A PDE Approach to Numerical Fractional Diffusion

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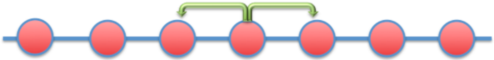
Outline

Local jump random walk

- We consider a random walk of a particle along the real line.
- $\mathbf{h}\mathbb{Z} := \{hz : z \in \mathbb{Z}\}$ — possible states of the jumping particle.
- $u(x, t)$ — probability of the particle to be at $x \in \mathbf{h}\mathbb{Z}$ at time $t \in \tau\mathbb{N}$.
- Local jump random walk: at each time step of size τ, the particle jumps to the left or right with probability $1/2$.



$$u(x, t+\tau) = \frac{1}{2}u(x+h, t) + \frac{1}{2}u(x-h, t)$$

If we consider $\tau = 2h^2$, then we obtain

$$\frac{u(x, t+\tau) - u(x, t)}{\tau} = \frac{u(x+h, t) + u(x-h, t) - 2u(x, t)}{h^2}$$

Letting $h, \tau \downarrow 0$, we have

heat equation: $u_t - \Delta u = 0.$

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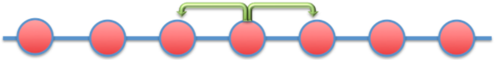

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Long jump random walk

- The probability that the particle jumps from the point $hk \in \mathbf{h}\mathbb{Z}$ to the point $hl \in \mathbf{h}\mathbb{Z}$ is $\mathcal{K}(k-l) = \mathcal{K}(l-k)$.

$$u(x, t+\tau) = \sum_{k\in\mathbb{Z}} \mathcal{K}(k) u(x+hk, t),$$

which, together with $\sum_{k\in\mathbb{Z}} \mathcal{K}(k) = 1$ yield

$$u(x, t+\tau) - u(x,t) = \sum_{k\in\mathbb{Z}} \mathcal{K}(k)\left(u(x+hk,t) - u(x,t)\right)$$

- Let $\mathcal{K}(y) = |y|^{-(n+2s)}$ with $s \in (0,1)$.
- Choose $\tau = h^{2s}$, then $\frac{\mathcal{K}(k)}{\tau} = h^n \mathcal{K}(kh)$

Letting $h, \tau \downarrow 0$,

$$\partial_t u = \int_{\mathbb{R}} \frac{u(x+y,t) - u(x,t)}{|y|^{n+2s}} dy \iff \partial_t u = -(-\Delta)^s u$$

Fractional heat equation: Singular integrals naturally arise as a continuous limit of discrete, long jump random walks.

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Applications I

Nonlocal operators and fractional diffusion appear in:

- Modeling anomalous diffusion (Metzler, Klafter 2004).
- Biophysics (Bueno-Orovio, Kay, Grau, Rodriguez, Burrage 2014)
- Turbulence (Chen 2006).
- Image processing (Gilboa, Osher 2008)
  Based on our PDE approach: Gatto, Hesthaven (2014).
- Nonlocal field theories (Eringen 2002).
- Materials science (Bates 2006).
- Peridynamics (Silling 2000; Du, Gunzburger 2012).
- Lévy processes (Bertoin 1996).
- Fractional Navier Stokes equation (Li et al 2012; Debbi 2014):

$$u_t + (-\Delta)^s u + u\nabla u - \nabla p = 0$$

- Fractional Cahn Hilliard equation (Segatti, 2014).

Outline

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The linear elliptic problem

Let Ω be a bounded domain with Lipschitz boundary and

$$\mathcal{L}u = -\nabla\cdot(a\nabla u) + cu$$

be a second order, symmetric, elliptic differential operator.
Let $s \in (0,1)$. Given $f : \Omega \to \mathbb{R}$, find u such that

$$\mathcal{L}^s u = f \quad \text{in } \Omega$$

where $\mathcal{L}^s$ denotes the fractional power of $\mathcal{L}$ supplemented with homogeneous Dirichlet boundary conditions.

Difficulty: $\mathcal{L}^s$ is a nonlocal operator.
Goal: design efficient solution techniques for problems involving $\mathcal{L}^s$.

From now on $\mathcal{L} = -\Delta$.
All our results hold for a general operator!

Spectral theory

We consider the definition of $(-\Delta)^s$ based on spectral theory:

- $-\Delta : H^2(\Omega) \cap H_0^1(\Omega) \subset L^2(\Omega) \to L^2(\Omega)$ is symmetric, closed and unbounded and its inverse is compact.
- The eigenpairs $\{\lambda_k, \varphi_k\}$, i.e.

$$-\Delta\varphi_k = \lambda_k\varphi_k, \qquad \varphi_k|_{\partial\Omega} = 0$$

  form an orthonormal basis of $L^2(\Omega)$.
- For u sufficiently smooth:

$$u = \sum_{k=1}^{\infty} u_k\varphi_k \longmapsto (-\Delta)^s u := \sum_{k=1}^{\infty} u_k\lambda_k^s\varphi_k$$

- $(-\Delta)^s : \mathbb{H}^s(\Omega) \to \mathbb{H}^{-s}(\Omega)$, $\mathbb{H}^s(\Omega) = [H_0^1(\Omega), L^2(\Omega)]_{1-s}$.

Spectral and integral methods

Spectral method: Given $f \in L^2(\Omega)$,

$$f = \sum_{k=1}^{\infty} f_k \varphi_k : \quad (-\Delta)^s u = f \implies \quad u_k = f_k \lambda_k^{-s}$$

Algorithm:

- Compute $\{\lambda_k, \varphi_k\}_{k=1}^N$ and the Fourier coefficients f_k.
- Compute $u_k = f_k \lambda_k^{-s}$.

Disadvantages:

- Quite expensive to compute N eigenpairs when N is large!

Integral method: extend u by zero outside Ω and compute

$$(-\Delta)^s u(x) = c_{n,s} \text{p.v.} \int_{\mathbb{R}^n} \frac{u(x) - u(z)}{|x - z|^{n+2s}} \, \mathrm{d}z,$$

which is equivalent to $\mathcal{F}((-\Delta)^s u)(\xi) = |\xi|^{2s} \mathcal{F}(u)$.

Discretization: Write a weak form and use a Galerkin method.

Disadvantages:

- Nonlocality $\implies$ dense matrix!
- Singularity $\implies$ complicated quadrature procedures!

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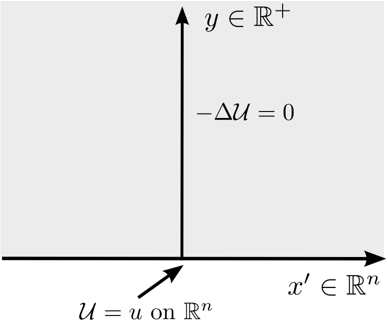
$(-\Delta)^{1/2}$: The Dirichlet-to-Neumann operator

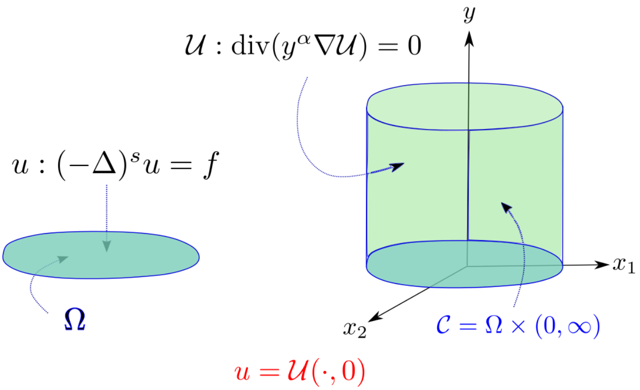


- DtN: $T : u \mapsto -\partial_y \mathcal{U}(\cdot, 0)$ is such that

$$T^2 u = \partial_y \left(\partial_y \mathcal{U}(\cdot, 0)\right) = -\Delta_{x'} \mathcal{U}(\cdot, 0) = -\Delta_{x'} u.$$

- T is positive, then $T = (-\Delta_{x'})^{\frac{1}{2}}$ and $(-\Delta_{x'})^{\frac{1}{2}} u = \partial_\nu \mathcal{U}$.

