

A posteriori error estimation in the FEniCSx finite element software and application to the fractional Laplacian.

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February 24, 2022



DRIVEN



FENICS
PROJECT

Background



2010-2013 **Bachelor in Mathematics**

at Université de Bourgogne Franche-Comté (FR).

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2014 **CAPES** (competitive exam)
of Mathematics.

2010-2013 **Bachelor in Mathematics**
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2016 **Agrégation** (competitive exam)
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2015-2017 Master in Advanced Mathematics

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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.
- 2015-2017 Master in Advanced Mathematics**
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 - Adaptive mesh refinement
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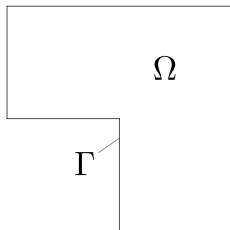
The Bank–Weiser estimator

The Bank–Weiser estimator

A reaction diffusion problem

Let $f \in L^2(\Omega)$ and $a \in \mathbb{R}^{+*}$, we look for u s.t.

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



The Bank–Weiser estimator

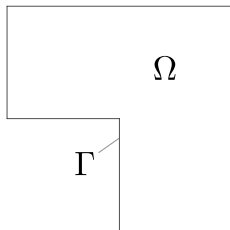
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In weak formulation, find u in $H_0^1(\Omega)$ such that

$$\int_{\Omega} uv + a \int_{\Omega} \nabla u \cdot \nabla v = \int_{\Omega} fv, \quad \forall v \in H_0^1(\Omega).$$



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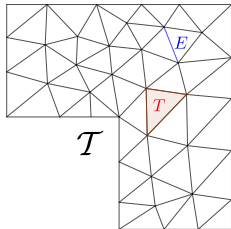
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Lagrange finite element discretization of order k , find u_k in V^k such that

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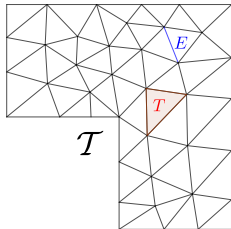
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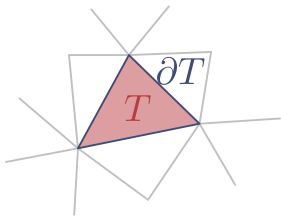
$$\int_{\Omega} u_k v_k + a \int_{\Omega} \nabla u_k \cdot \nabla v_k = \int_{\Omega} f v_k, \quad \forall v_k \in V^k.$$

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



The Bank–Weiser estimator

Definition

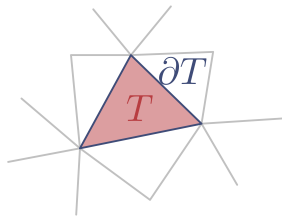


On a cell T , the Bank–Weiser problem is given by: find e_T^{bw} in \mathbf{V}_T^{bw} such that

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

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The Bank–Weiser estimator is defined as

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

The Bank–Weiser estimator

Definition

What is V_T^{bw} ?

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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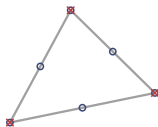
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Examples:

V_T^2

V_T^1



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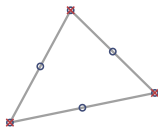
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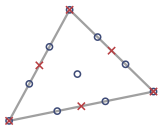
V_T^2

V_T^1



V_T^3

V_T^2



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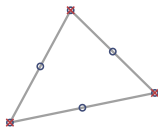
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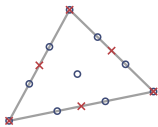
V_T^2

V_T^1



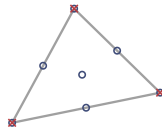
V_T^3

V_T^2



$V_T^3 + \text{Span}\{\psi_T\}$

V_T^1



The Bank–Weiser estimator

Implementation

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

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

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Problem: the space V_T^{bw} is not provided by DOLFIN/x.

