

Sparse spectral methods for fractional PDEs

PDE CDT Students & Alumni Reunion Event



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¹Imperial College London; ²University of Oxford; ³UCL

My timeline

Sep 2017 – PDE CDT
Cohort 4

Sep 2018 – Started DPhil project
with Patrick Farrell & Endre Süli

July 2021 – Postdoc
Position at ICL

Sep 2021 – DPhil
viva

July 2022 – Speaking at the
reunion event

My timeline

MSc

- Mathematical modelling and scientific computing

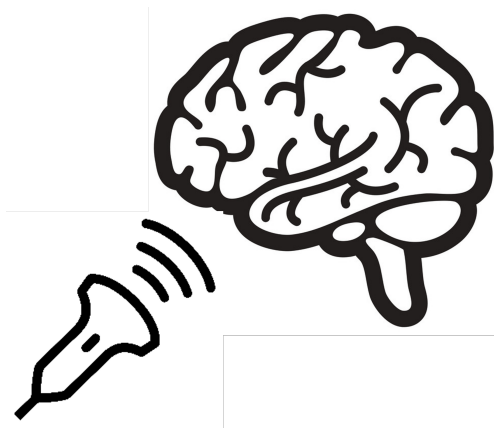
PDE CDT

- Nonconvex optimisation problems with PDE constraints
- Existence, regularity & FEM analysis

Postdoc

- Fractional PDEs & spectral methods

Are fractional PDEs physical?



FPDEs describe wave absorption in the brain¹.

¹Images from <https://clipart.world/brain-clipart/black-and-white-brain-clipart/>,
https://www.kindpng.com/imgv/iRoiRR_sound-wave-clipart-ultrasound-ultrasound-clip-art-hd/.

Other applications?

- Equilibrium measures;
- Dispersive transport of ions;
- Replacing total variation regularization in imaging;
- Geophysics problems with long range effects;
- Neural networks where all the layers are connected to every other layer.

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The problem

The PDE

Find $u \in H^{1/2}(\mathbb{R})$ that satisfies, for $\lambda \in \mathbb{R}$: $(\lambda \mathcal{I} + (-\Delta)^{1/2})u = f$.

$(-\Delta)^{1/2}$

Ten (or more) equivalent definitions of the fractional Laplacian over \mathbb{R}^d . E.g. for $s \in (0, 1)$,

$$(-\Delta)^s u(x) := c_{d,s} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x - y|^{d+2s}} dy$$

or

$$\mathcal{F}[(-\Delta)^s u](\omega) = |\omega|^{2s} \mathcal{F}[u](\omega).$$

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Fractional PDEs

Observation

Solutions of fractional PDEs are “nonlocal” and can exhibit singularities.

Consequence

The solutions can be difficult to approximate numerically.

Challenge

How do we compute them with fast convergence?

Our proposal

A spectral method based on a so-called sum space.

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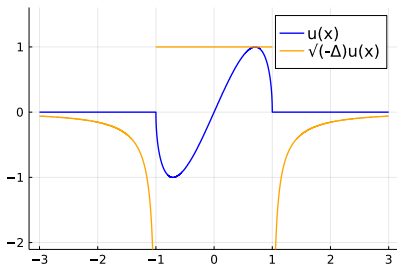
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Singularities and non-locality

The fractional Laplacian is not local. E.g.



Nonlocal

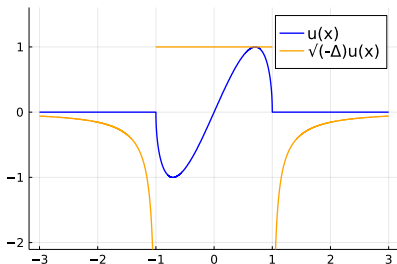
$u(x) = 0$ for $|x| \geq 1$ but $(-\Delta)^{1/2}u(x) \neq 0$ for all $x \in \mathbb{R}$.

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As $x \downarrow 1$ and $x \uparrow -1$, then $|(-\Delta)^{1/2}u(x)| \rightarrow \infty$.

