

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

**Raphaël Bulle**

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Franz Chouly, Alexei Lozinski

University of Luxembourg

Université de Bourgogne Franche-Comté

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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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**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**  
at Université de Bourgogne Franche-Comté.
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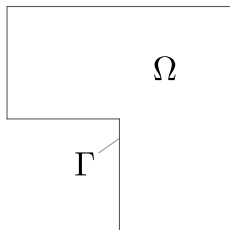
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# The Bank–Weiser estimator

## 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

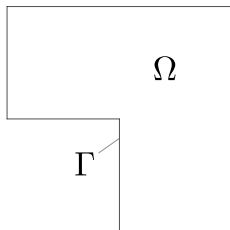
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$$\int_{\Omega} \nabla u \cdot \nabla v = \int_{\Omega} f v, \quad \forall v \in H_0^1(\Omega).$$



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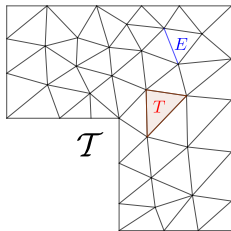
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Lagrange finite element discretization of order  $k$ , find  $u_k$  in  $V^k$  such that

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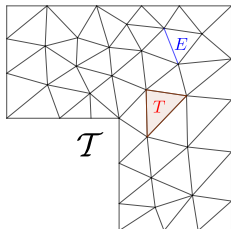
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**Goal:** estimate  $\eta_{\text{err}} = \|\nabla(u_k - u)\|_{\Omega}$  i.e. find a computable quantity  $\eta_{\text{bw}}$  such that  $\eta_{\text{bw}} \approx \eta_{\text{err}}$ .



# The Bank–Weiser estimator

## Definition

On a cell  $T$ , the Bank–Weiser problem is given by:  
find  $e_T^{\text{bw}}$  in  $V_T^{\text{bw}}$  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  $V_T^{\text{bw}}$  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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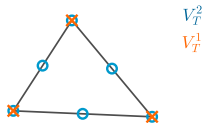
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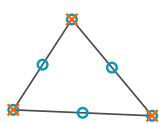
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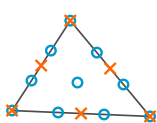
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Examples:



$V_T^2$   
 $V_T^1$



$V_T^3$   
 $V_T^2$



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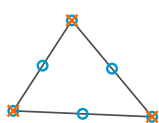
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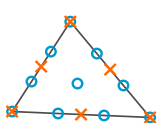
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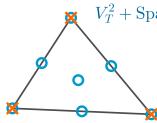
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$V_T^2 + \text{Span}\{\psi_T\}$   
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  - FEniCS and FEniCSx (Python, C++) [Bulle et al., 2021].

# Implementation

## Method details

We need to compute the matrix  $A_T^{\text{bw}}$  and vector  $b_T^{\text{bw}}$  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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**Problem:** the space  $V_T^{\text{bw}}$  is not provided by DOLFIN(x).

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

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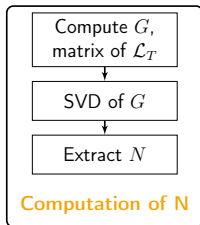
since  $V_T^+$  is provided by DOLFIN(x) and we look for a matrix  $N$  such that:

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



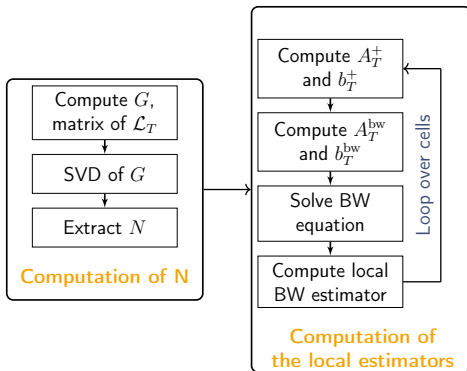
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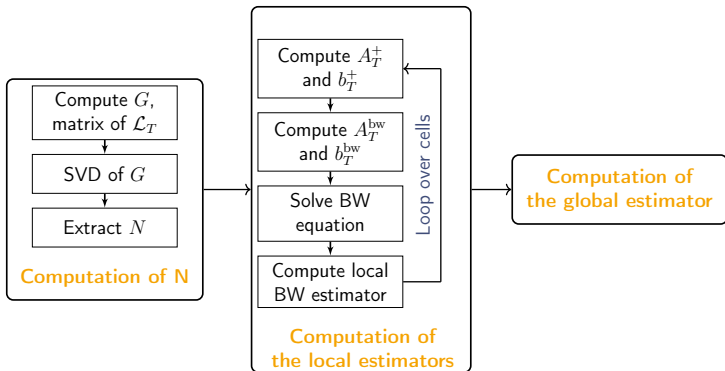
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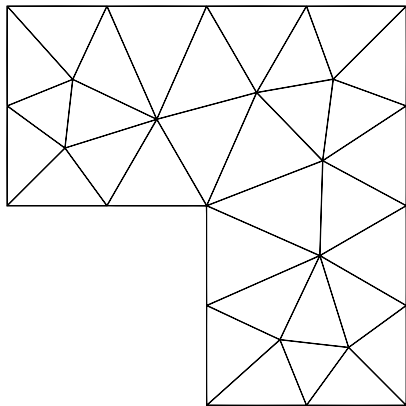


# Implementation

## Numerical results

Adaptive finite elements for a Poisson problem:

$-\Delta u = 0$  in  $\Omega$ ,  $u = u_D$  on  $\Gamma$ . Linear finite elements.

