An a Posteriori Error Estimator for the Spectral Fractional Power of the Laplacian

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Outline

- Contributions
- Problem setting
- Discretization
  - Rational approximation
  - Finite element method
- Error estimation
  - Rational approximation
  - Finite element approximation
- Adaptive refinement and numerical results
  - Mesh refinement
  - Rational scheme adaptation
- Future work

Outline

Contributions

Bulle, R., Barrera, O., Bordas, S. P. A., Chouly, F., and Hale, J. S. (2023a). An a posteriori error estimator for the spectral fractional power of the Laplacian. *Computer Methods in Applied Mechanics and Engineering*, 407:115943.

Contributions:

- A novel a posteriori error estimator of the FE error in the discretization of the fractional Laplacian.
- An algorithm combining FE mesh refinement and rational scheme adaptation.
- Implementation in FEniCSx.

Outline

Problem setting

Let $\Omega \subset \mathbb{R}^d$ for $d = 2, 3$, a bounded open domain with polygonal/polyhedral boundary, $s \in (0, 1)$ and

$$(-\Delta)^s u = f \quad \text{in } \Omega, \qquad u = 0 \quad \text{on } \partial\Omega. \tag{1}$$

We consider the *spectral* definition of the fractional Laplacian, the solution to eq. (1) reads

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

where $\{(\lambda_i, \psi_i)\}_{i=1}^{+\infty} \subset \mathbb{R}^{+,*} \times L^2(\Omega)$ is the spectrum of $-\Delta$ over Ω with homogeneous zero Dirichlet boundary conditions.

Outline

Contributions

Problem setting

Discretization
- Rational approximation
- Finite element method

Error estimation
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Adaptive refinement and numerical results
- Mesh refinement
- Rational scheme adaptation

Future work

Discretization: Rational approximation

Let us consider the following rational function defined $\forall \lambda \in \mathbb{R}^{+*}$

$$\mathcal{Q}_s^N(\lambda) := C_1 + C_2 \sum_{l=1}^{N} a_l (b_l + c_l \lambda)^{-1},$$

where $C_1, C_2, (a_l)_l, (b_l)_l$ and $(c_l)_l$ are well-chosen real numbers such that $\forall s \in (0,1)$ and $\forall \lambda \geqslant \lambda_0 > 0$,

$$|\lambda^{-s} - \mathcal{Q}_s^N(\lambda)| \leqslant \varepsilon(\lambda_0, s, N) \underset{N \to +\infty}{\longrightarrow} 0.$$

Discretization: Rational approximation

$$\mathcal{Q}_s^N(\lambda) := C_1 + C_2 \sum_{l=1}^{N} a_l (b_l + c_l \lambda)^{-1},$$

Many such rational functions are available in the litterature. We can cite:

- BURA methods[1] [Harizanov et al., 2020],
- integral representation methods[1] [Bonito and Pasciak, 2015],
- Dirichlet-to-Neumann mappings [Chen et al., 2015],
- time stepping methods [Vabishchevich, 2015].

More details about these schemes can be found in [Hofreither, 2020].

[1] For these methods $\varepsilon(\lambda_0, s, N)$ converges to zero exponentially fast.

Discretization: Rational approximation

Replacing λ_i^{-s} by its rational approximation we have

$$
\begin{aligned}
u &= \sum_{i=1}^{+\infty} \lambda_i^{-s} \left(f, \psi_i\right)_{L^2} \psi_i \\
&\simeq \sum_{i=1}^{+\infty} \mathcal{Q}_s^N(\lambda_i) \left(f_i, \psi_i\right)_{L^2(\Omega)} \psi_i \\
&\simeq C_1 \sum_{i=1}^{+\infty} \left(f_i, \psi_i\right)_{L^2(\Omega)} \psi_i \qquad + C_2 \sum_{l=1}^{N} a_l \left(\sum_{i=1}^{+\infty} (b_l + c_l \lambda_i)^{-1} \left(f_i, \psi_i\right)_{L^2(\Omega)} \psi_i \right) \\
&\simeq C_1 f \qquad + C_2 \sum_{l=1}^{N} a_l u_l,
\end{aligned}
$$

where $(u_l)_l \subset H_0^1(\Omega)$ are solutions to

$$
b_l \int_\Omega u_l v + c_l \int_\Omega \nabla u_l \cdot \nabla v = \int_\Omega f v \qquad \forall v \in H_0^1(\Omega).
$$

Discretization: Rational approximation

$$u \simeq u_N := C_1 f + C_2 \sum_{l=1}^{N} a_l u_l.$$

The function u_N ***is not a discrete function***.

