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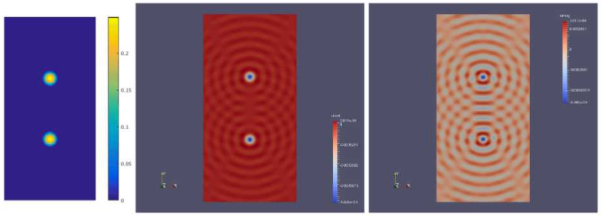

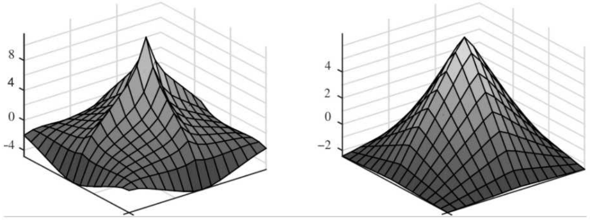

Fractional Differential Operators to Detect Multiscale Geophysical Features

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Goal:

Determine exponents of fractional differential operators from sparse EM measurements to characterize multiscale subsurface features.

Outline:

- Motivation
- Mathematical formulation
- Implementation details
- Preliminary numerical results
- Summary

Canonical Fractional Helmholtz Problem

$$\begin{aligned} (-\Delta)^s u - k^2 u = f \quad & \text{in } \Omega, \\ \alpha \partial_n u + \beta u = g \quad & \text{on } \Gamma. \end{aligned}$$

For mixed (Robin) boundary conditions, need to split u = v + w

$$\begin{aligned} (-\Delta)^s v - k^2 (v + w) = f \quad & \text{in } \Omega, \\ \partial_n v = 0 \quad & \text{on } \Gamma, \end{aligned}$$

$$\begin{aligned} (-\Delta)^s w = 0 \quad & \text{in } \Omega, \\ \alpha \partial_n w = g - \beta (v + w) \quad & \text{on } \Gamma. \end{aligned}$$

Fractional Laplace Eq can be replaced with a more easily handled classical Laplace E

$$\begin{aligned} (-\Delta) w = 0 \quad & \text{in } \Omega, \\ \alpha \partial_n w = g - \beta (v + w) \quad & \text{on } \Gamma, \end{aligned}$$

… but this still leaves the coupled Helmholtz system, which now possesses homogeneous BCs that are much easier to deal with.

Canonical Fractional Helmholtz Problem

$$\boxed{\begin{aligned} (-\Delta)^s v - k^2 (v + w) &= f \quad \text{in } \Omega, \\ \partial_n v &= 0 \quad \text{on } \Gamma, \end{aligned}}$$

Dunford-Taylor integral representation

$$\begin{aligned} (-\Delta)^{-s} &= \frac{\sin s\pi}{\pi} \int_{-\infty}^{\infty} e^{(1-s)y} \left(e^{y} - \Delta\right)^{-1} \, \mathrm{d}y, \\ &\approx \frac{\sin s\pi}{\pi} m \sum_{\ell=-N^-}^{N^+} e^{(1-s)y_\ell} \left(e^{y_\ell} - \Delta\right)^{-1}. \end{aligned}$$

Sinc-quadrature expansion of v

$$v = \frac{\sin s\pi}{\pi} m \sum_{\ell=-N^-}^{N^+} e^{(1-s)y_\ell} v_\ell$$

Equate term-by term to arrive at a large, coupled system Eq’s

$$v_\ell - \left(e^{y_\ell} - \Delta\right)^{-1} k^2 (v + w) = \left(e^{y_\ell} - \Delta\right)^{-1} f$$

$$\boxed{\left(e^{y_\ell} - \Delta\right) v_\ell - k^2 (v + w) = f}$$

Discrete, fully coupled finite element system of Eqs

$$\begin{pmatrix} \mathbf{A}_0 & d_1\,\mathbf{M}_2 & d_2\,\mathbf{M}_2 & \cdots & d_L\mathbf{M}_2 & \mathbf{M}_2 \\ d_0\,\mathbf{M}_2 & \mathbf{A}_1 & d_2\,\mathbf{M}_2 & \cdots & d_L\mathbf{M}_2 & \mathbf{M}_2 \\ d_0\,\mathbf{M}_2 & d_1\,\mathbf{M}_2 & \mathbf{A}_2 & \cdots & d_L\mathbf{M}_2 & \mathbf{M}_2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ d_0\,\mathbf{M}_2 & d_1\,\mathbf{M}_2 & d_2\,\mathbf{M}_2 & \cdots & \mathbf{A}_L & \mathbf{M}_2 \\ d_0\,\mathbf{M}_3 & d_1\,\mathbf{M}_3 & d_2\,\mathbf{M}_3 & \cdots & d_L\,\mathbf{M}_3 & \mathbf{B} \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_{-N^-} \\ \boldsymbol{v}_{1-N^-} \\ \boldsymbol{v}_{2-N^-} \\ \vdots \\ \boldsymbol{v}_{N^+} \\ \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{f} \\ \boldsymbol{f} \\ \vdots \\ \boldsymbol{f} \\ \boldsymbol{g}_\alpha \end{pmatrix}$$

Block dense, but the blocks are sparse

System size = N(FE) * (Nquad + 1)

Path to 3D necessitates HPC parallelization

Which hurts more: this or brute force discretization? TBD!

