

Hierarchical a posteriori error estimation in the FEniCS finite element software and applications to fractional PDEs.

Raphaël Bulle

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Background

2010-2013 **Bachelor in Mathematics**

at Université de Bourgogne Franche-Comté (FR).

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2014 **CAPES** (competitive exam)
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Background

- 
- 2017-2022** **PhD student in Computational Engineering and Applied Mathematics**
at University of Luxembourg and Université de Bourgogne Franche-Comté
Supervision: S. P. A. Bordas, F. Chouly, J. S. Hale and A. Lozinski.
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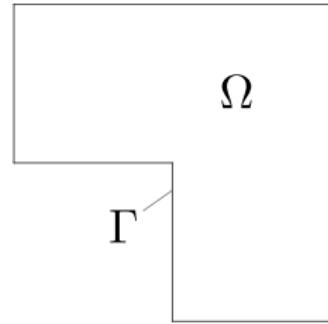
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- The spectral fractional Laplacian
 - Problem setting
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The Bank–Weiser estimator

Toy problem setting

Let $f \in L^2(\Omega)$, we look for u with sufficient regularity s.t.

$$-\Delta u = f \text{ in } \Omega, \quad u = 0 \text{ on } \Gamma.$$



The Bank–Weiser estimator

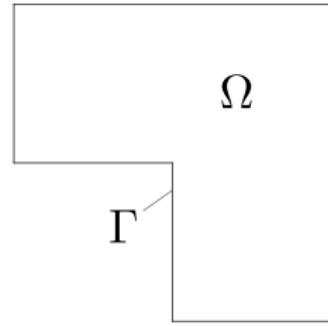
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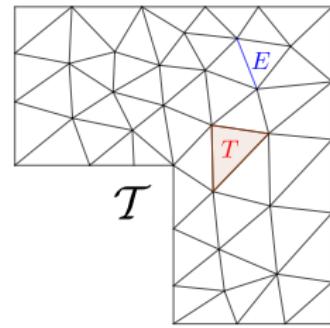
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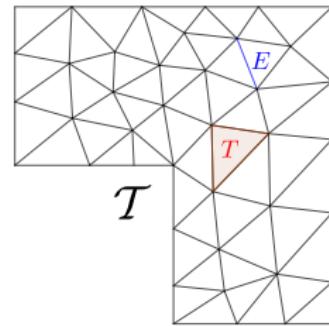
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Goal: estimate $\eta_{\text{err}} = \|\nabla(u_k - u)\|_{\Omega}$ i.e. find a computable quantity η_{bw} such that $\eta_{\text{bw}} \approx \eta_{\text{err}}$.



The Bank–Weiser estimator

Definition

On a cell T , the Bank–Weiser problem is given by:
find e_T^{bw} in V_T^{bw} such that

$$\int_T \nabla e_T^{\text{bw}} \cdot \nabla v_T^{\text{bw}} = \int_T r_T v_T^{\text{bw}} + \sum_{E \in \partial T} \frac{1}{2} \int_E J_E v_T^{\text{bw}} \quad \forall v_T^{\text{bw}} \in V_T^{\text{bw}}.$$

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The Bank–Weiser estimator is defined as

$$\eta_{\text{bw}}^2 := \sum_{T \in \mathcal{T}} \eta_{\text{bw},T}^2, \quad \eta_{\text{bw},T} := \|\nabla e_T^{\text{bw}}\|_T.$$

The Bank–Weiser estimator

Definition

How is V_T^{bw} defined ?

Let $V_T^- \subsetneq V_T^+$ be two finite element spaces and

$$\mathcal{L}_T : V_T^+ \longrightarrow V_T^-,$$

be the local Lagrange interpolation operator,

$$V_T^{\text{bw}} := \ker(\mathcal{L}_T) = \{v_T^+ \in V_T^+, \mathcal{L}_T(v_T^+) = 0\}.$$

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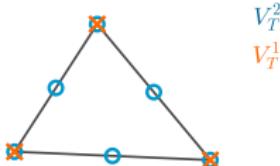
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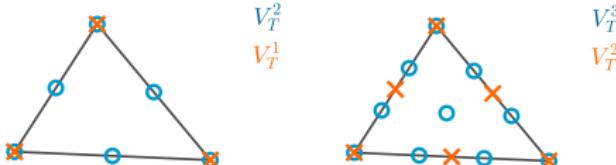
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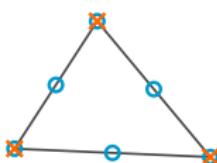
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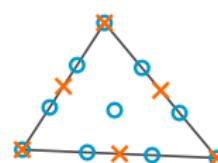
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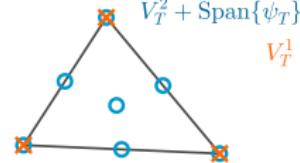
$$V_T^2$$

$$V_T^1$$



$$V_T^3$$

$$V_T^2$$



$$V_T^2 + \text{Span}\{\psi_T\}$$

$$V_T^1$$

The Bank–Weiser estimator

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 - FEniCS and FEniCSx (Python, C++) [Bulle et al., 2021].

