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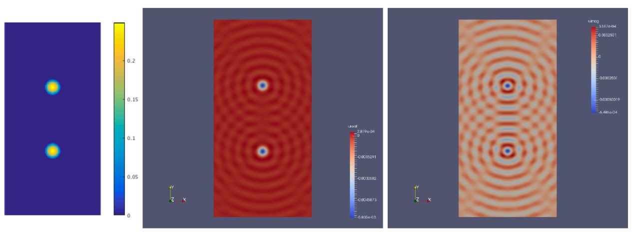

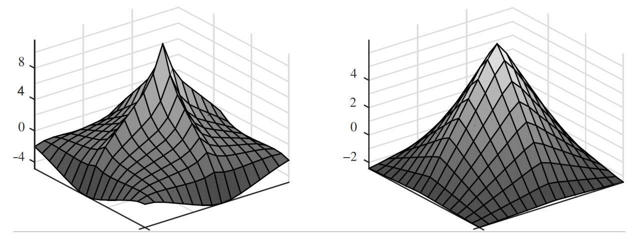

Fractional Differential Operators to Detect Multiscale Geophysical Features

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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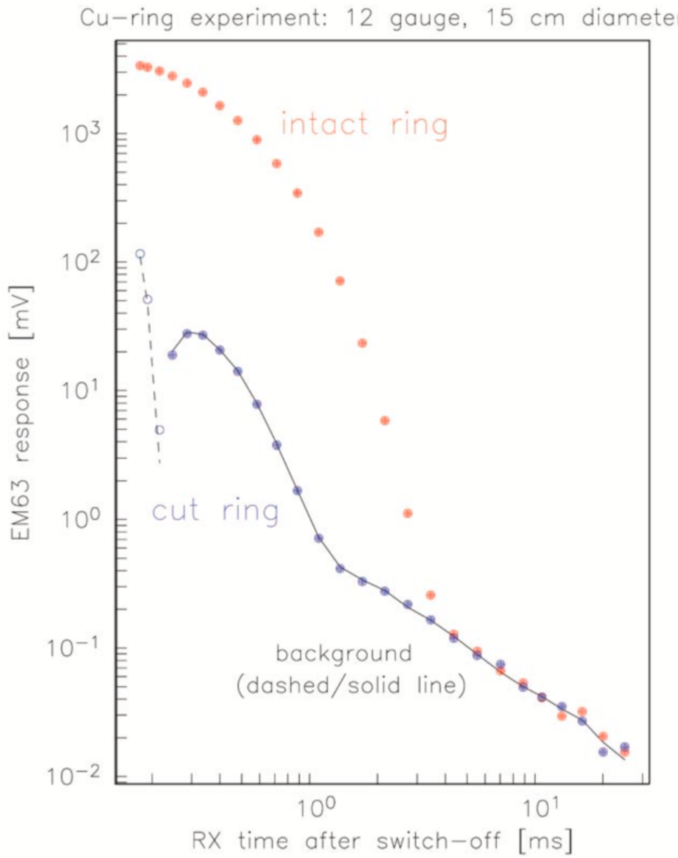
Motivation