The Bank–Weiser estimator

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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

The Bank–Weiser estimator

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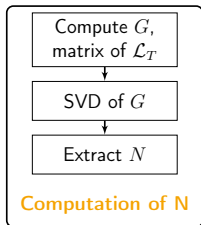
$$\int_T e_T^+ v_T^+ + a \int_T \nabla e_T^+ \cdot \nabla v_T^+ = \int_T r_T v_T^+ + \sum_{E \in \partial T} \frac{1}{2} \int_E J_E v_T^+ \quad \forall v_T^+ \in V_T^+,$$

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

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

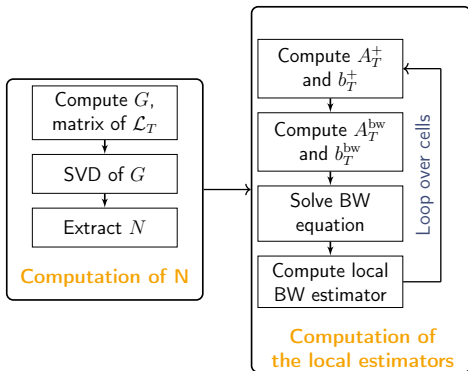
The Bank–Weiser estimator

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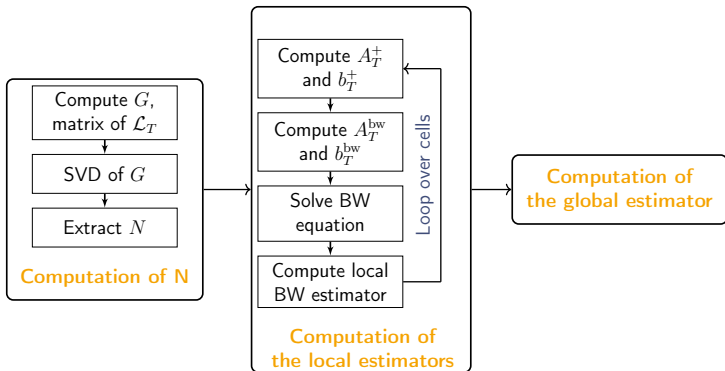
The Bank–Weiser estimator

Implementation



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The Bank–Weiser estimator

Pros and cons

Pros

Cons

The Bank–Weiser estimator

Pros and cons

Pros

Local efficiency

$$\eta_{\text{bw},T} \leq C\eta_{\text{err},T} + \text{h.o.t.}|_T$$

[Bank and Weiser, 1985, Nochetto, 1993,

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The Bank–Weiser estimator

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Reliability $\eta_{\text{err}} \leq c\eta_{\text{bw}} + \text{h.o.t.}$

under some conditions

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Not asymptotically exact in general

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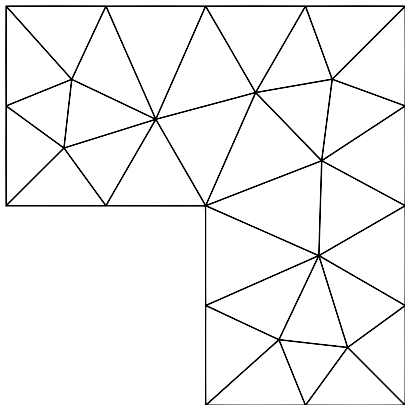
No convergence proof when used for adaptive mesh refinement
[Carstensen et al., 2014].

The Bank–Weiser estimator

Numerical results

Adaptive finite elements for a Poisson problem:

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

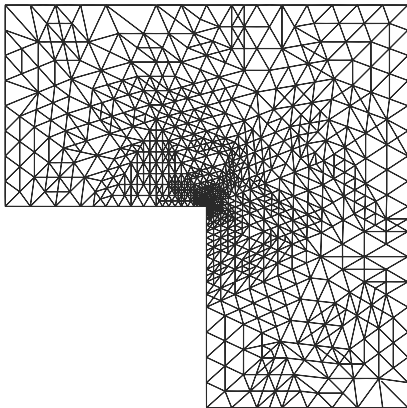


The Bank–Weiser estimator

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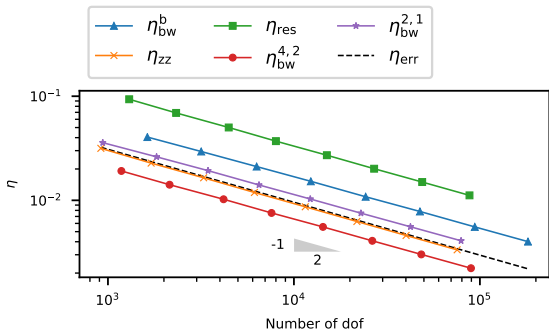
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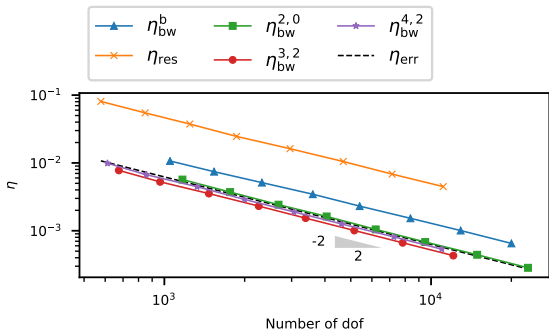
Notation	V_T^+	V_T^-
$\eta_{bw}^{k_+, k_-}$	$V_T^{k_+}$	$V_T^{k_-}$
η_{bw}^b	$V_T^2 + \text{bubble}$	V_T^1