Implementation

Method details

We need to compute the matrix A_T^{bw} and vector b_T^{bw} from

$$\int_T \nabla e_T^{\text{bw}} \cdot \nabla v_T^{\text{bw}} = \int_T r_T v_T^{\text{bw}} + \sum_{E \in \partial T} \frac{1}{2} \int_E J_E v_T^{\text{bw}} \quad \forall v_T^{\text{bw}} \in V_T^{\text{bw}}.$$

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Idea: we rely on the matrix A_T^+ and vector b_T^+ from

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since V_T^+ is provided by DOLFIN(x)

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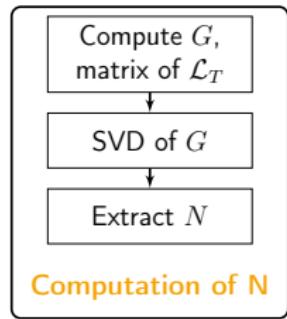
$$\int_T \nabla e_T^+ \cdot \nabla v_T^+ = \int_T r_T v_T^+ + \sum_{E \in \partial T} \frac{1}{2} \int_E J_E v_T^+ \quad \forall v_T^+ \in V_T^+,$$

since V_T^+ is provided by DOLFIN(x) and we look for a matrix N such that:

$$A_T^{\text{bw}} = N^t A_T^+ N, \quad \text{and} \quad b_T^{\text{bw}} = N^t b_T^+.$$

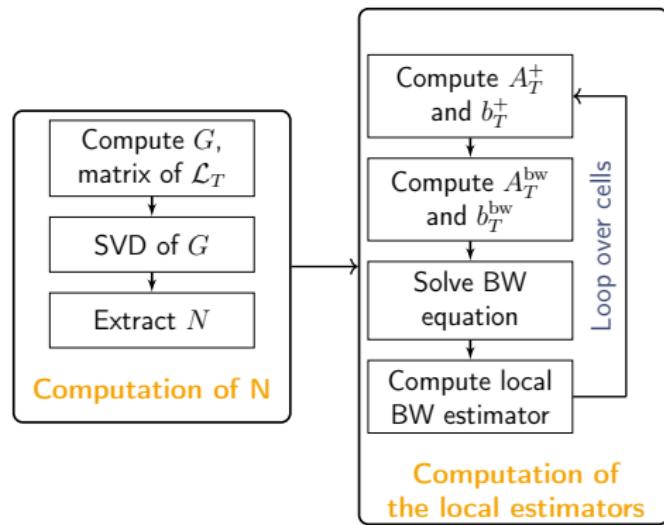
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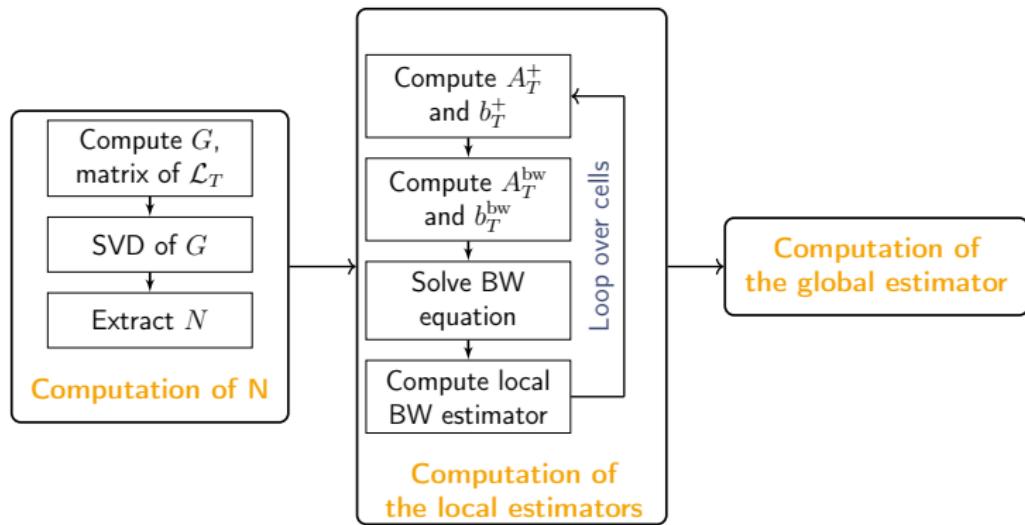
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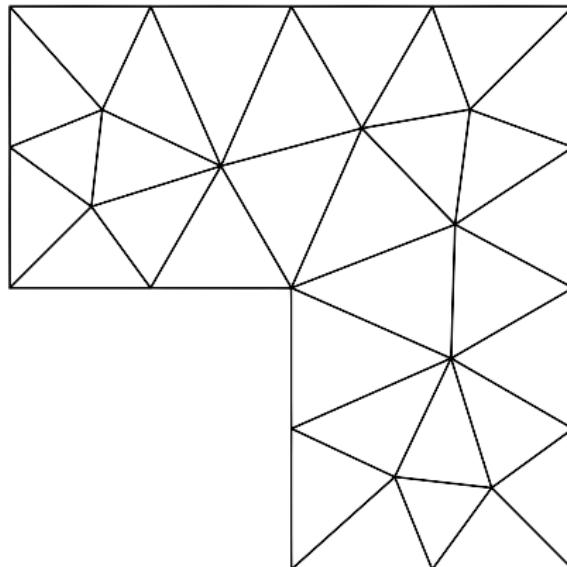


