# A PDE approach to spectral fractional diffusion 

Abner J. Salgado<br>Department of Mathematics, University of Tennessee

January 28, 2021

## Outline

Motivation: Fractional powers of an operator

Direct discretization approach

Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension

## Outline

Motivation: Fractional powers of an operator

## Direct discretization approach

## Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension

## Back to linear algebra I

- If $A$ is symmetric, that is

$$
A^{\top}=A,
$$

then it is diagonalizable.

- This means that there are $Q$ orthogonal, and $\Lambda$ diagonal, such that

$$
A=Q^{\top} \Lambda Q, \quad Q^{\top}=Q^{-1}, \quad \Lambda=\operatorname{diag}\left\{\lambda_{1}, \ldots, \lambda_{n}\right\}
$$

- In this case, the action $\mathbf{w}=A \mathbf{v}$ can be described as follows:
- $\tilde{\mathbf{v}}=Q \mathbf{v}$ is a change of basis.
$\circ \overline{\mathbf{v}}=\Lambda \tilde{\mathbf{v}}$ is a scaling in this new basis.
- $\mathbf{w}=Q^{\top} \Lambda \overline{\mathbf{v}}$ is returning to the original basis.
- If, in addition, $A$ is positive, that is

$$
\mathbf{v}^{\top} A \mathbf{v}>0
$$

then all its eigenvalues are positive $\lambda_{i}>0$.

## Back to linear algebra II

Why do we care about this? If $A \in \mathbb{R}^{n \times n}$ is symmetric:

- With this we can define almost any function of a matrix via

$$
f(A)=Q^{\top} f(\Lambda) Q, \quad f(\Lambda)=\operatorname{diag}\left\{f\left(\lambda_{1}\right), \ldots, f\left(\lambda_{n}\right)\right\}
$$

- Solution of ODEs:

$$
\dot{\mathbf{y}}(t)=A \mathbf{y}, t>0 \quad \mathbf{y}(0)=\mathbf{y}_{0} \quad \Longrightarrow \quad \mathbf{y}(t)=\exp (t A) \mathbf{y}_{0} .
$$

- Theory of iterative schemes: To solve $A \mathbf{x}=\mathbf{f}$ we can use a two-layer implicit scheme

$$
B \frac{\mathbf{x}^{k+1}-\mathbf{x}^{k}}{\alpha}+A \mathbf{x}^{k}=\mathbf{f}
$$

with SPD preconditioner $B$. The analysis of such schemes can be reduced to that of the explicit one

$$
\frac{\mathbf{v}^{k+1}-\mathbf{v}^{k}}{\alpha}+C \mathbf{v}^{k}=\mathbf{g}
$$

where

$$
\mathbf{v}^{k}=B^{1 / 2} \mathbf{x}^{k}, \quad C=B^{-1 / 2} A B^{-1 / 2}, \quad \mathbf{g}=B^{-1 / 2} \mathbf{f}
$$

## Spectral theory 101

Question: What happens in infinite dimensions? In particular, for differential operators?
A (the?) basic partial differential operator that expresses diffusion is the Laplacian

$$
-\Delta=-\sum_{i=1}^{n} \frac{\partial^{2}}{\partial x_{i}^{2}}
$$

- Integration by parts shows that $-\Delta$ is positive

$$
\int_{\Omega}-\Delta v v \mathrm{~d} x=\int_{\Omega}|\nabla v|^{2} \mathrm{~d} x>0, \quad \forall v \in C_{0}^{\infty}(\Omega) .
$$

- One can show that $(-\Delta)^{-1}: L^{2}(\Omega) \rightarrow L^{2}(\Omega)$ is compact:
- There exist $\left\{\lambda_{k}, \varphi_{k}\right\}_{k \in \mathbb{N}} \subset \mathbb{R}^{+} \times L^{2}(\Omega)$ such that:

$$
-\Delta \varphi_{k}=\lambda_{k} \varphi_{k}, \quad \varphi_{k \mid \partial \Omega}=0
$$

and $\left\{\varphi_{k}\right\}_{k \in \mathbb{N}}$ is an orthonormal basis of $L^{2}(\Omega)$.

- This means that if $w \in L^{2}(\Omega)$, then it has the following representation

$$
w=\sum_{k=1}^{\infty} w_{k} \varphi_{k} \quad w_{k}=\int_{\Omega} w \varphi_{k} \mathrm{~d} x
$$

## The spectral fractional Laplacian I

- In addition, if $w$ is sufficiently nice, then we have that

$$
-\Delta w=\sum_{k=1}^{\infty} w_{k} \lambda_{k} \varphi_{k}, \quad w_{k}=\int_{\Omega} w \varphi_{k} \mathrm{~d} x
$$

which is an analogue of the matrix case:

- The term $w_{k}$ is a change of basis.
- Multiplication by the eigenvalue $\lambda_{k}$ is a diagonal scaling.
- The outer sum is returning to the original basis.
- We can now define functions of $-\Delta$. For instance, if $s \in(0,1)$ and $w$ is sufficiently nice,

$$
(-\Delta)^{s} w=\sum_{k=1}^{\infty} w_{k} \lambda_{k}^{s} \varphi_{k}
$$

Questions: Why do we care? What is the domain of this operator? What is its range?

## The spectral fractional Laplacian II

- The heat equation

$$
\partial_{t} u-\Delta u=0, \quad u_{\mid t=0}=v
$$

smoothens and smears the initial condition $v$. This could be used, for instance, in image denoising. However, the effect of $-\Delta$ is too strong. Thus, it can be weakened by

$$
\partial_{t} u+(-\Delta)^{s} u=0, \quad u_{\mid t=0}=v
$$

- Some special cases of random walks also lead to the fractional heat equation ${ }^{\boldsymbol{B}}$.
- Models in phase transition ${ }^{\text {E }}$ : fractional Allen Cahn ( $\alpha=0$, $\beta \in(0,1))$ and Cahn Hilliard $(\alpha, \beta \in(0,1))$ equations

$$
\partial_{t} u+(-\Delta)^{\alpha}\left(\varepsilon^{2}(-\Delta)^{\beta} u+F^{\prime}(u)\right)=0
$$

[^0]
## The spectral fractional Laplacian III



- Original, noisy, regularized images for $L^{2}$ and $H^{-1}$ fidelity terms.
- Top: $s=0.42$
- Bottom: $s=0.35$
- Stolen from ${ }^{\boldsymbol{\theta}}$.


## Spectral theory 102

- Let $\mathcal{L}$ be a symmetric second order elliptic operator, i.e.,

$$
\mathcal{L} w=-\nabla \cdot(a \nabla w)+c w
$$

with $a \in L^{\infty}\left(\Omega, \mathbb{S}_{+}^{d}\right)$ uniformly positive definite and $0 \leq c \in L^{\infty}(\Omega)$.

- In a similar way we can define $\mathcal{L}_{0}^{s}$, the fractional powers of $\mathcal{L}$ supplemented with homogeneous Dirichlet (or Neumann) boundary conditions.
- From now on, and for simplicity only, we will only deal with the Laplacian. Everything that we will say applies to $\mathcal{L}_{0}^{s}$.


## Goal

- Given a suitable $f$ find $u$ such that

$$
(-\Delta)^{s} u=f
$$

in the sense described above.

- Where's the catch? The domain $\Omega$ can be quite general, so the spectrum of $-\Delta$ is not readily available.


## Domain, range, and regularity I

- Because of the way that we defined the fractional Laplacian we have

$$
(-\Delta)^{s}: \mathbb{H}^{s}(\Omega) \rightarrow \mathbb{H}^{-s}(\Omega)
$$

where

$$
\mathbb{H}^{s}(\Omega)=\left\{w=\sum_{k=1}^{\infty} w_{k} \varphi_{k}: \sum_{k=1}^{\infty} \lambda_{k}^{s}\left|w_{k}\right|^{2}<\infty\right\}
$$

- It turns out that

$$
\mathbb{H}^{s}(\Omega)= \begin{cases}H^{s}(\Omega), & s \in\left(0, \frac{1}{2}\right) \\ H_{00}^{1 / 2}(\Omega), & s=\frac{1}{2} \\ H_{0}^{s}(\Omega), & s \in\left(\frac{1}{2}, 1\right)\end{cases}
$$

where the zero subindices mean "zero boundary values".

- The fact that the domain has fractional Sobolev regularity reinforces the idea that we are taking fractional order derivatives.


## Domain, range, and regularity II

If we wish to develop a rigorous numerical approximation of $u$, then we must understand its regularity.

- From the definition it follows that, if $f \in \mathbb{H}^{r}(\Omega)$, then $u \in \mathbb{H}^{r+2 s}(\Omega)$, for all $r \in \mathbb{R}$.
- If $r \geq-s$ this means that, at least for $\omega \Subset \Omega$,

$$
u \in H^{r+2 s}(\omega)
$$

- What about near the boundary? For $x \in \bar{\Omega}$ let $\operatorname{dist}(x, \partial \Omega)$ be the distance of $x$ to $\partial \Omega$ :
- If $s \neq \frac{1}{2}$ then ${ }^{\boldsymbol{\theta}}$ there is a smooth function $v$ such that

$$
u(x) \approx v(x)+\operatorname{dist}(x, \partial \Omega)^{\min \{1,2 s\}}
$$

- If $s=\frac{1}{2}$ then we have the exceptional case ${ }^{\text {B }}$

$$
u(x) \approx v(x)+\operatorname{dist}(x, \partial \Omega)|\log \operatorname{dist}(x, \partial \Omega)|
$$

[^1]
## Outline

Motivation: Fractional powers of an operator

Direct discretization approach

## Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension

## Direct discretization

Given $f \in \mathbb{H}^{-s}(\Omega)$,

$$
f=\sum_{k=1}^{\infty} f_{k} \varphi_{k}: \quad(-\Delta)^{s} u=f \Longrightarrow \quad u_{k}=f_{k} \lambda_{k}^{-s}
$$

Algorithm:

- Compute a "sufficiently large" number of eigenpairs $\left\{\lambda_{k}, \varphi_{k}\right\}_{k=1}^{N}$.
- Compute the Fourier coefficients $f_{k}$.
- Find the solution: $u_{k}=f_{k} \lambda_{k}^{-s}$.

But

- How to choose $N$ ?
- VERY time consuming!
- Error analysis?


## Error analysis I

The eigenpairs can only be computed approximately (read, via finite elements). The error analysis in this case is as follows ${ }^{\boldsymbol{\theta}}$ :

- Let $X$ be a Hilbert space and $A$ be a positive definite self-adjoint operator on $X$.
- Let $\left\{X_{h}\right\}_{h>0}$ be a family of closed subspaces of $X$ and $A_{h}$ is a positive definite bounded self-adjoint operator on $X_{h}$.
- Inverse estimate: There is $\varepsilon: \mathbb{R}_{+} \rightarrow \mathbb{R}_{+}$with $\lim _{h \rightarrow 0} \varepsilon(0)=0$ such that

$$
\left\|A_{h}\right\| \lesssim \frac{1}{\varepsilon(h)}
$$

- Approximability: If $P_{h}$ is the orthogonal projection onto $X_{h}$

$$
\left\|\left(A_{h}^{-1} P_{h}-A^{-1}\right) f\right\|_{X} \lesssim \varepsilon(h)\|f\|_{X}
$$

- In this case, for $s \in(0,1)$, we have

$$
\left\|\left(A_{h}^{-s} P_{h}-A^{-s}\right) f\right\|_{X} \lesssim \varepsilon(h)^{s}\|f\|_{X}
$$

[^2]
## Error analysis II

In our case:

- $X=L^{2}(\Omega), X_{h}$ is a (piecewise linear) finite element space, $A=-\Delta$, and $A_{h}=-\Delta_{h}$.
- Since $X_{h}$ consists of piecewise polynomials

$$
\left\|A_{h}\right\| \lesssim \frac{1}{h^{2}}, \quad \Longrightarrow \quad \varepsilon(h)=h^{2}
$$

- For $f \in L^{2}(\Omega)$ we have

$$
u=(-\Delta)^{-1} f \in H^{2}(\Omega) \cap H_{0}^{1}(\Omega)
$$

and, if $u_{h} \in X_{h}$ is its finite element approximation: $u_{h}=\left(-\Delta_{h}\right)^{-1} P_{h} f$, then Aubin-Nitsche duality yields

$$
\left\|u-u_{h}\right\|_{L^{2}(\Omega)} \lesssim h^{2}|u|_{H^{2}(\Omega)} \lesssim h^{2}\|f\|_{L^{2}(\Omega)}
$$

- The previous theory then gives

$$
\left\|(-\Delta)^{-s} f-\left(-\Delta_{h}\right)^{-s} P_{h} f\right\|_{L^{2}(\Omega)} \lesssim h^{2 s}\|f\|_{L^{2}(\Omega)}
$$

We still need to compute $\left(-\Delta_{h}\right)^{-s}$ !