Discrete, fully coupled finite element system of Eqs

SPARSIFIED: include redundant vector v, but enforce compatibility with v_l

$$\begin{pmatrix} \tilde{\mathbf{A}}_0 & \mathbf{0} & \cdots & \cdots & \mathbf{0} & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \tilde{\mathbf{A}}_1 & \mathbf{0} & \cdots & \mathbf{0} & \mathrm{M}_2 & \mathrm{M}_2 \\ \vdots & & \ddots & & \vdots & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \cdots & \mathbf{0} & \tilde{\mathbf{A}}_{L-1} & \mathbf{0} & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & \tilde{\mathbf{A}}_L & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} & \mathrm{B} & \mathrm{M}_3 \\ -d_0\mathbf{M}_1 & \cdots & \cdots & \cdots & -d_L\mathbf{M}_1 & \mathbf{0} & \mathrm{M}_1 \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_{-N-} \\ \boldsymbol{v}_{1-N-} \\ \boldsymbol{v}_{2-N-} \\ \vdots \\ \boldsymbol{v}_{N+} \\ \boldsymbol{w} \\ \boldsymbol{v} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{f} \\ \boldsymbol{f} \\ \vdots \\ \boldsymbol{f} \\ \boldsymbol{g}_\alpha \\ \mathbf{0} \end{pmatrix}$$

Far fewer blocks → fewer computations for matrix-vector products

Discrete, fully coupled finite element system of Eqs

SPARSIFIED: include redundant vector v, but enforce compatibility with v_l *and* scale solution vectors by prefactors d_l to minimize ill-conditioning

$$\begin{pmatrix} \tilde{\mathbf{A}}'_0 & \mathbf{0} & \cdots & \cdots & \mathbf{0} & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \tilde{\mathbf{A}}'_1 & \mathbf{0} & \cdots & \mathbf{0} & \mathrm{M}_2 & \mathrm{M}_2 \\ \vdots & & \ddots & & \vdots & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \cdots & \mathbf{0} & \tilde{\mathbf{A}}'_{L-1} & \mathbf{0} & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \cdots & \cdots & \mathbf{0} & \tilde{\mathbf{A}}'_L & \mathrm{M}_2 & \mathrm{M}_2 \\ \mathbf{0} & \cdots & \cdots & \cdots & \mathbf{0} & \mathbf{B} & \mathrm{M}_3 \\ -\mathrm{M}_1 & \cdots & \cdots & \cdots & -\mathrm{M}_1 & \mathbf{0} & \mathrm{M}_1 \end{pmatrix} \begin{pmatrix} \boldsymbol{v}'_{-N-} \\ \boldsymbol{v}'_{1-N-} \\ \boldsymbol{v}'_{2-N-} \\ \vdots \\ \boldsymbol{v}'_{N+} \\ \boldsymbol{w} \\ \boldsymbol{v} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{f} \\ \boldsymbol{f} \\ \vdots \\ \boldsymbol{f} \\ \boldsymbol{g}_\alpha \\ \mathbf{0} \end{pmatrix}$$