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



Motivation: Putting it all together at the macroscopic level

Pulse propagation

Classical Gaussian ”anomalous” fractional

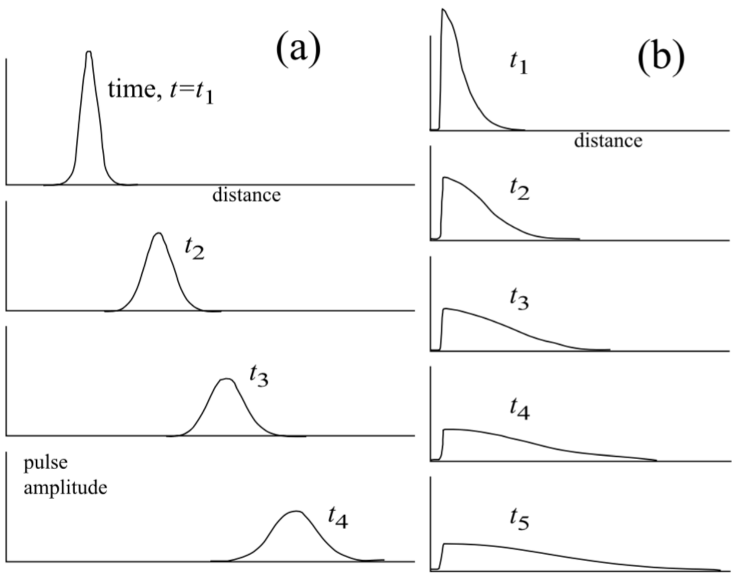
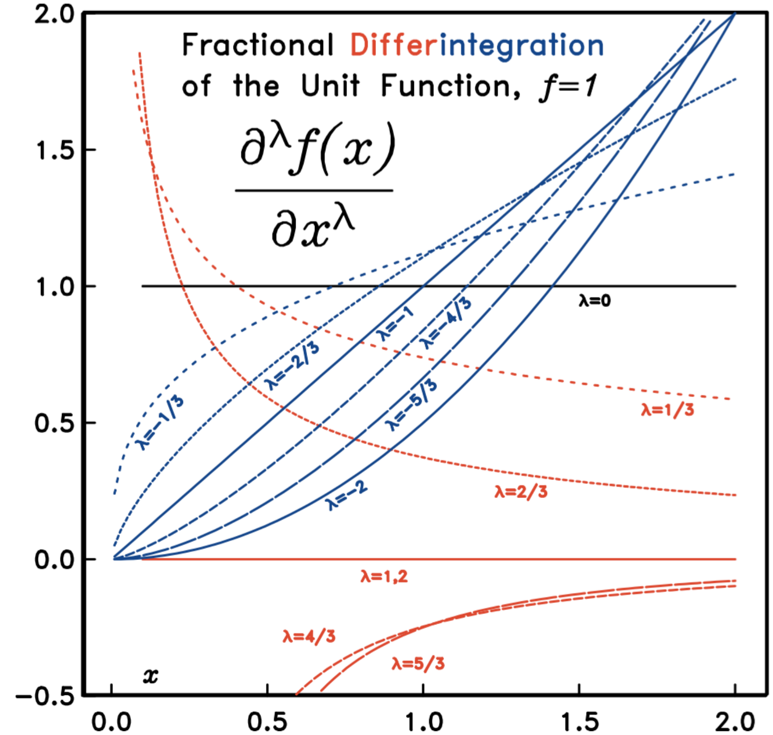


Figure 1. (a) Propagation of a Gaussian pulse $G(x,t)$ undergoing classical diffusion. (b) Propagation of a CTRW pulse $A(x,t)$ undergoing anomalous diffusion (after the work of *Scher and Montroll* [1975]).



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

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

Outline

- Maxwell's
- Fractional Laplacian and time operator
- Target optimization problem
- Solution strategy
- Implementation
- Summary

Maxwell's to Fractional Helmholtz

$$\frac{\partial \vec{\mathcal{B}}}{\partial t} + \nabla \times \vec{\mathcal{E}} = 0,$$
$$\frac{\partial \vec{\mathcal{D}}}{\partial t} - \nabla \times \vec{\mathcal{H}} = -\vec{\mathcal{J}},$$
$$\nabla \cdot \vec{\mathcal{D}} = \rho,$$
$$\nabla \cdot \vec{\mathcal{B}} = 0,$$

$$\nabla \times \vec{E} = i\omega\mu_0 \vec{H}$$
$$\nabla \times \vec{H} = -i\omega\epsilon_0 n^2(\vec{x})\vec{E}$$

First order Maxwell's

$$\nabla \times \nabla \times E = i\omega\mu_0 \nabla \times \vec{H} = \omega^2 \mu_0 \epsilon_0 n^2 \vec{E}$$

$$(\nabla^2 + k^2 n^2)\vec{E} = -\nabla[\vec{E} \cdot \nabla \ln n^2(\vec{x})]$$

Curl Curl system

$$\begin{aligned} -c^2 \Delta u(x) - \omega^2 u(x) &= f, \quad \in \Omega \\ u(x) &= 1, \quad \in \Gamma_1 \end{aligned}$$

$$-i\omega u(x) + c\frac{\partial u(x)}{\partial n} = 0 \quad \in \Gamma_2$$

Helmholtz

$$-c^2 \Delta u + (i\omega)^{2\alpha} = f \quad \in \Omega$$
$$-(iw)^\alpha u + c\frac{\partial u(x)}{\partial n} = 0 \quad \text{on } \Gamma$$