## Outline

## Motivation: Fractional powers of an operator

## Direct discretization approach

Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension

## Computing the discrete spectrum

Evaluating the eigenvalues of $-\Delta_{h}$ is time consuming: MTT, Lanczos, $\ldots$ Best uniform rational approximation (BURA) ${ }^{\boldsymbol{E}}$ : Assume we need to solve

$$
\mathcal{A}^{s} \mathbf{u}=\mathbf{f}
$$

where $\mathcal{A}$ is a rescaled version of $\left(-\Delta_{h}\right)^{s}$ so that its spectrum lies in $(0,1]$.

- Let $r_{s}$ be analytic on $(0,1]$ and, for some constant $\varepsilon>0$ satisfies

$$
\sup _{t \in(0,1]}\left|r_{s}(t)-t^{1-s}\right| \leq \varepsilon
$$

then, for every $\gamma \in \mathbb{R}$ and $\mathbf{F} \in \mathbb{R}^{N}$ we have

$$
\left\|\left(r_{s}(\mathcal{A})-\mathcal{A}^{1-s}\right) \mathbf{F}\right\|_{\mathcal{A}^{\gamma}} \leq \varepsilon\|\mathbf{F}\|_{\mathcal{A}^{\gamma}}
$$

- The previous result implies that, if $\mathbf{u}_{r}=r_{s}(\mathcal{A}) \mathcal{A}^{-1} \mathbf{f}$, then

$$
\left\|\mathbf{u}_{r}-\mathbf{u}\right\|_{\mathcal{A}^{\gamma}} \leq \varepsilon\|\mathbf{f}\|_{\mathcal{A}^{-1}}
$$

- Taking into account the discretization error, then $(\gamma=0)$

$$
\left\|u-u_{h, r}\right\|_{L^{2}(\Omega)} \lesssim h^{2 s}+\varepsilon .
$$

- Question: What is a suitable $r_{s}$ ?

[^3]
## BURA

- We choose $r_{s}$ as the best uniform $(m, k)$-approximation to $t^{1-s}$.
- Apply a partial fraction decomposition to $t^{-1} r_{s}(t)$ :

$$
t^{-1} r_{s}(t)=\sum_{j=0}^{m-k-1} b_{j} t^{j}+\frac{c_{0}}{t}+\sum_{j=1}^{p_{1}} \frac{c_{j}}{t-d_{j}}+\sum_{j=1}^{p_{2}} \frac{B_{j} t+C_{j}}{\left(t-F_{j}\right)^{2}+D_{j}^{2}}
$$

where $k=p_{1}+2 p_{2}$.

- To compute $\mathbf{u}_{r}=\mathcal{A}^{-1} r_{s}(\mathcal{A}) \mathbf{f}$ we need to evaluate

$$
\begin{aligned}
\mathcal{A}^{-1} r_{s}(\mathcal{A}) \mathbf{f} & =\sum_{j=0}^{m-k-1} b_{j} \mathcal{A}^{j} \mathbf{f}+c_{0} \mathcal{A}^{-1} \mathbf{f}+\sum_{j=1}^{p_{1}} c_{j}\left(\mathcal{A}-d_{j} \mathcal{I}\right)^{-1} \mathbf{f} \\
& +\sum_{j=1}^{p_{2}}\left(B_{j} \mathcal{A}+C_{j} \mathcal{I}\right)\left(\left(\mathcal{A}-F_{j} \mathcal{I}\right)^{2}+D_{j}^{2} \mathcal{I}\right)^{-1} \mathbf{f}
\end{aligned}
$$

- How do we choose $m$ and $k$ ? This is classical in rational approximation. For the optimal choice we have $m=k$ and

$$
\varepsilon \lesssim 4^{2-s}|\sin \pi(1-s)| e^{-2 \pi \sqrt{(1-s) k}}
$$

so that, for this choice, the error decays exponentially in the polynomial degree.

## Outlook

To solve

$$
(-\Delta)^{s} u=f
$$

with BURA we must:

- Solve $\mathcal{O}(|\log h|)$ problems of the type $\left(-\Delta_{h}+c \mathcal{I}\right) \mathbf{w}=\mathbf{g}$.
- Embarrassingly parallelizable.
- Error estimate

$$
\left\|u-u_{h, r}\right\|_{L^{2}(\Omega)} \lesssim h^{2 s} .
$$

Questions:

- Other norms?
- Other types of problems? Time-dependent? Nonlinear?
- Stability? It is known that rational approximations are very sensitive to numerical rounding.


## Outline

## Motivation: Fractional powers of an operator

## Direct discretization approach

## Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension

## The Balakrishnan formula

- Notice that, for $\lambda>0$ and $\theta \in(0,1)$

$$
\frac{\sin \pi \theta}{\pi} \int_{0}^{\infty} t^{\theta-1}(\lambda+t)^{-1} \mathrm{~d} t=\lambda^{\theta-1}
$$

- Functional calculus then says that, if $X$ is a Hilbert space and $A$ is a self-adjoint and positive operator on $X$ :

$$
A^{\theta}=A A^{\theta-1}=A \frac{\sin \pi \theta}{\pi} \int_{0}^{\infty} t^{\theta-1}(A+t \mathcal{I})^{-1} \mathrm{~d} t
$$

- Let $X=L^{2}(\Omega)$ and $A=-\Delta$, then

$$
\begin{aligned}
(-\Delta)^{-s} & =(-\Delta)^{-1}(-\Delta)^{1-s} \\
& =(-\Delta)^{-1}(-\Delta) \frac{\sin \pi(1-s)}{\pi} \int_{0}^{\infty} t^{1-s-1}(t \mathcal{I}-\Delta)^{-1} \mathrm{~d} t \\
& =\frac{\sin \pi s}{\pi} \int_{0}^{\infty} t^{-s}(t \mathcal{I}-\Delta)^{-1} \mathrm{~d} t
\end{aligned}
$$

where we used the previous formula with $\theta=1-s$.

## Numerical scheme

Using

$$
(-\Delta)^{-s}=\frac{\sin \pi \theta}{\pi} \int_{0}^{\infty} t^{-s}(t \mathcal{I}-\Delta)^{-1} \mathrm{~d} t
$$

we can formulate the following game plan to devise a numerical scheme ${ }^{{ }^{\boldsymbol{e}} \text { : }}$

- Step 1: Use a quadrature for the $t$ variable:

$$
(-\Delta)^{-s} f \approx \frac{\sin \pi s}{\pi} k \sum_{j=0}^{J} t_{j}^{-s}\left(t_{j} \mathcal{I}-\Delta\right)^{-1} f
$$

- Step 2: Use standard finite element methods on the same mesh to approximate

$$
\begin{aligned}
& \quad w_{j} \in H_{0}^{1}(\Omega): \quad t_{j} w_{j}-\Delta w_{j}=f \quad \text { in } \quad \Omega, \\
& \text { i.e., } w_{j}=\left(t_{j} \mathcal{I}-\Delta\right)^{-1} f .
\end{aligned}
$$

- Step 3: Gather all contributions.


## Step 1: Sinc quadrature

- Change of variable: Let $t=e^{y}$ to get

$$
u=(-\Delta)^{-s} f=\frac{\sin (\pi s)}{\pi} \int_{-\infty}^{\infty} e^{(1-s) y}\left(e^{y} I-\Delta\right)^{-1} f \mathrm{~d} y
$$

- Quadrature: Given $N \in \mathbb{N}$, define $k=1 / \sqrt{N}, y_{j}=j k$ and the quadrature approximation

$$
u^{N}=Q^{N} f=\frac{\sin (\pi s)}{\pi} k \sum_{j=-N}^{N} e^{(1-s) y_{j}}\left(e^{y_{j}} I-\Delta\right)^{-1} f
$$

- Exponential convergence: Let $s \in[0,1)$ and $r \in[0,1]$. If $f \in \mathbb{H}^{r}(\Omega)$, then

$$
\left\|u-u^{N}\right\|_{\mathbb{H}^{r}(\Omega)} \lesssim e^{-c \sqrt{N}}\|f\|_{\mathbb{H}^{r}(\Omega)}
$$

## Steps 2 and 3: Finite element approximation and parallelization

- Let $X_{h}$ be a finite element space over $\Omega$, and assume that the mesh is quasiuniform.
- $w_{h}^{j} \in X_{h}$ are the finite element solutions of

$$
\left(e^{y_{j}} \mathcal{I}-\Delta\right) w=f
$$

- These can be solved independently (embarrassingly parallelizable) and then gathered to obtain

$$
u_{h}^{N}=\frac{\sin (\pi s)}{\pi} k \sum_{j=-N}^{N} e^{(1-s) y_{j}} w_{h}^{j}
$$

## Error analysis

For simplicity, assume that $\Omega$ is convex.

- For $r \leq 2 s$ define

$$
\alpha_{\star}=\frac{1}{2}(\alpha+\min \{1-r, \alpha\}), \quad \sigma=\max \left\{2 \alpha_{\star}-2 s, 0\right\}
$$

If $f \in \mathbb{H}^{\sigma}(\Omega)$ then

$$
\left\|u-u_{h}^{N}\right\|_{\mathbb{H}^{r}(\Omega)} \lesssim h^{2 \alpha_{\star}}|\log h|\|f\|_{\mathbb{H}^{\sigma}(\Omega)}
$$

- Setting $r=s$ we get

$$
\left\|u-u_{h}^{N}\right\|_{\mathbb{H}^{s}(\Omega)} \lesssim h^{2-s}\|f\|_{\mathbb{H}^{2-2 s}(\Omega)}
$$

which is "optimal" in order $2-s$ and regularity $f \in \mathbb{H}^{2-2 s}(\Omega)$. However, this requires $u \in \mathbb{H}^{2}(\Omega)$, which is not generic!

## Outlook

To solve

$$
(-\Delta)^{s} u=f
$$

with the Balakrishnan formula we must:

- Solve $\mathcal{O}(|\log h|)$ problems of the type $\left(e^{y} \mathcal{I}-\Delta\right) w=f$.
- Embarrassingly parallelizable.
- Error estimate

$$
\left\|u-u_{h}^{N}\right\|_{\mathbb{H}^{s}(\Omega)} \lesssim h^{2-s}\|f\|_{\mathbb{H}^{2-2 s}(\Omega)},
$$

Questions:

- Other types of problems? Time-dependent? Nonlinear?
- Lower regularity on $f$ ? How can we capture the boundary singularities of $u$ ?