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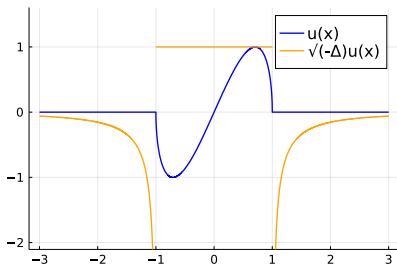
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Spectral methods

Pick an orthogonal set of polynomials, e.g. the so-called *Chebyshev* T polynomials, denoted $\{T_n(x)\}$. These satisfy

$$\int_{-1}^1 \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}} dx = \delta_{nm}; \quad T_0(x) = 1, \quad T_1(x) = x, \quad T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x).$$

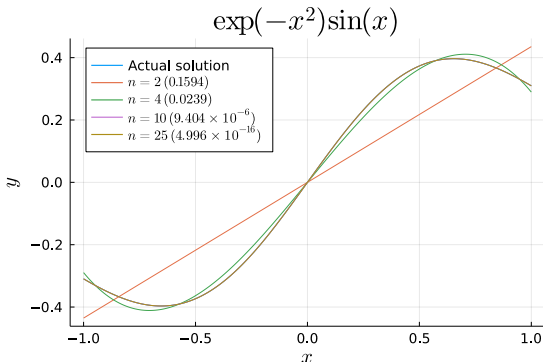
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Sparse spectral methods

Many spectral methods for differential equations induce *dense* matrices **X**. Consider solving

$$-u'(x) = f(x), \quad u(-1) = 0.$$

A spectral method recipe 📖:

- 1 Expand $f(x)$ in the ChebyshevT polynomial basis, truncate, and collect the coefficients in vector \mathbf{f} .
- 2 Construct the differential operator D via a collocation method. D is **dense**.
- 3 Solve $D\mathbf{u} = \mathbf{f}$ for the coefficients \mathbf{u} in the ChebyshevT expansion of $u(x)$.

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An observation

Let $\{U_n\}$ denote the *ChebyshevU* orthogonal polynomial basis. Then, for $n \geq 1$, $T'_n(x) = nU_{n-1}(x)$. Or in *quasimatrix* form:

$$(T'_0(x) \ T'_1(x) \ T'_2(x) \ \dots) \begin{pmatrix} 0 & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & \ddots \end{pmatrix} = (U_0(x) \ U_1(x) \ U_2(x) \ \dots)$$

A **sparse** spectral method recipe :

- 1 Expand $f(x)$ in the **ChebyshevU** polynomial basis, truncate, and collect the coefficients in vector \mathbf{f} .
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Sparse spectral method for FPDE

ChebyshevT

$T_n(x)$ = ChebyshevT, polynomials of order n , $x \in [-1, 1]$, orthogonal w.r.t. $1/\sqrt{1-x^2}$. Extend by 0 to \mathbb{R} outside $[-1, 1]$.

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Extended Chebyshev functions on \mathbb{R}

$\tilde{T}_n(x)$ and $\tilde{U}_n(x)$ are carefully chosen extensions of $T_n(x)$ and $U_n(x)$, respectively, for $x \in \mathbb{R}$.

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$$\tilde{U}_n(x) := \tilde{T}_n(x) - \tilde{U}_{n-2}(x), \quad n \geq 0,$$

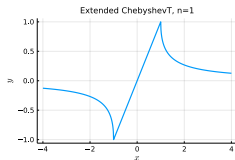
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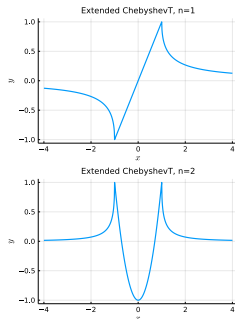
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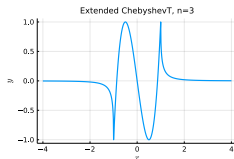
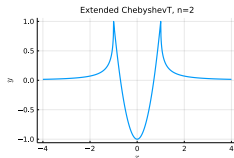
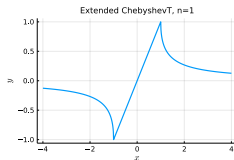
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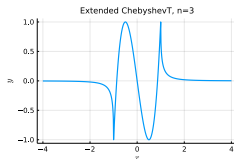
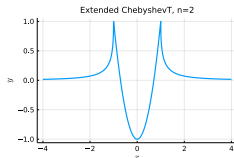
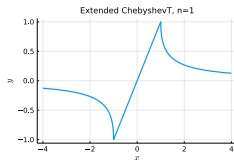
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Motivation for choice of functions

Denote the Hilbert transform: $\mathcal{H}[u](x) := \frac{1}{\pi} \int_{\mathbb{R}} \frac{u(y)}{x-y} dy$. Let
 $W_n(x) := (1 - x^2)_+^{1/2} U_n(x)$.