The Bank–Weiser estimator

Numerical results

Adaptive finite elements for a Poisson problem:

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



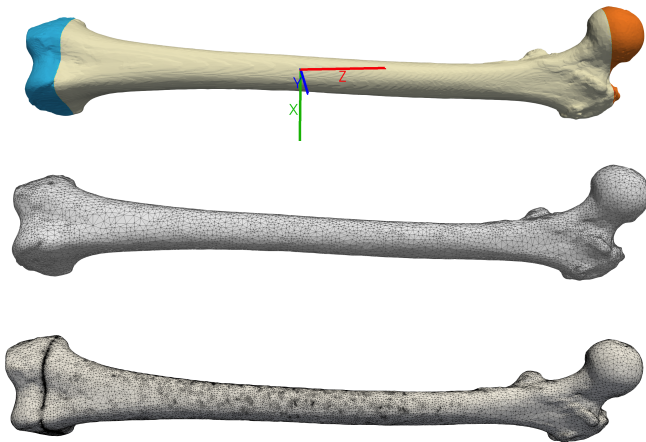
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The Bank–Weiser estimator

Numerical results

GO AFEM for a linear elasticity problem:

we used a technique from [Khan et al., 2019] and [Becker et al., 2011] to compute the estimators. The goal functional is defined by $J(\mathbf{u}, p) := \int_{\Gamma} \mathbf{u} \cdot \mathbf{n} c$, where c is a Gaussian weight centered on the middle of the bone.

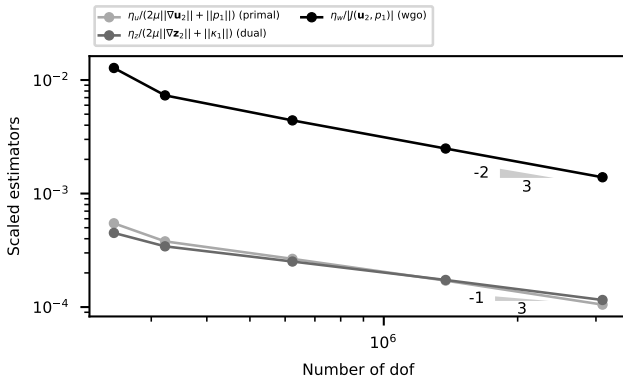


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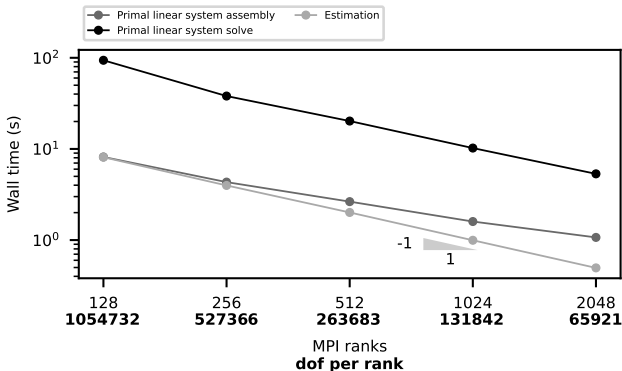
Timescale study:

strong scaling study on the Uni Lu cluster [Varrette et al., 2014].

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

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

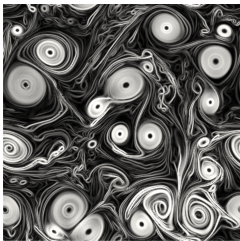
The problem size is fixed around 135 million dof.