## Outline

## Motivation: Fractional powers of an operator

Direct discretization approach

Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension
The Caffarelli-Silvestre extension
Regularity
Discretization
Tensor Product FEMs
Outlook
$(-\Delta)^{1 / 2}:$ The Dirichlet to Neumann operator I

- Let $u: \mathbb{R}^{n} \rightarrow \mathbb{R}$.
- Extend it harmonically to $\mathbb{R}_{+}^{n+1}$

$$
-\Delta \mathcal{U}=0, \text { in } \mathbb{R}_{+}^{n_{1}}, \quad \mathcal{U}(\cdot, 0)=u
$$

- The Dirichlet to Neumann map is

$$
\text { DtN : } u \mapsto-\partial_{y} \mathcal{U}(\cdot, 0)
$$



## $(-\Delta)^{1 / 2}$ : The Dirichlet to Neumann operator II

The Dirichlet to Neumann map

$$
\text { DtN : } u \mapsto-\partial_{y} \mathcal{U}(\cdot, 0) .
$$

has the following properties:

- $\mathrm{DtN}^{2}=-\Delta$ : Indeed, since $-\Delta_{x^{\prime}, y} \mathcal{U}=-\Delta_{x^{\prime}} \mathcal{U}-\partial_{y}^{2} \mathcal{U}=0$,

$$
\operatorname{DtN}^{2} u=\partial_{y}\left(\partial_{y} \mathcal{U}(\cdot, 0)\right)=-\Delta_{x^{\prime}} \mathcal{U}(\cdot, 0)=-\Delta_{x^{\prime}} u
$$

- DtN is positive: Since $\mathcal{U}$ is harmonic

$$
0=-\int_{\mathbb{R}_{+}^{n+1}} \Delta \mathcal{U} \mathcal{U} \mathrm{~d} x \mathrm{~d} y=\int_{\mathbb{R}_{+}^{n+1}}|\nabla \mathcal{U}|^{2} \mathrm{~d} x \mathrm{~d} y+\int_{\mathbb{R}^{n}} \partial_{y} \mathcal{U} \mathcal{U} \mathrm{~d} x .
$$

On the other hand

$$
\int_{\mathbb{R}^{n}} u \operatorname{DtN} u \mathrm{~d} x=-\int_{\mathbb{R}^{n}} \partial_{y} \mathcal{U} \mathcal{U} \mathrm{~d} x>0 .
$$

Thus, we define

$$
\operatorname{DtN}=\left(-\Delta_{x}\right)^{\frac{1}{2}}, \quad\left(-\Delta_{x}\right)^{\frac{1}{2}} u=\partial_{\nu} \mathcal{U} .
$$

## Outline

## Motivation: Fractional powers of an operator

## Direct discretization approach

## Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension
The Caffarelli-Silvestre extension
Regularity
Discretization
Tensor Product FEMs Outlook

## The $\alpha$-harmonic extension I

The previous extension property can be generalized to any $s \in(0,1)^{\boldsymbol{l}}$


$$
u=\mathcal{U}(\cdot, 0)
$$

- $s \in(0,1)$ and $\alpha=1-2 s \in(-1,1)$.
- $\partial_{\nu^{\alpha}} \mathcal{U}=-\lim _{y \downarrow 0} y^{\alpha} \partial_{y} \mathcal{U}=d_{s} f$ on $\Omega \times\{0\}$.
- $d_{s}=2^{\alpha} \Gamma(1-s) / \Gamma(s)$.


## The $\alpha$-harmonic extension II

Fractional powers of $-\Delta$ can be realized as a generalization of the Dirichlet to Neumann operator:

$$
\left\{\begin{array}{ll}
\partial_{y y}^{2} \mathcal{U}+\frac{\alpha}{y} \partial_{y} \mathcal{U}+\Delta_{x} \mathcal{U}=0 & \text { in } \mathcal{C} \\
\mathcal{U}=0 & \text { on } \partial_{L} \mathcal{C} \\
\partial_{\nu^{\alpha}} \mathcal{U}=d_{s} f & \text { on } \Omega \times\{0\}
\end{array} \Longleftrightarrow(-\Delta)^{s} u=f \text { in } \Omega\right.
$$

$$
u=\mathcal{U}(\cdot, 0)
$$

Here:

- $\mathcal{C}=\Omega \times(0, \infty)$.
- $\alpha=1-2 s \in(-1,1)$.
- $\partial_{\nu} \alpha \mathcal{U}=-\lim _{y \downarrow 0} y^{\alpha} \partial_{y} \mathcal{U}=$ $d_{s} f$.
- $d_{s}=2^{\alpha} \Gamma(1-s) / \Gamma(s)$.



## The $\alpha$-harmonic extension III

Why does this make sense?

- For $\lambda>0$ and $g \in \mathbb{R}$ consider the ODE:

$$
\begin{cases}\psi^{\prime \prime}+\frac{1-2 s}{y} \psi^{\prime}-\lambda \psi=0, & \text { in }(0, \infty), \\ -\lim _{y \downarrow 0} y^{1-2 s} \psi^{\prime}=d_{s}, & \lim _{y \uparrow \infty} \psi(y)=0 .\end{cases}
$$

- This is a Bessel equation with solution

$$
\psi(y)=C_{s} \lambda^{-s}(\sqrt{\lambda} y)^{s} K_{s}(\sqrt{\lambda} y)
$$

where $K_{s}$ is the modified Bessel function of the second kind.

- It is well known that $K_{s}(z)=a z^{-s}+o\left(z^{-s}\right)$, with $a>0$ as $z \downarrow 0$. Thus

$$
\psi(y)=c_{s} \lambda^{-s}(\sqrt{\lambda} y)^{s}\left(a(\sqrt{\lambda} y)^{-s}\right) \rightarrow a c_{s} \lambda^{-s}, \quad y \downarrow 0
$$

- Choosing $C_{s}$ appropriately we get $\psi(0)=\lambda^{-s}$.


## The $\alpha$-harmonic extension IV

- Recall that

$$
f=\sum_{k=1}^{\infty} f_{k} \varphi_{k} \in \mathbb{H}^{-s}(\Omega), \quad(-\Delta)^{s} u=f, \quad \Longrightarrow u=\sum_{k=1}^{\infty} \lambda_{k}^{-s} f_{k} \varphi_{k}
$$

- Applying separation of variables to the extension problem ${ }^{\text {E }}$

$$
u(x)=\sum_{k=1}^{\infty} u_{k} \varphi_{k}(x) \Longrightarrow \mathcal{U}(x, y)=\sum_{k=1}^{\infty} u_{k} \varphi_{k}(x) \psi_{k}(y)
$$

where the functions $\psi_{k}$ solve

$$
\psi_{k}^{\prime \prime}+\frac{\alpha}{y} \psi_{k}^{\prime}=\lambda_{k} \psi_{k}, \text { in }(0, \infty), \quad \psi_{k}(0)=1, \quad \lim _{y \rightarrow \infty} \psi_{k}(y)=0
$$

so that, as before,

$$
\psi_{k}(y)=c_{s}\left(\sqrt{\lambda_{k}} y\right)^{s} K_{s}\left(\sqrt{\lambda_{k}} y\right)
$$

## Weak formulation

- Multiply $\nabla \cdot\left(y^{\alpha} \nabla \mathcal{U}\right)$ by a test function $\phi$ and integrate over the cylinder $\mathcal{C}$ to obtain a possible weak formulation

$$
\int_{\mathcal{C}} y^{\alpha} \nabla \mathcal{U} \cdot \nabla \phi \mathrm{d} x \mathrm{~d} y=d_{s} \int_{\Omega} f \phi(x, 0) \mathrm{d} x, \quad \forall \phi \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right)
$$

- Where the energy space is

$$
\begin{aligned}
L^{2}\left(y^{\alpha}, \mathcal{C}\right) & =\left\{w: \int_{\mathcal{C}}|w|^{2} y^{\alpha} \mathrm{d} x \mathrm{~d} y<\infty\right\} \\
\stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right) & =\left\{w \in L^{2}\left(y^{\alpha}, \mathcal{C}\right): \nabla w \in L^{2}\left(y^{\alpha}, \mathcal{C}\right),\left.w\right|_{\partial_{L} \mathcal{C}}=0\right\}
\end{aligned}
$$



The weight $y^{\alpha}$ is degenerate $(\alpha>0)$ or singular $(\alpha<0)$ !

## Muckenhoupt weights

For every $a, b \in \mathbb{R}$, with $a<b$,

$$
\frac{1}{b-a} \int_{a}^{b}|y|^{\alpha} \mathrm{d} y \cdot \frac{1}{b-a} \int_{a}^{b}|y|^{-\alpha} \mathrm{d} y \lesssim 1
$$

which means $y^{\alpha}$ belongs to the Muckenhoupt class $A_{2}$.
This condition, essentially, means that $y^{\alpha}$ behaves like a constant at every scale!
Since $y^{\alpha} \in A_{2}$ :

- The Hardy-Littlewood maximal operator is continuous on $L^{2}\left(y^{\alpha}, \mathcal{C}\right)$.
- Singular integral operators are continuous on $L^{2}\left(y^{\alpha}, \mathcal{C}\right)$.
- $L^{2}\left(y^{\alpha}, \mathcal{C}\right) \hookrightarrow L_{\text {loc }}^{1}(\mathcal{C})$.
- $H^{1}\left(y^{\alpha}, \mathcal{C}\right)$ is Hilbert and $\mathcal{C}_{b}^{\infty}(\mathcal{C})$ is dense.
- Traces on $\partial_{L} \mathcal{C}$ are well defined.


## Weighted Sobolev spaces

- Weighted Poincaré inequality:

$$
\int_{\mathcal{C}} y^{\alpha}|w|^{2} \mathrm{~d} x \mathrm{~d} y \lesssim \int_{\mathcal{C}} y^{\alpha}|\nabla w|^{2} \mathrm{~d} x \mathrm{~d} y \quad \forall w \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right) .
$$

- Surjective trace operator $\operatorname{tr}_{\Omega}: \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right) \rightarrow \mathbb{H}^{s}(\Omega)$.
- Lax-Milgram $\Rightarrow$ existence and uniqueness for every $f \in \mathbb{H}^{-s}(\Omega)$. Also

$$
\|\mathcal{U}\|_{H_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right)}^{2}=\|u\|_{\mathbb{H}^{s}(\Omega)}^{2}=d_{s}\|f\|_{\mathbb{H}^{-s}(\Omega)}^{2} .
$$

We will discretize the $\alpha$-harmonic extension!

$$
\mathcal{U} \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right): \quad \begin{cases}\nabla \cdot\left(y^{\alpha} \nabla \mathcal{U}\right)=0 & \text { in } \mathcal{C} \\ \mathcal{U}=0 & \text { on } \partial_{L} \mathcal{C} \\ \partial_{\nu^{\alpha}} \mathcal{U}=d_{s} f & \text { on } \Omega \times\{0\}\end{cases}
$$

## Advantages and disadvantages

Advantages:

- Implementation requires standard numerical PDE components.
- It is very flexible as we will see later.

Disadvantages:

- One extra dimension! We have efficient solvers, and we will see later how to minimize the effect of $y$.
- Singular/degenerate weight $y^{\alpha}$ ? The weight $y^{\alpha} \in A_{2}$ for which there is a very well developed theory.


## Outline

> Motivation: Fractional powers of an operator

> Direct discretization approach

> Best uniform rational approximation

> The Balakrishnan formula

The Caffarelli-Silvestre extension
The Caffarelli-Silvestre extension
Regularity
Discretization
Tensor Product FEMs
Outlook

## Solution representation

- Recall that we found, via separation of variables

$$
u(x)=\sum_{k=1}^{\infty} \lambda_{k}^{-s} f_{k} \varphi_{k}(x) \Longrightarrow \mathcal{U}(x, y)=\sum_{k=1}^{\infty} \lambda_{k}^{-s} f_{k} \varphi_{k}(x) \psi_{k}(y),
$$

- The pairs $\left\{\lambda_{k}, \varphi_{k}\right\}_{k=1}^{\infty}$ are the eigenpairs of the Laplacian.
- The $\psi_{k}$ are

$$
\psi_{k}(y)=c_{s}\left(\sqrt{\lambda_{k}} y\right)^{s} K_{s}\left(\sqrt{\lambda_{k}} y\right)
$$

where $K_{s}$ is the modified Bessel function of the second kind.