In order to obtain a fully discrete approximation to u we use a finite element method to discretize the functions $(u_l)_l$ and f.

Discretization: Finite element method

Let $\mathcal{T}$ be a mesh over Ω, $p \in \mathbb{N}$ and V_p be the continuous Lagrange finite element space of degree p associated to $\mathcal{T}$.
We consider the finite element approximations $(u_{l,p})_l$, solutions to

$$b_l \int_\Omega u_{l,p} v_p + c_l \int_\Omega \nabla u_{l,p} \cdot \nabla v_p = \int_\Omega f v_p \qquad \forall v_p \in V_p.$$

Then,

$$u \simeq \underbrace{u_N := C_1 f + C_2 \sum_{l=1}^{N} a_l u_l}_{\text{Rational approximation}} \simeq \underbrace{u_{N,p} := C_1 f_p + C_2 \sum_{l=1}^{N} a_l u_{l,p}}_{\text{Finite element approximation}},$$

where f_p is the L^2 projection of f onto V_p.

Outline

Error estimation

How can we control the discretization(s) error(s) ?

Using the triangle inequalities we have

$$\|u - u_{N,p}\|_{L^2(\Omega)} \leqslant \|u - u_N\|_{L^2(\Omega)} + \|u_N - u_{N,p}\|_{L^2(\Omega)},$$

and

$$\left| \|u - u_N\|_{L^2(\Omega)} - \|u_N - u_{N,p}\|_{L^2(\Omega)} \right| \leqslant \|u - u_{N,p}\|_{L^2(\Omega)},$$

where

- $\|u - u_N\|_{L^2(\Omega)}$ is the rational approximation error,
- $\|u_N - u_{N,p}\|_{L^2(\Omega)}$ is the finite element approximation error.

Error estimation: Rational approximation

The rational error can be reduced to a 1D scalar function approximation error.
If $\forall i \in \mathbb{N}^* \ \lambda_i \geqslant \lambda_0$,

$$\|u - u_N\|_{L^2(\Omega)} \leqslant \max_{\lambda \geqslant \lambda_0} (\lambda^{-s} - \mathcal{Q}_s^N(\lambda)) \|f\|_{L^2(\Omega)}.$$

In practice, for certain schemes this maximum is reached for λ close to λ_0, thus computing an approximation η_N^{ra} of $\max_{\lambda \geqslant \lambda_0} (\lambda^{-s} - \mathcal{Q}_s^N(\lambda)) \|f\|_{L^2(\Omega)}$ is an easy task compared to the finite element error approximation.

Error estimation: Finite element approximation

$$(-\Delta)^s u = f \quad \longrightarrow \quad \begin{aligned} b_1 \int_\Omega u_{1,p} v_p + c_1 \int_\Omega \nabla u_{1,p} \cdot \nabla v_p &= \int_\Omega f v_p \quad \longrightarrow \quad \text{Error estimator} \\ &\cdots \\ b_N \int_\Omega u_{N,p} v_p + c_N \int_\Omega \nabla u_{N,p} \cdot \nabla v_p &= \int_\Omega f v_p \quad \longrightarrow \quad \text{Error estimator} \end{aligned}$$

Error estimation: Finite element approximation

By linearity we have,

$$u_{N|T} - u_{N,p|T} = C_1(f_{|T} - f_{p|T}) + C_2 \sum_{l=1}^{N} a_l(u_{l|T} - u_{l,p|T}).$$

We are looking for computable local functions h_T and $e^{\mathrm{bw}}_{l,T}$ such that for each $T \in \mathcal{T}$,

$$u_{N|T} - u_{N,p|T} \simeq C_1 h_T + C_2 \sum_{l=1}^{N} a_l e^{\mathrm{bw}}_{l,T}.$$

For example, we can consider $h_T := f_{p+1|T} - f_{p|T}$, where f_{p+1} is the L^2 projection of f onto V_{p+1}.