Implementation

Numerical results

Adaptive finite elements for a Poisson problem:

$-\Delta u = 0$ in Ω , $u = u_D$ on Γ . Linear finite elements.

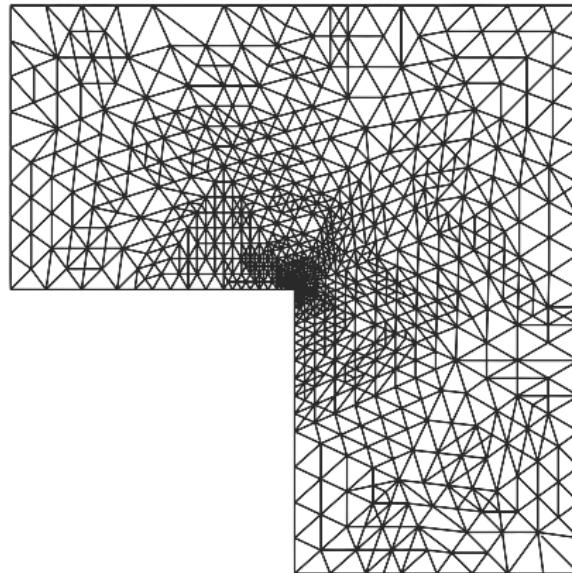


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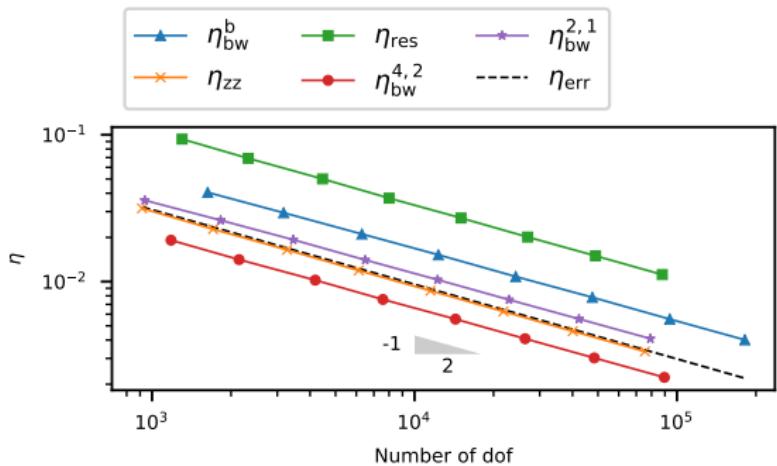


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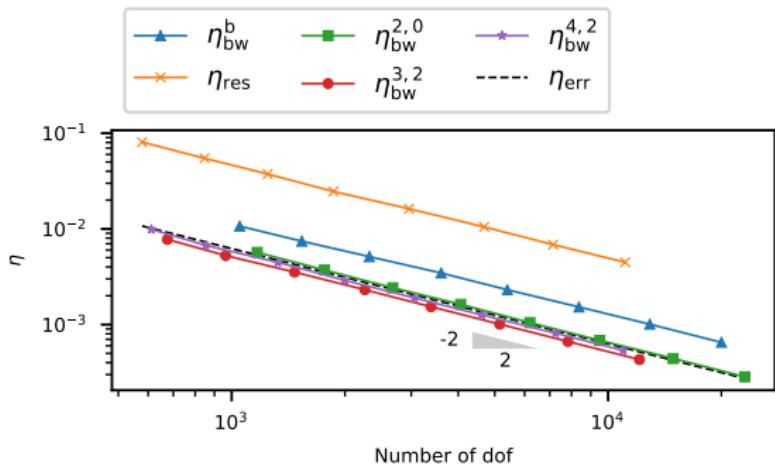
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η_{bw}^b	$V_T^2 + \text{bubble}$	V_T^1