Fractional Helmholtz

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

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

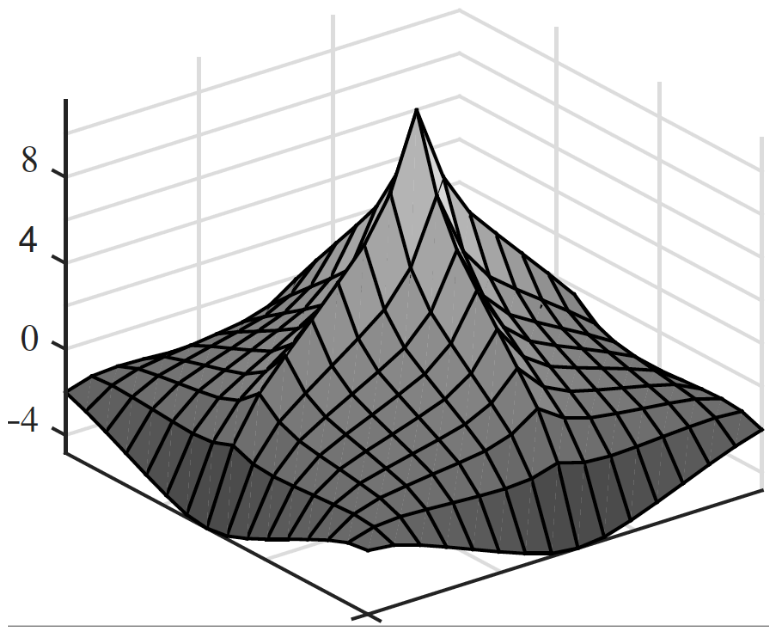
and let $u \in C_0^\infty(\Omega)$. Then

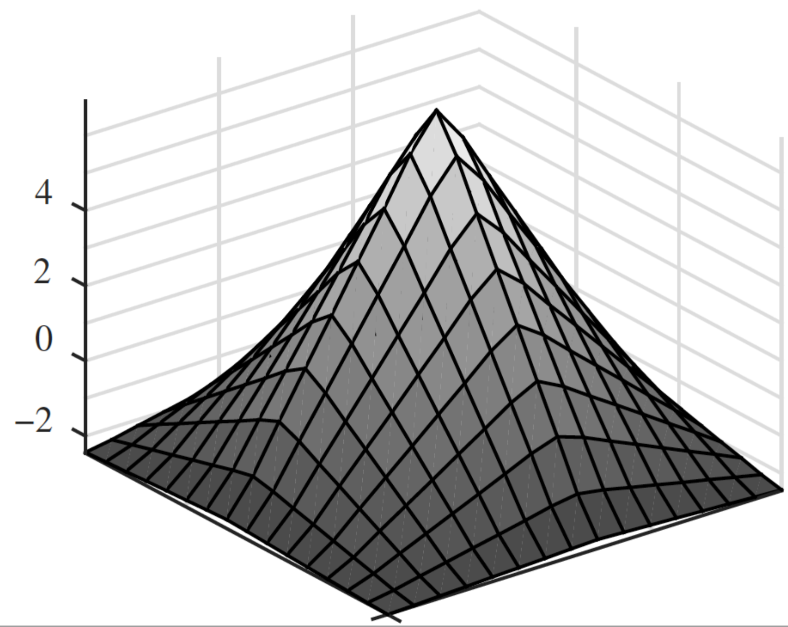
$$u = \sum_{k=1}^{\infty} u_k \varphi_k \longmapsto (-\Delta_D)^s u := \sum_{k=1}^{\infty} u_k \lambda_k^s \varphi_k.$$

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: $\rightarrow$ Requires several solves of standard diffusion equation.
    - Extension approach, see Caffarelli et al '07, Stinga et al '10, Nochetto et al 16': $\rightarrow$ local problem but one extra dimension with degenerate/singular coefficients.

