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Hybrid Finite Element - Spectral Method for the Spectral Fractional Laplacian

Approximation Theory and Efficient Solver

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Motivation

- Fractional and non-local models allow for a more accurate description of phenomena in a wide range of applications:
  - anomalous diffusion [2],
  - material science [14, 1],
  - image processing [7, 8],
  - finance [16],
  - electromagnetic fluids [9].
- Space-Fractional equations arise naturally as the limit of discrete diffusion governed by stochastic processes with long jumps [10].

Efficient solution of fractional equations in complex domains is of great practical interest.

Fractional Laplacian in $\mathbb{R}^d$

On full space $\mathbb{R}^d$, it is straightforward to define

$$(-\Delta)^s u = \mathcal{F}^{-1}\left[|\xi|^{2s}\,\mathcal{F}u\right].$$

Rewritten in integral form (for $s \in (0,1)$)

$$(-\Delta)^s u(\vec{x}) = C(d,s)\,\text{p. v.}\int_{\mathbb{R}^d} d\vec{y}\,\frac{u(\vec{x}) - u(\vec{y})}{|\vec{x}-\vec{y}|^{d+2s}},$$

with p. v. the Cauchy principal value and $C(d,s)$ a normalization constant.

Fractional Laplacians on bounded domains

$$(-\Delta)^s u(\vec{x}) = C(d,s)\,\text{p.v.}\int_{\mathbb{R}^d} d\vec{y}\,\frac{u(\vec{x}) - u(\vec{y})}{|\vec{x}-\vec{y}|^{d+2s}}, \quad \vec{x}\in\mathbb{R}^d$$

No unique way of defining the fractional Laplacian on bounded domain $\Omega \in C^2$ (or polyhedral):

- Integral fractional Laplacian: use full-space operator, enforce $u = 0$ on Ω^c (homogeneous Dirichlet condition)
- Regional fractional Laplacian: use full-space operator, set flux from Ω^c to zero (homogeneous Neumann condition)
- Spectral fractional Laplacian: define operator via spectral decomposition of regular Laplacian:

$$(-\Delta)^s u = \sum_m \lambda_m^s u_m \phi_m, \qquad \text{where } -\Delta\phi_m = \lambda_m\phi_m + \text{B.C.}$$

Fractional Laplacians on bounded domains

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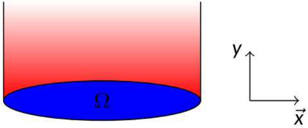
Fractional Poisson problem with homogeneous Dirichlet condition:

$$\begin{aligned}(-\Delta)^s u &= f \quad \text{in } \Omega,\\ u &= 0 \quad \text{on } \partial\Omega.\end{aligned}$$

Computing eigenpairs $(\lambda_m,\ \phi_m)$ with the required accuracy is inefficient.

Extension approach [5], [15]

Reformulate as $(d+1)$-dimensional integer-order problem:



$$\begin{cases} -\nabla \cdot y^{\alpha} \nabla U(\vec{x}, y) &= 0, & (\vec{x}, y) \in \mathcal{C} := \Omega \times [0, \infty), \\ U(\vec{x}, y) &= 0, & (\vec{x}, y) \in \partial_L \mathcal{C} := \partial\Omega \times [0, \infty), \\ \frac{\partial U}{\partial \nu^{\alpha}}(\vec{x}) &= d_s f(\vec{x}), & \vec{x} \in \Omega, \end{cases}$$

where $\alpha = 1 - 2s$, $d_s = 2^{1-2s} \frac{\Gamma(1-s)}{\Gamma(s)}$, and

$$\frac{\partial U}{\partial \nu^{\alpha}}(\vec{x}) = - \lim_{y \to 0^+} y^{\alpha} \frac{\partial U}{\partial y}(\vec{x}, y),$$

with the solution to the fractional Poisson problem recovered by taking the trace of U on Ω, i.e. $u = \mathrm{tr}_{\Omega} U$.