Solver requirements

non-symmetric matrices

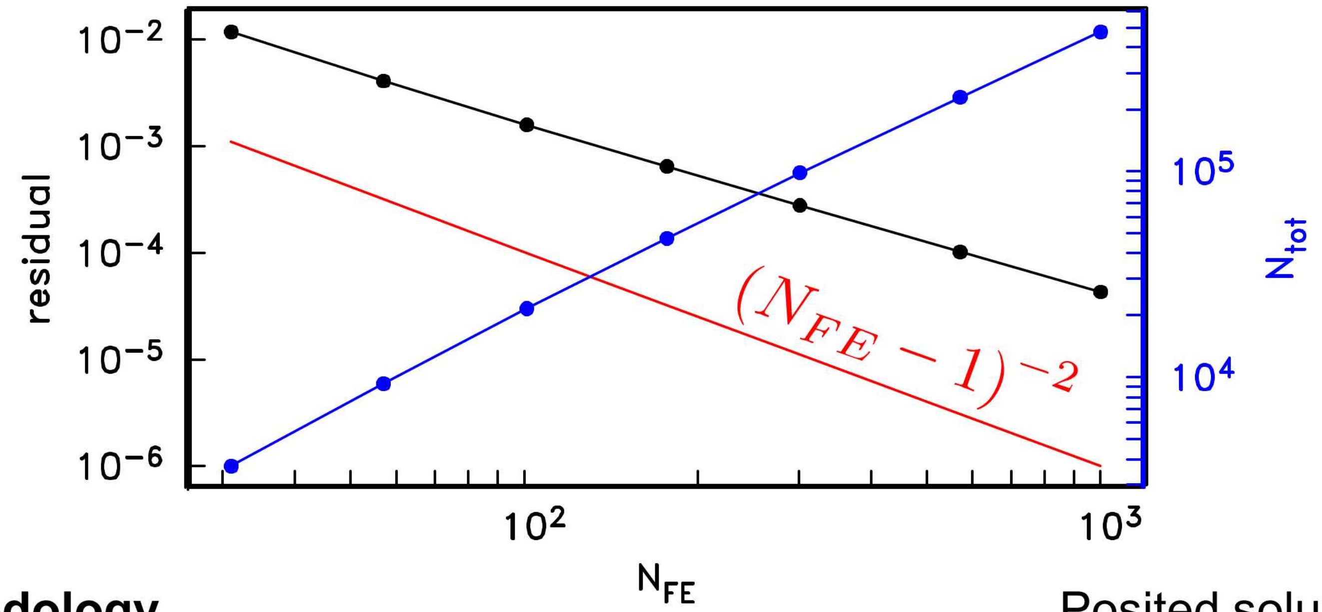
Solver preferences

complex arithmetic, exploit sparsity, easily preconditioned, minimal memory footprint, HPC scalable

Testing the Theoretical Convergence Rate

$$(-\Delta)^s u(x) - u(x) = \left(\left(4\pi^2\right)^s - 1 \right) \cos 2\pi x$$

$$\partial_x u + u = 1 \quad x = 0, 1$$



MMS methodology

Posit a solution to the PDE
Algebraically evaluate the RHS
Discretize the RHS and solve
Compare posited solution to recovered, discrete solution

Posited solution

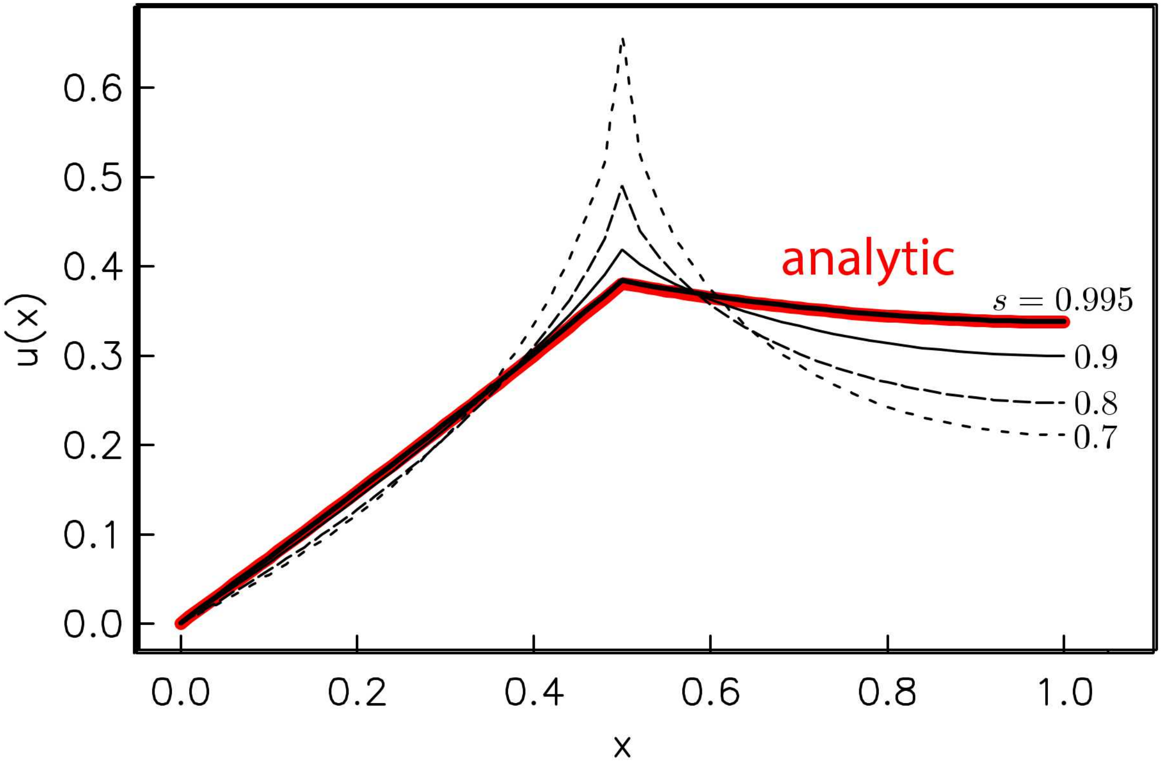
$$u(x) = \cos(2\pi x)$$

BiCG-STAB solver,
matrix-free, Jacobi scaling

Reality Check: Does the fractional Helmholtz converge to classical for s=1?