We need an error estimation method that computes the local functions $e^{\mathrm{bw}}_{l,T}$.
We use the hierarchical a posteriori error estimation method derived in [Bank and Weiser, 1985].

Error estimation: Finite element approximation

First, we notice that the functions $u_l - u_{l,p}$ satisfy the following equation

$$b_l \int_{\Omega} (u_l - u_{l,p}) v + c_l \int_{\Omega} \nabla (u_l - u_{l,p}) \cdot \nabla v = \sum_{T \in \mathcal{T}} R_T(v_{|T}) \quad \forall v \in H_0^1(\Omega),$$

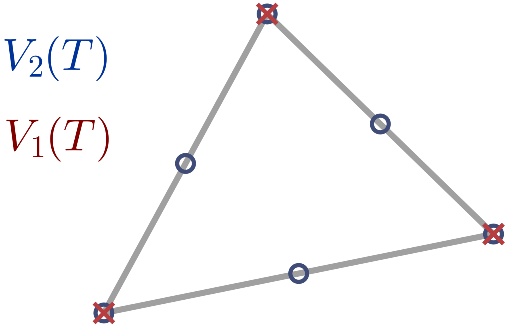
where R_T is a linear form that depends on $u_{l,p}$ but *not on* u_l.
The idea behind Bank-Weiser error estimation is to localize and discretize the previous equation into

$$b_l \int_{T} e^{\mathrm{bw}}_{l,T} v^{\mathrm{bw}}_T + c_l \int_{T} \nabla e^{\mathrm{bw}}_{l,T} \cdot \nabla v^{\mathrm{bw}}_T = R_T(v^{\mathrm{bw}}_T) \quad \forall v^{\mathrm{bw}}_T \in V^{\mathrm{bw}}(T).$$

Error estimation: Finite element approximation

If $\mathcal{I}_T : V_{p+1}(T) \longrightarrow V_p(T)$ is the local Lagrange interpolation operator, then the Bank-Weiser space is defined as

$$V^{\mathrm{bw}}(T) := \left\{ v_{p+1,T} \in V_{p+1}(T),\, \mathcal{I}(v_{p+1,T}) = 0 \right\} = \ker(\mathcal{I}_T).$$



Error estimation: Finite element approximation

Then, the local fractional a posteriori error estimator is given by

$$\|u_{N|T} - u_{N,p|T}\|_{L^2(T)} \simeq \eta^{\text{bw}}_{N,T} := \left\| C_1 h_T + C_2 \sum_{l=1}^{N} a_l e^{\text{bw}}_{l,T} \right\|_{L^2(T)},$$

and the corresponding global estimator is given by

$$\|u_N - u_{N,p}\|^2_{L^2(\Omega)} \simeq {\eta^{\text{bw}}_N}^2 := \sum_{T\in\mathcal{T}} {\eta^{\text{bw}}_{N,T}}^2.$$

Error estimation

To summarize,

	Rational scheme	FE method
Exact errors	$\|u - u_N\|_{L^2(\Omega)}$	$\|u_N - u_{N,p}\|_{L^2(\Omega)}$
Estimators	η_N^{ra} Approx. of the max of a 1D function	η_N^{bw} Hierarchical error estimator of Bank–Weiser type
Properties	”Easily” computable	Fully local and computable in parallel wrt l and T.

Outline

Adaptive refinement and numerical results: Mesh refinement

We can use the Bank-Weiser error estimator to drive an adaptive mesh refinement algorithm.

$$\cdots \longrightarrow \text{Solve} \longrightarrow \text{Estimate} \longrightarrow \text{Mark} \longrightarrow \text{Refine} \longrightarrow \cdots$$

When the rational scheme is not adapted, we assume that N is large enough so that the rational error can be neglected.
Rational schemes tested:

- BP (Bonito-Pasciak) [Bonito and Pasciak, 2015].
- BURA (with `baryrat`[1]) [Harizanov et al., 2020, Hofreither, 2021].

The numerical results are obtained using the FEniCSx software [Alnæs et al., 2015] and our FEniCSx library[2] [Bulle et al., 2023b]. A minimal example code is available here[3].