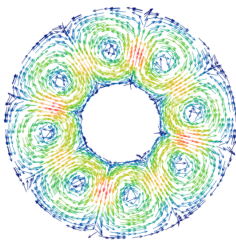


The spectral fractional Laplacian

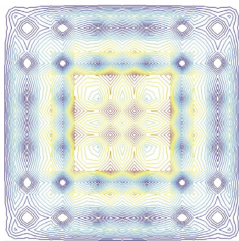
The spectral fractional Laplacian



[Bonito and Nazarov, 2021]



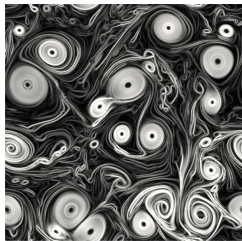
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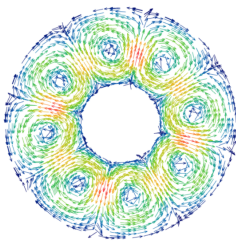
[Sumelka, 2015]

Fractional models are more and more popular and are used in a wide range of fields such as statistics, hydrogeology, finance, physics...

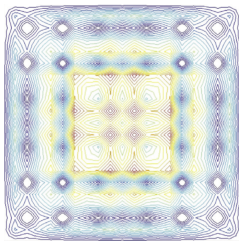
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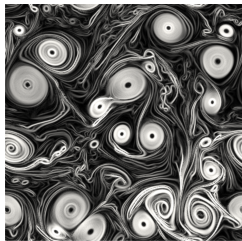


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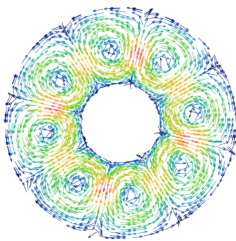
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- **Main advantage:** they are nonlocal.

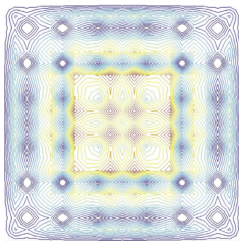
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Fractional models are more and more popular and are used in a wide range of fields such as statistics, hydrogeology, finance, physics...

- **Main advantage:** they are nonlocal.
- **Main drawback:** they are nonlocal.

The spectral fractional Laplacian

Problem setting

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

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

The spectral fractional Laplacian

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The solution u is defined by

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

where $\{\psi_i, \lambda_i\}_{i=1}^{+\infty} \subset L^2(\Omega) \times \mathbb{R}^+$ is the spectrum of $-\Delta$.

The spectral fractional Laplacian

Problem setting

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

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If $f \in L^2(\Omega)$, then $u \in \mathbb{H}^{2s}(\Omega)$ and

$$\|u\|_{\mathbb{H}^{2s}}^2 = \|f\|_{L^2}^2.$$

The spectral fractional Laplacian

Discretization

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

How to solve this equation numerically ?

The spectral fractional Laplacian

Discretization

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

How to solve this equation numerically ?

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

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

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

The spectral fractional Laplacian

Discretization

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

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The spectral fractional Laplacian

Discretization

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

For $l = 1, \dots, N$,

$$u_l - b_l \Delta u_l = f, \quad \text{in } \Omega, \quad (1)$$

$$u_l = 0, \quad \text{on } \Gamma. \quad (2)$$

The spectral fractional Laplacian

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

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The spectral fractional Laplacian

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However, $u_{Q_s^N}$ **is not a discrete function**. To get a full discretization, we use a FE method. We reformulate (1) and (2) in weak form

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

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and write its FE discretization

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

The spectral fractional Laplacian

Discretization

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

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- it is easily parallelizable,
- it involves “standard” FE machinery,
- it is well-suited to three-dimensional problems.

The spectral fractional Laplacian

Error estimation

How can we bound the discretization error ?

$$\|u - u_{Q_s^N}^k\| \leq \|u - u_{Q_s^N}\| + \|u_{Q_s^N} - u_{Q_s^N}^k\|.$$

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

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The spectral fractional Laplacian

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The spectral fractional Laplacian

Error estimation

Quantification of the rational approximation error $\|u - u_{Q_s^N}\|$.

The spectral fractional Laplacian

Error estimation

Quantification of the rational approximation error $\|u - u_{Q_s^N}\|$.

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

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

then, [Bonito and Pasciak, 2015]

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

The spectral fractional Laplacian

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

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

In particular, there exists an approximation Q_s^N such that $\varepsilon_s(N)$ is fully computable and [Bonito and Pasciak, 2015]

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

The spectral fractional Laplacian

Error estimation

Quantification of the rational approximation error $\|u - u_{Q_s^N}\|$.