Laplacian with different exponents





$\alpha = 0.5$ $\alpha = 1.0$

Fractional time operator

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

Implementation Issues:

- Straight forward except…..
- Need real and imaginary part
- Boundary condition requires fractional exponent
- Complex value exponent needs to calculated a priori
- Optimization requires multiple frequencies to recover fractional Brownian motion

Target Optimization Problem

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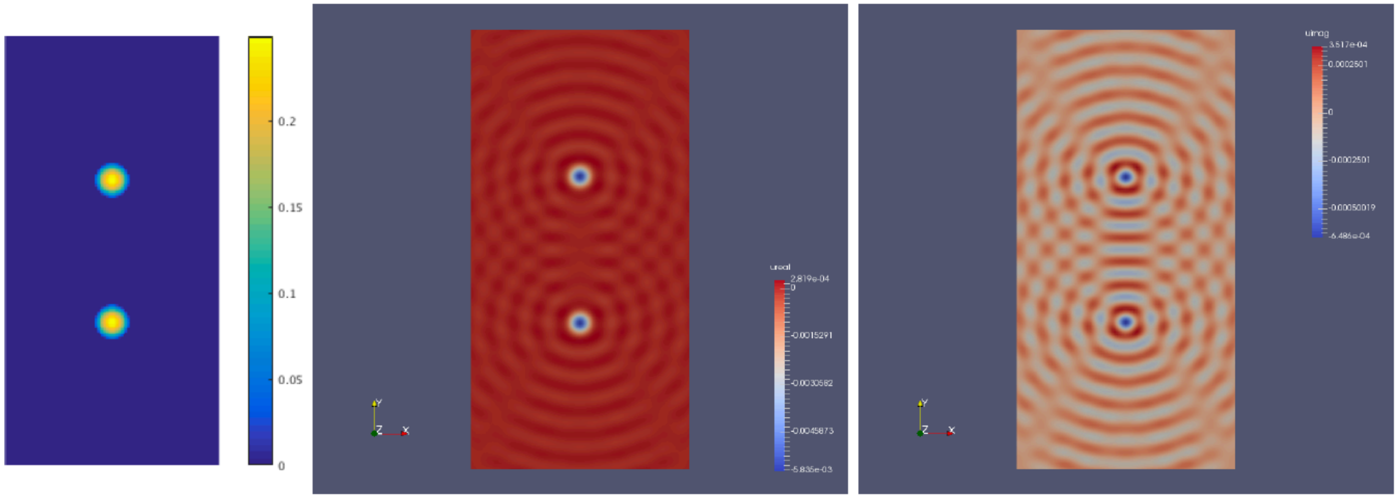
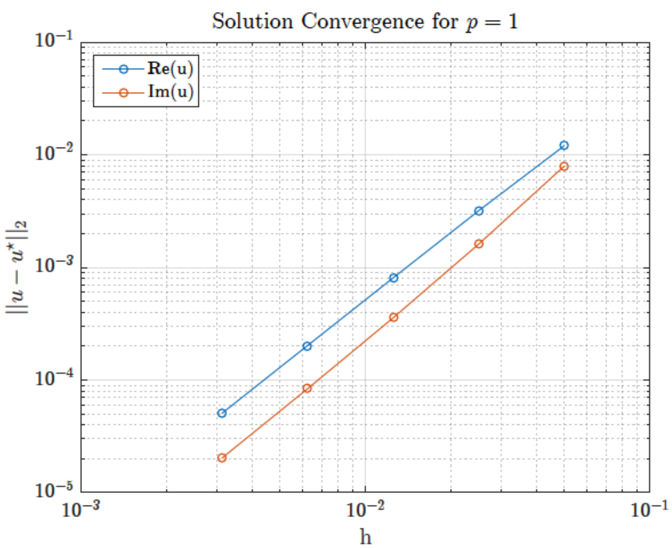
$$\min_{\alpha} \ \mathcal{J} = \frac{1}{2}\int_{\Omega} (u-u^*)^2 \delta(x-x^*) dx + \frac{\beta}{2}\int_{\Omega} \alpha^2 dx$$

$$\text{where } u \text{ solves: } -c^2\Delta u + (i\omega)^{2\alpha} = f \quad \in \Omega$$

$$-(iw)^{\alpha} u + c\frac{\partial u(x)}{\partial n} = 0 \quad \text{on } \Gamma$$