Discretization

Discretization options explored in the literature:

- Dunford-Taylor integral representation of the solution [3, 4],
- Graded meshes or adaptivity on a truncated cylinder [12, 6], [11],

Define (semi-)norms

$$\|U\|_{L^2_\alpha}^2 = \int_{\mathcal{C}} y^\alpha |U|^2, \qquad |U|_{H^1_\alpha}^2 = \int_{\mathcal{C}} y^\alpha |\nabla U|^2,$$
$$\|U\|_{H^1_\alpha}^2 = \|U\|_{L^2_\alpha}^2 + |U|_{H^1_\alpha}^2,$$

along with the associated weighted spaces

$$L^2_\alpha(\mathcal{C}) = \left\{U \text{ measurable } \mid \|U\|_{L^2_\alpha} < \infty\right\}, \quad H^1_\alpha(\mathcal{C}) = \left\{U \in L^2_\alpha(\mathcal{C}) \mid \|U\|_{H^1_\alpha} < \infty\right\}.$$

Find $U \in \mathcal{H}^1_\alpha(\mathcal{C}) := \left\{V \in H^1_{y^\alpha}(\mathcal{C}) \mid V = 0 \text{ on } \partial_L \mathcal{C}\right\}$ such that

$$\int_{\mathcal{C}} y^\alpha \nabla U \cdot \nabla V = d_s \langle f, \operatorname{tr}_\Omega V\rangle \quad \forall V \in \mathcal{H}^1_\alpha(\mathcal{C}).$$

Eigenfunctions of the Extruded Problem

The eigenfunction associated with the eigenvalue λ_m^s is given by

$$\phi_m(\vec{x})\,\psi_m(y)\,.$$

Here, $(\phi_m,\ \lambda_m)$ is an eigenpair of the standard integer-order Poisson problem, and

$$\psi_m(y) := c_s\left(\lambda_m^{1/2}y\right)^s K_s\left(\lambda_m^{1/2}y\right),$$

where $c_s = 2^{1-s}/\Gamma(s)$.

$$\int_0^\infty y^\alpha \psi_m\psi_n = \begin{cases} d_s\frac{\lambda_m^s-\lambda_n^s}{\lambda_m-\lambda_n} & \text{if } m\neq n,\\ sd_s\lambda_m^{s-1} & \text{if } m=n,\end{cases}, \quad \int_0^\infty y^\alpha \psi_m'\psi_n' = \begin{cases} d_s\frac{\lambda_m\lambda_n^s-\lambda_n\lambda_m^s}{\lambda_m-\lambda_n} & \text{if } m\neq n,\\ (1-s)d_s\lambda_m^s & \text{if } m=n.\end{cases}$$

The solution to the extruded problem with right-hand side f is then given by

$$f(\vec{x}) = \sum_{m=0}^\infty f_m\phi_m(\vec{x}),$$

$$U(\vec{x},y) = \sum_{m=0}^\infty u_m\phi_m(\vec{x})\psi_m(y) \quad \text{where } u_m = \lambda_m^{-s}f_m.$$

Hybrid Finite Element - Spectral Approach

Use finite elements for discretization in $\vec{x}$, and functions resembling ψ_m in y.

Discretization of the Extruded Problem

Take some approximation $\widetilde{\lambda}_m \approx \lambda_m$ and set

$$\widetilde{\psi}_m(y) := c_s \left(\widetilde{\lambda}_m^{1/2} y\right)^s K_s \left(\widetilde{\lambda}_m^{1/2} y\right),$$

let $\mathcal{T}_h$ be a shape regular, globally quasi-uniform triangulation of Ω, and let

$$V_h = \left\{ v_h \in H_0^1(\Omega) \mid v_h\big|_K \in \mathbb{P}_k(K) \ \forall K \in \mathcal{T}_h \right\},$$

$$\mathcal{V}_M = \left\{ V_M = \sum_{m=0}^{M-1} v_m(\vec{x})\, \widetilde{\psi}_m(y) \mid v_m \in H_0^1(\Omega) \right\} \subset \mathcal{H}_\alpha^1(\mathcal{C}),$$

$$\mathcal{V}_{h,M} = \left\{ V_{h,M} = \sum_{m=0}^{M-1} v_{h,m}(\vec{x})\, \widetilde{\psi}_m(y) \mid v_{h,m} \in V_h \right\} \subset \mathcal{H}_\alpha^1(\mathcal{C})$$