- The function $\psi_{k}$ satisfies, as $y \rightarrow \infty$,

$$
\psi_{k}(y) \approx\left(\sqrt{\lambda_{k}} y\right)^{s-1 / 2} e^{-\sqrt{\lambda_{k}} y}
$$

- The function $\psi_{k}$ satisfies, as $y \rightarrow 0$,

$$
\psi_{k}^{\prime}(y) \approx y^{-\alpha}, \quad \psi_{k}^{\prime \prime}(y) \approx y^{-\alpha-1}
$$

## Global Sobolev Regularity

- Compatible data: Let $f \in \mathbb{H}^{1-s}(\Omega)$, which means that $f$ has a vanishing trace for $s<\frac{1}{2}$.
- Space regularity:

$$
\left\|\Delta_{x} \mathcal{U}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)}^{2}+\left\|\partial_{y} \nabla_{x} \mathcal{U}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)}^{2}=d_{s}\|f\|_{\mathbb{H}^{1-s}(\Omega)}^{2}
$$

- Regularity in extended variable $y$ : If $s \neq \frac{1}{2}$ and $\beta>2 \alpha+1$ then

$$
\left\|\partial_{y y} \mathcal{U}\right\|_{L^{2}\left(y^{\beta}, \mathcal{C}\right)} \lesssim\|f\|_{L^{2}(\Omega)} .
$$

If $s=\frac{1}{2}$, then

$$
\|\mathcal{U}\|_{H^{2}(\mathcal{C})} \lesssim\|f\|_{\mathbb{H}^{1 / 2}(\Omega)}
$$

- Elliptic pick-up regularity: If $\Omega$ convex, then

$$
\|w\|_{H^{2}(\Omega)} \lesssim\left\|\Delta_{x} w\right\|_{L^{2}(\Omega)} \quad \forall w \in H^{2}(\Omega) \cap H_{0}^{1}(\Omega)
$$

Under this assumption, we further have

$$
\left\|D_{x}^{2} \mathcal{U}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} \lesssim\|f\|_{\mathbb{H}^{1-s}(\Omega)}
$$

## Analytic Regularity

- Behavior of $\psi(z)=c_{s} z^{s} K_{s}(z)$ near $z=0$ :

$$
\left|\frac{\mathrm{d}^{\ell}}{\mathrm{d} z^{\ell}} \psi(z)\right| \leq C d_{s} \ell!z^{2 s-\ell}
$$

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

- Behavior of $\psi(z)$ for $z$ large:

$$
\left|\frac{\mathrm{d}^{\ell}}{\mathrm{d} z^{\ell}} \psi(z)\right| \leq C_{\epsilon, s} \ell!\epsilon^{-\ell} z^{s-\ell-\frac{1}{2}} e^{-(1-\epsilon) z}
$$

- Global regularity of $\mathcal{U}$ : If $0 \leq \tilde{\nu}<s$ and $0 \leq \nu<1+s$, then there exists $\kappa>1$ such that

$$
\begin{aligned}
\left\|\partial_{y}^{\ell+1} \mathcal{U}\right\|_{L^{2}\left(\omega_{\alpha+2 \ell-2 \tilde{\nu}, \gamma}, \mathcal{C}\right)} & \lesssim \kappa^{\ell+1}(\ell+1)!\|f\|_{\mathbb{H}^{-s+\tilde{\nu}}(\Omega)}, \\
\left\|\nabla_{x} \partial_{y}^{\ell+1} \mathcal{U}\right\|_{L^{2}\left(\omega_{\alpha+2(\ell+1)-2 \nu, \gamma}, \mathcal{C}\right)} & \lesssim \kappa^{\ell+1}(\ell+1)!\|f\|_{\mathbb{H}^{-s+\nu}(\Omega)} \\
\left\|\Delta_{x} \partial_{y}^{\ell+1} \mathcal{U}\right\|_{L^{2}\left(\omega_{\alpha+2(\ell+1)-2 \nu, \gamma}, \mathcal{C}\right)} & \lesssim \kappa^{\ell+1}(\ell+1)!\|f\|_{\mathbb{H}^{1-s+\nu}(\Omega)},
\end{aligned}
$$

with weight $\omega_{\beta, \gamma}(y)=y^{\beta} e^{\gamma y}, 0 \leq \gamma<2 \sqrt{\lambda_{1}}$.

## Outline

## Motivation: Fractional powers of an operator

## Direct discretization approach

## Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension
The Caffarelli-Silvestre extension
Regularity
Discretization
Tensor Product FEMs
Outlook

## Domain truncation

The domain $\mathcal{C}$ is infinite. We need to consider a truncated problem.
Theorem (exponential decay)
For every $\mathcal{y}>0$

$$
\|\mathcal{U}\|_{\dot{H}_{L}^{1}\left(y^{\alpha}, \Omega \times(y, \infty)\right)} \lesssim e^{-\sqrt{\lambda_{1}} y / 2}\|f\|_{\mathbb{H}-s(\Omega)}
$$

Let $v$ solve

$$
\begin{cases}\nabla \cdot\left(y^{\alpha} \nabla v\right)=0 & \text { in } \mathcal{C}_{y}=\Omega \times(0, \mathscr{y}), \\ v=0 & \text { on } \partial_{L} \mathcal{C}_{y} \cup \Omega \times\{\mathscr{y}\}, \\ \partial_{\nu^{\alpha}} v=d_{s} f & \text { on } \Omega \times\{0\}\end{cases}
$$

Theorem (exponential convergence)
For all $y>0$,

$$
\|\mathcal{U}-v\|_{\stackrel{H}{L}_{1}^{L}\left(y^{\alpha}, \mathcal{C}_{y}\right)} \lesssim e^{-\sqrt{\lambda_{1}} y / 4}\|f\|_{\mathbb{H}^{-s}(\Omega)} .
$$

## Finite element method I: Mesh

Let $\mathscr{T}_{\Omega}=\{K\}$ be triangulation of $\Omega$ (simplices or cubes)

- $\mathscr{T}_{\Omega}$ is conforming and shape regular.

Let $\mathscr{T}_{y}=\{T\}$ be a triangulation of $\mathcal{C}_{y}$ into cells of the form

$$
T=K \times I, \quad K \in \mathscr{T}_{\Omega}, \quad I=(a, b) .
$$

$\mathcal{U}_{y y} \approx y^{-\alpha-1}$ as $y \approx 0+$ so we consider anisotropic elements


Shape regularity condition does NOT hold!

## Finite element method II: Spaces

We only require that if $T=K \times I$ and $T^{\prime}=K^{\prime} \times I^{\prime}$ are neighbors

$$
\frac{|I|}{\left|I^{\prime}\right|} \approx 1,
$$

This weak condition allows us to consider anisotropic meshes Define

$$
\mathbb{V}\left(\mathscr{T}_{y}\right)=\left\{W \in \mathcal{C}^{0}\left(\overline{\mathcal{C}}_{y}\right): W_{\mid T} \in \mathcal{P}_{1}(K) \otimes \mathbb{P}_{1}(I), W_{\mid \Gamma_{D}}=0\right\}
$$

with $\Gamma_{D}=\partial_{L} \mathcal{C} \cup \Omega \times\{\mathscr{Y}\}$, and

$$
\mathbb{U}\left(\mathscr{T}_{\Omega}\right)=\operatorname{tr}_{\Omega} \mathbb{V}\left(\mathscr{T}_{Y}\right)=\left\{W \in \mathcal{C}^{0}(\bar{\Omega}): W_{\mid K} \in \mathcal{P}_{1}(K), W_{\mid \partial \Omega}=0\right\}
$$

Here $\mathcal{P}_{1}=\mathbb{P}_{1}$ if $K$ is a simplex and $\mathcal{P}_{1}=\mathbb{Q}_{1}$ if is a "brick".

## Finite element method III: Discrete problem

- Galerkin method for the extension: Find $V_{\mathscr{T}_{y}} \in \mathbb{V}\left(\mathscr{T}_{Y}\right)$ such that

$$
\int_{\mathcal{C}_{y}} y^{\alpha} \nabla V_{\mathscr{T}_{y}} \nabla W \mathrm{~d} x \mathrm{~d} y=d_{s} \int_{\Omega} f W(x, 0) \mathrm{d} x, \quad \forall W \in \mathbb{V}\left(\mathscr{T}_{y}\right) .
$$

- Define

$$
U_{\mathscr{T}_{\Omega}}=V_{\mathscr{T}_{r}}(\cdot, 0) \in \mathbb{U}\left(\mathscr{T}_{\Omega}\right) .
$$

- A trace estimate and Cèa's Lemma imply quasi-best approximation:

$$
\left\|u-U_{\mathscr{T}_{\Omega}}\right\|_{\mathbb{H}^{s}(\Omega)} \lesssim\left\|v-V_{\mathscr{Y}_{y}}\right\|_{\stackrel{\circ}{L}_{1}^{L}\left(y^{\alpha}, \mathcal{C}_{y}\right)}=\inf _{W \in \mathbb{V}\left(\mathscr{F}_{Y}\right)}\|v-W\|_{\stackrel{\circ}{L}_{1}^{1}\left(y^{\alpha}, \mathcal{C}_{Y}\right)}
$$

We reduced the error analysis to a question of approximation theory in weighted spaces. Usually we set $W=\Pi v \in \mathbb{V}\left(\mathscr{T}_{y}\right)$ where $\Pi$ is a suitable interpolation operator.

## The quasi-interpolation operator

We introduce an averaged interpolation operator $\Pi^{\boldsymbol{\theta}}$

$$
\Pi \phi(z)=Q_{z}^{m} \phi(z) .
$$

where $Q_{z}^{m} \phi$ is an averaged Taylor polynomial of $\phi$ of degree $m$. Notice that:

- This is defined for all polynomial degree $m$ and any element shape (simplices or rectangles).
- We do not go back to the reference element - This is important for anisotropic estimates.
If the mesh is rectangular and Cartesian If $R$ and $S$ are neighbors

$$
h_{R}^{i} / h_{S}^{i} \lesssim 1, \quad i=\overline{1, N}
$$



[^4]
## Error estimates on rectangles ${ }^{\text {E }}$

Theorem

$$
\begin{aligned}
& \text { If } \varpi \in A_{p}\left(\mathbb{R}^{N}\right) \text {, and } \phi \in W_{p}^{1}\left(\varpi, S_{R}\right) \\
& \qquad\|\phi-\Pi \phi\|_{L^{p}(\varpi, R)} \lesssim \sum_{i=1}^{N} h_{R}^{i}\left\|\partial_{i} \phi\right\|_{L^{p}\left(\varpi, S_{R}\right)} .
\end{aligned}
$$

If $\phi \in W_{p}^{2}\left(\varpi, S_{R}\right)$

$$
\begin{aligned}
\left\|\partial_{j}(\phi-\Pi \phi)\right\|_{L^{p}(\varpi, R)} & \lesssim \sum_{i=1}^{N} h_{R}^{i}\left\|\partial_{i} \partial_{j} \phi\right\|_{L^{p}\left(\varpi, S_{R}\right)}, \\
\|\phi-\Pi \phi\|_{L^{p}(\varpi, R)} & \lesssim \sum_{i, j=1}^{N} h_{R}^{i} h_{R}^{j}\left\|\partial_{i} \partial_{j} \phi\right\|_{L^{p}\left(\varpi, S_{R}\right)}
\end{aligned}
$$

- Directional estimates: note the products of the form $h_{R}^{i} h_{R}^{j}\left\|\partial_{i} \partial_{j} \phi\right\|_{L^{p}\left(\varpi, S_{R}\right)}$.
- Estimates on simplicial elements, different metrics and applications.


## Error estimates. Quasiuniform meshes

On quasiuniform meshes $h_{T} \approx h_{K} \approx h_{I}$ for all $T \in \mathscr{T}_{y}$, then
Theorem (error estimates)
The following estimate holds for all $\epsilon>0$

$$
\begin{aligned}
\left\|\nabla\left(v-V_{\mathscr{T}_{Y}}\right)\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}_{y}\right)} & \lesssim h_{K}\left\|\partial_{y} \nabla_{x^{\prime}} v\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)}+h_{I}^{s-\epsilon}\left\|\partial_{y y} v\right\|_{L^{2}\left(y^{\beta}, \mathcal{C}\right)} \\
& \lesssim h^{s-\epsilon}\|f\|_{\mathbb{H}^{1-s}(\Omega)} .
\end{aligned}
$$

Consequently,

$$
\left\|u-U_{\mathscr{T}_{\Omega}}\right\|_{\mathbb{H}^{s}(\Omega)} \lesssim h^{s-\epsilon}\|f\|_{\mathbb{H}^{1-s}(\Omega)} .
$$

- This is suboptimal in terms of order (only order $s-\epsilon$ )
- Is it sharp?