Property 1

- $\mathcal{H}[W_n](x) = \tilde{T}_{n+1}(x)$ for all $x \in \mathbb{R}$.
- $\mathcal{H}[\tilde{T}_{n+1}](x) = -W_n(x)$ for all $x \in \mathbb{R}$.

Property 2

Modulo some assumptions: $\frac{d}{dx} \mathcal{H} = (-\Delta)^{1/2}$ in 1D.

Property 3

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Denote the Hilbert transform: $\mathcal{H}[u](x) := \frac{1}{\pi} \int_{\mathbb{R}} \frac{u(y)}{x-y} dy$. Let
 $W_n(x) := (1 - x^2)_+^{1/2} U_n(x)$.

Property 1

- $\mathcal{H}[W_n](x) = \tilde{T}_{n+1}(x)$ for all $x \in \mathbb{R}$.
- $\mathcal{H}[\tilde{T}_{n+1}](x) = -W_n(x)$ for all $x \in \mathbb{R}$.

Property 2

Modulo some assumptions: $\frac{d}{dx} \mathcal{H} = (-\Delta)^{1/2}$ in 1D.

Property 3

- $\frac{d}{dx} [W_n](x) = (n+1)(1-x^2)_+^{-1/2} T_{n+1}(x)$.
- $\frac{d}{dx} [\tilde{T}_{n+1}](x) = n\tilde{U}_{n-1}(x)$.

$(-\Delta)^{1/2}$

$$\begin{aligned}\{(1-x^2)_+^{1/2} U_n(x)\} &\xrightarrow{(-\Delta)^{1/2}} \{\tilde{U}_n(x)\}, \\ \{\tilde{T}_n(x)\} &\xrightarrow{(-\Delta)^{1/2}} \{(1-x^2)_+^{-1/2} T_n(x)\}.\end{aligned}$$

Identity

$$\begin{aligned}\{(1-x^2)_+^{1/2} U_n(x)\} &\xrightarrow{\mathcal{I}} \{(1-x^2)_+^{-1/2} T_n(x)\}, \\ \{\tilde{T}_n(x)\} &\xrightarrow{\mathcal{I}} \{\tilde{U}_n(x)\}.\end{aligned}$$

A sparse spectral method for an FPDE

Key idea: use sum space $\{\tilde{T}_n(x)\} \cup \{(1-x^2)_+^{1/2} U_n(x)\}$.

$$\lambda \mathcal{I} + (-\Delta)^{1/2}$$

$$\underbrace{\{\tilde{T}_n(x)\} \cup \{(1-x^2)_+^{1/2} U_n(x)\}}_{\text{sum space}} \xrightarrow{\lambda \mathcal{I} + (-\Delta)^{1/2}} \underbrace{\{\tilde{U}_n(x)\} \cup \{(1-x^2)_+^{-1/2} T_n(x)\}}_{\text{dual sum space}}.$$

A **sparse** spectral method recipe 🍷:

- 1 Expand f in the **dual sum space**, truncate, and collect coefficients in vector \mathbf{f} .
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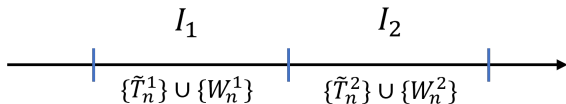
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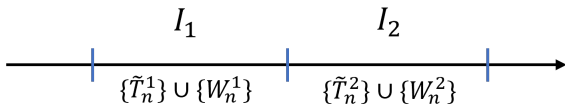
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Combining different intervals



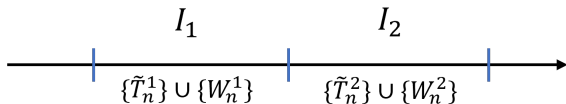
- $\{\tilde{T}_n^i\}$ and $\{W_n^i\}$, $i = 1, 2$, are the spaces of affine transformed functions of the spaces $\{\tilde{T}_n\}$ and $\{\sqrt{1-x^2}U_n\}$, respectively, centred at the interval midpoints of I_1 and I_2 .
- W_n^i are supported on I_i , $i = 1, 2$.
- \tilde{T}_n^i are not only supported on I_i and interact with other functions centred on other intervals.