$$(-\Delta)^s u(x) + u(x) = \delta\left(x - \frac{1}{2}\right)$$

$$u(0) = 0, \quad \partial_x u(1) = 0$$

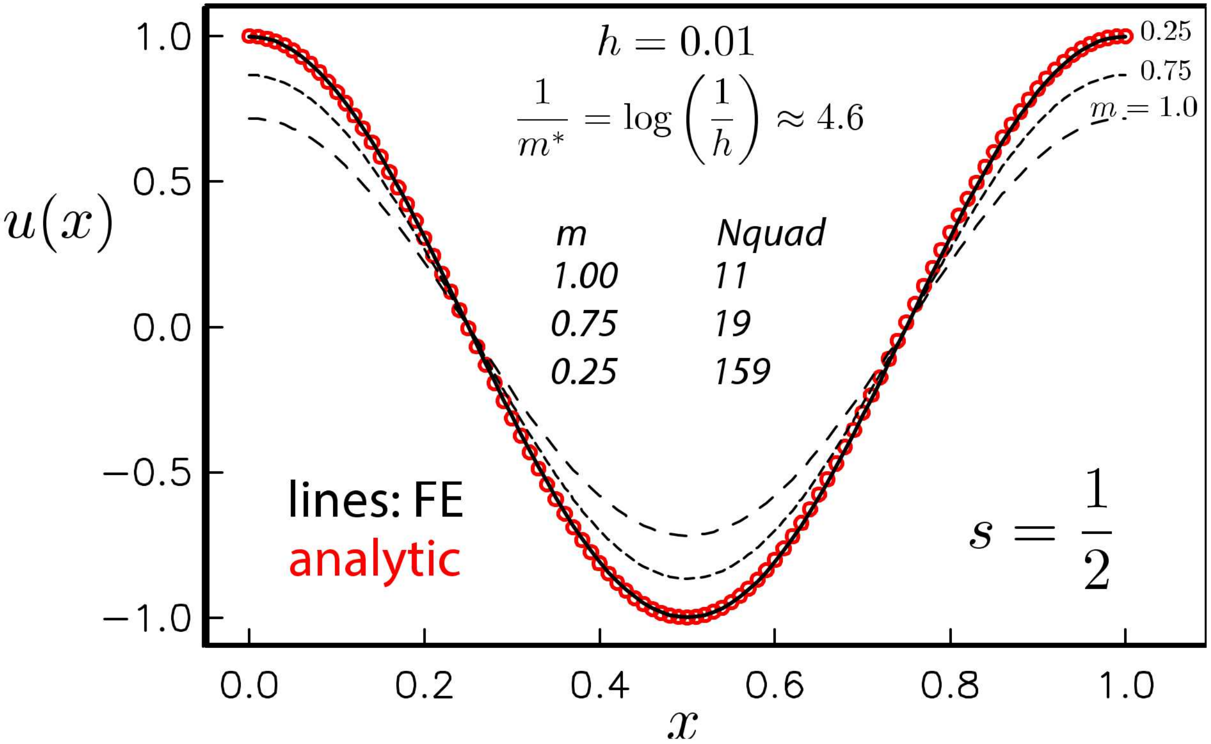


As s → 0, the support of the Helmholtz operator becomes more local, as expecte

Sinc quadrature: number of quad nodes balanced with FE discretization

$$(-\Delta)^s u(x) - u(x) = \left(\left(4\pi^2\right)^s - 1\right)\cos 2\pi x$$

$$\partial_x u = 0 \quad x = 0, 1$$