The Galerkin approximation consists of seeking $U_{h,M} \in \mathcal{V}_{h,M}$ such that

$$\int_{\mathcal{C}} y^\alpha \nabla U_{h,M} \cdot \nabla V = d_s \langle f, \mathrm{tr}_\Omega V \rangle \quad \forall V \in \mathcal{V}_{h,M},$$

with the approximate solution of the fractional Poisson problem given by

$$u_{h,M} := \mathrm{tr}_\Omega U_{h,M}.$$

Approximations $\widetilde{\lambda}_m$ need to be chosen (efficiently)

A priori error estimate – semi-discrete case

Lemma

Let $M \in \mathbb{N}$ and $U \in \mathcal{H}^1_\alpha(\mathcal{C})$ be the solution of the extruded problem. Then

$$\inf_{V_M \in \mathcal{V}_M} \|U - V_M\|^2_{\mathcal{H}^1_\alpha} = d_s \sum_{m=0}^{\infty} \beta_m u_m^2 \lambda_m^s,$$

where

$$\beta_m = \begin{cases} g\left(s, \widetilde{\lambda}_m/\lambda_m\right) & m = 0, \dots, M-1, \\ 1 & m \geq M, \end{cases} \qquad g(s,\rho) = 1 - \frac{1}{(1-s)\rho^s + s\rho^{s-1}}.$$

Lemma

Let $s \in (0,1)$, $0 \leq \varepsilon \leq \min\left\{\frac{e}{2}\frac{\min\{s,1-s\}}{\max\{s,1-s\}}, 1\right\}$ and $\kappa_s = \sqrt{\frac{2}{e}\frac{1}{s(1-s)}}$. If

$$|\log\rho| \leq \kappa_s\sqrt{\varepsilon} \quad \text{then} \quad g(s,\rho) \leq \varepsilon \text{ and } \max\{\rho^s, \rho^{s-1}\} \leq e.$$

A priori error estimate – fully discrete case

Theorem

Let $f \in \widetilde{H}^r(\Omega)$, *for* $r \geq -s$, *and choose* M *sufficiently large such that* $\lambda_M^{-(r+s)/2} \sim h^{\min\{k,r+s\}}$. *Assume that for* $0 \leq m \leq M-1$ *it holds that*

$$\mathbf{g}\left(\mathbf{s}, \widetilde{\lambda}_{\mathbf{m}}/\lambda_{\mathbf{m}}\right) \leq \lambda_{\mathbf{m}}^{\mathbf{r+s}} \mathbf{h}^{\mathbf{2}\min\{\mathbf{k},\mathbf{r+s}\}}, \qquad \left(\frac{\widetilde{\lambda}_m}{\lambda_m}\right)^s, \left(\frac{\lambda_m}{\widetilde{\lambda}_m}\right)^{1-s} \leq c_\sigma^2$$

with a positive constant c_σ *that is independent of* h. *Moreover, assume that there exist positive constants* C_0, C_1 *independent of* h *such that the following two inequalities hold for any* $\vec{\gamma} \in \mathbb{R}^M$:

$$\sum_{m,n=0}^{M-1} \gamma_m \gamma_n \int_\Omega (\phi_m - \pi_h \phi_m)(\phi_n - \pi_h \phi_n) \leq C_0 \log(\lambda_M) \sum_{m=0}^{M-1} \gamma_m^2 \|\phi_m - \pi_h \phi_m\|_{L^2}^2,$$

$$\sum_{m,n=0}^{M-1} \gamma_m \gamma_n \int_\Omega \nabla(\phi_m - \pi_h \phi_m) \cdot \nabla(\phi_n - \pi_h \phi_n) \leq C_1 \log(\lambda_M) \sum_{m=0}^{M-1} \gamma_m^2 \|\nabla(\phi_m - \pi_h \phi_m)\|_{L^2}^2,$$