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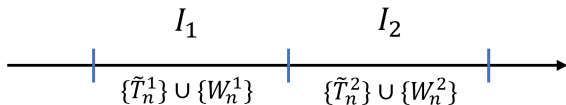
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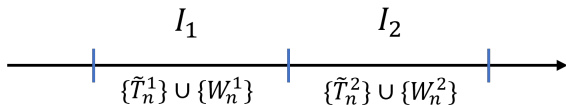
$\lambda \mathcal{I} + (-\Delta)^{1/2}$ induces a block-diagonal matrix. Each block corresponds to the sum space centred at one interval.

$$\begin{pmatrix} D_1 & \\ & D_2 \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \end{pmatrix}.$$

This decomposes to

$$D_1 \mathbf{u}_1 = \mathbf{f}_1, \quad D_2 \mathbf{u}_2 = \mathbf{f}_2.$$

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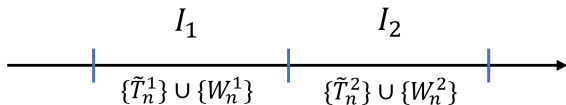
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Example: the Gaussian

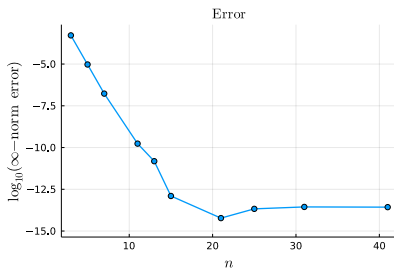
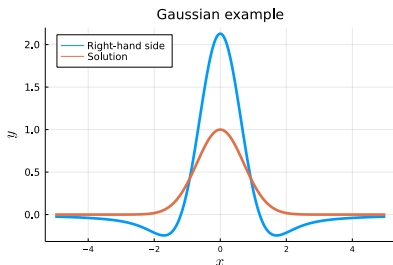
$$(\mathcal{I} + (-\Delta)^{1/2})u(x) = e^{-x^2} + \frac{2}{\sqrt{\pi}} {}_1F_1(1; 1/2; -x^2).$$

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Example: wave propagation

Consider the FPDE ($u(x, t) \rightarrow 0$ as $|x| \rightarrow \infty$):

$$[(-\Delta)^{1/2} + \mathcal{H} + \frac{\partial^2}{\partial t^2}]u(x, t) = (1 - x^2)_+^{1/2} U_4(x) e^{-t^2}.$$

A Fourier transform in time gives ($\hat{u}(x, \omega) \rightarrow 0$ as $|x| \rightarrow \infty$):

$$[(-\Delta)^{1/2} + \mathcal{H} - \omega^2]\hat{u}(x, \omega) = \sqrt{\pi}(1 - x^2)_+^{1/2} U_4(x) e^{-\omega^2/4}.$$

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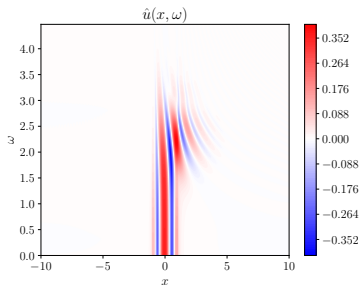
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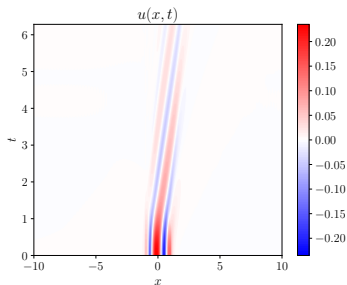
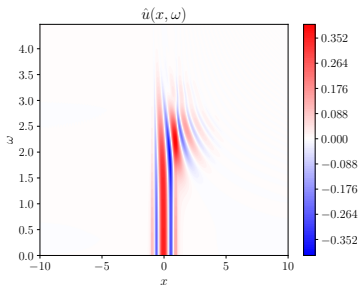
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Still to come

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Thank you for listening!

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