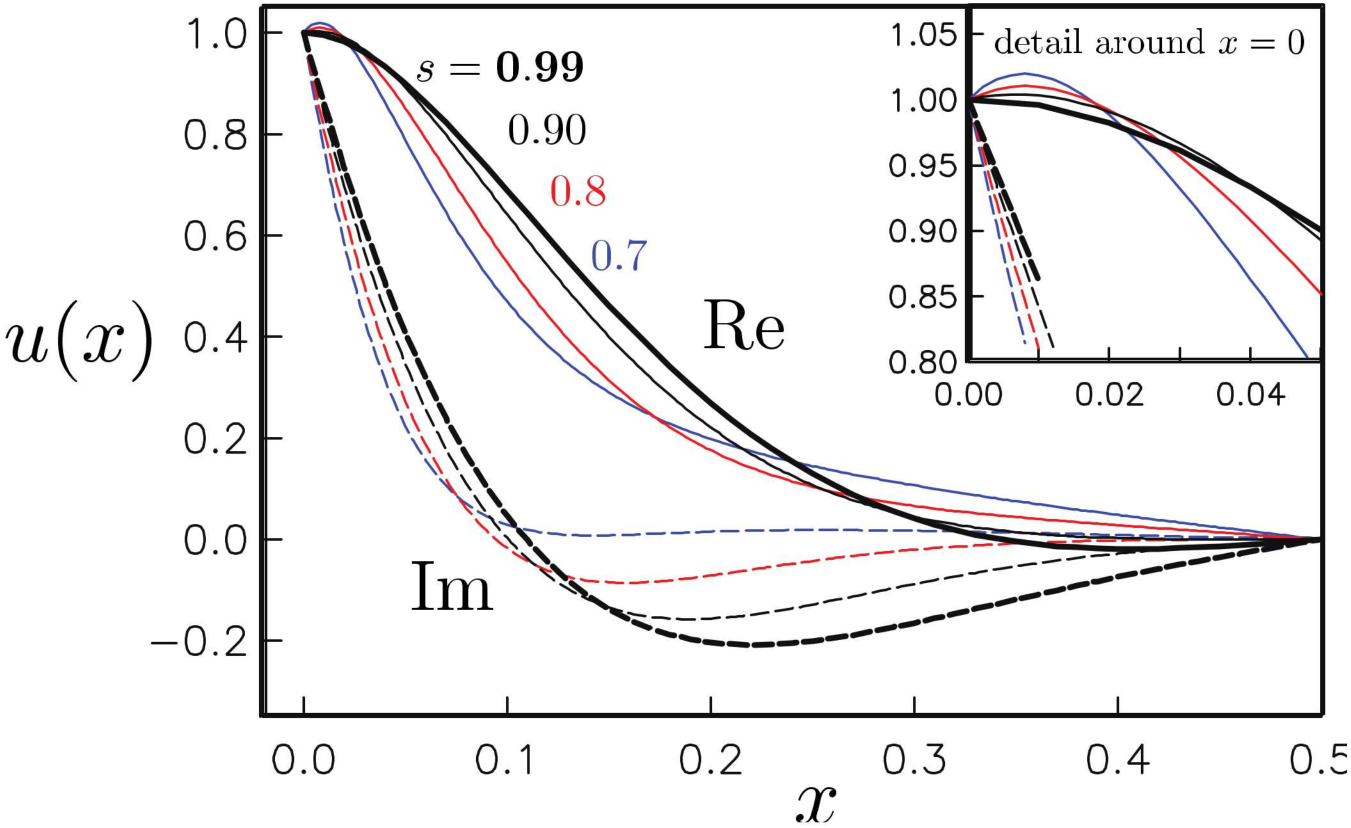


No obvious shortcuts for reducing Nquad!

1D Magnetotelluric Response of Fractional Helmholtz Earth

$$(-\Delta)^s\, u(x) + \mathrm{i}k^2\, u(x) = 0$$

$$u(0) = \sqrt{2\mathrm{i}} \qquad u(1) = -\sqrt{2\mathrm{i}}$$

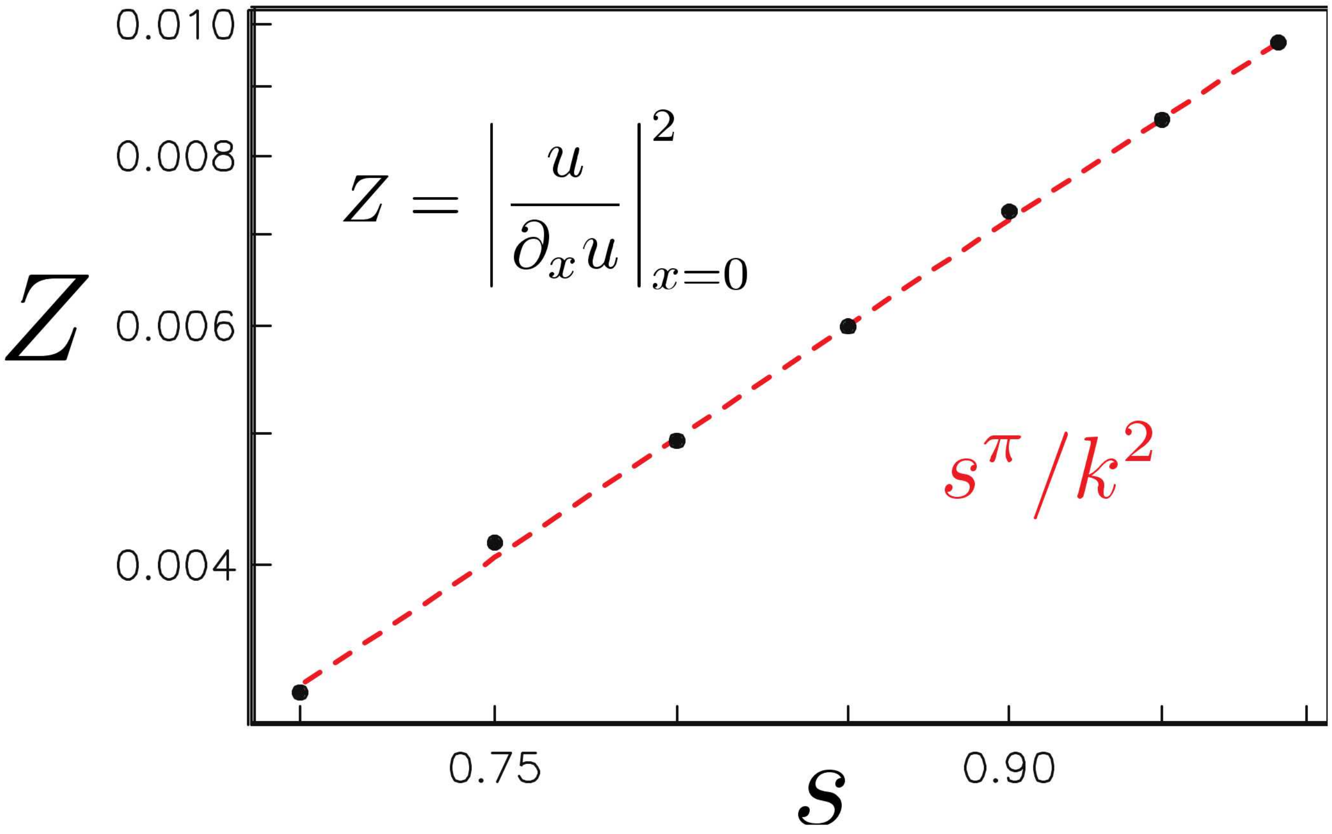


As s increases, the curvature in u is concentrated near the air/earth interface x=0.