where π_h *is the Scott-Zhang interpolant [13]. Then, the solution* $u_{h,M}$ *to the fractional Poisson problem and the solution* $U_{h,M}$ *to the discretized extruded problem satisfy*

$$\left\|u - u_{h,M}\right\|_{\widetilde{H}^s} \leq C \left\|U - U_{h,M}\right\|_{\mathcal{H}^1_\alpha} \leq C\,|f|_{\widetilde{H}^r}\, h^{\min\{k,r+s\}} \sqrt{|\log h|},$$

where C *is independent of* h.

Choice of approximate eigenvalues – upper part of the spectrum

A cheap eigenvalue approximation: Weyl's asymptotic law

$$\widetilde{\lambda}_m^{\text{Weyl}} := C_d \left(\frac{m}{|\Omega|} \right)^{2/d} \qquad \text{with } C_d = 4\pi\Gamma\left(1 + d/2\right)^{2/d}.$$

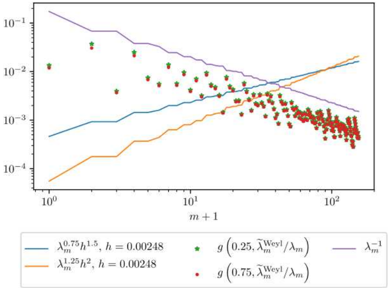


Figure: Theorem requires $g\left(s, \widetilde{\lambda}_m^{\text{Weyl}}/\lambda_m\right) \leq \lambda_m^{r+s} h^{2\min\{k,r+s\}}$.
We display $g\left(s, \widetilde{\lambda}_m^{\text{Weyl}}/\lambda_m\right)$ and $\lambda_m^{r+s} h^{2\min\{k,r+s\}}$ for $r+s \in \{0.75, 1.25\}$ and $k = 1$.
Here, h corresponds to a triangulation of the unit disc with about one million nodes.

All eigenvalues λ_m, $m \geq m_0$ are well approximated by Weyl's law (and m_0 can be estimated).

Choice of approximate eigenvalues – lower part of the spectrum

We will be constructing a multigrid preconditioner for a FE discretization of the integer-order Laplacian on a mesh of size h.

$\rightarrow$ Compute eigenvalue approximations based on coarse representation on mesh of size $H > h$.

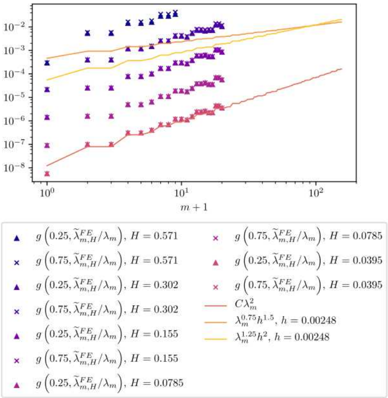


Figure: Theorem requires $g\left(s, \widetilde{\lambda}^{FE}_{m,H}/\lambda_m\right) \leq \lambda_m^{r+s} h^{2\min\{k,r+s\}}$.

We display $g\left(s, \widetilde{\lambda}^{FE}_{m,H}/\lambda_m\right)$ for several choices of coarsened mesh sizes H against $\lambda_m^{r+s} h^{2\min\{k,r+s\}}$ for $r+s \in \{0.75, 1.25\}$ and $k = 1$.

Here, h corresponds to a triangulation of the unit disc with about one million nodes.

Complexity

Remember

$$\widetilde{\psi}_m(y) = c_s \left(\widetilde{\lambda}_m^{1/2} y\right)^s K_s\left(\widetilde{\lambda}_m^{1/2} y\right),$$

$$\mathcal{V}_{h,M} = \left\{ v_{h,M} = \sum_{m=0}^{M-1} v_{h,m}(\vec{x})\, \widetilde{\psi}_m(y) \mid v_{h,m} \in V_h \right\}.$$

If $\widetilde{\lambda}_m \neq \widetilde{\lambda}_n$, then

$$\mathcal{N} := \dim \mathcal{V}_{h,M} = nM, \qquad \text{where } n = \dim V_h.$$

Theorem + Weyl's law: $M \sim n^{\min\{1,k/(r+s)\}} \to \mathcal{N} \sim n^p$, $p \in (1,2]$.