The α-harmonic extension



Here:

- $s \in (0, 1)$ and $\alpha = 1 - 2s \in (-1, 1)$.
- $\partial_{\nu^\alpha} \mathcal{U} = -\lim_{y \downarrow 0} y^\alpha \partial_y \mathcal{U} = d_s f$ on $\Omega \times \{0\}$.
- $d_s = 2^\alpha \Gamma(1 - s)/\Gamma(s)$.
- References: Caffarelli, Silvestre (2007), Cabré, Tan (2010), Capella et al. (2011), Stinga Torrea (2010–2012).

The α-harmonic extension

Fractional powers of $-\Delta$ can be realized as a DtN operator:

$$\begin{cases} \nabla\cdot(y^\alpha \nabla \mathcal{U}) = 0 & \text{in } \mathcal{C} \\ \mathcal{U} = 0 & \text{on } \partial_L \mathcal{C} \\ \partial_{\nu^\alpha} \mathcal{U} = d_s f & \text{on } \Omega \times \{0\} \end{cases} \iff \begin{cases} (-\Delta)^s u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

$$u = \mathcal{U}(\cdot, 0).$$

Here:

- $\mathcal{C} = \Omega \times (0, \infty)$
- $\alpha = 1 - 2s \in (-1, 1)$
- $\partial_{\nu^\alpha} \mathcal{U} = -\lim_{y\downarrow 0} y^\alpha \partial_y \mathcal{U} = d_s f$
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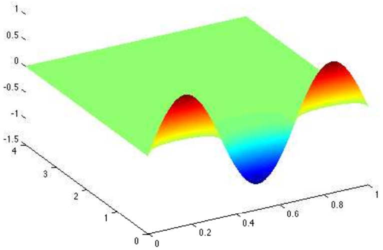


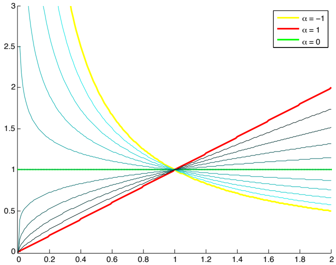
Weak formulation

A possible weak formulation reads

$$\int_{\mathcal{C}} y^{\alpha} \nabla \mathcal{U} \cdot \nabla \phi = d_s \langle f, tr_{\Omega} \phi \rangle_{\mathbb{H}^{-s}(\Omega), \mathbb{H}^{s}(\Omega)}, \quad \forall \phi \in \mathring{H}^1_L(y^{\alpha}, \mathcal{C}),$$

where

$$\mathring{H}^1_L(y^{\alpha}, \mathcal{C}) = \left\{ w \in L^2(y^{\alpha}, \mathcal{C}) : \ \nabla w \in L^2(y^{\alpha}, \mathcal{C}), \ w|_{\partial_L \mathcal{C}} = 0 \right\}.$$



The weight y^{α} is degenerate $(\alpha > 0)$ or singular$(\alpha < 0)$!

Muckenhoupt weights

There is a constant C such that for every $a, b \in \mathbb{R}$, with $a > b$,

$$\frac{1}{b-a}\int_a^b |y|^\alpha \,\mathrm{d}y \cdot \frac{1}{b-a}\int_a^b |y|^{-\alpha}\,\mathrm{d}y \leq C$$

which means y^α belongs to the Muckenhoupt class A_2. Then

- The Hardy-Littlewood maximal operator is continuous on $L^2(y^\alpha, \mathcal{C})$.
- Singular integral operators are continuous on $L^2(y^\alpha, \mathcal{C})$.
- $L^2(y^\alpha, \mathcal{C}) \hookrightarrow L^1_{loc}(\mathcal{C})$.
- $H^1(y^\alpha, \mathcal{C})$ is Hilbert and $C_b^\infty(\mathcal{C})$ is dense.
- Traces on $\partial_L \mathcal{C}$ are well defined.

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- Traces on $\partial_L \mathcal{C}$ are well defined.

Weighted Sobolev spaces

- Weighted Poincaré inequailty: There is a constant C, s.t.

$$\int_{\mathcal{C}} y^{\alpha}|w|^2 \leq C \int_{\mathcal{C}} y^{\alpha}|\nabla w|^2 \quad \forall w \in \mathring{H}_L^1(y^{\alpha}, \mathcal{C}).$$

- Surjective trace operator $tr_{\Omega} : \mathring{H}_L^1(y^{\alpha}, \mathcal{C}) \to \mathbb{H}^s(\Omega)$.

- Lax-Milgram $\Longrightarrow$ existence and uniqueness for every $f \in \mathbb{H}^{-s}(\Omega)$. Also

$$\|\mathcal{U}\|_{\mathring{H}_L^1(y^{\alpha}, \mathcal{C})} = \|u\|_{\mathbb{H}^s(\Omega)} = d_s\|f\|_{\mathbb{H}^{-s}(\Omega)}.$$

We will discretize the α-harmonic extension!

$$\mathcal{U} \in \mathring{H}_L^1(y^{\alpha}, \mathcal{C}) : \quad \begin{cases} \nabla\cdot(y^{\alpha}\nabla\mathcal{U}) = 0 & \text{in } \mathcal{C} \\ \mathcal{U} = 0 & \text{on } \partial_L\mathcal{C} \\ \partial_{\nu^{\alpha}}\mathcal{U} = d_s f & \text{on } \Omega \times \{0\} \end{cases}$$

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Separation of Variables

- Apply separation of variables (Capella et al. 2011)

$$u(x') = \sum_{k=1}^{\infty} u_k \varphi_k(x') \Longrightarrow \mathcal{U}(x', y) = \sum_{k=1}^{\infty} u_k \varphi_k(x') \psi_k(y),$$

where the functions ψ_k solve

$$\begin{cases} \psi_k'' + \dfrac{\alpha}{y}\psi_k' - \lambda_k \psi_k = 0, & \text{in } (0,\infty), \\ \psi_k(0) = 1, & \lim\limits_{y\to\infty} \psi_k(y) = 0. \end{cases}$$

- It turns out that

$$\psi_k(y) = c_s \left(\sqrt{\lambda_k} y\right)^s K_s(\sqrt{\lambda_k} y),$$

K_s – modified Bessel function of the second kind.

- Since

$$\psi_k'(y) \approx y^{-\alpha}, \quad y \downarrow 0 \quad \Longrightarrow \quad \mathcal{U} \notin H^1(\mathcal{C}).$$

Outline

Domain truncation

The domain $\mathcal{C}$ is infinite. We need to consider a truncated problem.

Theorem (exponential decay)

For every $\mathscr{Y} > 0$

$$\|\mathcal{U}\|_{\mathring{H}^1_L(y^\alpha,\Omega\times(\mathscr{Y},\infty))} \lesssim e^{-\sqrt{\lambda_1}\mathscr{Y}/2}\|f\|_{\mathbb{H}^{-s}(\Omega)}.$$

Let v solve

$$\begin{cases} \nabla\cdot(y^\alpha\nabla v) = 0 & \text{in } \mathcal{C}_\mathscr{Y} = \Omega\times(0,\mathscr{Y}), \\ v = 0 & \text{on } \partial_L\mathcal{C}_\mathscr{Y}\cup\Omega\times\{\mathscr{Y}\}, \\ \partial_{\nu^\alpha} v = d_s f & \text{on } \Omega\times\{0\}. \end{cases}$$

Theorem (exponential convergence)

For all $\mathscr{Y} > 0$,

$$\|\mathcal{U} - v\|_{\mathring{H}^1_L(y^\alpha,\mathcal{C}_\mathscr{Y})} \lesssim e^{-\sqrt{\lambda_1}\mathscr{Y}/4}\|f\|_{\mathbb{H}^{-s}(\Omega)}.$$

Finite element method I

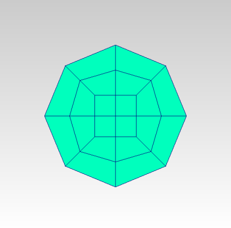
- Continuous solution. $\mathbb{V}$-Hilbert space. Find u s.t.