MMS verification $\alpha = 1.0$

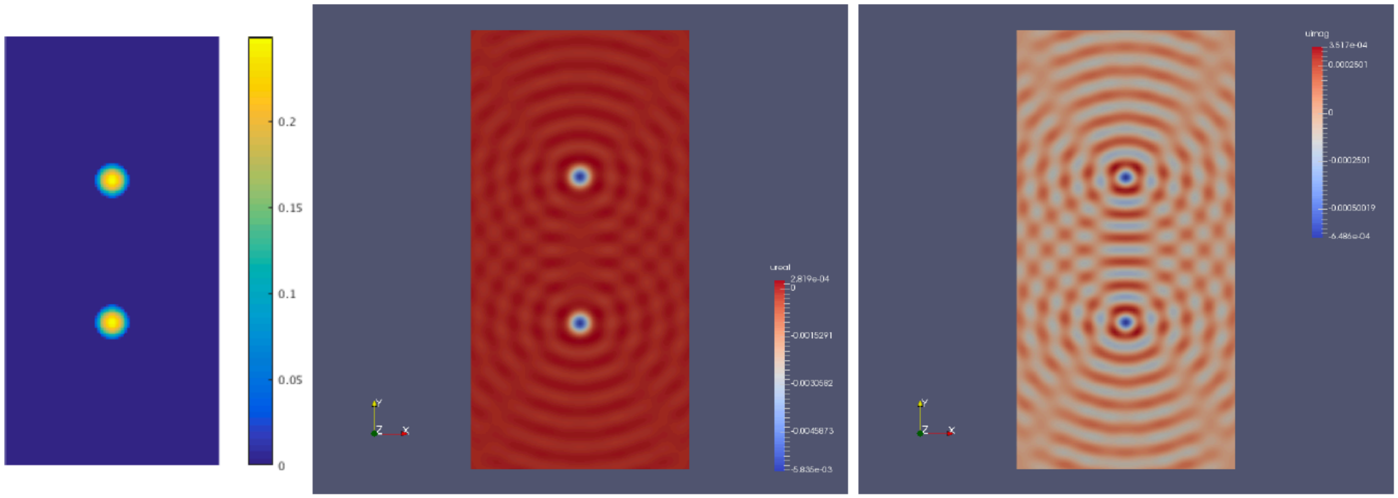




$$u^\star = (1+i)(\sin(2\pi x)\sin(2\pi y)), \quad c^2 = (x+i)^2, \quad \omega^2 = 1,$$

$$f = ((2-2x)(2\pi\cos(2\pi x)\sin(2\pi y)) + (8\pi^2(x^2-2x-1)-1)(\sin(2\pi x)\sin(2\pi y))) \\ + i((-2-2x)(2\pi\cos(2\pi x)\sin(2\pi y)) + (8\pi^2(x^2+2x-1)-1)(\sin(2\pi x)\sin(2\pi y))).$$