## Numerical experiment. Quasiuniform mesh

Let $\Omega=(0,1)$ and $f=\pi^{2 s} \sin (\pi x)$, then

$$
\mathcal{U}=\frac{2^{1-s} \pi^{s}}{\Gamma(s)} \sin (\pi x) y^{s} K_{s}(\pi y)
$$

If $s=0.2$, then


The energy error behaves like $D O F S^{-0.1} \approx h^{0.2}$, as predicted!

## Error estimates. Graded meshes

We use the principle of error equilibration. We use a graded mesh on $(0, y)$

$$
y_{j}=\mathcal{Y}\left(\frac{j}{M}\right)^{\gamma}, \quad j=\overline{0, M}, \quad \gamma>1
$$

$\mathcal{U}_{y y} \approx y^{-\alpha-1} \Longrightarrow$ energy equidistribution for $\gamma>3 /(1-\alpha)$.
Theorem (error estimates ${ }^{\left[{ }^{\boldsymbol{U}}\right.}$ )
If $f \in \mathbb{H}^{1-s}(\Omega)$ and $\mathcal{Y} \approx\left|\log \# \mathscr{T}_{y}\right|$,
$\left\|u-U_{\mathscr{T}_{\Omega}}\right\|_{\mathbb{H}^{s}(\Omega)}=\left\|\nabla\left(\mathcal{U}-V_{\mathscr{T}_{y}}\right)\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} \lesssim\left|\log \# \mathscr{T}_{Y}\right|^{s} \# \mathscr{T}_{9}^{-\frac{1}{n+1}}\|f\|_{\mathbb{H}^{1-s}(\Omega)}$,
or equivalently

$$
\left\|u-U_{\mathscr{T}_{\Omega}}\right\|_{\mathbb{H}^{s}(\Omega)} \lesssim\left|\log \mathscr{T}_{\Omega}\right|^{s} \mathscr{T}_{\Omega}^{-1 / n}\|u\|_{\mathbb{H}^{1+s}(\Omega)}
$$

- This is near optimal in terms of regularity of $u \in \mathbb{H}^{1+s}(\Omega)$ and almost linear decay rate in $h$.
- This is suboptimal in terms of total number of degrees of freedom $\# \mathscr{T}_{y} \approx \# \mathscr{T}_{\Omega}^{1+\frac{1}{n}} \gg \# \mathscr{T}_{\Omega}$ with respect to the degrees of freedom in

[^5]
## Numerical experiment

Experimental rates for circle and $s=0.3$ and $s=0.7$.
Set $\Omega=D(0,1) \subset \mathbb{R}^{2}, f=j_{1,1}^{2 s} J_{1}\left(j_{1,1} r\right)\left(A_{1,1} \cos (\theta)+B_{1,1} \sin (\theta)\right)$. With graded meshes:


The experimental convergence rate $-1 / 3$ is optimal!

## Outline

> Motivation: Fractional powers of an operator

> Direct discretization approach

> Best uniform rational approximation

> The Balakrishnan formula

The Caffarelli-Silvestre extension
The Caffarelli-Silvestre extension
Regularity
Discretization
Tensor Product FEMs
Outlook

## Diagonalization I

- Discretization in $y$ : Let $\mathcal{G}^{M}$ be an arbitrary mesh in $(0, \mathcal{Y})$ with $M=\# \mathcal{G}^{M}$ and let $S^{\mathbf{r}}\left(0, \mathcal{Y} ; \mathcal{G}^{M}\right)$ be a FE space of polynomial degree $\mathbf{r}$ in $y$.
- Define

$$
\mathbb{V}_{M}^{\mathrm{r}}\left(\mathcal{C}_{y}\right)=H_{0}^{1}(\Omega) \otimes S^{\mathbf{r}}\left(0, \mathscr{\mathscr { C }} ; \mathcal{G}^{M}\right)
$$

FE in $y$, continuous in $x$.

- Semidiscrete solution: $\mathcal{U}_{M} \in \mathbb{V}_{M}^{\mathbf{r}}\left(\mathcal{C}_{y}\right)$ satisfies

$$
\int_{\mathcal{C}_{y}} y^{\alpha} \nabla \mathcal{U}_{M} \nabla \phi \mathrm{~d} x \mathrm{~d} y=d_{s} \int_{\Omega} f \phi(x, 0) \mathrm{d} x \quad \forall \phi \in \mathbb{V}_{M}^{\mathrm{r}}\left(\mathcal{C}_{y}\right) .
$$

- Exponential convergence: Let $f \in \mathbb{H}^{-s+\nu}(\Omega)$ for $0<\nu<s$. If $\mathcal{Y} \approx M$, the mesh $\mathcal{G}^{M}$ is geometric towards $y=0$, and the polynomial degree $\mathbf{r}$ grows linearly from $y=0$, then there exists $b>0$ such that

$$
\left\|\nabla\left(\mathcal{U}-\mathcal{U}_{M}\right)\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} \lesssim e^{-b M}\|f\|_{\mathbb{H}^{-s+\nu}(\Omega)}
$$

## Diagonalization II

- Eigenvalue problem: Let $\mathcal{M}=\operatorname{dim} S^{\mathbf{r}}\left(0, \mathscr{\mathscr { F }} ; \mathcal{G}^{M}\right)$ and $\left(\mu_{i}, v_{i}\right)_{i=1}^{\mathcal{M}}$ be the (normalized) eigenpairs of

$$
\mu \int_{0}^{\mathscr{y}} y^{\alpha} v^{\prime}(y) w^{\prime}(y) \mathrm{d} y=\int_{0}^{y} y^{\alpha} v(y) w(y) \mathrm{d} y \quad \forall w \in S^{\mathbf{r}}\left(0, \mathscr{Y} ; \mathcal{G}^{M}\right)
$$

- Representation: If $\mathcal{U}_{M}(x, y)=\sum_{j=1}^{\mathcal{M}} U_{j}(x) v_{j}(y)$ with $U_{j} \in H_{0}^{1}(\Omega)$, then

$$
a_{\mu_{i}, \Omega}\left(U_{i}, V\right)=d_{s} v_{i}(0) \int_{\Omega} f V \mathrm{~d} x \quad \forall V \in H_{0}^{1}(\Omega)
$$

where $a_{\mu_{i}, \Omega}$ are the singularly perturbed bilinear forms

$$
a_{\mu_{i}, \Omega}(U, V):=\int_{\Omega}\left(\mu_{i} \nabla_{x} U \nabla_{x} V \mathrm{~d} x+U V\right) \mathrm{d} x
$$

## Tensor product discretization

- Ritz projections: $\Pi_{i} u \in S_{0}^{q}\left(\mathscr{T}_{\Omega}\right)$ satisfies

$$
a_{\mu_{i}, \Omega}\left(u-\Pi_{i} u, v\right)=0 \quad \forall v \in S_{0}^{q}\left(\mathscr{T}_{\Omega}\right),
$$

where $S_{0}^{q}\left(\mathscr{T}_{\Omega}\right) \subset H_{0}^{1}(\Omega)$ is the FE space of piecewise polynomials of degree $\leq q$ over $\mathscr{T}_{\Omega}$.

- Discrete solution: Let $U_{h, M} \in S_{0}^{q}\left(\mathscr{T}_{\Omega}\right) \otimes S^{\mathbf{r}}\left(0, \mathscr{\mathscr { G }} ; \mathcal{G}^{M}\right)$ satisfy

$$
\int_{\mathcal{C}_{y}} y^{\alpha} \nabla U_{h, M} \nabla V \mathrm{~d} x \mathrm{~d} y=d_{s} \int_{\Omega} f V(x, 0) \mathrm{d} x, \forall V \in S_{0}^{q}\left(\mathscr{T}_{\Omega}\right) \otimes S^{\mathbf{r}}\left(0, \mathscr{Y} ; \mathcal{G}^{M}\right)
$$

and note that it can be represented as follows

$$
U_{h, M}(x, y)=\sum_{i=1}^{\mathcal{M}} \Pi_{i} U_{i}(x) v_{i}(y)
$$

- Parallelization: This corresponds to solving $\mathcal{M}$ decoupled elliptic problems with the singularly perturbed bilinear form $a_{\mu_{i}, \Omega}$ for $i=1, \ldots, \mathcal{M}$.


## Tensor $\mathbb{P}_{1}$-FEM

- Assume that $f \in L^{2}(\Omega)$ where $\Omega \subset \mathbb{R}^{2}$ is a polygon with corners $\mathbf{c}$.
- The solution to

$$
\begin{gathered}
-\Delta_{x} w=f, \text { in } \Omega \quad w=0, \text { on } \partial \Omega \Longrightarrow \\
\|w\|_{H_{\beta}^{2}(\Omega)} \lesssim\|f\|_{L^{2}(\Omega)}, \quad|w|_{H_{\beta}^{2}(\Omega)}^{2}=\int_{\Omega} \prod_{\mathbf{c}}\left|x^{\prime}-\mathbf{c}\right|^{2 \beta}\left|D^{2} w\right|^{2} \mathrm{~d} x .
\end{gathered}
$$

- This type of singularity can be captured by using a graded mesh in $\Omega$ : Let $\mathscr{T}_{\Omega}$ be graded towards the re-entrant corners so that, if $N=\# \mathscr{T}_{\Omega}$ and $h=N^{-1 / 2}$, for any $w \in S_{0}^{1}\left(\mathscr{T}_{\Omega}\right)$

$$
N\|w-\Pi w\|_{L^{2}(\Omega)}^{2} \lesssim\|w\|_{H^{1}(\Omega)}^{2}, \quad N^{2}\|w-\Pi w\|_{L^{2}(\Omega)}^{2} \lesssim\|w\|_{H_{\beta}^{2}(\Omega)}^{2} .
$$

- With this construction we obtain that, if $\mathcal{G}_{\eta}^{M}$ is a suitably graded radical mesh $\left\{y_{i}=\left(\frac{i}{M}\right)^{\eta} \mathscr{Y}\right\}_{i=0}^{M}$, with $\eta s>1$ and $M \approx N^{\frac{1}{2}}=\left(\# \mathscr{T}_{\Omega}\right)^{\frac{1}{2}}$, the discrete solution $U_{h, M}$ satisfies

$$
\left\|u-\operatorname{tr}_{\Omega} U_{h, M}\right\|_{\mathbb{H}^{s}(\Omega)} \leq h\|f\|_{\mathbb{H}^{1-s}(\Omega)}
$$

and

$$
\operatorname{dim} \mathbb{V}_{h, M}^{1,1}\left(\mathscr{T}_{\Omega}, \mathcal{G}^{M}\right) \approx h^{-3} \log |\log h| \approx N_{\Omega}^{1+\frac{1}{2}} \log \log N_{\Omega}
$$

## Sparse grid FEM

- Complexity of tensor product: $N_{\Omega}^{1+\frac{1}{2}}$ is suboptimal.
- To overcome this we use a sparse grid space. Let

$$
\mathbb{V}_{L}^{1,1}\left(\mathcal{C}_{y}\right)=\sum_{\ell, \ell^{\prime} \geq 0, \ell+\ell^{\prime} \leq L} S_{0}^{1}\left(\mathscr{T}_{\Omega}^{\ell}\right) \otimes S^{1}\left(0, \mathscr{Y} ; \mathcal{G}_{\eta}^{2^{\ell^{\prime}}}\right)
$$

where $\mathscr{T}_{\Omega}^{\ell}$ and $\mathcal{G}_{\eta}^{2^{\ell^{\prime}}}$ are nested meshes of levels $\ell$ and $\ell^{\prime}$ graded towards corners $\mathbf{c}$ of $\Omega$ and $y=0$, respectively.

