\Omega)$ with $s < \delta \leq \min(2 - s, \sigma)$ and $\sigma < \frac{3}{2}$, there holds

$$|a(u, w) - a^N(u, w)| \lesssim e^{-c\sqrt{N}} \|u\|_{\mathbb{H}^\delta(\Omega)} \|w\|_{\mathbb{H}^s(\Omega)}.$$

Domain Truncation

- **Support of $v(u,\mu)$:** since this support is all of $\mathbb{R}^d$ we must truncate the domain to solve with FEMs.
- **Truncated domains:** The truncated domain diameter depends on the quadrature point y_j. If B is a ball enclosing Ω of diameter 1, then for a truncation parameter M, we define the dilated domains

$$B^M(\mu) := \begin{cases} \{y = \big(1+\mu(1+M)\big)x \ : x \in B\}, & \mu \geq 1, \\ \{y = (2+M)x \ : x \in B\}, & \mu < 1. \end{cases}$$

- **Truncated solution:** $v^M = v^M(u,\mu) \in H_0^1(B^W(\mu)) : v^M - \Delta v^M = -u.$
- **Truncated bilinear form:**

$$[\![u,w]\!]^{N,M} = \frac{\sin(s\pi)}{\pi} k \sum_{j=-N}^{N} e^{sy_j} \int_\Omega (u + v^M(u,\mu(y_j)))w \,\mathrm{d}x.$$

- **Error estimate:** the exponential decay of $v(u,\mu)$ at ∞ implies

$$\left| [\![u,w]\!] - [\![u,w]\!]^{N,M} \right| \lesssim e^{-cM} \|u\|_{L^2(\Omega)} \|w\|_{L^2(\Omega)}.$$

Finite Element Approximation

- **Domain:** Ω is polytopal in $\mathbb{R}^d$
- **Mesh of Ω:** conforming partition $\mathscr{T}$ shape regular and quasi-uniform
- **Mesh of $B^M(\mu)$:** conforming partition $\mathscr{T}_M$ which matches $\mathscr{T}$
- **Finite element spaces:** Compatible $\mathbb{U}(\mathscr{T})$ and $\mathbb{U}(\mathscr{T}_M)$.
- **Finite element solution:** given $U \in \mathbb{U}(\mathscr{T})$ let $V(U,\mu) \in \mathbb{U}(\mathscr{T}_M)$ be the FE approximation of $v^M(U)$.
- **Fully discrete bilinear form:**

$$[\![U,W]\!]^{N,M}_{\mathscr{T}} = \frac{\sin(s\pi)}{\pi} k \sum_{j=-N}^{N} e^{sy_j} \int_\Omega (U + V^M(U,\mu(y_j)))W \, \mathrm{d}x.$$

- **Finite element consistency:** If $\beta \in (s, 3/2)$, for all $V, W \in \mathbb{U}(\mathscr{T})$ we have

$$\left| [\![U,W]\!]^{N,M} - [\![U,W]\!]^{N,M}_{\mathscr{T}} \right| \lesssim |\log h| h^{\beta - s} \|U\|_{\mathbb{H}^\beta(\Omega)} \|W\|_{\mathbb{H}^s(\Omega)}.$$

Fully Discrete Scheme

- **Finite element solution:** find $U = U_{\mathscr{T}}^{N,M} \in \mathbb{U}(\mathscr{T})$ such that
$$[\![U, W]\!]_{\mathscr{T}}^{M,N} = \int_\Omega fW \quad \forall\, W \in \mathbb{U}(\mathscr{T}).$$
This bilinear form is elliptic provided $e^{-c\sqrt{N}} h^{s-\delta} \le C$ and $\delta = \min(2-s, \beta)$.

- **Error estimate:** Let $\beta \in (s, 3/2)$. Then
$$\|u - U\|_{\mathbb{H}^s(\Omega)} \lesssim \left(e^{-c\sqrt{N}} + e^{-cM} + |\log h| h^{\beta - s} \right) \|u\|_{\mathbb{H}^\beta(\Omega)}.$$

- **Order:** Take $\beta = s + \frac{1}{2} - \epsilon$, which is consistent with the regularity of $u \in \mathbb{H}^{\frac{1}{2}+s-\epsilon}(\Omega)$ and $M \approx |\log h|$, $N \approx |\log h|^2$ to obtain
$$\|u - U\|_{\mathbb{H}^s(\Omega)} \lesssim h^{\frac{1}{2}-\epsilon} \|u\|_{\mathbb{H}^{\frac{1}{2}+s-\epsilon}(\Omega)}.$$

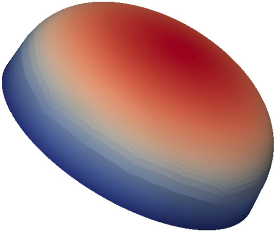
- **Comparison with integral method:**
  - Similar convergence rate for quasi-uniform $\mathscr{T}$
  - Effect of locally refined meshes towards $\partial\Omega$ remains open.