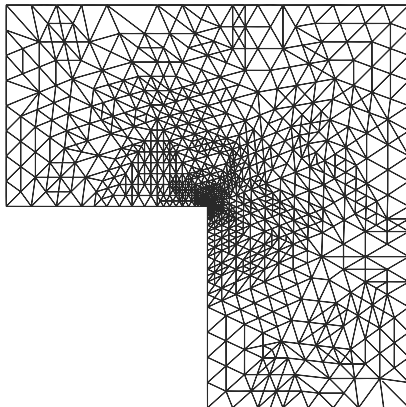


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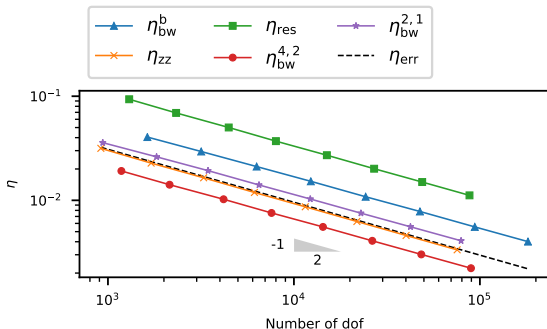


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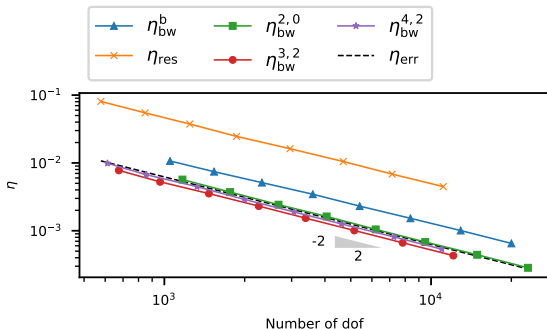
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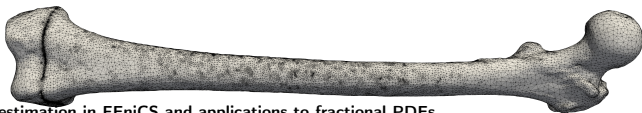
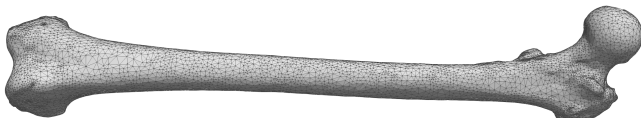
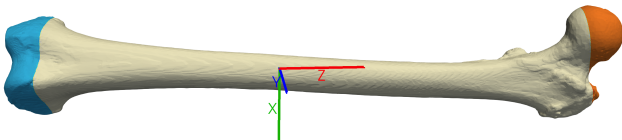
# Implementation

## Numerical results

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  $J(\mathbf{u}_2, p_1) := \int_{\Gamma} \mathbf{u}_2 \cdot \mathbf{n} c$ .





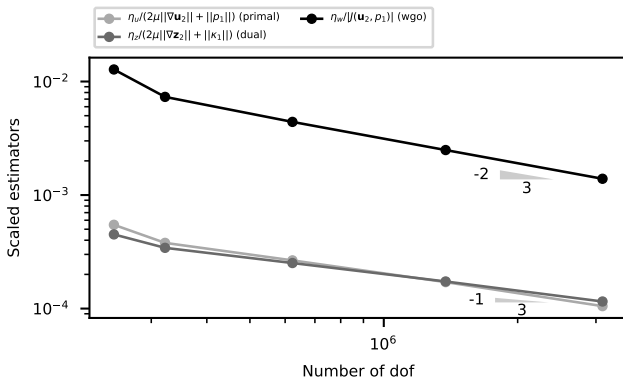
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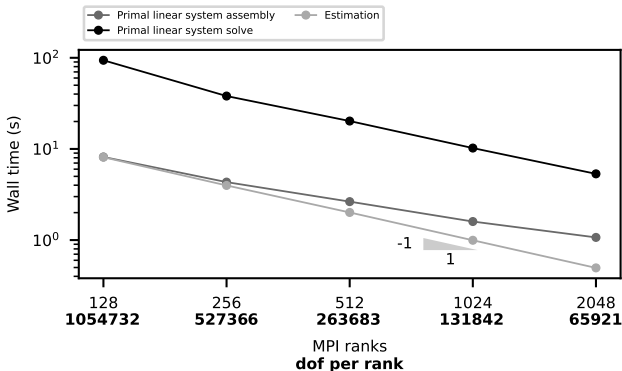
### Timescale study:

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

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

Fractional operators are used in a wide range of different fields such as statistics, hydrogeology, finance, physics...