The method does not have optimal complexity!

Eigenvalue decimation

Build a smaller approximation space $\mathcal{V}_{h,M}$ from FE and Weyl approximations $\left\{\widetilde{\lambda}_m\right\}$:

$$\widehat{\lambda}_0 = \widetilde{\lambda}_0, \qquad \widehat{\lambda}_m = \begin{cases} \widehat{\lambda}_{m-1} & \text{if } \widehat{\lambda}_{m-1} \text{ satisfies criteria of Theorem,} \\ \widetilde{\lambda}_m & \text{otherwise} \end{cases}$$

Experimentally, we observe that the number of distinct eigenvalues $\widetilde{M} = \mathcal{O}\left(\log^p n\right)$ for some $p \geq 0$, and hence $\mathcal{N} = \mathcal{O}\left(n \log^p n\right)$.

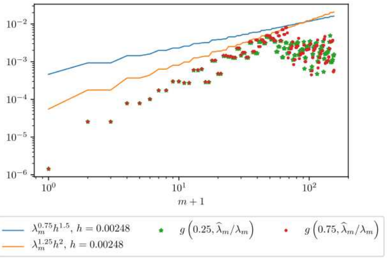


Figure: Theorem requires $g\left(s, \widehat{\lambda}_m/\lambda_m\right) \leq \lambda_m^{r+s} h^{2\min\{k,r+s\}}$.
We display $g\left(s, \widehat{\lambda}_m/\lambda_m\right)$ and $\lambda_m^{r+s} h^{2\min\{k,r+s\}}$ for $r+s \in \{0.75, 1.25\}$ and $k = 1$.

Number of DoFs scales quasi-optimally, but we need to solve efficiently as well!

Solution of the linear system

Set Φ_i, $i = 0, \ldots, n$ the finite element basis functions, and

$$\mathbf{M}_{FE} = \left(\int_\Omega \Phi_i \Phi_j \right), \qquad \mathbf{S}_{FE} = \left(\int_\Omega \nabla \Phi_i \nabla \Phi_j \right),$$

$$\mathbf{M}_\sigma = \left(\int_0^\infty y^\alpha \widetilde{\psi}_m \widetilde{\psi}_n \right), \qquad \mathbf{S}_\sigma = \left(\int_0^\infty y^\alpha \widetilde{\psi}'_m \widetilde{\psi}'_n \right),$$

$$\vec{F}_{h,M} = \vec{f}_h \otimes \vec{1}_{\widetilde{M}}, \qquad \vec{f}_h = \left(d_s \langle f_h, \Phi_i \rangle \right).$$

Linear system to be solved:

$$\left(\mathbf{M}_{FE} \otimes \mathbf{S}_\sigma + \mathbf{S}_{FE} \otimes \mathbf{M}_\sigma \right) \vec{U}_{h,M} = \vec{F}_{h,M},$$

Cholesky factorisation:	$\mathbf{M}_\sigma = \mathbf{L}\mathbf{L}^T$
Eigen-decomposition:	$\mathbf{S}_\sigma = \mathbf{L}\mathbf{P}\mathbf{\Lambda}\mathbf{P}^T\mathbf{L}^T$

Then

$$\left(\mathbf{M}_{FE} \otimes \mathbf{S}_\sigma + \mathbf{S}_{FE} \otimes \mathbf{M}_\sigma \right)^{-1} = \left[\mathbf{I} \otimes \left(\mathbf{L}^{-T}\mathbf{P} \right) \right] \left[\mathbf{M}_{FE} \otimes \mathbf{\Lambda} + \mathbf{S}_{FE} \otimes \mathbf{I} \right]^{-1} \left[\mathbf{I} \otimes \left(\mathbf{P}^T \mathbf{L}^{-1} \right) \right].$$

i.e. solution of a sequence of systems $\mathbf{M}_{FE} \mathbf{\Lambda}_{mm} + \mathbf{S}_{FE}$. We use conjugate gradients preconditioned with geometric multigrid.