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

The spectral fractional Laplacian

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What we can prove [Bulle, 2022]:

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

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

The spectral fractional Laplacian

Error estimation

Quantification of the finite element error $\|u_{Q_s^N} - u_{Q_s^N}^k\|$.

The spectral fractional Laplacian

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The spectral fractional Laplacian

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The spectral fractional Laplacian

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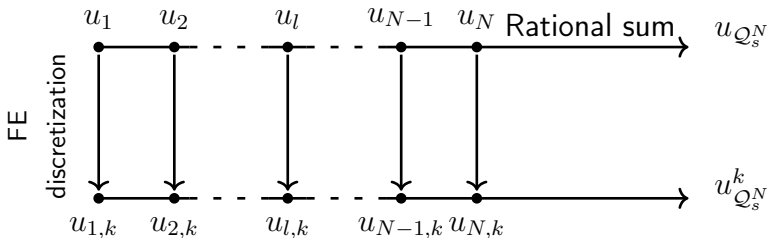
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- A posteriori error estimate for $\|\cdot\|_{\mathbb{H}^s}$ is an ongoing work.

The spectral fractional Laplacian

Error estimation

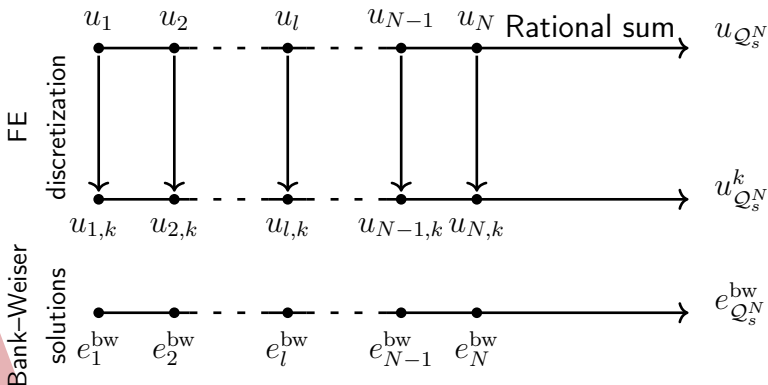
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The spectral fractional Laplacian

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The spectral fractional Laplacian

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Quantification of the finite element error $\|u_{Q_s^N} - u_{Q_s^N}^k\|$.

For each cell $T \in \mathcal{T}_h$ and each parametric problem $l \in \llbracket 1, N \rrbracket$, we solve the Bank–Weiser equation to estimate the difference

$$u_l|_T - u_{l,k}|_T \simeq e_{l,T}^{\text{bw}}.$$

The spectral fractional Laplacian

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Then,

$$\left(u_{Q_s^N} - u_{Q_s^N}^k\right)|_T = C_s(N) \sum_{l=1}^N a_l (u_l - u_{l,k}) \simeq C_s(N) \sum_{l=1}^N a_l e_{l,T}^{\text{bw}} =: e_{Q_s^N, T}^{\text{bw}},$$

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Quantification of the finite element error $\|u_{Q_s^N} - u_{Q_s^N}^k\|$.

For each cell $T \in \mathcal{T}_h$ and each parametric problem $l \in \llbracket 1, N \rrbracket$, we solve the Bank–Weiser equation to estimate the difference

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and finally, we expect that:

$$\|u_{Q_s^N} - u_{Q_s^N}^k\|_{L^2}^2 \simeq \|e_{Q_s^N}^{\text{bw}}\|_{L^2}^2 = \sum_{T \in \mathcal{T}} \|e_{Q_s^N, T}^{\text{bw}}\|_{L^2(T)}^2.$$

The spectral fractional Laplacian

Adaptive mesh refinement

Fractional Laplacian problems show a particular sensibility to **boundary layers effect**. Thus, even for smooth data, the mesh might need to be adaptively refined near the boundary Γ [Banjai et al., 2019].

The spectral fractional Laplacian

Adaptive mesh refinement

Fractional Laplacian problems show a particular sensibility to **boundary layers effect**. Thus, even for smooth data, the mesh might need to be adaptively refined near the boundary Γ [Banjai et al., 2019].

We can use the Bank–Weiser error estimator to steer an adaptive refinement algorithm.