# 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

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

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The solution  $u$  is defined by

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



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## 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

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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  $\lambda$ .

# The spectral fractional Laplacian

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We denote

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

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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  $u$

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

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

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

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

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  $\mathcal{Q}_s^N$  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  $\varepsilon$ .

# A posteriori error estimation

Finite element error

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

# 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].

# 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  $\eta$  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

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



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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

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

# A posteriori error estimation

## Finite element error

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We use the Bank–Weiser solution to quantify

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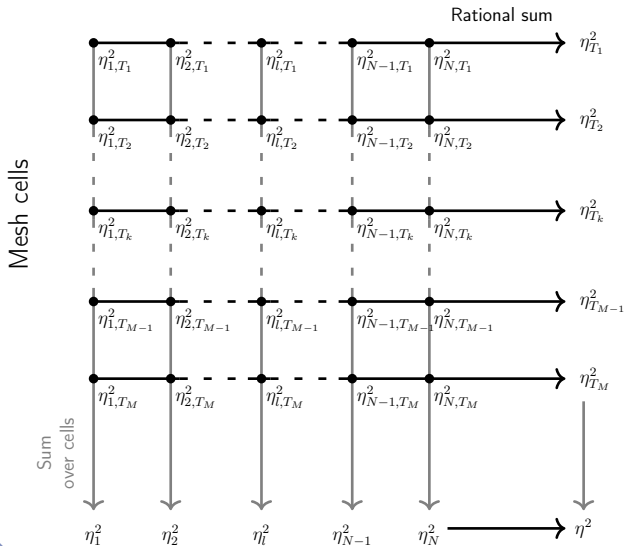
where  $\| \| v \| \|_l^2 := \|v\|_{L^2}^2 + b_l |v|_{H^1}^2$ . Then, we hope that:

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

# A posteriori error estimation

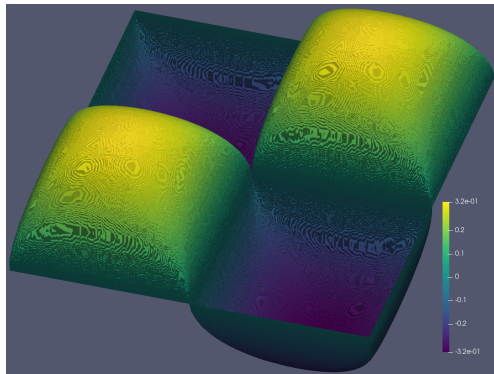
Finite element error

Parametric problems



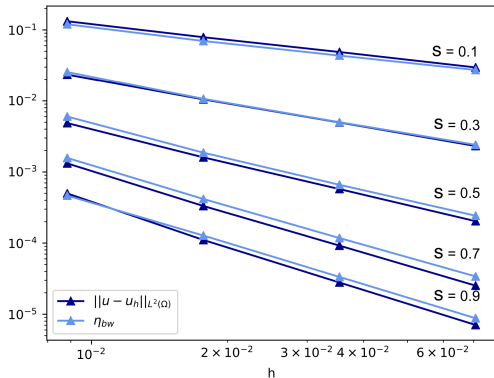
# Numerical results

$(-\Delta)^s u = f$ , in  $[0, 1]^2$ ,  $u = 0$ , on  $\Gamma$ ,  
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.

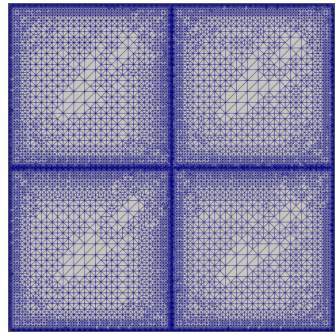
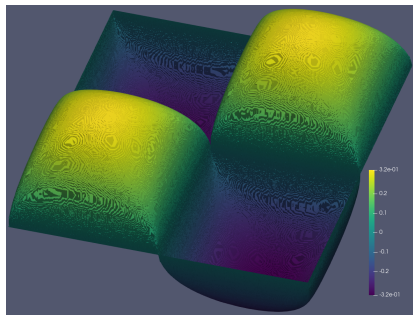


$s$	0.1	0.3	0.5	0.7	0.9
Th. slope	0.7	1.1	1.5	1.9	2.0
Err. slope	0.71	1.11	1.52	1.9	2.04
Est. slope	0.71	1.13	1.54	1.84	1.91

[Bonito and Pasciak, 2015]

# Numerical results

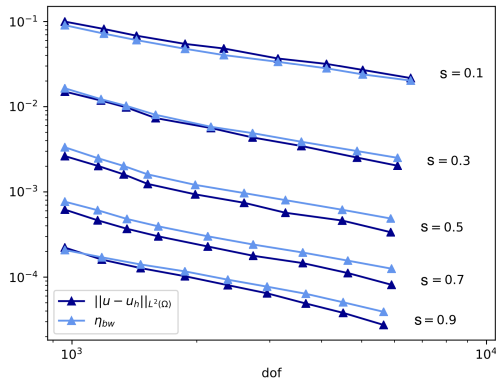
Adaptive mesh refinement.





# 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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