Implementation

Numerical results

Adaptive finite elements for a Poisson problem:

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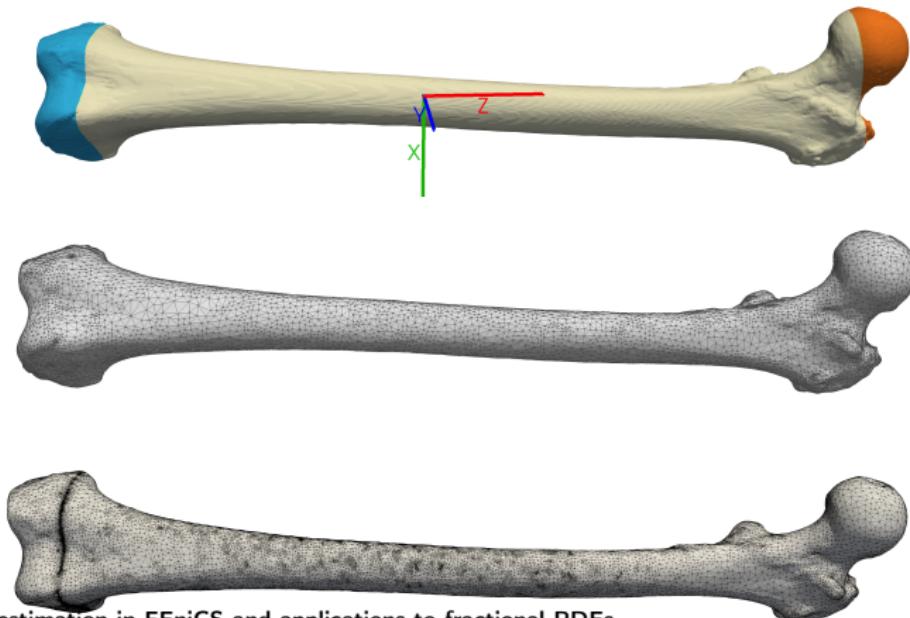
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GO AFEM for a linear elasticity problem:

we used a technique from [Khan et al., 2019] to compute the estimators.

The goal functional is defined by $J(\mathbf{u}_2, p_1) := \int_{\Gamma} \mathbf{u}_2 \cdot \mathbf{n} c$.



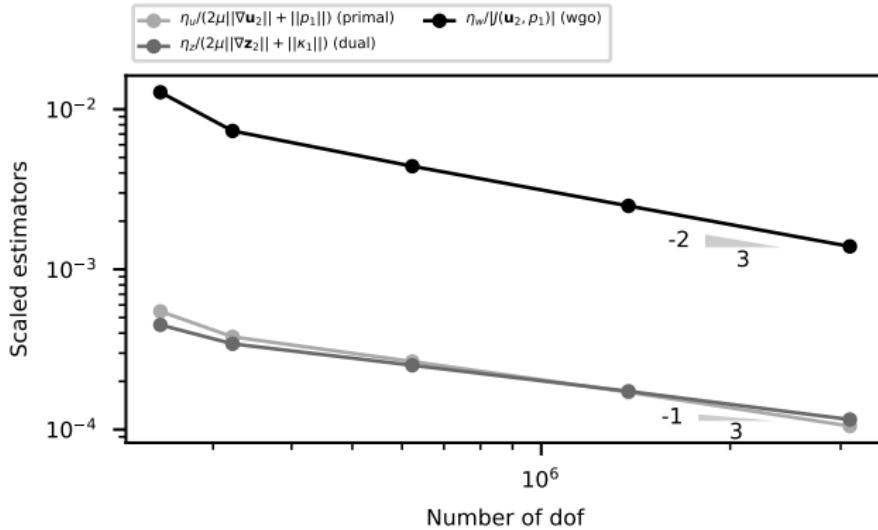
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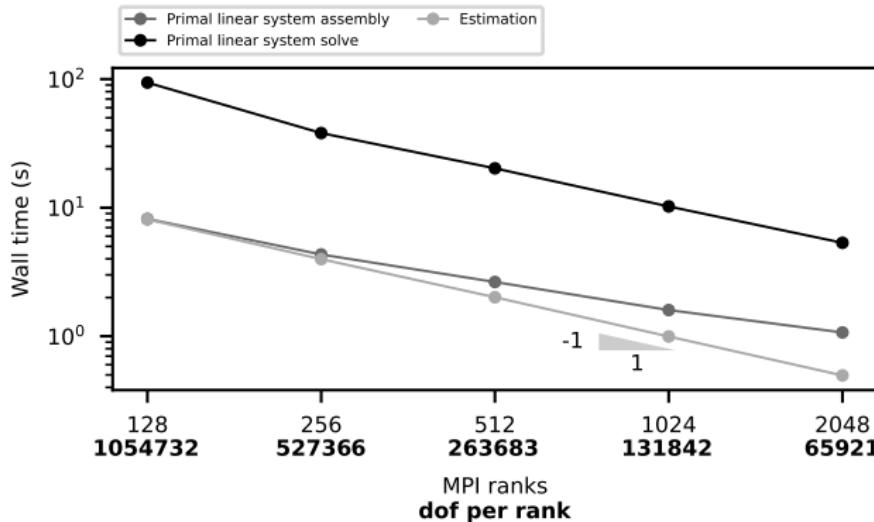
Timescale study:

strong scaling study of the DOLFINx version on the Uni Lu cluster.

$-\Delta u = f$ on $[0, 1]^3$, $u = 0$ on Γ . \mathcal{P}_2 Lagrange elements.

The Bank–Weiser estimator is $\eta_{\text{bw}}^{3,2}$.

The problem size is fixed around 135 million dof.



The spectral fractional Laplacian

Problem setting

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Let $\Omega \subset \mathbb{R}^d$, $s \in (0, 1)$ and $f \in L^2(\Omega)$.

$$(-\Delta)^s u = f \quad \text{in } \Omega, \quad u = 0 \quad \text{on } \Gamma.$$

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Let $\{\psi_i, \lambda_i\}_{i=1}^{+\infty} \subset L^2(\Omega) \times \mathbb{R}^+$ be such that

$$-\Delta \psi_i = \lambda_i \psi_i \quad \text{in } \Omega, \quad \psi_i = 0 \quad \text{on } \Gamma, \quad \forall i = \llbracket 1, +\infty \rrbracket.$$

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The solution u is defined by

$$u := \sum_{i=1}^{+\infty} \lambda_i^{-s} (f, \psi_i)_{L^2}.$$

The spectral fractional Laplacian

Problem setting

The natural Sobolev space associated with this problem is

$$\mathbb{H}^s(\Omega) := \left\{ v \in L^2(\Omega), \sum_{i=1}^{+\infty} \lambda_i^s (v, \psi_i)_{L^2}^2 < +\infty \right\},$$

of natural norm

$$\|v\|_{\mathbb{H}^s}^2 := \sum_{i=1}^{+\infty} \lambda_i^s (v, \psi_i)_{L^2}^2.$$

The spectral fractional Laplacian

Discretization

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

How to solve this equation numerically ?

The spectral fractional Laplacian

Discretization

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

How to solve this equation numerically ?

Considering

$$u := (-\Delta)^{-s} f = \sum_{i=1}^{+\infty} \lambda_i^{-s} (f, \psi_i)_{L^2},$$

we use a rational approximation

$$\lambda^{-s} \simeq \mathcal{Q}_s^N(\lambda) := C_s(N) \sum_{l=1}^N a_l (1+b_l \lambda)^{-1}, \quad \forall \lambda \in [\lambda_1, +\infty),$$

where $(a_l)_l$ and $(b_l)_l$ are positive coefficients and $C_s(N)$ is independent of λ .

The spectral fractional Laplacian

Discretization

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The spectral fractional Laplacian

Discretization

$$\begin{aligned} u = (-\Delta)^{-s} f &= \sum_{i=1}^{+\infty} \lambda_i^{-s} (f, \psi_i)_{L^2} \\ &\simeq \sum_{i=1}^{+\infty} \mathcal{Q}_s^N(\lambda_i) (f, \psi_i)_{L^2} \end{aligned}$$

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The spectral fractional Laplacian

Discretization

$$u = (-\Delta)^{-s} f \quad \longrightarrow \quad u_l = (\text{Id} - b_l \Delta)^{-1} f, \quad \forall l \in [1, N].$$

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$$u \simeq u^N := C_s(N) \sum_{l=1}^N a_l u_l.$$

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However, u^N is not a discrete function. To get a full discretization, we use a FE method. We reformulate the problems in the weak form

$$\int_{\Omega} u_l v + b_l \int_{\Omega} \nabla u_l \cdot \nabla v = \int_{\Omega} f v, \quad \forall v \in H_0^1(\Omega), \forall l \in [1, N],$$