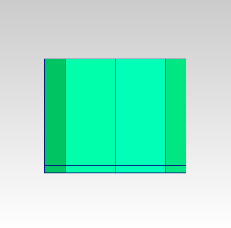
$$\mathscr{B}[u, v] = \mathscr{F}[v], \qquad \forall v \in \mathbb{V}.$$

$\mathscr{B}$-continuous and coercive bilinear form, and $\mathscr{F}$-continuous linear functional.

- Approximate solution. Let $\mathbb{V}_{\mathrm{N}}$ be a finite dimensional space. Find U_{N} s.t.

$$\mathscr{B}[U_{\mathrm{N}}, V_{\mathrm{N}}] = \mathscr{F}[V_{\mathrm{N}}], \qquad \forall v \in \mathbb{V}_{\mathrm{N}}.$$





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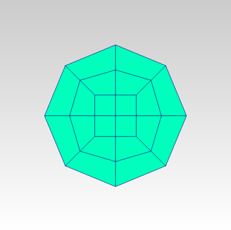

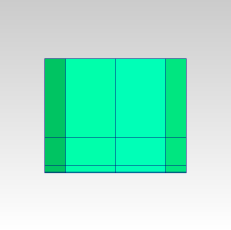

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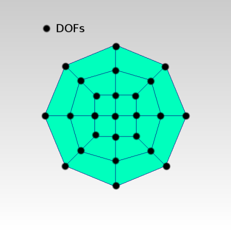

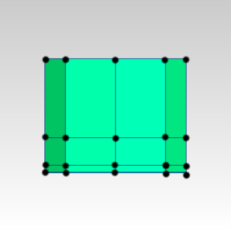

Finite element method II

- Continuous solution. $\mathbb{V}$-Hilbert space. Find u s.t.

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  $\mathscr{B}$-continuous and coercive bilinear form, and $\mathscr{F}$-continuous linear functional.

- Approximate solution. Let $\mathbb{V}_{\mathrm{N}}$ be a finite dimensional space. Find U_{N} s.t.

$$\mathscr{B}[U_{\mathrm{N}}, V_{\mathrm{N}}] = \mathscr{F}[V_{\mathrm{N}}], \qquad \forall v \in \mathbb{V}_{\mathrm{N}}.$$

- Error estimates.
  - A priori. Convergence, a rate of convergence, and know the depende of the error on different factors. Typical estimate:

$$\|u - U_{\mathrm{N}}\|_{\mathbb{V}} \lesssim N^{-a}\|u\| \approx h^b\|u\|$$

  - A posteriori. Information beyond asymptotics; computable in terms of $\mathscr{F}$ and U_{N}. Quality assessment; adaptivity.

Galerkin method: mesh

Let $\mathscr{T}_\Omega = \{K\}$ be triangulation of Ω (simplices or cubes)

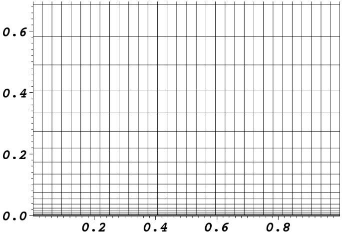
- $\mathscr{T}_\Omega$ is conforming and shape regular.

Let $\mathscr{T}_\mathcal{Y} = \{T\}$ be a triangulation of $\mathcal{C}_\mathcal{Y}$ into cells of the form

$$T = K \times I, \quad K \in \mathscr{T}_\Omega, \quad I = (a, b).$$

Why? Natural on the cylinder $\mathcal{C}_\mathcal{Y}$, deal.ii, and $\mathcal{U}_{yy} \approx y^{-\alpha-1}$ as $y \approx 0+$

Approximation of singular functions $\Longrightarrow$ anisotropic elements



Shape regularity condition does NOT hold!

Galerkin method: discrete spaces

We only require that if $T = K \times I$ and $T' = K' \times I'$ are neighbors

$$\frac{|I|}{|I'|} \simeq 1,$$

so the lengths of I and I' are comparable. This weak condition allows us to consider anisotropic meshes

Define:

$$\mathbb{V}(\mathscr{T}_{\mathcal{Y}}) = \left\{ W \in \mathcal{C}^0(\overline{\mathcal{C}_{\mathcal{Y}}}) : \ W|_T \in \mathcal{P}_1(T), \quad W|_{\Gamma_D} = 0 \right\}$$

with $\Gamma_D = \partial_L \mathcal{C} \cup \Omega \times \{\mathcal{Y}\}$, and

$$\mathbb{U}(\mathscr{T}_\Omega) = tr_\Omega \mathbb{V}(\mathscr{T}_{\mathcal{Y}}) = \left\{ W \in \mathcal{C}^0(\bar{\Omega}) : \ W|_K \in \mathcal{P}_1(K), \ W_{\partial\Omega} = 0 \right\}$$

Galerkin method: discrete problem

Galerkin method for the extension: Find $V_{\mathscr{T}_\mathcal{Y}} \in \mathbb{V}(\mathscr{T}_\mathcal{Y})$ such that

$$\int_{\mathcal{C}_\mathcal{Y}} y^\alpha \nabla V_{\mathscr{T}_\mathcal{Y}} \nabla W = d_s \langle f, tr_\Omega W \rangle_{\mathbb{H}^{-s}(\Omega),\mathbb{H}^s(\Omega)}, \quad \forall W \in \mathbb{V}(\mathscr{T}_\mathcal{Y})$$

Define:

$$\boxed{U_{\mathscr{T}_\Omega} = tr_\Omega V_{\mathscr{T}_\mathcal{Y}} \in \mathbb{U}(\mathscr{T}_\Omega)}$$

A trace estimate and Cèa's Lemma imply quasi-best approximation:

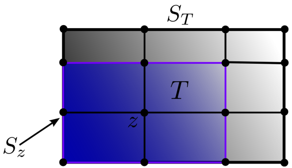
$$\begin{aligned}\|u - U_{\mathscr{T}_\Omega}\|_{\mathbb{H}^s(\Omega)} &\lesssim \|v - V_{\mathscr{T}_\mathcal{Y}}\|_{\mathring{H}_L^1(y^\alpha,\mathcal{C}_\mathcal{Y})} \\ &= \inf_{W \in \mathbb{V}(\mathscr{T}_\mathcal{Y})} \|v - W\|_{\mathring{H}_L^1(y^\alpha,\mathcal{C}_\mathcal{Y})}\end{aligned}$$

Setting $W = \Pi v \in \mathbb{V}(\mathscr{T}_\mathcal{Y}) \implies$ interpolation analysis!

Outline

The averaged Taylor polynomial

Consider $\omega \in A_2(\mathbb{R}^N)$ and $\phi \in L^2(\omega, D)$, with $D \subset \mathbb{R}^N$. Given a node z of the mesh, we define



Given $m \in \mathbb{N}$, we define

$$Q_z^m \phi(y) = \int \sum_{|\alpha| \leq m} \frac{1}{\alpha!} D^\alpha \phi(x)(y-x)^\alpha \psi_z(x) \, \mathrm{d}x.$$

A weighted Poincaré inequailty yields

$$\|\phi - Q_z^0 \phi\|_{L^2(\omega, S_z)} \lesssim \mathrm{diam}(S_z) \|\nabla \phi\|_{L^2(\omega, S_z)},$$

which, via an induction argument, allows us to derive

$$|\phi - Q_z^m \phi|_{H^k(\omega, S_z)} \lesssim \mathrm{diam}(S_z)^{m+1-k} |\phi|_{H^{m+1}(\omega, S_z)}, \quad k = 0, 1, \ldots, m+1$$

Extension to the weighted case! Simple argument!