1D Magnetotelluric Response of Fractional Helmholtz Earth

$$(-\Delta)^s u(x) + \mathrm{i}k^2 u(x) = 0$$

$$u(0) = \sqrt{2\mathrm{i}} \qquad u(1) = -\sqrt{2\mathrm{i}}$$



Magnitude of surface impedance is a function of fractional Helmholtz exponent, s

Implementation Strategies

- **Integral and regional** Laplacians require sophisticated quadrature to approximate the singular integrals. This is especially challenging in more than 1D. See Acosta et al '16 and Ainsworth et al '17.
- **Spectral** Laplacian can be realized using:
  - FFT in rectangular domains, see Antil et al '17.
  - In general domains, there are three approaches:
    - Compute the eigenvalues (λ_k) and eigenvectors (φ_k): $\rightarrow$ can be challenging, see Karniadakis et al '17.
    - Dunford-Taylor approach, see Bonito et al '15: → Requires several solves of standard diffusion equation.
    - Extension approach, see Caffarelli et al '07, Stinga et al '10, Nochetto et al 16': → local problem but one extra dimension with degenerate/singular coefficients.

Summary

- Implemented fractional Helmholtz
- Developed decomposition of Helmholtz with BCs
- Reformulation for computational improvements
- Implemented MMS verification
- Demonstrated Magnetotelluric application

Next steps:

- *Implement solution to adjoint formulation*
- *Extend fractional operator to Maxwell's*
- *Test inversion on multiscale realizations*

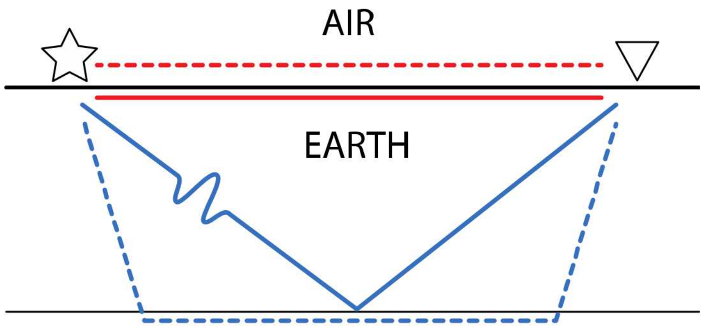
Thank you!

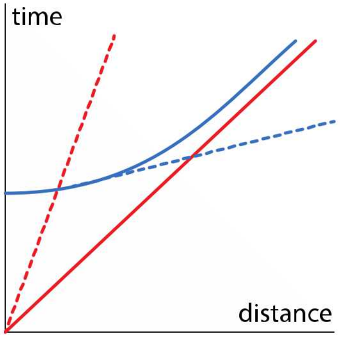
Motivation III:

subsurface imaging and predictive modeling for realistic, complex geology – conditions motivate the resolution of fine features

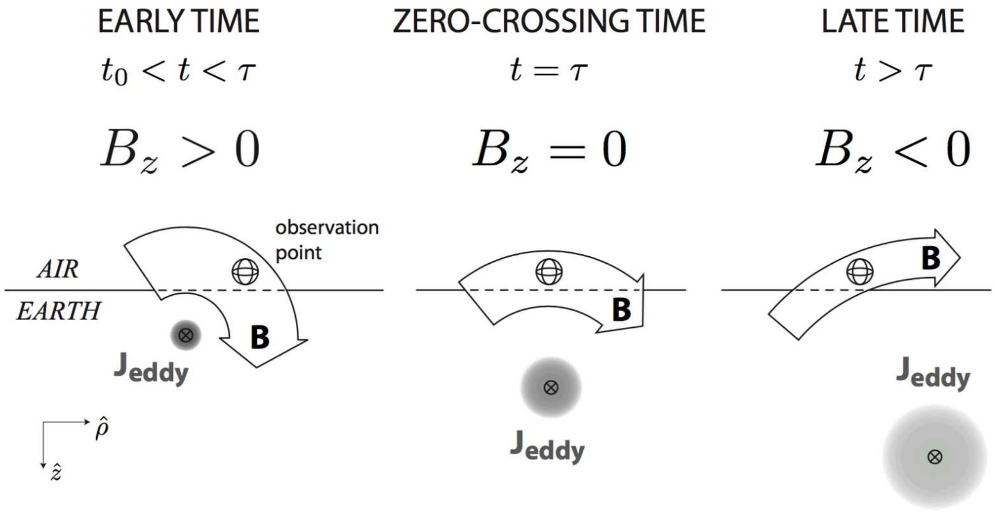
Exposures with high and low fracture frequency at same stratigraphic level