- We have the error estimate: Let $1<\nu<1+s, \eta(\nu-1) \geq 1$, and $y \approx\left|\log h_{L}\right|$. If $f \in \mathbb{H}^{-s+\nu}(\Omega)$, then $\mathcal{U}_{L} \in \mathbb{V}_{L}^{1,1}\left(\mathcal{C}_{y}\right)$ satisfies

$$
\begin{aligned}
\left\|\mathcal{U}-\mathcal{U}_{L}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} & \lesssim h_{L}\left|\log h_{L}\right|\|f\|_{\mathbb{H}^{-s+\nu}(\Omega)} \\
\operatorname{dim} \mathbb{V}_{L}^{1,1}\left(\mathcal{C}_{y}\right) & \lesssim N_{\Omega} \log \log N_{\Omega}
\end{aligned}
$$

- The complexity of sparse grids is quasi-optimal in terms of $N_{\Omega}$.


## $h p$-FEM in $y$ and $\mathbb{P}_{1}$-FEM in $\Omega$

- Graded geometric mesh: Let $\mathcal{G}_{\sigma}^{M}=\left\{\mathcal{V} \sigma^{M-i}\right\}_{i=1}^{M}$ with $\sigma<1$.
- Data regularity: $f \in \mathbb{H}^{1-s}(\Omega)$ and $\Omega \subset \mathbb{R}^{2}$ is a polygon with corners c.
- FE space: $\mathbb{V}_{h, M}^{1, \mathbf{r}}\left(\mathscr{T}_{\Omega}, \mathcal{G}_{\sigma}^{M}\right)$ is the space of piecewise polynomials of degree one over $\mathscr{T}_{\Omega}$ and piecewise polynomials of degree $\mathbf{r}$ growing linearly from 1 over $\mathcal{G}_{\sigma}^{M}$.
- Error estimates: Let $\mathscr{T}_{\Omega}$ be a suitably graded mesh towards the re-entrant corners $\mathbf{c}$. If $\mathscr{y} \approx|\log h|$ and $U_{h, M} \in \mathbb{V}_{h, M}^{1, \mathbf{r}}\left(\mathscr{T}_{\Omega}, \mathcal{G}_{\sigma}^{M}\right)$ is the Galerkin solution, then

$$
\begin{aligned}
\left\|\nabla\left(\mathcal{U}-U_{h, M}\right)\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} & \lesssim h\|f\|_{\mathbb{H}^{1-s}(\Omega)} \\
\operatorname{dim} \mathbb{V}_{h, M}^{1, \mathbf{r}}\left(\mathscr{T}_{\Omega}, \mathcal{G}_{\sigma}^{M}\right) & \approx h^{-2}|\log h|^{2} \approx N_{\Omega}\left|\log N_{\Omega}\right|
\end{aligned}
$$

- Complexity: This is quasi-optimal in terms of $N_{\Omega}$.


## $h p-F E M$ in $y$ and $\Omega$

- Data regularity: The domain $\Omega \subset \mathbb{R}^{2}$ and $f$ are analytic.
- Graded mesh in $\Omega$ : The mesh $\mathscr{T}_{\Omega}$ is anisotropic and graded towards $\partial \Omega$ so that it resolves the smallest scale $\mu_{\mathcal{M}}$ of the singularly perturbed problems originating from the diagonalization.
- Graded mesh in $y$ : Let $\mathcal{G}_{\sigma}^{M}=\left\{\mathscr{g} \sigma^{M-i}\right\}_{i=1}^{M}$ with $\sigma<1$.
- Error estimate: If $\mathcal{y} \approx M, \mathbf{r}$ grows linearly from $y=0$, then the Galerkin solution $U_{h, M} \in S_{0}^{q}\left(\mathscr{T}_{\Omega}\right) \otimes S^{\mathbf{r}}\left(\mathcal{G}_{\sigma}^{M}\right)$ and the total number $N_{\Omega, y}$ of degrees of freedom satisfy

$$
\begin{aligned}
\left\|\nabla\left(\mathcal{U}-U_{h, M}\right)\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} & \lesssim M^{2} e^{-b q}+e^{-b M} \\
N_{\Omega, y} & \approx q^{2} M^{3} .
\end{aligned}
$$

- Exponential rate of convergence: If $q \approx M$, then

$$
\left\|\nabla\left(\mathcal{U}-U_{h, M}\right)\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)} \lesssim e^{-b^{\prime} N_{\Omega, \gamma^{\prime}}^{1 / 5}} .
$$

## Numerical experiment. Performance of tensor FEMs

- Data: $\Omega$ L-shaped domain in $\mathbb{R}^{2} ; f=1 ; s=3 / 4$.
- Error: It is always measured in the energy space $\mathbb{H}^{s}(\Omega)$.

- Conclusions: Both sparse grid FEM and $h p$-FEM reduced substantially the DOFs relative to tensor FEM and deliver quasi-optimal complexity.


## Outline

## Motivation: Fractional powers of an operator

## Direct discretization approach

## Best uniform rational approximation

The Balakrishnan formula

The Caffarelli-Silvestre extension
The Caffarelli-Silvestre extension
Regularity
Discretization
Tensor Product FEMs
Outlook

## Outlook I

- PDE approach. The extension converts the nonlocal problem into a local PDE problem in one higher dimension. This is very flexible:
- Parabolic problems ${ }^{\text {E }}$ Details
- Stationary ${ }^{\boldsymbol{\theta}}$ Details and time dependent ${ }^{\text {星 }}$ Details obstacle problems.
- We have a complete and quasi-optimal a priori error analysis over anisotropic meshes. The complexity, in terms of total degrees of freedom, is:
- $\mathbb{P}_{1}-\mathbb{P}_{1}$-elements: suboptimal complexity and linear rate for $\Omega$ convex and compatible data. Extension to non-convex domains.
- Sparse tensor $\mathbb{P}_{1}-\mathbb{P}_{1}$-elements: quasi-optimal complexity and linear rate for $\Omega$ polygonal with compatible data.
- hp-elements: quasi-optimal complexity and exponential rate for analytic but incompatible data.
- We also have multigrid methods ${ }^{\text {D }}$ Details , a posteriori error estimators Details

[^6]
## Outlook II

Questions:

- Adaptivity: Convergence and optimality is still open (issue is anisotropic meshes and lack of shape regularity).
- 3d-computations: A virtual implementation of extended variable is open.
- Theory and implementation of $3 d h p$-FEM are open.


## Outline

A posteriori error analysis Motivation
A fundamental difficulty
Anisotropic error estimation

## Multilevel methods

Time dependent problems

Elliptic obstacle problem

Parabolic obstacle problem

## Outline

A posteriori error analysis Motivation
A fundamental difficulty
Anisotropic error estimation

## Multilevel methods

## Time dependent problems

Elliptic obstacle problem

Parabolic obstacle problem

## Adaptivity

Adaptivity is motivated by:

- Computational efficiency: extra $n+1$-dimension.
- The a priori theory requires:
- Regularity of the datum: $f \in \mathbb{H}^{1-s}(\Omega)$.
- Regularity of the domain: $\Omega$ is $C^{1,1}$ or a convex polygon.
- If one of these conditions is violated, the solution $\mathcal{U}$ may have singularities in $\Omega$ which lead to fractional regularity.
- Quasiuniform refinement of $\Omega$ would not result in an efficient solution technique.
- We need anisotropic a posteriori error estimators.


## Adaptive Loop

We consider an almost standard adaptive loop:

$$
\text { SOLVE } \rightarrow \text { ESTIMATE } \rightarrow \text { MARK } \rightarrow \text { REFINE }
$$

except for the statements in red below:

- SOLVE: Finds the Galerkin solution $V_{\mathscr{T}_{r}}$.
- ESTIMATE: Computes a star-indicator $\mathcal{E}_{z^{\prime}}$ for every node $z^{\prime} \in \Omega$.
- MARK: For $\theta \in(0,1)$ choose a minimal subset of nodes $\mathcal{M}$ :

$$
\mathcal{E}_{\mathcal{M}}^{2}=\sum_{z^{\prime} \in \mathcal{M}} \mathcal{E}_{z^{\prime}}^{2} \geq \theta^{2} \mathcal{E}_{\mathscr{T}}^{2}
$$

- REFINE: Given a set of marked nodes $\mathcal{M}$
- Refine the cells $K \ni z^{\prime}$ for all $z^{\prime} \in \mathcal{M}$ to get $\widetilde{\mathscr{T}_{\Omega}}$.
- Create an anisotropic mesh $\left\{y_{j}\right\}_{j=1}^{M}$ so that grading $y_{j}=\mathcal{Y}\left(\frac{j}{M}\right)^{\gamma}$ holds.
- The refined mesh is $\widetilde{\mathscr{T}_{y}}=\widetilde{\mathscr{T}_{\Omega}} \times\{\widetilde{I}\}$ with $\widetilde{I}=\left[y_{j-1}, y_{j}\right]$.


## Outline

A posteriori error analysis

## Motivation

A fundamental difficulty
Anisotropic error estimation

Multilevel methods

Time dependent problems

Elliptic obstacle problem

Parabolic obstacle problem

## Isotropic a posteriori error indicators

- Residual error indicator: If we were to integrate by parts the discrete problem over an element $T \in \mathscr{T}_{9}$, we would get

$$
\int_{T} y^{\alpha} \nabla V \nabla W=\int_{\partial T} y^{\alpha} W \nabla V \cdot \boldsymbol{\nu}-\int_{T} \nabla \cdot\left(y^{\alpha} \nabla V\right) W
$$

Since $\alpha \in(-1,1)$, the boundary integral is meaningless for $y=0$.

- Alternative error indicators: Residual indicators are not the only possibility:
- Local problems on stars: $\quad \mathcal{E}_{z}^{2}=\int_{S_{z}} y^{\alpha}|\nabla Z|^{2} \quad(Z$ solution of a BVP in $S_{z}$ ).
- Zienkiewicz-Zhu estimators.
- Hypercircle estimators.
- Local problems on stars: We prove for all nodes $z \in \mathcal{N}$

$$
\mathcal{E}_{z}^{2} \lesssim\|\nabla(v-V)\|_{L^{2}\left(y^{\alpha}, S_{z}\right)}^{2} \lesssim \mathcal{E}_{z}^{2}+\operatorname{osc}\left(y^{\alpha}, V, f, S_{z}\right)^{2}
$$

## Numerical Experiment with Isotropic Refinement

- Set $\mathcal{C}_{y}=(0,1) \times(0,4)$ and $u=\sin (\pi x)$
- Experimental convergence rates:

- The error decays like $\left(\# \mathscr{T}_{\gamma}\right)^{-(1-|\alpha|) / 4}$ as in uniform/isotropic refinement!
- Does adaptivity help?


## Outline

A posteriori error analysis

## Motivation

A fundamental difficulty
Anisotropic error estimation

## Multilevel methods

## Time dependent problems

Elliptic obstacle problem

Parabolic obstacle problem

## Anisotropic Error Estimation

- Anisotropic a posteriori error estimator: we need to distinguish the behavior on the extended variable $y$ from the rest.
- The theory of a posteriori error estimation (and adaptivity) on anisotropic discretizations is still in its infancy.
- Cylindrical stars: We propose an error estimator based on solving local problems on sets $\mathcal{C}_{z^{\prime}}=S_{z^{\prime}} \times(0, \mathscr{Y})$ as depicted in red in the figure:



## An Ideal A Posteriori Error Estimator

- Local space: For $z^{\prime} \in \Omega$ a node, let $\mathcal{C}_{z^{\prime}}=S_{z^{\prime}} \times(0, \mathcal{Y})$ and define

$$
\mathcal{W}\left(\mathcal{C}_{z^{\prime}}\right)=\left\{w \in H^{1}\left(y^{\alpha}, \mathcal{C}_{z^{\prime}}\right): w=0 \text { on } \partial \mathcal{C}_{z^{\prime}} \backslash \Omega \times\{0\}\right\} .
$$

- Local star indicator: The error indicator $\eta_{z^{\prime}} \in \mathcal{W}\left(\mathcal{C}_{z^{\prime}}\right)$ is given by

$$
\int_{\mathcal{C}_{z^{\prime}}} y^{\alpha} \nabla \eta_{z^{\prime}} \nabla w \mathrm{~d} x \mathrm{~d} y=d_{s} \int_{\Omega} f w(x, 0) \mathrm{d} x-\int_{\mathcal{C}_{z^{\prime}}} y^{\alpha} \nabla V \nabla w \mathrm{~d} x \mathrm{~d} y
$$

for every $w \in \mathcal{W}\left(\mathcal{C}_{z^{\prime}}\right)$.