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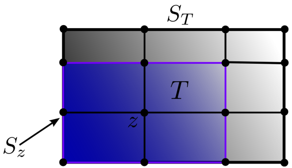

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The quasi-interpolant operator

We introduce an averaged interpolation operator Π *á la* Duran Lombardi, 2005 (Sobolev 1950, Dupont Scott 1980)

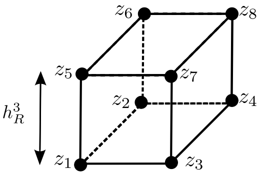
$$\Pi\phi(z) = Q_z^m \phi(z).$$

Notice that:

- This is defined for all polynomial degree m and any element shape (simplices or rectangles).
- We do not go back to the reference element — This is important for anisotropic estimates.

The mesh is rectangular and Cartesian. If R and S are neighbors

$$h_R^i / h_S^i \lesssim 1, \qquad i = \overline{1, N}.$$



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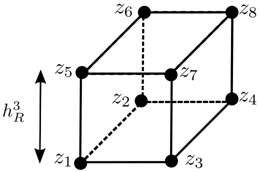

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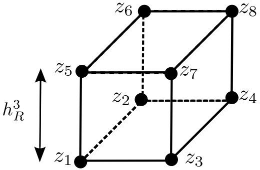

Error estimates on rectangles

Theorem

If $\phi \in H^1(\omega, S_R)$

$$\|\phi - \Pi\phi\|_{L^2(\omega,R)} \lesssim \sum_{i=1}^{N} h_R^i \|\partial_i \phi\|_{L^2(\omega,S_R)}.$$

If $\phi \in H^2(\omega, S_R)$

$$\|\partial_j(\phi - \Pi\phi)\|_{L^2(\omega,R)} \lesssim \sum_{i=1}^{N} h_R^i \|\partial_i \partial_j \phi\|_{L^2(\omega,S_R)},$$

$$\|\phi - \Pi\phi\|_{L^2(\omega,R)} \lesssim \sum_{i,j=1}^{N} h_R^i h_R^j \|\partial_i \partial_j \phi\|_{L^2(\omega,S_R)}.$$

Error estimates on rectangles

Theorem

If $\omega \in A_p(\mathbb{R}^N)$, *and* $\phi \in \cancel{H^1(\omega, S_R)}$ $W_p^1(\omega, S_R)$

$$\|\phi - \Pi\phi\|_{L^p(\omega,R)} \lesssim \sum_{i=1}^{N} h_R^i \|\partial_i \phi\|_{L^p(\omega,S_R)}.$$

If $\phi \in \cancel{H^2(\omega, S_R)}$ $W_p^2(\omega, S_R)$

$$\|\partial_j(\phi - \Pi\phi)\|_{L^p(\omega,R)} \lesssim \sum_{i=1}^{N} h_R^i \|\partial_i \partial_j \phi\|_{L^p(\omega,S_R)},$$

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Estimates on simplicial elements, different metrics and applications in RHN, EO, AJS. *Piecewise polynomial interpolation in Muckenhoupt weighted Sobolev spaces and applications*, *Numer. Math.* (2015)

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Estimates on simplicial elements, different metrics and applications in RHN, EO, AJS. *Piecewise polynomial interpolation in Muckenhoupt weighted Sobolev spaces and applications, Numer. Math. (2015)*

Outline

Regularity of Extension $\mathcal{U}$

Using properties of Bessel functions we obtain

$$\psi_k''(y) \approx y^{-\alpha-1}, \quad y \downarrow 0 \qquad \Longrightarrow \qquad \mathcal{U} \notin H^2(\mathcal{C}, y^\alpha).$$

But

Theorem (regularity of the extension)

If $f \in \mathbb{H}^{1-s}(\Omega)$ and Ω is $C^{1,1}$ or a convex polygon

$$\|\Delta_{x'}\mathcal{U}\|^2_{L^2(\mathcal{C},y^\alpha)} + \|\partial_y \nabla_{x'}\mathcal{U}\|^2_{L^2(\mathcal{C},y^\alpha)} = d_s\|f\|^2_{\mathbb{H}^{1-s}(\Omega)}$$

If $\beta > 1 + 2\alpha$

$$\|\partial_{yy}\mathcal{U}\|_{L^2(\mathcal{C},y^\beta)} \lesssim \|f\|_{L^2(\Omega)}$$

Anisotropic estimates compensate singular behavior!

Error Estimates: Quasi-uniform Meshes

On uniform meshes $h_T \approx h_K \approx h_I$ for all $T \in \mathscr{T}_{\mathcal{Y}}$, then

Theorem (error estimates)

The following estimate holds for all $\epsilon > 0$

$$\|\nabla(v - V_{\mathscr{T}_{\mathcal{Y}}})\|_{L^2(\mathcal{C}_{\mathcal{Y}}, y^\alpha)} \lesssim h_K \|\partial_y \nabla_{x'} v\|_{L^2(\mathcal{C}, y^\alpha)} + h_I^{s-\epsilon} \|\partial_{yy} v\|_{L^2(\mathcal{C}, y^\beta)}$$
$$\lesssim h^{s-\epsilon} \|f\|_{\mathbb{H}^{1-s}(\Omega)}$$

Consequently,

$$\|u - U_{\mathscr{T}_\Omega}\|_{\mathbb{H}^s(\Omega)} \lesssim h^{s-\epsilon} \|f\|_{\mathbb{H}^{1-s}(\Omega)}.$$

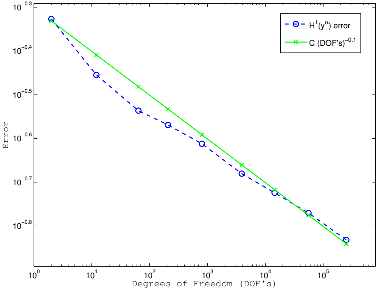
- This is suboptimal in terms of order (only order $s - \epsilon$)
- It cannot be improved as numerical experimentation reveals!

Numerical Experiment: Quasi-uniform Mesh

Let $\Omega = (0,1)$ and $f = \pi^{2s}\sin(\pi x)$, then

$$\mathcal{U} = \frac{2^{1-s}\pi^s}{\Gamma(s)} \sin(\pi x') y^s K_s(\pi y)$$

If $s = 0.2$, then



The energy error behaves like $DOFS^{-0.1} \approx h^{0.2}$, as predicted!

Error Estimates: Graded Meshes

We use the principle of error equilibration. Mesh on $(0, \mathscr{Y})$

$$y_j = \mathscr{Y}\left(\frac{j}{M}\right)^{\gamma}, \quad j = \overline{0, M}, \quad \gamma > 1$$

$\psi_k''(y) \approx y^{-\alpha-1} \Longrightarrow$ energy equidistribution for $\gamma > 3/(1-\alpha)$.

Theorem (error estimates)

If $f \in \mathbb{H}^{1-s}(\Omega)$ and $\mathscr{Y} \approx |\log N|$,

$$\begin{aligned}\|u - U_{\mathscr{T}_\Omega}\|_{\mathbb{H}^s(\Omega)} &= \|\nabla(\mathcal{U} - V_{\mathscr{T}_\mathscr{Y}})\|_{L^2(\mathcal{C}, y^\alpha)} \\ &\lesssim |\log N|^s N^{-\frac{1}{n+1}} \|f\|_{\mathbb{H}^{1-s}(\Omega)},\end{aligned}$$

or equivalently

$$\|u - U_{\mathscr{T}_\Omega}\|_{\mathbb{H}^s(\Omega)} \lesssim |\log N_\Omega|^s N_\Omega^{-1/n} \|u\|_{\mathbb{H}^{1+s}(\Omega)}.$$