Numerical examples in 2D

Consider the problem

$$\begin{cases} (-\Delta)^s u & = f \qquad \text{in } \Omega = B(0,1) \subset \mathbb{R}^2 \\ u & = 0 \qquad \text{on } \partial\Omega, \end{cases}$$

where

- $f = \left(1 - |\vec{x}|^2\right)^{r-1/2} \in \widetilde{H}^{r-\varepsilon}(\Omega)$, for all $\varepsilon > 0$,
- $r \in \{0.5, 2\}$,
- $s \in \{0.25, 0.75\}$,
- piecewise linear finite elements (i.e. $k = 1$).

Since eigenpairs are known, errors in $\mathcal{H}^1_\alpha$-norm can be computed via a convergent series.

Numerical Examples in 2D – Errors wrt mesh size

Predicted by Theorem: $h^{\min\{k,r+s\}}\sqrt{|\log h|} \sim n^{-\min\{k,r+s\}/d}\sqrt{|\log n|}$

Expected after decimation: $\mathcal{N}^{-\min\{k,r+s\}/d}\,|\log^p \mathcal{N}|$

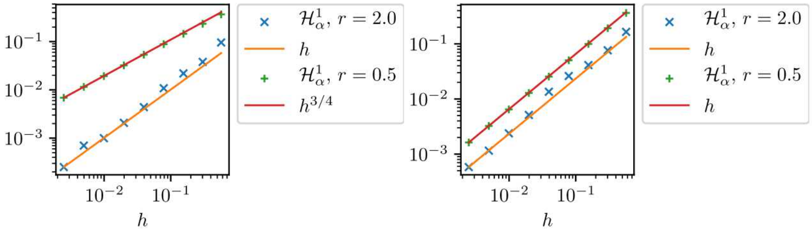


Figure: $\mathcal{H}^1_\alpha$-error for the fractional Poisson problem with right-hand side $f = \left(1 - |\vec{x}|^2\right)^{r-1/2}$ on the unit disc with piecewise linear finite elements ($k = 1$). $s = 0.25$ on the left, $s = 0.75$ on the right.

Numerical Examples in 2D – Errors wrt total #DoFs

Predicted by Theorem: $h^{\min\{k,r+s\}}\sqrt{|\log h|} \sim n^{-\min\{k,r+s\}/d}\sqrt{|\log n|}$

Expected after decimation: $\mathcal{N}^{-\min\{k,r+s\}/d}\,|\log^p \mathcal{N}|$

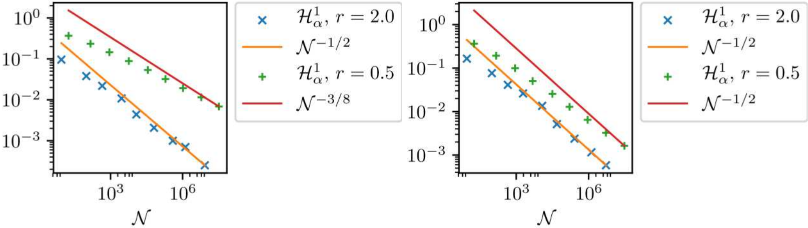
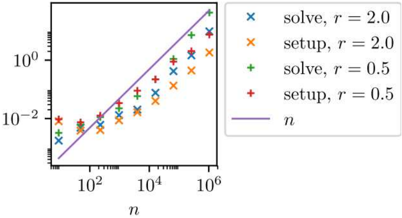


Figure: $\mathcal{H}^1_\alpha$-error with respect to the total number of degrees of freedom $\mathcal{N}$ on the unit disc with piecewise linear finite elements ($k = 1$). $s = 0.25$ on the left, $s = 0.75$ on the right. Quasi-optimal convergence is obtained.