[1] `https://github.com/c-f-h/baryrat`

[2] `https://github.com/jhale/fenicsx-error-estimation`

[3] `https://figshare.com/articles/software/Example_of_a_posteriori_error_estimation_of_fractional_partial_differential_equation_in_FEniCSx_Error_Estimation_FEniCSx-EE_/19086695/3`

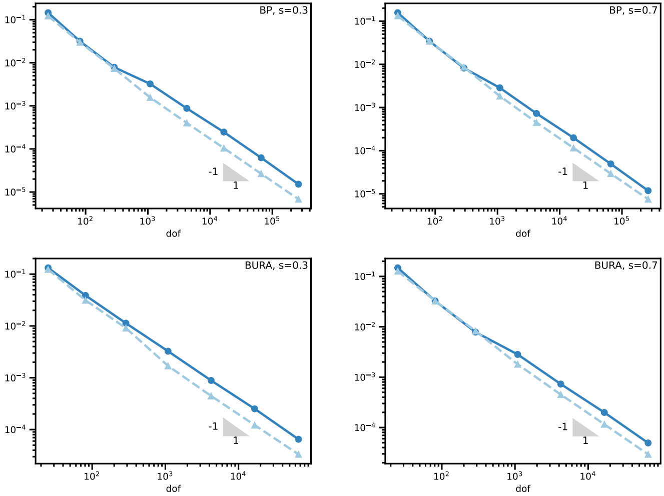
Adaptive refinement and numerical results: Mesh refinement

Choose a tolerance $\mathrm{tol} > 0$, an initial mesh $\mathcal{T}_{n=0}$ and a rational scheme $\mathcal{Q}_s^N$ s.t. $\|u - u_N\|_{L^2} \ll \mathrm{tol}$.
Generate $\mathcal{Q}_s^N$ coefficients
while $\eta_N^{\mathrm{bw}} > \mathrm{tol}$ **do** (Refinement loop)
  for $l \in [\![1, N]\!]$ **do** (Rational scheme loop)
    Compute $u_{l,p}$ on $\mathcal{T}_n$
    Add $a_l u_{l,p}$ to $u_{N,p}$
    for $T \in \mathcal{T}_n$ **do** (Local FE error estimation loop)
      Compute $e_{l,T}^{\mathrm{bw}}$
      Add $a_l e_{l,T}^{\mathrm{bw}}$ to $e_{N,T}^{\mathrm{bw}}$
    end for
  end for
  Multiply $u_{N,p}$ and $e_{N,T}^{\mathrm{bw}}$ by C_2
  Compute f_{V^p} the L^2 projection of f onto V^p and add $C_1 f_{V^p}$ to $u_{\mathcal{Q}_s,p}$
  Compute $f_{V^{p+1}}$ the L^2 projection of f onto V^{p+1} and add $C_1 (f_{V^{p+1}} - f_{V^p})_{|T}$
  Compute $\eta_{N,T}^{\mathrm{bw}} := \|e_{N,T}^{\mathrm{bw}}\|_{L^2(T)}$ for all $T \in \mathcal{T}_n$ and $\eta_N^{\mathrm{bw}} := \sqrt{\sum_T {\eta_{N,T}^{\mathrm{bw}}}^2}$
  if $\eta_N^{\mathrm{bw}} < \mathrm{tol}$ **then**
    Return $u_{N,p}$
  else
    Mark the mesh $\mathcal{T}_n$ using $\{\eta_{N,T}^{\mathrm{bw}}\}_T$
    Refine the mesh $\mathcal{T}_n$ to obtain $\mathcal{T}_{n+1}$
  end if
end while

Adaptive refinement and numerical results: Mesh refinement

2D problem with analytical solution

$(-\Delta)^s u = f$ in $[0,\pi]^2$, $u = 0$ on Γ, with $f(x,y) = (2/\pi)\sin(x)\sin(y)$. Exact solution $u(x,y) = 2^{-s} f(x,y)$.