Outline

Numerical Experiments: Meshes for Circle and $s = 0.3$

Set $\Omega = D(0,1) \subset \mathbb{R}^2$,

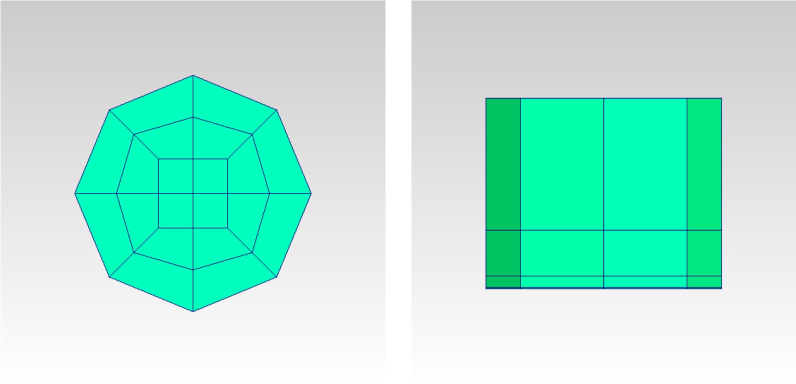
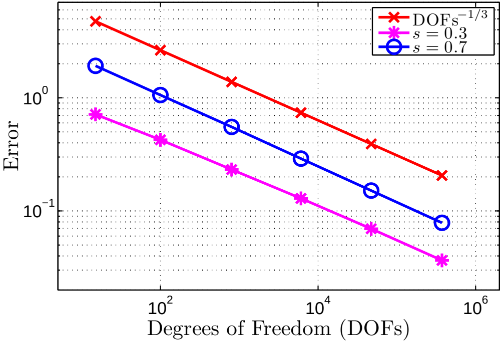


Figure : Uniform mesh in x' and anisotropic mesh in y

Experimental Rates for Circle and $s = 0.3$ and $s = 0.7$

Set $\Omega = D(0,1) \subset \mathbb{R}^2$, $f = j_{1,1}^{2s} J_1(j_{1,1} r)(A_{1,1}\cos(\theta) + B_{1,1}\sin(\theta))$.
With graded meshes:



The experimental convergence rate $-1/3$ is optimal!

RHN, EO, AJS. *A PDE approach to fractional diffusion in general domains: a priori error analysis*, Found. Comput. Math. (2014).

Outline

Adaptivity

Adaptivity is motivated by

- Computational efficiency: extra $n+1$-dimension.
- The a priori theory requires
  - regularity of the datum: $f \in \mathbb{H}^{1-s}(\Omega)$.
  - regularity of the domain: Ω is $C^{1,1}$ or a convex polygon.
- If one of these conditions is violated, the solution $\mathcal{U}$ may have singularities in Ω and exhibit fractional regularity.
- Quasi-uniform refinement of Ω would not result in an efficient solution technique.
- We need an adaptive loop.

An adaptive loop

Our adaptive loop is *almost* standard:

$$\mathit{SOLVE} \rightarrow \mathit{ESTIMATE} \rightarrow \mathit{MARK} \rightarrow \mathit{REFINE}$$

with

- **SOLVE**: Finds $V_{\mathscr{T}_{\mathcal{Y}}}$, the Galerkin solution.
- **ESTIMATE**: Compute $\mathcal{E}_{z'}$ for every node $z' \in \Omega$.
- **MARK**: For $\theta \in (0,1)$ choose a minimal subset of nodes $\mathcal{M}$:

$$\sum_{z' \in \mathcal{M}} \mathcal{E}_{z'}^2 \geq \theta^2 \mathcal{E}_{\mathscr{T}}^2.$$

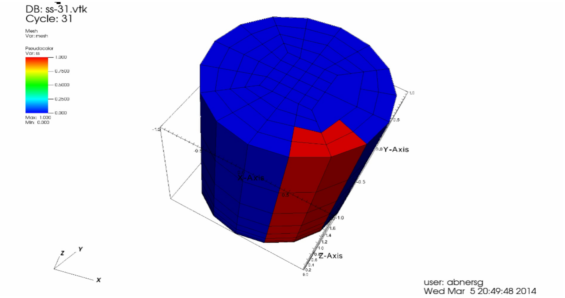
- **REFINE**: Given $\mathcal{M}$:
  1. $\forall z' \in \mathcal{M}$ refine the cells $K \ni z'$ to get $\tilde{\mathscr{T}}_\Omega$.
  2. Create an anisotropic mesh $\{\tilde{I}\}$ with M so that grading holds.
  3. The refined mesh is $\tilde{\mathscr{T}}_{\mathcal{Y}} = \tilde{\mathscr{T}}_\Omega \times \{\tilde{I}\}$.

Adaptivity

- One of the main ingredients of our adaptive loop is an a posteriori error estimator.

Despite of what might be claimed, the theory of a posteriori error estimation on anisotropic discretizations is still in its infancy.

We propose an error estimator based on solving local problem on stars:



An ideal error estimator

Define

$$\mathbb{W}(\mathcal{C}_{z'}) = \left\{ w \in H^1(y^\alpha, \mathcal{C}_{z'}) : \; w = 0 \text{ on } \partial\mathcal{C}_{z'} \setminus \Omega \times \{0\} \right\}.$$

For $z' \in \Omega$ a node, we define the ideal estimator $\zeta_{z'} \in \mathbb{W}(\mathcal{C}_{z'})$:

$$\int_{\mathcal{C}_{z'}} y^\alpha \nabla \zeta_{z'} \nabla \psi = d_s \langle f, tr_\Omega \psi \rangle_{\mathbb{H}^{-s}(\Omega)\times\mathbb{H}^s(\Omega)} - \int_{\mathcal{C}_{z'}} y^\alpha \nabla V \nabla \psi$$

for all $\psi \in \mathbb{W}(\mathcal{C}_{z'})$, and

$$\tilde{\mathcal{E}}_{\mathscr{T}_\mathcal{Y}} = \left(\sum_{z'} \tilde{\mathcal{E}}_{z'}^2 \right)^{1/2}, \quad \mathcal{E}_{z'} = \|\nabla \zeta_{z'}\|_{L^2(y^\alpha, \mathcal{C}_{z'})}.$$

Theorem (ideal estimator)

We have

$$\|\nabla e\|_{L^2(y^\alpha, \mathcal{C}_\mathcal{Y})} \lesssim \tilde{\mathcal{E}}_{\mathscr{T}_\mathcal{Y}}$$

and, for every node $z' \in \Omega$

$$\tilde{\mathcal{E}}_{z'} \leq \|\nabla e\|_{L^2(y^\alpha, \mathcal{C}_{z'})}.$$

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Local Problems on Stars

- Discretization based on $\mathbb{P}_2$: Discrete space $\mathcal{W}(\mathcal{C}_{z'})$. Then, we define

$$\mathcal{E}_{z'}^2 := \int_{\mathcal{C}_{z'}} y^\alpha |\nabla W_{z'}|^2, \qquad \mathcal{E}_{\mathscr{T}_\Omega}^2 := \sum_{z'} \mathcal{E}_{z'}^2.$$

- Define the data oscillation. If $f_{z'|K} = \frac{1}{|K|}\int_K f$ then

$$\operatorname{osc}_{\mathscr{T}_\Omega}(f)^2 = \sum_{z'} \operatorname{osc}_{z'}(f)^2, \quad \operatorname{osc}_{z'}(f)^2 = d_s h_{z'}^{2s} \| f - f_{z'} \|_{L^2(S_{z'})}^2$$

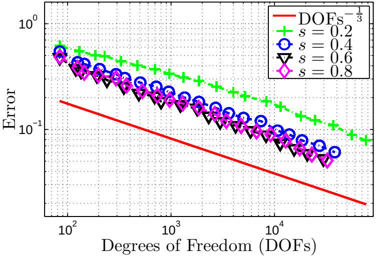
Theorem (computable estimator)

$$\mathcal{E}^2 \lesssim \|\nabla(v - V_{\mathscr{T}_\mathcal{Y}})\|_{L^2(y^\alpha, \mathcal{C}_\mathcal{Y})}^2 \lesssim \mathcal{E}^2 + \operatorname{osc}(y^\alpha, V_{\mathscr{T}_\mathcal{Y}}, f, \mathcal{C}_{z'})^2$$

- Is this enough for convergence and optimality?

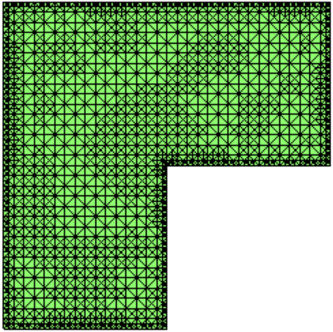
L-shaped domain with incompatible data

- Ω is the standard L-shaped domain. $f = 1$. For $s < \frac{1}{2}$ the data is not compatible with the problem.
- The nature of the singularity of the solution is not known for this problem.