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and write its FE discretization

$$\int_{\Omega} u_{l,k} v_k + b_l \int_{\Omega} \nabla u_{l,k} \cdot \nabla v_k = \int_{\Omega} f v_k, \quad \forall v_k \in V^1, \forall l \in [1, N].$$

The spectral fractional Laplacian

Discretization

Solving these classical FE problems we finally get a fully discrete approximation of u

$$u \simeq u^N := C_s(N) \sum_{l=1}^N a_l u_l \simeq \textcolor{red}{C}_s(N) \sum_{l=1}^N a_l u_{l,k} =: \textcolor{red}{u}_k^N$$

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The main advantages of this kind of methods is that they are easily parallelizable and involve "standard" FE machinery.

A posteriori error estimation

Rational approximation error

The next question is:

how can we bound the discretization error ?

$$\text{err} := \|u - u_k^N\| \leq \|u - u^N\| + \|u^N - u_k^N\|.$$

A posteriori error estimation

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Two sources of error:

- the rational approximation error $\|u - u^N\|$,
- the finite element error $\|u^N - u_k^N\|$.

where $\|\cdot\| = \|\cdot\|_{L^2}$, or $\|\cdot\|_{\mathbb{H}^s}$.

A posteriori error estimation

Rational approximation error

If there exists $\varepsilon(N) \xrightarrow[N \rightarrow +\infty]{} 0$ such that

$$|\lambda^{-s} - Q_s^N(\lambda)| \leq \varepsilon(N), \quad \forall \lambda \in [\lambda_1, +\infty),$$

then, [Bonito and Pasciak, 2015]

$$\|u - u^N\|_{L^2} \leq \varepsilon(N) \|f\|_{L^2}.$$

Moreover, if $f \in \mathbb{H}^s(\Omega)$, then [Bonito and Pasciak, 2016]

$$\|u - u^N\|_{\mathbb{H}^s} \leq \varepsilon(N) \|f\|_{\mathbb{H}^s}.$$

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$$\|u - u^N\|_{\mathbb{H}^s} \leq \varepsilon(N) \|f\|_{\mathbb{H}^s}.$$

In particular, there exists an approximation Q_s^N such that
[Bonito and Pasciak, 2015]

$$\varepsilon(N) = \mathcal{O}_{N \rightarrow +\infty} \left(e^{-(\pi^2/2\sqrt{2})\sqrt{N}} \right).$$

A posteriori error estimation

Rational approximation error

Conjecture: $\|u - u^N\|_{\mathbb{H}^s} \leq \varepsilon(N) \|f\|_{L^2}.$

A posteriori error estimation

Rational approximation error

Conjecture: $\|u - u^N\|_{\mathbb{H}^s} \leq \varepsilon(N) \|f\|_{L^2}$.

What we can prove currently (not published yet):

$$\|u - u^N\|_{\mathbb{H}^s} \leq \tilde{\varepsilon}(N) \|f\|_{L^2},$$

where $\tilde{\varepsilon}(N) \xrightarrow[N \rightarrow +\infty]{} 0$ with a possibly slower convergence rate than ε .

A posteriori error estimation

Finite element error

What about $\|u^N - u_k^N\|$?

A posteriori error estimation

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A priori error estimates in [Bonito and Pasciak, 2015] and [Bonito and Pasciak, 2016].

A posteriori error estimation

Finite element error

What about $\|u^N - u_k^N\|$?

A priori error estimates in [Bonito and Pasciak, 2015] and [Bonito and Pasciak, 2016].

We are looking for a computable quantity η such that

$$\|u^N - u_k^N\| \simeq \eta.$$

A posteriori error estimation

Finite element error

Heuristics L^2 case:

$$u^N - u_k^N = C_s(N) \sum_{l=1}^N a_l(u_l - u_{l,k}),$$

We use the Bank–Weiser solution to quantify

$$u_l - u_{l,k} \simeq e_l^{\text{bw}}.$$

A posteriori error estimation

Finite element error

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Then,

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Finally, we hope that:

$$\|u^N - u_k^N\|_{L^2} \simeq \|e^{\text{bw},N}\|_{L^2}.$$

A posteriori error estimation

Finite element error

Heuristics \mathbb{H}^s case:

$$u^N - u_k^N = C_s(N) \sum_{l=1}^N a_l (u_l - u_{l,k}),$$

We use the Bank–Weiser solution to quantify

$$\|u_l - u_{l,k}\|_l \simeq \|e_l^{\text{bw}}\|_l,$$

where $\|v\|_l^2 := \|v\|_{L^2}^2 + b_l |v|_{H^1}^2$.