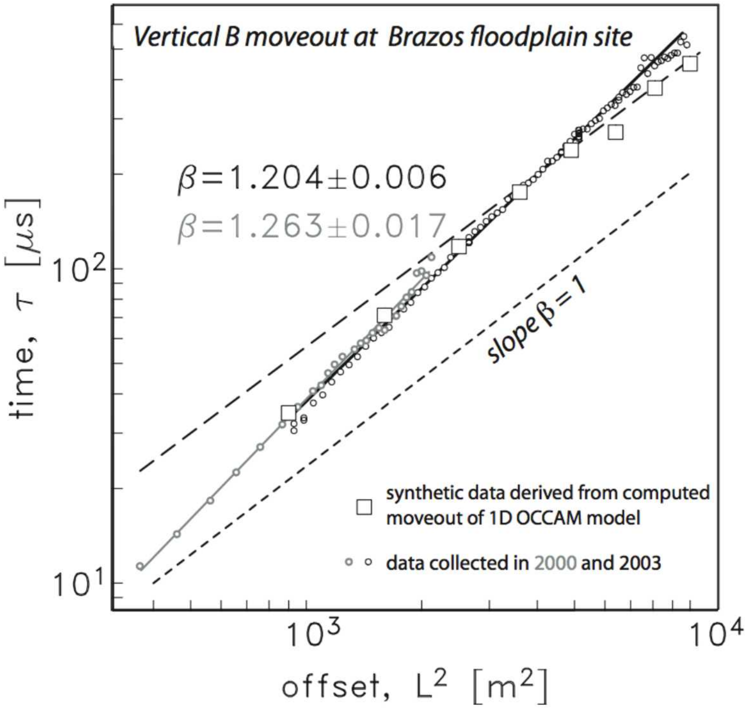
Anomalous Diffusion Experimental Evidence





Similar to seismic travel time analysis, the arrival time of the EM pulse is analyzed for consistency with classical diffusion.





Fractional Laplacian

Definition 1: (integral) Let $u \in C_0^\infty(\Omega)$ and extend it by zero outside of Ω. Then

$$(-\Delta_{I,0})^s u(x) = C_{n,s}\text{p.v.} \int_{\mathbb{R}^n} \frac{u(x) - u(z)}{|x - z|^{n+2s}}\, dz$$

where $C_{n,s}$ is a constant and p.v. is the Cauchy principal value.

Definition 2: (regional) Let $u \in C_0^\infty(\Omega)$. Then

$$(-\Delta_{\Omega,0})^s u(x) = C_{n,s}\text{p.v.} \int_{\Omega} \frac{u(x) - u(z)}{|x - z|^{n+2s}}\, dz$$

Definition 3: (Spectral) Let φ_k amd λ_k solve

$$-\Delta_{D,0}\varphi_k = \lambda_k \varphi_k, \qquad \varphi_k|_{\partial\Omega} = 0,$$

and let $u \in C_0^\infty(\Omega)$. Then

$$u = \sum_{k=1}^{\infty} u_k \varphi_k \longmapsto (-\Delta_D)^s u := \sum_{k=1}^{\infty} u_k \lambda_k^s \varphi_k .$$

Motivation: Putting it all together at the macroscopic level

Pulse propagation

Classical Gaussian ”anomalous” fractional

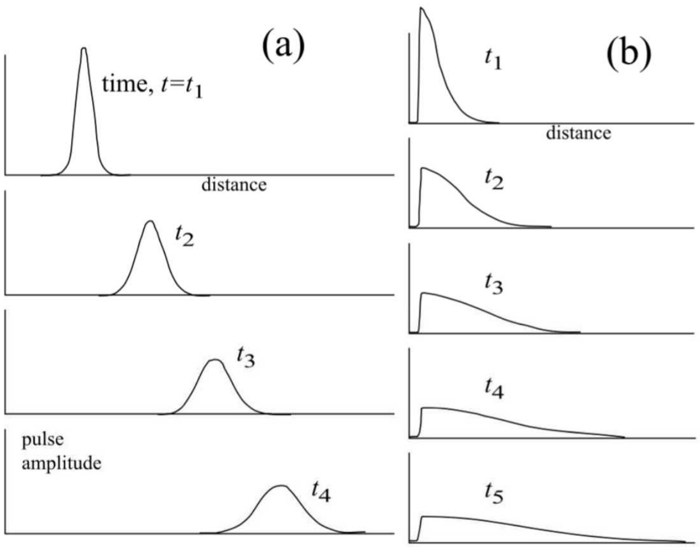
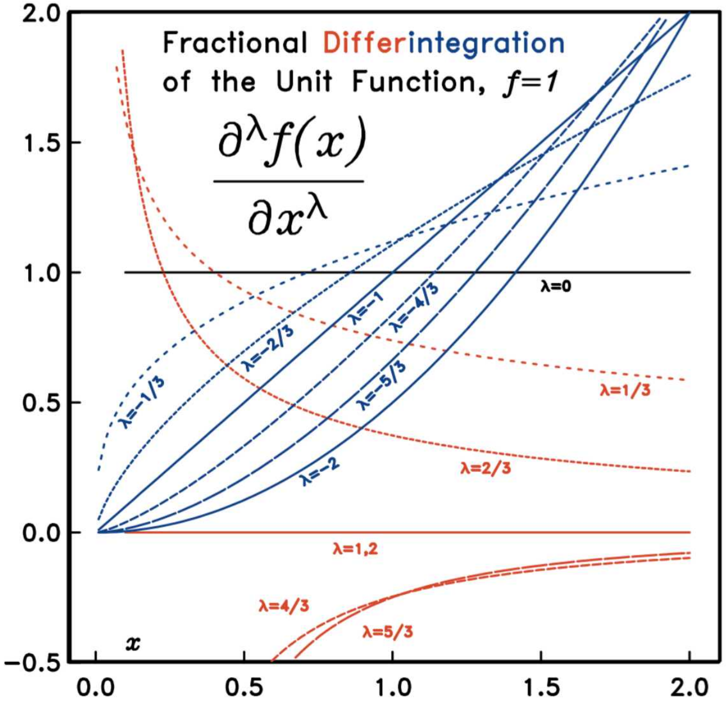