- Global error estimator:

$$
\mathcal{E}_{\mathscr{S}_{\Omega}}=\left(\sum_{z^{\prime}} \mathcal{E}_{z^{\prime}}^{2}\right)^{1 / 2}, \quad \mathcal{E}_{z^{\prime}}=\left\|\nabla \eta_{z^{\prime}}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}_{z^{\prime}}\right)} .
$$

## Anisotropic a posteriori error analysis

- Efficiency: For every node $z^{\prime} \in \Omega$ we have

$$
\mathcal{E}_{z^{\prime}} \leq\|\nabla e\|_{L^{2}\left(y^{\alpha}, \mathcal{C}_{z^{\prime}}\right)}
$$

- Data oscillation: If $f_{z^{\prime} \mid K}=\frac{1}{|K|} \int_{K} f \mathrm{~d} x$ for every element $K \subset S_{z^{\prime}}$, then

$$
\operatorname{osc}_{\mathscr{T}_{\Omega}}(f)^{2}=\sum_{z^{\prime}} \operatorname{osc}_{z^{\prime}}(f)^{2}, \quad \operatorname{osc}_{z^{\prime}}(f)^{2}=d_{s} h_{z^{\prime}}^{2 s}\left\|f-f_{z^{\prime}}\right\|_{L^{2}\left(S_{z^{\prime}}\right)}^{2}
$$

- Reliability:

$$
\|\nabla e\|_{L^{2}\left(y^{\alpha}, \mathcal{C}_{y}\right)}^{2} \lesssim \mathcal{E}_{\mathscr{T}_{\Omega}}^{2}+\operatorname{osc}_{\mathscr{T}_{\Omega}}(f)^{2} .
$$

- Computable estimator: Restrict $\mathcal{W}\left(\mathcal{C}_{z^{\prime}}\right)$ to a discrete subspace

$$
\left\{W \in \mathcal{W}\left(\mathcal{C}_{z^{\prime}}\right):\left.W\right|_{T} \in \mathcal{P}_{2}(K) \otimes \mathbb{P}_{2}(I), \forall T=K \times I\right\}
$$

$\mathcal{P}_{2}(K)=\mathbb{Q}_{2}(K)$ for rectangles, $\mathcal{P}_{2}(K)=\mathbb{P}_{2}(K) \oplus \mathbb{B}_{3}(K)$ for simplices.

## Numerical experiment I

- $\Omega$ is the standard L -shaped domain in 2 d .
- $f=1$ which, for $s<\frac{1}{2}$, is incompatible with the problem and creates a boundary layer.
- Experimental error and estimator: error computed against a very fine discrete solution.

- Optimal decay rate: We get $D O F^{-1 / 3}$ for all $s$.


## Numerical experiment II: Meshes

- Meshes: For $s<1 / 2$ the solution exhibits a boundary layer.


$$
s=0.2
$$



$$
s=0.8
$$

- Question: Is there any theory on anisotropic adaptive approximation ${ }^{\boldsymbol{\theta}}$ ?


## Outline

## A posteriori error analysis

Multilevel methods

## Time dependent problems

## Elliptic obstacle problem

Parabolic obstacle problem

## Multilevel methods

If you do not diagonalize, How do you solve the equations? We use multilevel methods.

- We have a sequence of nested meshes $\mathscr{T}_{0} \preceq \mathscr{T}_{1} \preceq \cdots \preceq \mathscr{T}_{J}$ which induces a sequence of nested FE spaces

$$
\mathbb{V}_{0} \subset \mathbb{V}_{1} \subset \cdots \subset \mathbb{V}_{J}=\mathbb{V}
$$

- Introduce the space macro and micro decomposition

$$
\mathbb{V}=\sum_{k=0}^{J} \mathbb{V}_{k}=\sum_{k=0}^{J} \sum_{j=1}^{\mathcal{M}_{k}} \mathbb{V}_{k, j}
$$

- Define a multigrid algorithm as a standard $\mathrm{SSC}^{\boldsymbol{\theta}}$ over this decomposition.
- This setting allows for point and line smoothers.


## Properties of the decomposition

Lemma (stability and inverse inequality)
Let $v \in \mathbb{V}$ and $v=\sum_{i=1}^{\mathcal{N}} v_{i}$ be the line decomposition of $v$. Then we have the norm equivalence

$$
\sum_{i=1}^{\mathcal{N}}\left\|v_{i}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)}^{2} \lesssim\|v\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)}^{2} \lesssim \sum_{i=1}^{\mathcal{N}}\left\|v_{i}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}\right)}^{2}
$$

Moreover, for every $K \in \mathscr{T}_{\Omega}$ we have

$$
\|\nabla v\|_{L^{2}\left(y^{\alpha}, K \times(0, y)\right)} \lesssim h_{K}^{-1}\|v\|_{L^{2}\left(y^{\alpha}, K \times(0, y)\right)}
$$

In both inequalities the hidden constant is independent of $J$ and depends on $y^{\alpha}$ only through $C_{2, y^{\alpha}}$.

- The proof relies fundamentally on the fact that $y^{\alpha} \in A_{2}$.


## Convergence rate ${ }^{\text {E }}$

Theorem (convergence of multigrid)
The contraction rate of the multigrid algorithm is

$$
\delta \leq 1-\frac{1}{1+C J}
$$

where the constant $C$ is independent of the mesh size, and it depends on $y^{\alpha}$ only through $C_{2, y^{\alpha}}$.

Back

## Outline

## A posteriori error analysis

## Multilevel methods

Time dependent problems

## Elliptic obstacle problem

Parabolic obstacle problem

## Space-time fractional parabolic problem

Let $T>0$ be some positive time. Given $f: \Omega \rightarrow \mathbb{R}$ and $u_{0}: \Omega \rightarrow \mathbb{R}$ find $u$ such that

$$
\partial_{t}^{\gamma} u+(-\Delta)^{s} u=f \text { in } \Omega \times\left.(0, T] \quad u\right|_{t=0}=u_{0} \quad \text { in } \Omega
$$

Here $\gamma \in(0,1]$.
For $\gamma=1$ this is the usual time derivative, if $\gamma<1$ we consider the Caputo derivative

$$
\partial_{t}^{\gamma} u(x, t)=\frac{1}{\Gamma(1-\gamma)} \int_{0}^{t} \frac{\partial_{r} u(x, r)}{(t-r)^{\gamma}} \mathrm{d} r=\left[I^{1-\gamma} \partial_{r} u(x, \cdot)\right](t)
$$

where $I^{\sigma}$ is the Riemann-Liouville fractional integral of order $\sigma$.
Nonlocality in space and time!
We will overcome the nonlocality in space using the Caffarelli-Silvestre extension.

## Extended evolution problem

The Caffarelli-Silvestre extension turns our problem into a quasistationary elliptic problem with dynamic boundary condition

$$
\begin{cases}-\nabla \cdot\left(y^{\alpha} \nabla \mathcal{U}\right)=0, & \text { in } \mathcal{C}, t \in(0, T), \\ \mathcal{U}=0, & \text { on } \partial_{L} \mathcal{C}, t \in(0, T), \\ d_{s} \partial_{t}^{\gamma} \mathcal{U}+\frac{\partial \mathcal{U}}{\partial \nu^{\alpha}}=d_{s} f, & \text { on } \Omega \times\{0\}, t \in(0, T), \\ \mathcal{U}=\mathrm{u}_{0}, & \text { on } \Omega \times\{0\}, t=0\end{cases}
$$

Connection: $\mathbf{u}=\mathcal{U}(x, 0), \alpha=1-2 s$.
Nonlocality just in time!
Weak formulation: seek $\mathcal{U} \in \mathbb{V}$ such that for a.e. $t \in(0, T)$,

$$
\left\{\begin{array}{l}
\int_{\Omega} \partial_{t}^{\gamma} \mathcal{U}(x, 0) \phi(x, 0) \mathrm{d} x+a(w, \phi)=\int_{\Omega} f \phi(x, 0) \mathrm{d} x \\
\mathcal{U}_{\mid t=0}=\mathbf{u}_{0}
\end{array}\right.
$$

for all $\phi \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right)$, where

$$
a(w, \phi)=\frac{1}{d_{s}} \int_{\mathcal{C}} y^{\alpha} \nabla w \cdot \nabla \phi \mathrm{~d} x \mathrm{~d} y .
$$

## Discretization

- As in the elliptic case $\mathcal{C}$ is infinite, but we have exponential decay.
- This allows us to consider a truncated problem.
- In doing so we commit only an exponentially small error

$$
I^{1-\gamma}\left\|\operatorname{tr}_{\Omega}(\mathcal{U}-v)\right\|_{L^{2}(\Omega)}^{2}+\|\nabla(\mathcal{U}-v)\|_{L^{2}\left(0, T ; L^{2}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)}^{2} \lesssim e^{-\sqrt{\lambda_{1} \gamma}} .
$$

- For $\gamma=1^{\boldsymbol{l}}$, we consider backward Euler:
- We initialize by setting $V^{0}(x, 0)=\mathrm{u}_{0}$.
- For $k=0, \ldots, \mathcal{K}-1$, we find $V^{k+1} \in \dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)$ solution of

$$
\tau^{-1}\left(V^{k+1}(\cdot, 0)-V^{k}(\cdot, 0), W(\cdot, 0)\right)_{L^{2}(\Omega)}+a\left(V^{k+1}, W\right)=\left(f^{k+1}, W(\cdot, 0)\right)_{L^{2}(\Omega}
$$

for all $W \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)$, where $f^{k+1}=f\left(t^{k+1}\right)$.

- Unconditional stability:

$$
\left\|V^{\tau}(\cdot, 0)\right\|_{\ell^{\infty}\left(L^{2}(\Omega)\right)}^{2}+\left\|V^{\tau}\right\|_{\ell^{2}\left(\dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)}^{2} \lesssim\left\|\mathrm{u}_{0}\right\|_{L^{2}(\Omega)}^{2}+\left\|f^{\tau}\right\|_{\ell^{2}\left(\mathbb{H}^{-s}(\Omega)\right)}^{2}
$$

## Error estimates for fully discrete schemes ${ }^{\text {E }}$

Discretization in time and space: stability + consistency yield

- Error estimates for $\mathcal{U}: s \in(0,1)$ and $\gamma \in(0,1)$

$$
\begin{aligned}
{\left[I^{1-\gamma}\left\|t_{\Omega}\left(v^{\tau}-V_{\mathscr{T}_{y}}^{\tau}\right)\right\|_{L^{2}(\Omega)}^{2}(T)\right]^{\frac{1}{2}} } & \lesssim \tau^{\theta}+\left|\log \# \mathscr{T}_{y}\right|^{2 s} \# \mathscr{T}_{\gamma}^{\frac{-(1+s)}{n+1}} \\
\left\|v^{\tau}-V_{\mathscr{T}_{y}}^{\tau}\right\|_{\ell^{2}\left(H_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)} & \lesssim \tau^{\theta}+\left|\log \# \mathscr{T}_{y}\right|^{s} \# \mathscr{T}_{y^{\frac{-1}{n+1}}}
\end{aligned}
$$

- Error estimates for $u: s \in(0,1)$ and $\gamma \in(0,1)$

$$
\begin{aligned}
{\left[I^{1-\gamma}\left\|u^{\tau}-U^{\tau}\right\|_{L^{2}(\Omega)}^{2}(T)\right]^{\frac{1}{2}} } & \lesssim \tau^{\theta}+\left|\log \# \mathscr{T}_{y}\right|^{2 s} \# \mathscr{T}_{\gamma}^{\frac{-(1+s)}{n+1}} \\
\left\|u^{\tau}-U^{\tau}\right\|_{\ell^{2}\left(H^{s}(\Omega)\right)} & \lesssim \tau^{\theta}+\left|\log \# \mathscr{T}_{y}\right|^{s} \# \mathscr{T}_{r}^{\frac{-1}{n+1}}
\end{aligned}
$$

where $\theta<\frac{1}{2}$.