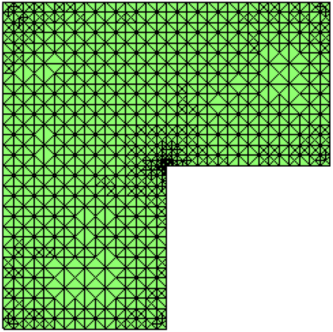


L-shaped domain with incompatible data

Some meshes:



$s = 0.2$



$s = 0.8$

A posteriori error analysis and adaptivity

LC, RHN, EO, AJS: *A PDE approach to fractional diffusion in general domains: a posteriori error analysis* . J. Comput. Phys. (2015).

- Question: Is there any theory on anisotropic error estimators? (Cohen Mirebeau 2010-2012) (Petrushev 2007-2009)?
- A posteriori error estimators, convergence of AFEM, convergence rates for AFEM are still open questions.

Outline

Outline

Space-time fractional parabolic problem

Let $T > 0$ be some positive time. Given $f : \Omega \to \mathbb{R}$ and $u_0 : \Omega \to \mathbb{R}$ the problem reads: Find u such that

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

Here $\gamma \in (0, 1]$. For $\gamma = 1$ this is the usual time derivative, if $\gamma < 1$ we consider the Caputo derivative

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

Nonlocality in space and time!

We will overcome the nonlocality in space using the Caffarelli-Silvestre extension.

Outline

Extended evolution problem

The Caffarelli-Silvestre extension turns our problem into a quasi stationary elliptic problem with dynamic boundary condition

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

Connection: $\mathrm{u}=tr_{\Omega}\,\mathcal{U}$, $\alpha=1-2s$.

Nonlocality just in time!

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

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

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

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

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

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

Truncation

$\mathcal{C}$ is infinite, but we have exponential decay.

Theorem

Let $\gamma \in (0,1]$ and $s \in (0,1)$. If $\mathcal{Y} > 1$ then

$$\|\nabla \mathcal{U}\|_{L^2(0,T;L^2(\Omega\times(\mathcal{Y},\infty),y^\alpha))} \lesssim e^{-\sqrt{\lambda_1}/2}$$

- This allows us to consider a truncated problem.
- In doing so we commit only an exponentially small error

$$I^{1-\gamma}\|tr_\Omega(\mathcal{U}-v)\|^2_{L^2(\Omega)} + \|\nabla(\mathcal{U}-v)\|_{L^2(0,T;L^2(\mathcal{C}_\mathcal{Y},y^\alpha))} \lesssim e^{-\sqrt{\lambda_1}\mathcal{Y}}$$

where I^σ is the *Riemann Liouville* fractional integral of order σ.

Outline

Time discretization for $\gamma = 1$

Time step $\tau = T/\mathcal{K}$. 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.
For $\gamma = 1$, we consider backward Euler

- We initialize by setting $tr_\Omega V^0 = \mathsf{u}_0$.
- For $k = 0, \ldots, \mathcal{K} - 1$, we find $V^{k+1} \in \mathring{H}_L^1(y^\alpha, \mathcal{C})$ solution of

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

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

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

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

For $\gamma \in (0,1)$, we consider the so-called L1 scheme

$$\begin{aligned}\partial_t^\gamma u(x, t_{k+1}) &= \frac{1}{\Gamma(1-\gamma)} \int_0^{t_{k+1}} \frac{\partial_r u(x,r)}{(t_{k+1}-r)^\gamma} \,\mathrm{d}r \\ &\approx \frac{1}{\Gamma(2-\gamma)} \sum_{j=0}^{k} a_j \frac{u(x, t_{k+1-j}) - u(x, t_{k-j})}{\tau^\gamma} \\ &= D^\gamma u(x)^{k+1}\end{aligned}$$

where $a_j = (j+1)^{1-\gamma} - j^{1-\gamma}$.
For $\gamma \in (0,1)$, the scheme reads

- We initialize by setting $tr_\Omega V^0 = \mathrm{u}_0$.
- For $k = 0, \ldots, \mathcal{K}-1$, we find $V^{k+1} \in \mathring{H}_L^1(\mathcal{C}, y^\alpha)$ solution of

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

Time discretization for $\gamma \in (0,1)$. Stability

The lack of fractional integration by parts makes it difficult to obtain energy estimates. We obtain new semidiscrete energy estimates for the L1 scheme

Theorem (stability)

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

Since these are uniform in τ and the scheme is consistent[1] we derive a novel continuous energy estimate

Theorem (energy estimates)

$$I^{1-\gamma}\|tr_\Omega \mathcal{U}\|^2_{L^2(\Omega)} + \|\mathcal{U}\|^2_{\ell^2(\mathring{H}^1_L(\mathcal{C},y^\alpha))} \leq I^{1-\gamma}\|\mathrm{u}_0\|^2_{L^2(\Omega)} + \|f^\tau\|^2_{\ell^2(\mathbb{H}^{-s}(\Omega))}.$$

[1] see next slide

Time discretization for $\gamma \in (0,1)$. Consistency

- The literature analyzes the L1 scheme assuming smoothness of the solution $u \in C^2([0,T],\mathbb{H}^{-s}(\Omega))$.
- However, in general, this assumption is not valid!
- We showed that

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

and

$$\partial_{tt} u \in L^2(t^\sigma,(0,T)),$$

for $\sigma > 3-2\gamma$. These are valid under realistic assumptions on f and u_0.

Time discretization for $\gamma \in (0,1)$. Consistency

- Using these new regularity estimates we can provide an analysis of the L1 scheme.
- Since
$$\partial_t^\gamma u(x, t_{k+1}) = D^\gamma u(x)^{k+1} + \mathrm{r}_\gamma^\tau$$
and the remainder satisfies
$$\|\mathrm{r}_\gamma^\tau\|_{\mathbb{H}^{-s}(\Omega)} \lesssim \tau^\theta \left(\|\mathrm{u}_0\|_{\mathbb{H}^{2s}(\Omega)} + \|f\|_{H^2(0,T;\mathbb{H}^{-s}(\Omega))} \right),$$
where $\theta < \frac{1}{2}$.
  - Key result: $u_t \in L \log L(0,T;\mathbb{H}^{-s}(\Omega))$. Hardy and Littlewood yields $I^{1-\gamma} : L \log L(0,T) \to L^{\frac{1}{\gamma}}(0,T)$ boundedly.

Error estimates for fully discrete schemes

Discretization in time and space: stability + consistency yield

- Error estimates for $\mathcal{U}$: $s \in (0,1)$ and $\gamma \in (0,1)$

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

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

- Error estimates for u: $s \in (0,1)$ and $\gamma \in (0,1)$

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

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

where $\theta < \frac{1}{2}$.

RHN, EO, AJS. *A PDE approach to space-time fractional parabolic problems*. SIAM J. Numer. Analysis. 2014 (submitted).

Outline

Outline

Classical obstacle problem

- Consider a surface given by the graph of a function u.
- u solves $\Delta u = 0$ for fixed boundary data (elastic membrane).

- Let us now slide an obstacle from below. The surface must stay above it.