Numerical Experiment

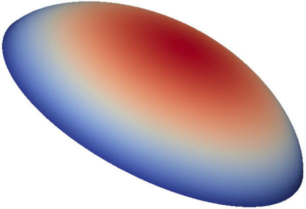
- **Setting:** Ω is the unit ball in $\mathbb{R}^2$ and the exact solution $u \in \mathbb{H}^s(\Omega)$ is

$$u(r) = \frac{2^{-2s}\Gamma(n/2)}{\Gamma(n/2+s)\Gamma(1+s)}(1-r^2)^s.$$

- **Regularity:** $u \in \mathbb{H}^\sigma(\Omega)$ with $\sigma = \min(2s, s + \frac{1}{2} - \epsilon)$.
- **FE solution for $s = 0.3$ and $s = 0.7$:**



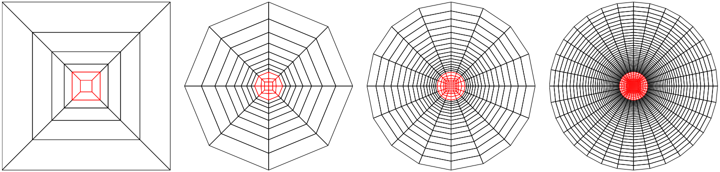
$s = 0.3$



$s = 0.7$

Space Discretization: Some Details

- **Implementation:**
  - Implementation tool: Deal.II Library
  - Four node quadrilateral bilinear element
- **Non-uniform extended mesh $\mathscr{T}_M$:**
  - The same nodes distribution as one dimensional case on each radial direction
  - The same number of nodes on angular direction.

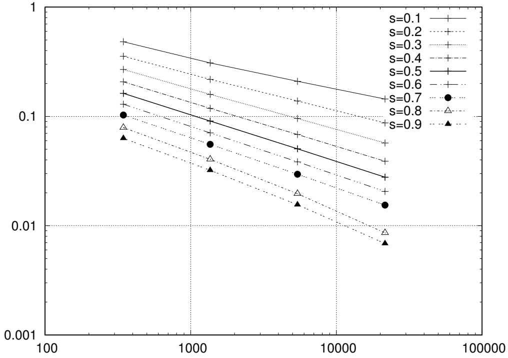


coarse grid refine once refine twice refine three times

  - $\mathbb{V}_h^M$ depends on μ and keeps the same number degree of freedom for all μ.

Finite Element Approximation: Quantitative Study

- **Parameters:** $M = 4,\ k = 0.25$
- **Computed error:** $\|u - U\|_{L^2(\Omega)}$
- **Expected rate:** $\min(s + \frac{1}{2}, 1)$
- **Simulations:**



number of DOFS of extended mesh $\mathscr{T}_M$

Outline

Space-Time Fractional PDEs

Multilevel Methods

Fractional Obstacle Problems

Spectral Fractional Laplacian: Balakrihsnan Formula

Integral Laplacian: Dunford-Taylor Formula

Conclusions

Conclusions about the Spectral Fractional Laplacian

- **PDEs with fractional time derivatives**
  - Global estimates: quasi-optimal in terms of regularity but suboptimal in terms of approximability.
  - Estimates for graded meshes is open; this may cure suboptimality.
  - Optimal local estimates for Balakhrisnan formula which degenerate for small t (Bonito, Lei, Pasciak (2017)).

- **Multilevel methods:**
  - Robust performance with respect to s and anisotropy; valid for Muckenhoupt weights.
  - Standard multilevel solvers usable for Balakhrisnan formula (Bonito, Pasciak (2015)).

- **Fractional obstacle problems:**
  - Optimal a priori error analysis for spectral method (thin obstacle). No a posteriori error analysis available.
  - A priori error analysis for integral method (Schwab, Matache, Nitsche (2005); a posteriori error analysis (N, von Petersdorff, Zhang (2010).
  - Open for Balakhrisnan formula.

Conclusions about Dunford-Taylor Approach

- **Spectral Dirichlet Laplacian: Balakrishnan formula**
  - Representation of the solution $(-\Delta)^{-\beta} f$ using the Balakrishnan formula
  - Exponential convergent SINC quadrature
  - Optimal FEM discretizations.
  - Applicable in $3d$.
  - A posteriori error analysis is open.

- **Fractional Laplacian:**
  - The Balakrishnan formula cannot be used to represent the solution
  - Derivation of the bilinear form using Fourier transform $\rightarrow$ non conforming method $\rightarrow$ Strang's lemma
  - Additional exponentially convergent domain truncation and sinc quadrature.
  - Applicable in $3d$.
  - A posteriori error analysis is open.