## Outline

## A posteriori error analysis

## Multilevel methods

## Time dependent problems

Elliptic obstacle problem

Parabolic obstacle problem

## Formulation

- Given $f \in \mathbb{H}^{-s}(\Omega)$ and an obstacle $\psi \in \mathbb{H}^{s}(\Omega) \cap C(\bar{\Omega})$ with $\psi \leq 0$ on $\partial \Omega$.
- Find $u \in \mathcal{K}$ such that

$$
\left\langle(-\Delta)^{s} u, u-w\right\rangle \leq\langle f, u-w\rangle \quad \forall w \in \mathcal{K}
$$

where

$$
\mathcal{K}:=\left\{w \in \mathbb{H}^{s}(\Omega): w \geq \psi \text { a.e. in } \Omega\right\} .
$$

- Nonlinear and (because of $(-\Delta)^{s}$ ) nonlocal problem!
- Use the Caffarelli-Silvestre extension.


## Thin obstacle problem

- We convert the fractional obstacle problem into a thin obstacle problem.

- The restriction $\mathcal{U}>\psi$ only applies when $y=0$ (thin obstacle).


## Truncation

- The domain $\mathcal{C}$ is infinite.
- The energy of the solution decays exponentially in $y$.
- We truncate the cylinder $\mathcal{C}_{y}=\Omega \times(0, \mathcal{Y})$ and consider a truncated problem.
- In doing this we only commit an exponentially small error

$$
\|\nabla(\mathcal{U}-\mathcal{V})\|_{L^{2}\left(y^{\alpha}, \mathcal{C}_{y}\right)} \lesssim e^{-\sqrt{\lambda_{1}} \boldsymbol{y} / 8}
$$

## Discretization

Discretize the truncation over an anisotropic mesh.
Theorem ( ${ }^{\text {E }}$ )
If $\mathcal{U}$ is the exact solution and $V_{\mathscr{T}_{y}}$ the discrete solution, then

$$
\left\|\mathcal{U}-V_{\mathscr{T}_{y}}\right\|_{\dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right)} \lesssim\left|\log \left(\# \mathscr{T}_{y}\right)\right|^{s}\left(\# \mathscr{T}_{y}\right)^{-1 /(n+1)}
$$

where $C$ depends on the Hölder moduli of smoothness of $\mathcal{U}$ and $\mathcal{V}$, $\|f\|_{\mathbb{H}^{-s}(\Omega)}$ and $\|\psi\|_{\mathbb{H}^{s}(\Omega)}$.

- Optimal regularity in $\Omega^{\Theta^{3}}: u \in C^{1, s}$.
- This implies that $\partial_{\nu}^{\alpha} \mathcal{U}(\cdot, 0) \in C^{0,1-s}$.
- For $y$ "small" use that ${ }^{\boldsymbol{\theta}}: s \leq \frac{1}{2} \Rightarrow \mathcal{V} \in C^{0,2 s}\left(\mathcal{C}_{y}\right)$ and $s>\frac{1}{2} \Rightarrow \mathcal{V} \in C^{1,2 s-1}\left(\mathcal{C}_{y}\right)$.
- For $y$ "big" use ${ }^{\boldsymbol{E}} \mathcal{V} \in H^{2}\left(y^{\beta}, \mathcal{C}_{y}\right)$ with $\beta>1+2 \alpha$.


## Back

[^7]
## Outline

## A posteriori error analysis

## Multilevel methods

Time dependent problems
Elliptic obstacle problem

Parabolic obstacle problem

## Formulation

- Define the energy

$$
\mathcal{J}(v)=\frac{1}{2}\|v\|_{\mathbb{H}^{s}(\Omega)}^{2}+\mathbf{1}_{\mathcal{K}}(v)
$$

- We will study the (sub)gradient flow

$$
u_{t}+\left.\partial \mathcal{J}(u) \ni f \quad u\right|_{t=0}=u_{0} .
$$

- Equivalently we have the evolution variational inequality

$$
\left(u_{t}, u-\phi\right)_{L^{2}(\Omega)}+\left\langle(-\Delta)^{s} u, u-\phi\right\rangle \leq(f, u-\phi)_{L^{2}(\Omega)} \quad \forall \phi \in \mathcal{K} .
$$

- Or the complementarity conditions

$$
\min \left\{u_{t}+(-\Delta)^{s} u-f, u-\psi\right\}=0
$$

## The Caffarelli-Silvestre extension and truncation

- We will again overcome the nonlocality with the Caffarelli-Silvestre extension and consider

$$
\begin{array}{r}
\left(\mathcal{U}_{t}(\cdot, 0),(\mathcal{U}-\phi)(\cdot, 0)\right)_{L^{2}(\Omega)}+\frac{1}{d_{s}} \int_{\mathcal{C}} y^{\alpha} \nabla \mathcal{U} \nabla(\mathcal{U}-\phi) \mathrm{d} x \mathrm{~d} y \leq \\
(f,(\mathcal{U}-\phi)(\cdot, 0))_{L^{2}(\Omega)}
\end{array}
$$

for all $\phi \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right)$ with $\phi(\cdot, 0) \in \mathcal{K}$.

- We consider, again, a truncated problem over $\mathcal{C}_{y}$ :

$$
\|(\mathcal{U}-\mathcal{V})(\cdot, 0)\|_{L^{\infty}\left(0, T ; L^{2}(\Omega)\right)}+\|\mathcal{U}-\mathcal{V}\|_{L^{2}\left(0, T ; \dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{\mathcal{Y}}\right)\right)} \lesssim e^{-\sqrt{\lambda_{1} y / 8}}
$$

## Time discretization

- The energy $\mathcal{J}$ is convex and lower semicontinuous $\Longrightarrow \partial \mathcal{J}$ is maximal monotone.
- We use the implicit Euler method:

$$
\begin{aligned}
& \left(\frac{V^{k+1}-V^{k}}{\tau}(\cdot, 0),\left(V^{k+1}-\phi\right)(\cdot, 0)\right)_{L^{2}(\Omega)} \\
+ & \frac{1}{d_{s}} \int_{\mathcal{C}_{y}} y^{\alpha} \nabla V^{k+1} \nabla\left(V^{k+1}-\phi\right) \mathrm{d} x \mathrm{~d} y \leq\left(f^{k+1},\left(V^{k+1}-\phi\right)(\cdot, 0)\right)_{L^{2}(\Omega)}
\end{aligned}
$$

for all $\phi \in \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}\right)$ with $\phi(\cdot, 0) \in \mathcal{K}$.

## Time discretization

The general theory of graident flows ${ }^{\boldsymbol{\theta}}$ yields:

- If $u_{0} \in \mathcal{K}$ and $f \in L^{2}\left(0, T ; L^{2}(\Omega)\right)$

$$
\|(\mathcal{V}-V)(\cdot, 0)\|_{L^{\infty}\left(0, T ; L^{2}(\Omega)\right)}+\|\mathcal{V}-V\|_{L^{2}\left(0, T ; \dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)} \lesssim \tau^{1 / 2}
$$

- If $u_{0} \in \mathcal{K} \cap \mathbb{H}^{2 s}(\Omega)$ and $f \in B V\left(0, T ; L^{2}(\Omega)\right)$

$$
\|(\mathcal{V}-V)(\cdot, 0)\|_{L^{\infty}\left(0, T ; L^{2}(\Omega)\right)}+\|\mathcal{V}-V\|_{L^{2}\left(0, T ; \dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)} \lesssim \tau
$$

These estimates are sharp!

## Space discretization I: Minimal regularity

- Discretize in space using finite elements over an anisotropic mesh $\mathscr{T}_{y}$.
- If the discrete initial condition $V_{\mathscr{S}_{y}}^{0}$ satisfies

$$
\left\|\nabla V_{\mathscr{T}_{2}}^{0}\right\|_{L^{2}\left(y^{\alpha}, \mathcal{C}_{y}\right)} \lesssim\left\|u_{0}\right\|_{\mathbb{H}^{s}(\Omega)} .
$$

then ${ }^{\text {e }}$

$$
\begin{array}{r}
\left\|\left(V-V_{\mathscr{F}_{\mathfrak{Y}}}\right)(\cdot, 0)\right\|_{L^{\infty}\left(0, T ; L^{2}(\Omega)\right)}+\left\|V-V_{\mathscr{F}_{Y}}\right\|_{L^{2}\left(0, T ; H_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)} \lesssim \\
\tau^{\theta}+\|\mathcal{V}-\Pi \mathcal{V}\|_{L^{2}\left(0, T ; H_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)}^{1 / 2}
\end{array}
$$

where $\theta \in\{1 / 2,1\}$ depends on the smoothness of $f$ and $u_{0}$

- No regularity assumptions!


## Space discretization II: Analysis with regularity

- Under certain conditions we have that ${ }^{\text {I }}$

$$
\begin{aligned}
& u_{t},(-\Delta)^{s} u \in \log \operatorname{Lip}\left((0, T], C^{1-s}(\bar{\Omega})\right) \quad s \leq \frac{1}{3} \\
& u_{t},(-\Delta)^{s} u \in C^{\frac{1-s}{2 s}}\left((0, T], C^{1-s}(\bar{\Omega})\right) \quad s>\frac{1}{3}
\end{aligned}
$$

- With this regularity ${ }^{\text {E }}$

$$
\begin{array}{r}
\left\|\left(V-V_{\mathscr{T}_{Y}}\right)(\cdot, 0)\right\|_{L^{\infty}\left(0, T ; L^{2}(\Omega)\right)}+\left\|V-V_{\mathscr{T}_{Y}}\right\|_{L^{2}\left(0, T ; \dot{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)} \lesssim \\
\tau+\left|\log \# \mathscr{T}_{y}\right|^{s}\left(\# \mathscr{T}_{y}^{-\frac{1}{n+1}}+\frac{\# \mathscr{T}_{y}^{-\frac{1+s}{n+1}}}{\tau^{1 / 2}}\right) \\
+\|\mathcal{V}-\Pi \mathcal{V}\|_{L^{2}\left(0, T ; \stackrel{\circ}{H}_{L}^{1}\left(y^{\alpha}, \mathcal{C}_{y}\right)\right)}
\end{array}
$$


[^0]:    E ${ }^{\text {Valdinoci }} 2017$
    ${ }^{\text {E }}$ Ainsworth and Mao 2017, Antil and Bartels 2018

[^1]:    ${ }^{\text {E }}$ Caffarelli, Stinga 2016
    Costabel, Dauge 1993

[^2]:    $\boldsymbol{E}_{\text {Matsuki, Ushijima }} 1993$

[^3]:    Harizanov, Lazarov, Margenov, Vutov 2016

[^4]:    E $_{\text {Durán, Lombardi 2005; Dupont, Scott 1980; Sobolev } 1950}$

[^5]:    ${ }^{\boldsymbol{E}}$ Nochetto, Otárola, AJS 2015

[^6]:    ${ }^{\text {E }}$ Nochetto, Otárola, AJS 2016
    ${ }^{\text {E }}$ Nochetto, Otárola, AJS 2015
    Elárola, AJS 2016
    ${ }^{\text {El }}$ Chen, Nochetto, Otárola, AJS 2016
    ${ }^{\text {E }}$ Chen, Nochetto, Otárola, AJS 2015

[^7]:    ${ }^{\text {E }}$ Nochetto, Otárola, AJS 2015
    ${ }^{[1}$ Caffarelli, Salsa and Silvestre 2008
    ${ }^{\text {E }}$ Allen, Lindgren, and Petrosyan 2014
    ${ }^{\text {E }}$ Nochetto, Otárola, AJS 2015