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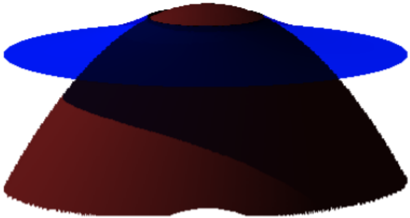

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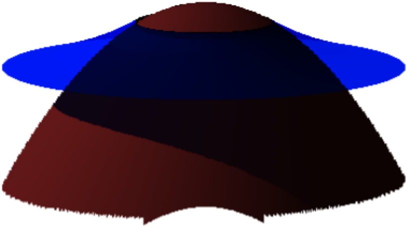

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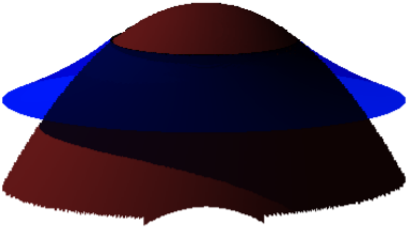
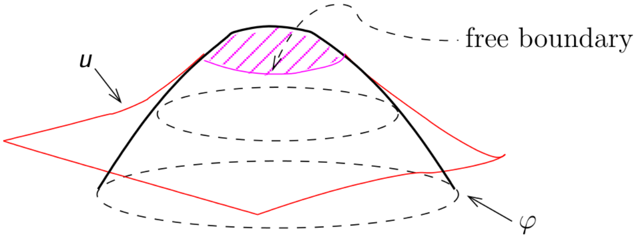


- Let us now slide an obstacle from below. The surface must stay above it.
- For a given obstacle ψ, we obtain a function $u \geq \psi$, that will try to be as harmonic as possible.

Classical obstacle problem

- $\Delta u = 0$ when $u > \psi$, since there u is free to move.
- $\Delta u \le 0$ everwhere, since the surface pushes down.
- $u \ge \psi$.
- Complementarity system:

$$\lambda = -\Delta u \ge 0, \quad u - \psi \ge 0, \quad \Delta u(u - \psi) = 0 \quad \text{a.e. in } \Omega.$$



Motivation for the fractional obstacle problem

- Consider

$$u = \sup_{\tau} E(\psi(X_\tau^x)),$$

where X_τ^x is a purely jump process starting at x and τ denotes any stopping time.

- Then

$$u \geq \psi, \quad Lu \geq 0, \quad Lu = 0 \text{ if } u > \psi,$$

where the operator L is

$$Lu(x) = \mathrm{P.V.} \int (u(x) - u(x+u))\mathcal{K}(y).$$

- Natural example: $\mathcal{K}(y) = |y|^{-(n+2s)}$ with $s \in (0,1)$ gives

$$(-\Delta)^s u = 0 \text{ where } u > \psi, \quad (-\Delta)^s u \geq 0 \text{ everywhere }, u \geq \psi$$

Outline

Motivation

The elliptic linear problem case

Space-time fractional parabolic problem

The fractional obstacle problem
- Motivation
- Formulation
- Truncation
- Error estimates

An optimal control problem

Conclusions and future work

The fractional obstacle problem

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

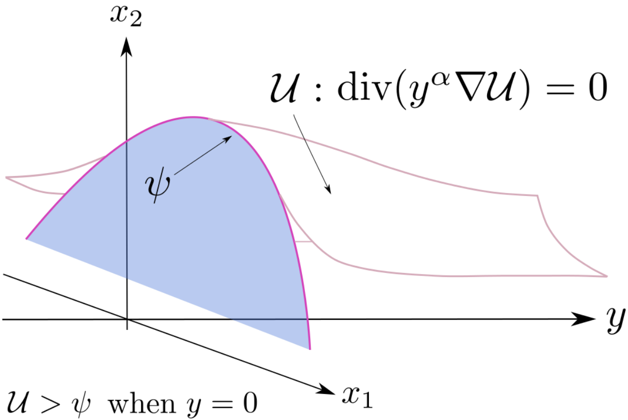
$$u \in \mathcal{K} : \quad \langle (-\Delta)^s u, u - w \rangle \leq \langle f, u - w \rangle \quad \forall w \in \mathcal{K}.$$

- $\mathcal{K} := \{ w \in \mathbb{H}^s(\Omega) : \ w \geq \psi \text{ a.e. in } \Omega \}$.
- Nonlinear and nonlocal problem since $(-\Delta)^s$!
- We use Caffarelli-Silvestre extension!

  In fact, the study of the regularites properties of the fractional obstacle problem motivated the Caffarelli-Silvestre extension.

Thin obstacle problem

- We convert the fractional obstacle problem in a thin obstacle problem.



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

Outline

Thin obstacle problem

- Truncation of the cylinder:

$$\|\nabla(\mathcal{U}-\mathcal{V})\|_{L^2(y^\alpha,\mathcal{C}_\mathcal{Y})} \lesssim e^{-\sqrt{\lambda_1}\mathcal{Y}/8}\left(\|\psi\|_{\mathbb{H}^s(\Omega)}+\|f\|_{\mathbb{H}^{-s}(\Omega)}\right).$$

- To derive an error estimate the following regularity results are fundamental:
  - $u \in C^{1,\alpha}$ for $\alpha < s$ by Silvestre (2007).
  - Optimal regularity: $u \in C^{1,s}$ by Cafarelli, Salsa and Silvestre (2008).
  - $\partial_\nu^\alpha \mathcal{U}(\cdot,0) \in C^{0,1-s}(\Omega)$.
  - Optimal regularity by Allen, Lindgren, and Petrosyan (2014) $s \le \frac{1}{2} \ \Rightarrow \mathcal{V} \in C^{0,2s}(\mathcal{C}_\mathcal{Y})$ and $s > \frac{1}{2} \ \Rightarrow \mathcal{V} \in C^{1,2s-1}(\mathcal{C}_\mathcal{Y})$.

Outline

Thin obstacle problem

- Nearly optimal error estimate:

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

  where C depends on the Hölder moduli of smoothness of $\mathcal{U}$ and $\mathcal{V}$, $\|f\|_{\mathbb{H}^{-s}(\Omega)}$ and $\|\psi\|_{\mathbb{H}^s(\Omega)}$.
- Same techniques can be applied for the Signori or thin obstacle problem.

RHN, EO, AJS. *Convergence rates for the obstacle problem: classical, thin and fractional*, Phil. Trans. R. Soc. A (2015).

Outline

Motivation: Cardiac Microstructure

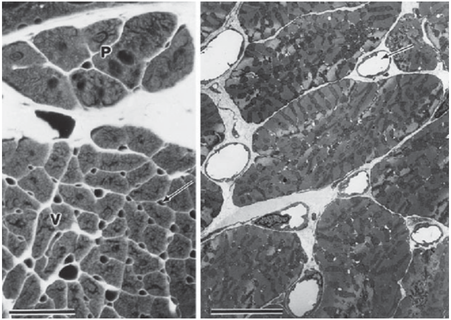
- The heart has its own internal electrical system that controls the rate and rhythm of heartbeat.
- Heartbeat produces an electrical signal that spreads from the top to the bottom: it causes the heart to contract and pump blood.
- Problems with this electrical system cause arrhythmia!
- Implantable cardioverter defibrillator (ICD): monitors the heart rhythm.
- If an irregular rhythm is detected, it will use low-energy electrical pulses to restore a normal rhythm.
- Fundamental modeling to understand the propagation of electrical excitation is:

$$\partial_t u - \Delta u = f$$

Motivation: Cardiac Microstructure

- This conventional model neglects the highly complex, heterogeneous nature of the underlying tissues.
- Bueno-Orovio, Kay, Grau, Rodriguez, and Burrage (2014):

$$\partial_t u + (-\Delta)^s u = f.$$



Outline

Problem Formulation

Define

$$J(\mathrm{u},\mathrm{z}) = \frac{1}{2}\|\mathrm{u}-\mathrm{u}_d\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|\mathrm{z}\|^2_{L^2(\Omega)}.$$

We are interested in the optimal control problem:

$$\min J(\mathrm{u},\mathrm{z})$$

subject to the non-local state equation

$$\mathcal{L}^s \mathrm{u} = \mathrm{z} \text{ in } \Omega, \qquad \mathrm{u} = 0 \text{ on } \partial\Omega,$$

and the control constraints

$$\mathrm{z} \in \mathrm{Z}_{\mathrm{ad}} := \{\mathrm{w} \in L^2(\Omega) : \mathrm{a}(x') \leq \mathrm{w}(x') \leq \mathrm{b}(x') \quad \text{a.e.} \quad x' \in \Omega\}.$$