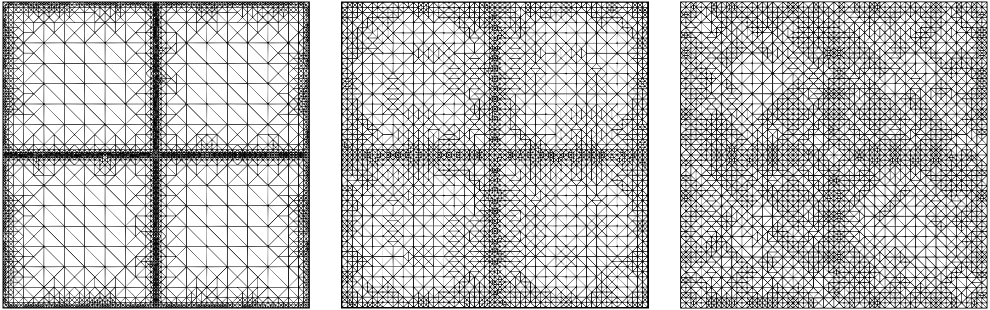


Solid line: Bank-Weiser estimator, dashed line: exact error.

Adaptive refinement and numerical results: Mesh refinement

2D checkerboard problem

$(-\Delta)^s u = f,$ 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. Initial mesh 4×4.

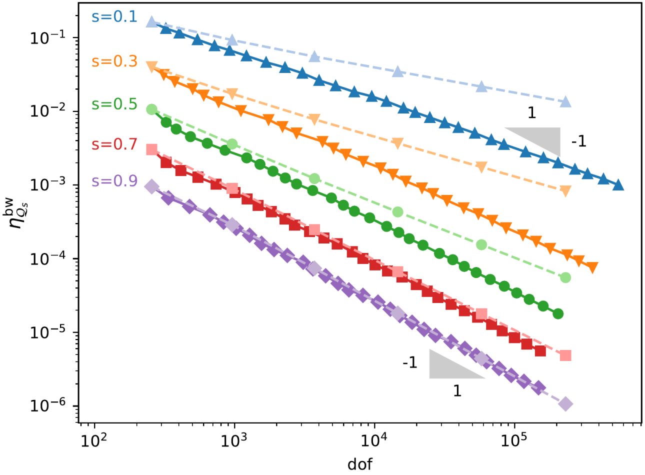


$s = 0.1$ $s = 0.5$ $s = 0.9$

Meshes after 10 adaptive refinement steps.

Adaptive refinement and numerical results: Mesh refinement

2D checkerboard problem



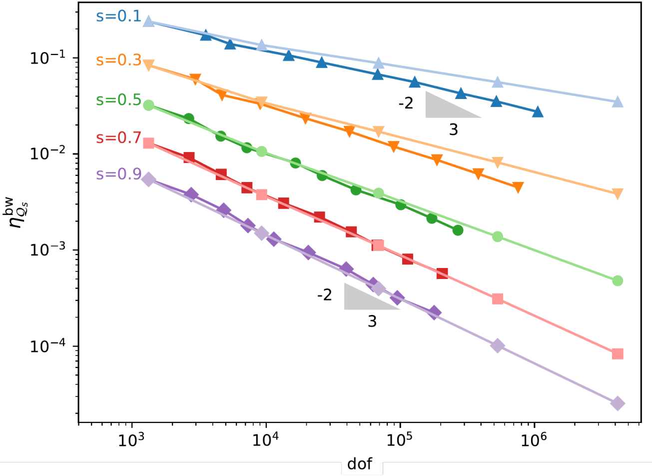
BP rational scheme.

Solid lines: BW estimator, adaptive ref. Dashed lines: BW estimator, uniform ref.

Adaptive refinement and numerical results: Mesh refinement

3D checkerboard problem (BP scheme)

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



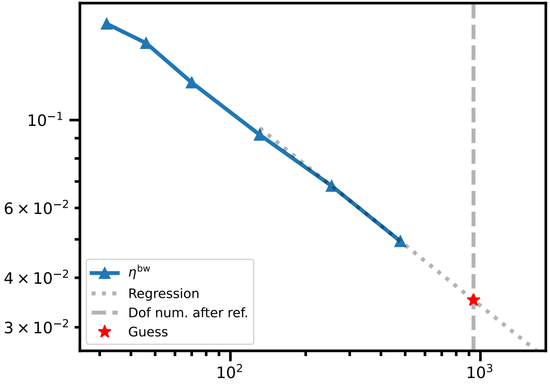
Light lines: BW estimator, uniform ref. Dark lines: BW estimator, adaptive ref.