Numerical Examples in 2D – Timings



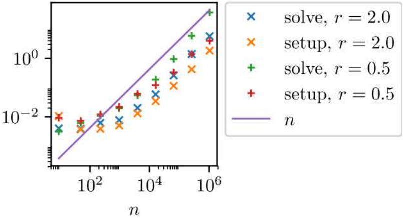
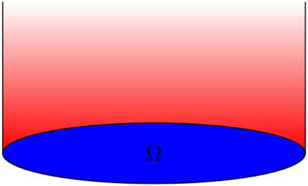


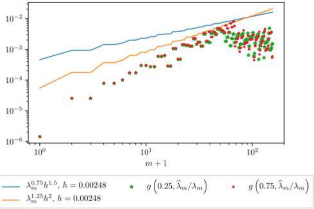
Figure: Timings of setup and solution. $s = 0.25$ on the left, $s = 0.75$ on the right. It can be seen that both setup of the solver, which includes the approximation of eigenvalues, and solution of the resulting linear system of equations scale roughly as $\mathcal{O}(n)$, where n is the number of degrees of freedom of the finite element discretization.

Conclusion

- Method with quasi-optimal complexity for the solution of a fractional Poisson problem.
- Allows use of standard iterative linear solvers.
- Works for any dimension (as long as we can solve standard Laplace problems).

Thanks for listening!





Numerical Examples in 3D – Errors wrt mesh size

Predicted by Theorem: $h^{\min\{k,r+s\}}\sqrt{|\log h|} \sim n^{-\min\{k,r+s\}/d}\sqrt{|\log n|}$

Expected after decimation: $\mathcal{N}^{-\min\{k,r+s\}/d}\,|\log^p \mathcal{N}|$

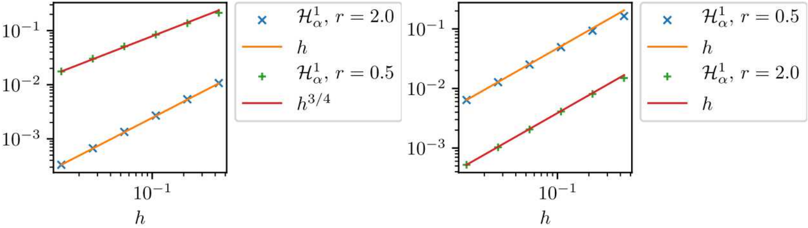


Figure: $\mathcal{H}^1_\alpha$-error for the fractional Poisson problem with right-hand side $f = [x_1x_2x_3(1-x_1)(1-x_2)(1-x_3)]^{r-1/2}$ on the unit cube with piecewise linear finite elements ($k = 1$). $s = 0.25$ on the left, $s = 0.75$ on the right.

Numerical Examples in 3D – Errors wrt total #DoFs

Predicted by Theorem: $h^{\min\{k,r+s\}}\sqrt{|\log h|} \sim n^{-\min\{k,r+s\}/d}\sqrt{|\log n|}$

Expected after decimation: $\mathcal{N}^{-\min\{k,r+s\}/d}\,|\log^p \mathcal{N}|$

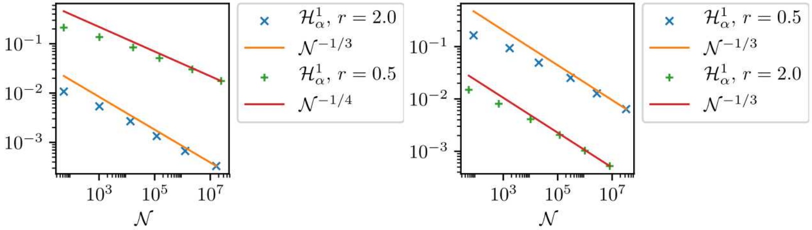


Figure: $\mathcal{H}^1_\alpha$-error with respect to the total number of degrees of freedom $\mathcal{N}$ on the unit cube with piecewise linear finite elements ($k = 1$). $s = 0.25$ on the left, $s = 0.75$ on the right. Quasi-optimal convergence is obtained.

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