A posteriori error estimation

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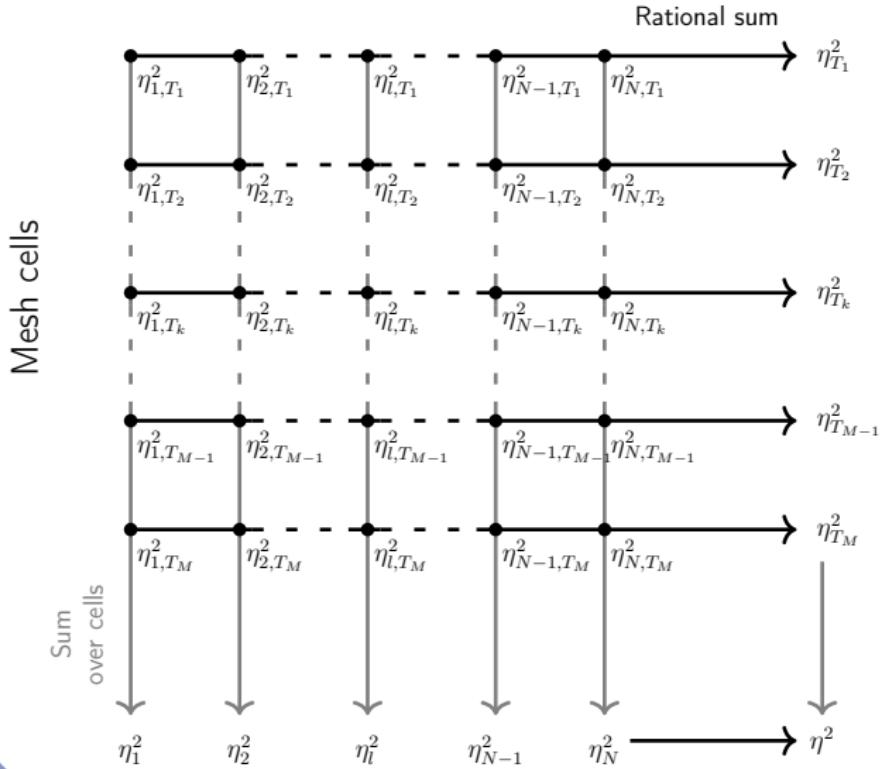
where $\|v\|_l^2 := \|v\|_{L^2}^2 + b_l |v|_{H^1}^2$. Then, we hope that:

$$\|u^N - u_k^N\|_{\mathbb{H}^s}^2 \simeq C_s(N) \sum_{l=1}^N a_l \|u_l - u_{l,k}\|_l^2 \simeq C_s(N) \sum_{l=1}^N a_l \|e_l^{\text{bw}}\|_l^2.$$