Adaptive refinement and numerical results: Rational scheme adaptation

Using an overly refined rational scheme is a waste of computational resources...
Is it possible to even the FE and rational discretization errors ?

$$\cdots \longrightarrow \text{Solve} \longrightarrow \text{Estimate} \longrightarrow \text{Mark} \longrightarrow \text{Refine} \longrightarrow \text{Adapt ra. sch.} \longrightarrow \cdots$$

At step m of refinement, we need to guess what will be the $m+1^{\text{th}}$ value of η^{bw} and try to match this value with η^{ra}.



Adaptive refinement and numerical results: Rational scheme adaptation

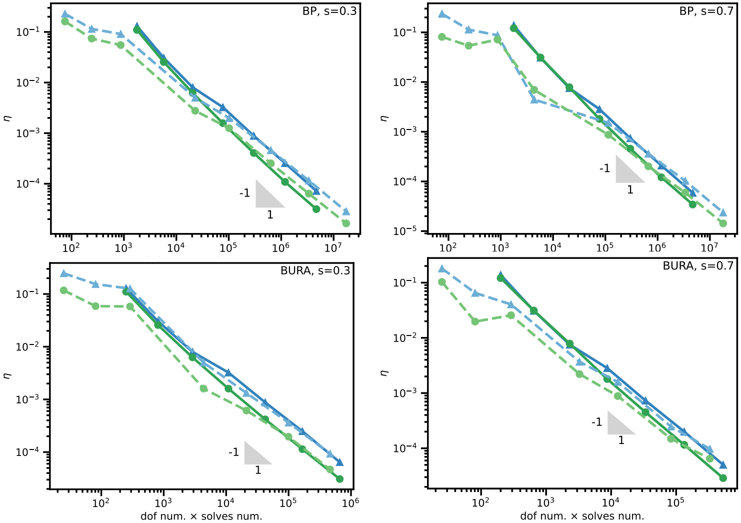
2D problem with analytical solution

	Frac. power	0.1	0.3	0.5	0.7	0.9
BP	Fixed ra. scheme	1155	497	427	497	1155
	Adaptive ra. scheme	504	209	178	199	358
BURA	Fixed ra. scheme	96	77	63	49	35
	Adaptive ra. scheme	42	33	29	20	17

Total number of parametric problems solves.

Adaptive refinement and numerical results: Rational scheme adaptation

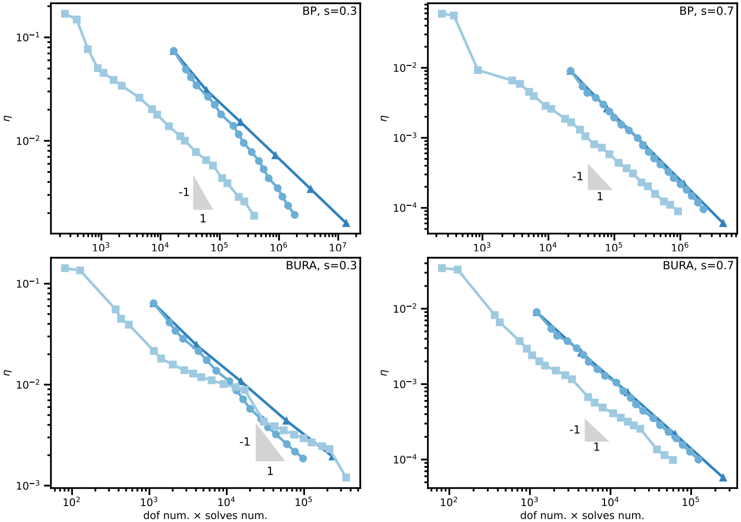
2D problem with analytical solution



Solid lines: fixed rational scheme, dashed lines: adaptive rational scheme.

Adaptive refinement and numerical results: Rational scheme adaptation

2D checkerboard problem



Dark blue lines: uniform mesh ref. & fixed rational scheme, medium blue lines: adaptive mesh ref. & fixed rational scheme, light blue lines: adaptive mesh ref. & adaptive rational scheme.

Outline

Future work

- Improve the mesh refinement method (e.g. multi–mesh, anisotropic refinement).
- Try other hierarchical a posteriori error estimators (following e.g. [Zhang and Naga, 2002]).
- Derive an estimator for the fractional Sobolev norm.
- Adapt the method to other fractional Laplacian definitions (e.g. integral Laplacian, following [Bonito et al., 2019]).

Thank you for your attention!

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