Figure 1. (a) Propagation of a Gaussian pulse $G(x,t)$ undergoing classical diffusion. (b) Propagation of a CTRW pulse $A(x,t)$ undergoing anomalous diffusion (after the work of *Scher and Montroll* [1975]).



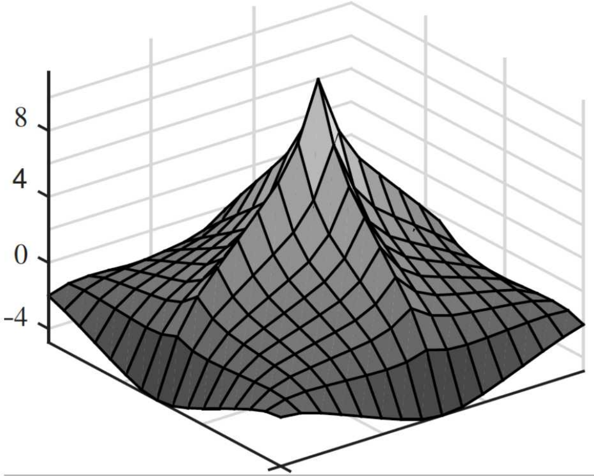
Fractional diffusion equation

$$\frac{\partial}{\partial t}A(x,t) = {}_0D_t^{1-\alpha}\left[v_\alpha \frac{\partial^2}{\partial x^2}A(x,t)\right]$$

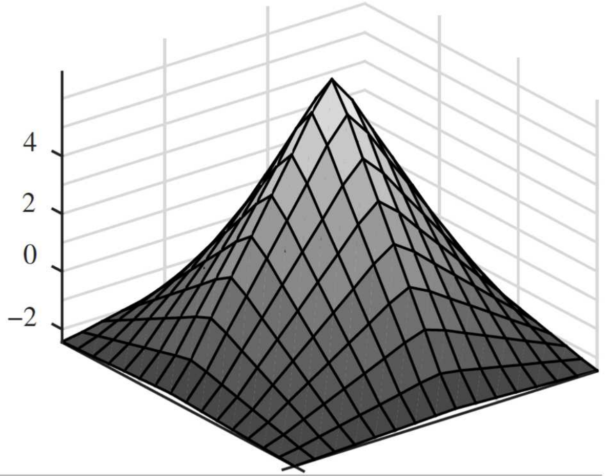
Riemann-Louiville convolution

$${}_0D_t^{1-\alpha}A(x,t) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\left[\int_0^t \frac{A(x,t')}{(t-t')^{1-\alpha}}\,\mathrm{d}t'\right]$$

Laplacian with different exponents using the extension problem strategy



RHS



$\alpha = 0.5$

Complications:
- Preconditioning for large scale systems

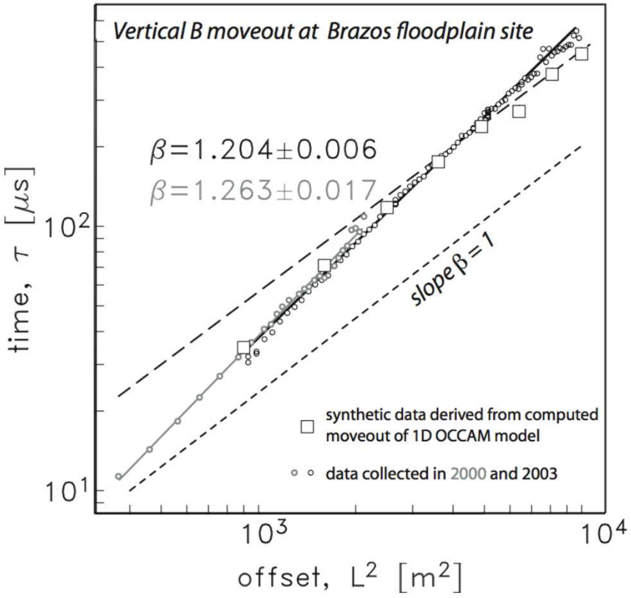
Fractional time operator

$$\mathcal{F}\left(\frac{d^n}{dt^n}f\right) = (i\omega)^n \mathcal{F}(f)$$

Complications:

- Optimization requires multiple frequencies to recover fractional Brownian motion
- Complex value exponent needs to be calculated a priori:

$$(i\omega)^\alpha = \gamma\omega + \beta i$$



alpha	gamma	beta
2	-1	0
0.5	0.7071	0.7071
0.25	0.9238	0.3826