A posteriori error estimation

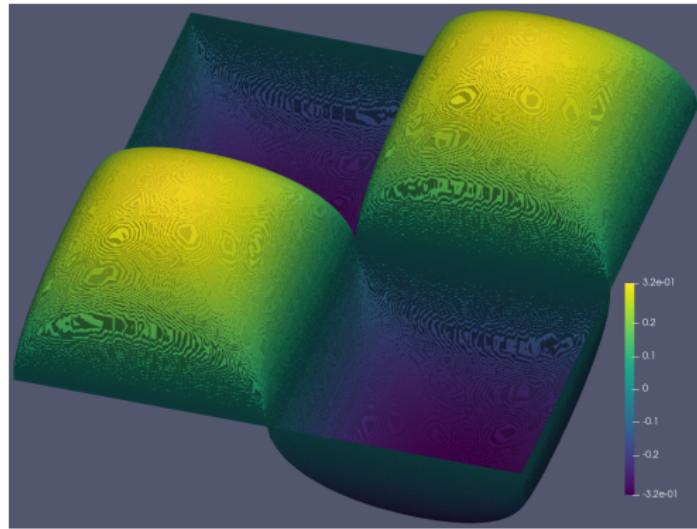
Finite element error

Parametric problems



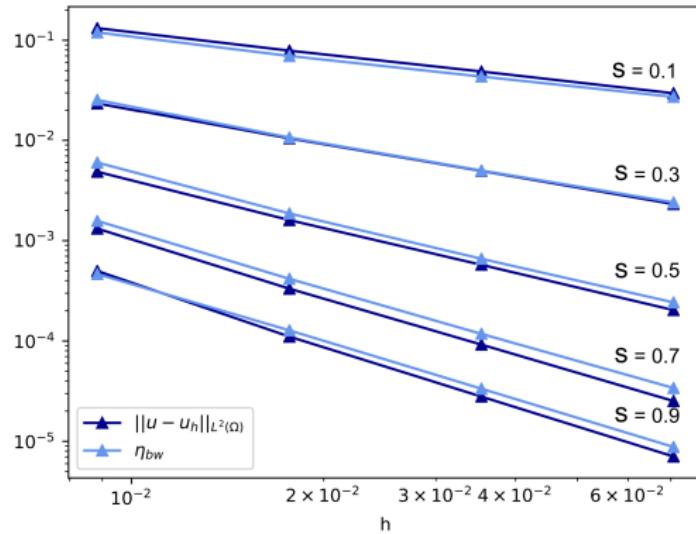
Numerical results

$(-\Delta)^s u = f$, in $[0, 1]^2$, $u = 0$, on Γ ,
with $f(x, y) = 1$ in $[0, 0.5]^2 \cup [0.5, 1]^2$, -1 otherwise.
We assume the rational approximation is negligible, i.e. $u = u^N$.



Numerical results

Uniform mesh refinement.

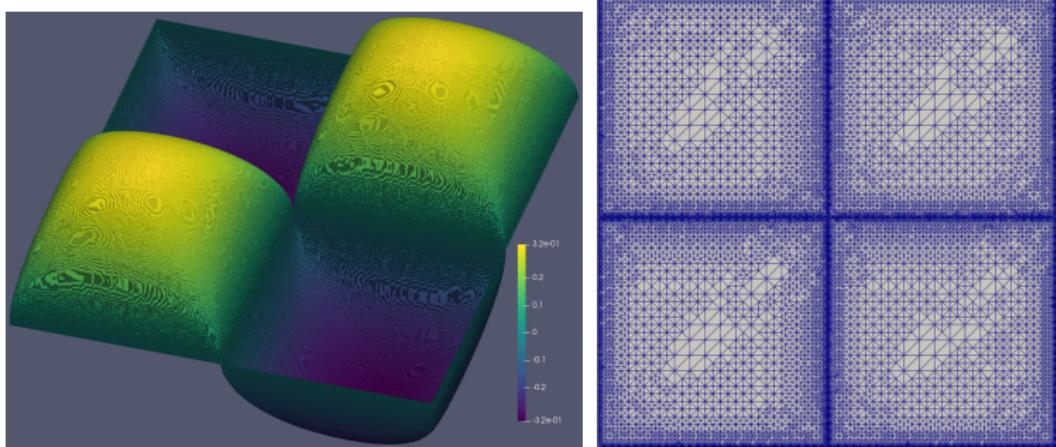


s	0.1	0.3	0.5	0.7	0.9
Th. slope	0.7	1.1	1.5	1.9	2.0
Err. slope	0.71	1.11	1.52	1.9	2.04
Est. slope	0.71	1.13	1.54	1.84	1.91

[Bonito and Pasciak, 2015]

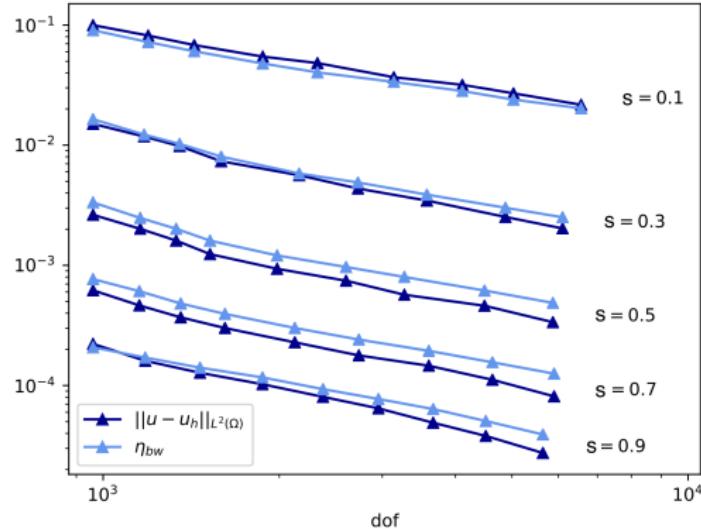
Numerical results

Adaptive mesh refinement.



Numerical results

Adaptive mesh refinement.



s	0.1	0.3	0.5	0.7	0.9
Th. slope (unif.)	0.35	0.55	0.75	0.95	1.0
Err. slope (adapt.)	0.71	0.81	0.86	0.88	0.99
Est. slope (adapt.)	0.72	0.79	0.85	0.89	0.96

[Bonito and Pasciak, 2015]

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Thank you for your attention!



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