Here,

$$\mathcal{L}w = -\nabla\cdot_{x'}(A\nabla_{x'} w) + cw.$$

Outline

An equivalent control problem

The Caffarelli-Silvestre result allows us to rewrite our control problem as follows:

$$\min \; J(tr_{\Omega}\mathcal{U}, \mathsf{z}) = \frac{1}{2}\|tr_{\Omega}\mathcal{U} - \mathsf{u}_d\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|\mathsf{z}\|^2_{L^2(\Omega)}$$

subject to the linear and local state equation

$$\frac{1}{d_s}\int_{\mathcal{C}} y^{\alpha}\nabla\mathcal{U}\cdot\nabla\phi = \langle \mathsf{z}, tr_{\Omega}\phi\rangle_{\mathbb{H}^{-s}(\Omega),\mathbb{H}^{s}(\Omega)}, \quad \forall \phi \in \mathring{H}^1_L(y^{\alpha},\mathcal{C}),$$

and the control constraints

$$\mathsf{z} \in \mathsf{Z}_{\mathrm{ad}} := \{\mathsf{w} \in L^2(\Omega) : \mathsf{a}(x') \leq \mathsf{w}(x') \leq \mathsf{b}(x') \quad \text{a.e.} \;\; x' \in \Omega\}.$$

Existence and uniquess of an optimal pair $(\bar{\mathsf{z}}, \bar{\mathcal{U}})$ follows standard arguments.

Outline

A truncated control problem

$$\min\ J(tr_\Omega v, \mathrm{r}) = \frac{1}{2}\|tr_\Omega v - \mathrm{u}_d\|^2_{L^2(\Omega)} + \frac{\lambda}{2}\|\mathrm{r}\|^2_{L^2(\Omega)},$$

subject to the truncated state equation

$$\frac{1}{d_s}\int_{\mathcal{C}_\mathcal{Y}} y^\alpha \nabla v \cdot \nabla \phi = \langle \mathrm{r}, tr_\Omega \phi \rangle_{\mathbb{H}^{-s}(\Omega)\times\mathbb{H}^s(\Omega)}, \quad \forall \phi \in \mathring{H}^1_L(y^\alpha, \mathcal{C}_\mathcal{Y}),$$

and the control constraints $\mathrm{r} \in \mathrm{Z}_{\mathrm{ad}}$.

First order necessary and sufficient optimality conditions:

$$\begin{cases} \bar{v} = \bar{v}(\bar{\mathrm{r}}) \in \mathring{H}^1_L(y^\alpha, \mathcal{C}_\mathcal{Y}) \text{ solution of state equation}, \\ \bar{p} = \bar{p}(\bar{\mathrm{r}}) \in \mathring{H}^1_L(y^\alpha, \mathcal{C}_\mathcal{Y}) \text{ solution of adjoint equation}, \\ \bar{\mathrm{r}} \in \mathrm{Z}_{\mathrm{ad}}, \quad (tr_\Omega \bar{p} + \lambda \bar{\mathrm{r}}, \mathrm{r} - \bar{\mathrm{r}})_{L^2(\Omega)} \geq 0 \quad \forall \mathrm{r} \in \mathrm{Z}_{\mathrm{ad}}. \end{cases}$$

Exponential convergence: For every $\mathcal{Y} \geq 1$, we have

$$\|\bar{\mathrm{r}} - \bar{\mathrm{z}}\|_{L^2(\Omega)} \lesssim e^{-\sqrt{\lambda_1}\mathcal{Y}/4}\left(\|\bar{\mathrm{r}}\|_{L^2(\Omega)} + \|\mathrm{u}_d\|_{L^2(\Omega)}\right),$$

$$\|\nabla(\bar{\mathcal{U}}(\bar{\mathrm{z}}) - \bar{v}(\bar{\mathrm{r}}))\|_{L^2(y^\alpha,\mathcal{C})} \lesssim e^{-\sqrt{\lambda_1}\mathcal{Y}/4}(\|\bar{\mathrm{r}}\|_{L^2(\Omega)} + \|\mathrm{u}_\mathrm{d}\|_{L^2(\Omega)}).$$

A truncated control problem

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subject to the truncated state equation

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$$\|\nabla(\bar{\mathcal{U}}(\bar{\mathrm{z}}) - \bar{v}(\bar{\mathrm{r}}))\|_{L^2(y^\alpha, \mathcal{C})} \lesssim e^{-\sqrt{\lambda_1}\mathcal{Y}/4}(\|\bar{\mathrm{r}}\|_{L^2(\Omega)} + \|\mathrm{u}_\mathrm{d}\|_{L^2(\Omega)}).$$

Error Estimates

- We propose a fully discrete scheme for the control problem based on the Cafarelli-Silvestre extension.
- The control is discretized with piecewise constants. The state is approximated as before.
- Error estimates for the control:

$$\|\bar{\mathsf{z}} - \bar{Z}\|_{L^2(\Omega)} \lesssim |\log N|^{2s} N^{\frac{-1}{(n+1)}}.$$

- Error estimates for the state:

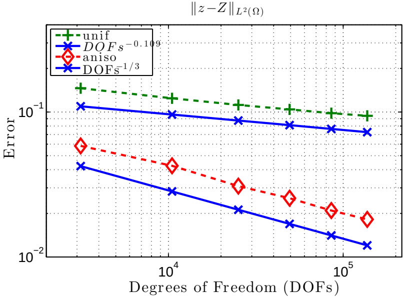
$$\|\bar{\mathsf{u}} - \bar{U}\|_{H^s(\Omega)} \lesssim |\log N|^{2s} N^{\frac{-1}{(n+1)}}.$$

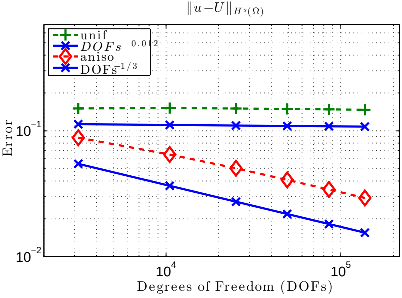
Uniform versus anisotropic refinement

#DOFs	$\|\bar{\mathsf{z}} - \bar{Z}\|_{L^2(\Omega)}$	$\|\bar{\mathsf{z}} - \bar{Z}\|_{L^2(\Omega)}$	$\|\bar{\mathsf{u}} - \bar{U}\|_{H^s(\Omega)}$	$\|\bar{\mathsf{u}} - \bar{U}\|_{H^s(\Omega)}$
3146	1.46088e-01	5.84167e-02	1.50840e-01	8.83235e-02
10496	1.24415e-01	4.25698e-02	1.51756e-01	6.49159e-02
25137	1.11969e-01	3.08367e-02	1.50680e-01	5.04449e-02
49348	1.04350e-01	2.54473e-02	1.49425e-01	4.07946e-02
85529	9.82338e-02	2.09237e-02	1.48262e-01	3.42406e-02
137376	9.41058e-02	1.81829e-02	1.47146e-01	2.93122e-02

Table : uniform - anisotropic - uniform - anisotropic.

Uniform versus anisotropic refinement





HA, EO: *A FEM for an optimal control problem of fractional powers of elliptic operators*, submmited to SIAM J. Control and Optim. (2014).

Outline

Conclusions

- Discretize nonlocal operators using local techniques.
- The analysis requires nonstandard ideas for FE:
  - Weighted spaces and weighted norm inequalities.
  - A posteriori error estimators on cylindrical stars.
  - Combination of Hölder and Sobolev regularity and growth conditions for obstacle problems.
  - ...

  but the implementation is "simple".
- Efficient solution techniques (multilevel and adaptivity).
- Provided an analysis of a commonly used but not properly analyzed scheme for Caputo time derivatives.
- These techniques have already found applications in control theory[2], image processing and others.

[2] HA, EO, AJS *A fractional space-time optimal control problem: analysis and discretization*. SIAM J. Control and Optimization, 2015 (submitted).

Future work

- Approximation classes for anisotropic adaptive methods.
- Multilevel methods for obstacle problems (with L. Chen UCI).
- Discretization of fractional powers of nondivergence form elliptic operators (with P.R. Stinga TU Austin).
- Applications.
- . . .

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