The spectral fractional Laplacian

Adaptive mesh refinement

- Choose a tolerance $\delta > 0$, an initial mesh $\mathcal{T}_{n=0}$ and N such that $\varepsilon_s(N)\|f\|_{L^2} \ll \delta$
- Generate the rational approximation Q_s^N coefficients
- Initialize the estimator $\eta_{Q_s^N}^{\text{bw}} = \delta + 1$

The spectral fractional Laplacian

Adaptive mesh refinement

Choose a tolerance $\delta > 0$, an initial mesh $\mathcal{T}_{n=0}$ and N such that $\varepsilon_s(N)\|f\|_{L^2} \ll \delta$

Generate the rational approximation Q_s^N coefficients

Initialize the estimator $\eta_{Q_s^N}^{\text{bw}} = \delta + 1$

While $\eta_{Q_s^N}^{\text{bw}} > \delta$:

Initialize the solution $u_{Q_s^N, k} = 0$

Initialize the local Bank–Weiser solutions $\{e_{Q_s^N, T}^{\text{bw}} = 0\}_T$

The spectral fractional Laplacian

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For each parametric problem $l \in \llbracket 1, N \rrbracket$:

Solve parametric problem on \mathcal{T}_n to obtain $u_{l,k}$

Add $u_{Q_s^N,k} + C_s(N)a_l u_{l,k}$

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For each cell T of \mathcal{T}_n :

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Add $e_{Q_s^N, T}^{\text{bw}} + C_s(N)a_l e_{l, T}^{\text{bw}}$

The spectral fractional Laplacian

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Choose a tolerance $\delta > 0$, an initial mesh $\mathcal{T}_{n=0}$ and N such that $\varepsilon_s(N)\|f\|_{L^2} \ll \delta$
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For each cell T of \mathcal{T}_n :

Solve BW local parametric problem on T to obtain $e_{l,T}^{\text{bw}}$

Add $e_{Q_s^N,T}^{\text{bw}} + C_s(N)a_l e_{l,T}^{\text{bw}}$

Compute $\{\eta_{Q_s^N,T}^{\text{bw}} = \|e_{Q_s^N,T}^{\text{bw}}\|_{L^2(T)}\}_T$

Take the square root of the sum of $\{\eta_{Q_s^N,T}^{\text{bw}}\}_T$ to obtain $\eta_{Q_s^N}^{\text{bw}}$

The spectral fractional Laplacian

Adaptive mesh refinement

Choose a tolerance $\delta > 0$, an initial mesh $\mathcal{T}_{n=0}$ and N such that $\varepsilon_s(N)\|f\|_{L^2} \ll \delta$
Generate the rational approximation Q_s^N coefficients
Initialize the estimator $\eta_{Q_s^N}^{\text{bw}} = \delta + 1$

While $\eta_{Q_s^N}^{\text{bw}} > \delta$:

Initialize the solution $u_{Q_s^N, k} = 0$

Initialize the local Bank-Weiser solutions $\{e_{Q_s^N, T}^{\text{bw}} = 0\}_T$

For each parametric problem $l \in \llbracket 1, N \rrbracket$:

Solve parametric problem on \mathcal{T}_n to obtain $u_{l, k}$

Add $u_{Q_s^N, k} + C_s(N)a_l u_{l, k}$

For each cell T of \mathcal{T}_n :

Solve BW local parametric problem on T to obtain $e_{l, T}^{\text{bw}}$

Add $e_{Q_s^N, T}^{\text{bw}} + C_s(N)a_l e_{l, T}^{\text{bw}}$

Compute $\{\eta_{Q_s^N, T}^{\text{bw}} = \|e_{Q_s^N, T}^{\text{bw}}\|_{L^2(T)}\}_T$

Take the square root of the sum of $\{\eta_{Q_s^N, T}^{\text{bw}}\}_T$ to obtain $\eta_{Q_s^N}^{\text{bw}}$

If $\eta_{Q_s^N}^{\text{bw}} > \delta$:

Mark the mesh using $\{\eta_{Q_s^N, T}^{\text{bw}}\}_T$

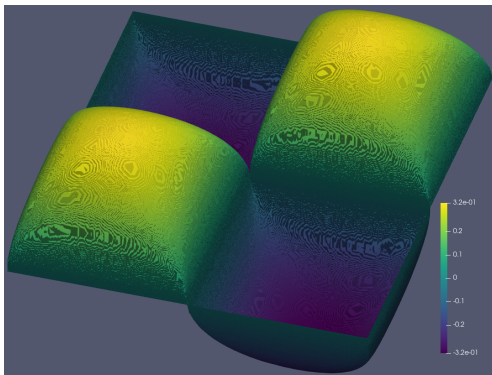
Refine the mesh and replace \mathcal{T}_n by \mathcal{T}_{n+1}

The spectral fractional Laplacian

Numerical results

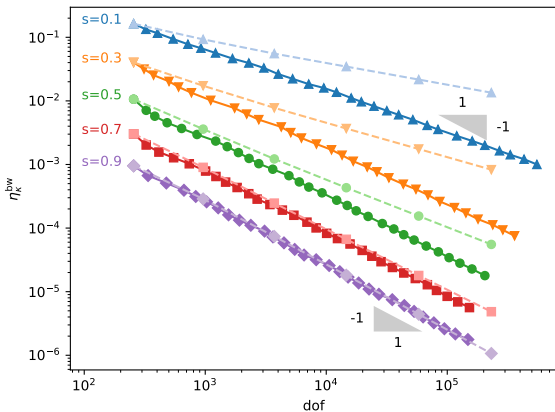
$(-\Delta)^s u = f$, in $[0, 1]^2$, $u = 0$, on Γ ,
with $f(x, y) = 1$ in $[0, 0.5]^2 \cup [0.5, 1]^2$, -1 otherwise.

We assume the rational approximation is negligible, i.e. $u = u_{Q_s^N}$.



The spectral fractional Laplacian

Numerical results



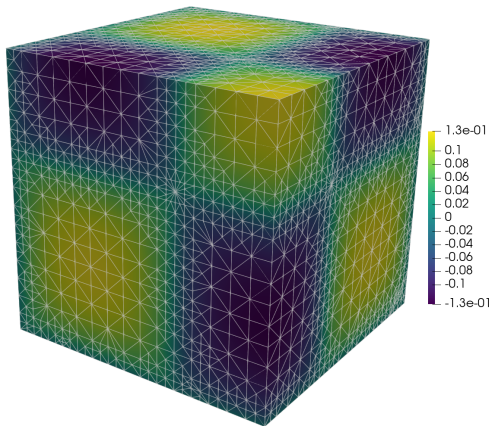
Frac. power	0.1	0.3	0.5	0.7	0.9
Theory [Bonito and Pasciak, 2015]	-0.35	-0.55	-0.75	-0.95	-1.00
Est. (unif.)	-0.35	-0.55	-0.76	-0.95	-1.00
Est. (adapt.)	-0.65	-0.84	-0.93	-0.97	-1.01

The spectral fractional Laplacian

Numerical results

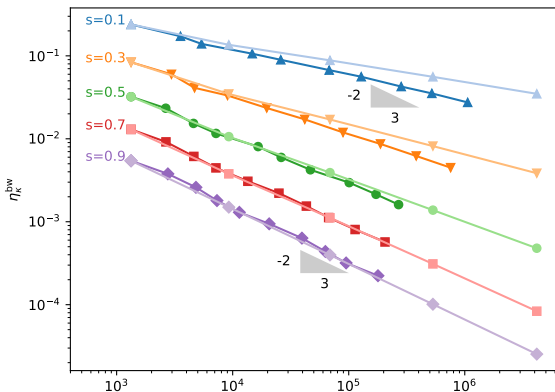
$$(-\Delta)^s u = f, \text{ in } [0, 1]^3, \quad u = 0, \text{ on } \Gamma.$$

We assume the rational approximation is negligible, i.e. $u = u_{Q_s^N}$.



The spectral fractional Laplacian

Numerical results



Frac. power	0.1	0.3	0.5	0.7	0.9
Theory [Bonito and Pasciak, 2015]	-0.23	-0.37	-0.50	-0.63	-0.67
Est. (unif.)	-0.24	-0.38	-0.52	-0.62	-0.67
Est. (adapt.)	-0.33	-0.46	-0.55	-0.65	-0.68

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Thank you for your attention!



I would like to acknowledge the support of the ASSIST research project of the University of Luxembourg. This presentation has been prepared in the framework of the DRIVEN project funded by the European Union's Horizon 2020 Research and Innovation programme under Grant Agreement No. 811099.