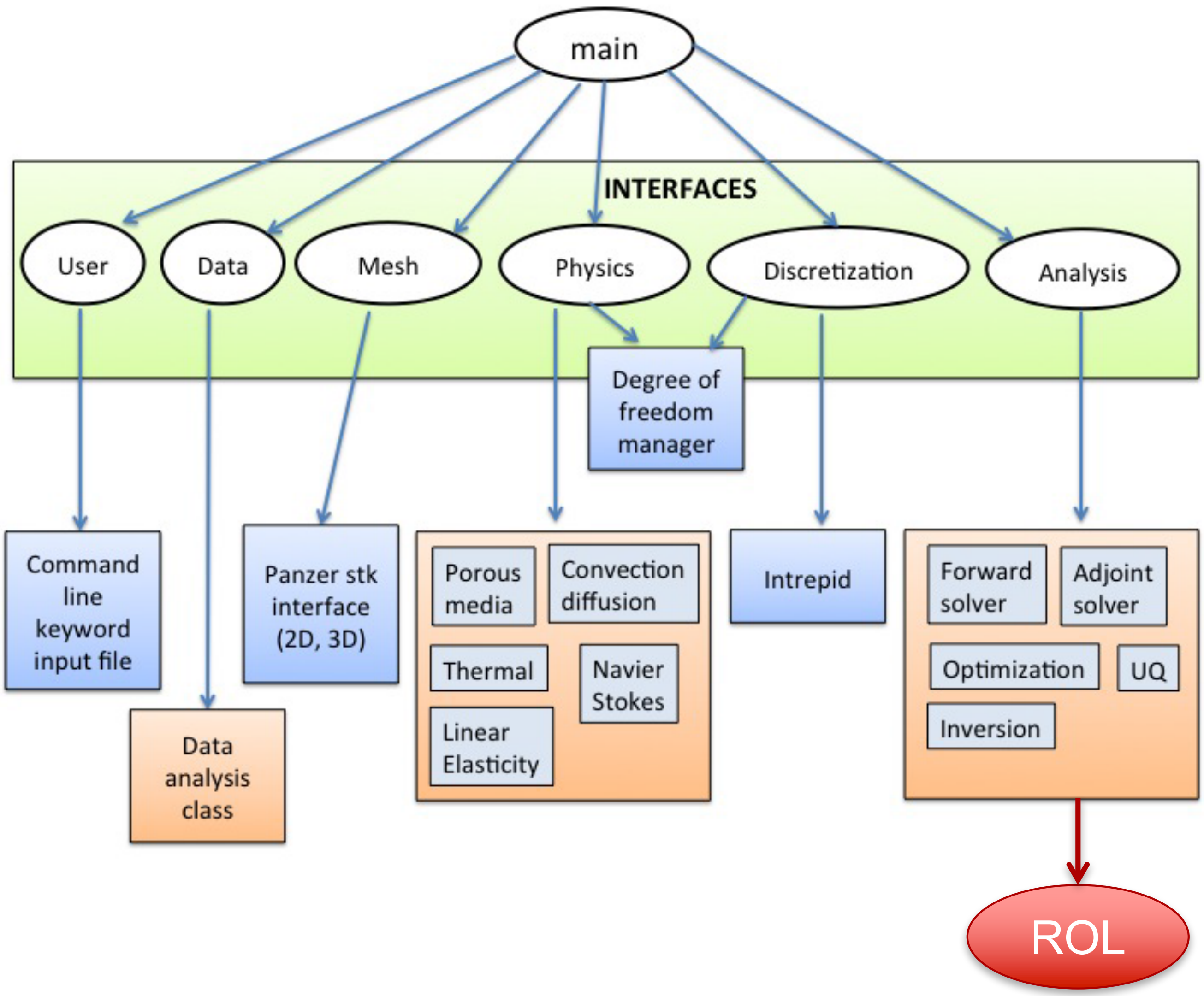
Fractional Inversion Results



Alpha true	Alpha Inverted	Error
1.0	1.0	0.0
0.5	0.49	0.01

Note:
- Synthetic sensors
- Add noise
- Invert for exponent

Multi scale/physics Interface for Large scale Optimization (MILO)



strong form:

$$\frac{\partial T}{\partial t} - D\frac{\partial T}{\partial dx} = f$$

weak form:

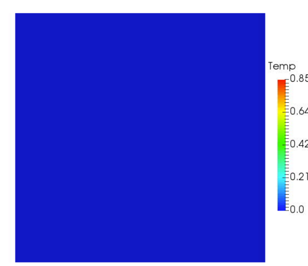
$$\int_\Omega \rho c_p \frac{\partial T}{\partial t} v + D\frac{\partial T}{\partial x}\frac{\partial v}{\partial x} - f \cdot v d\Omega = 0$$

code:

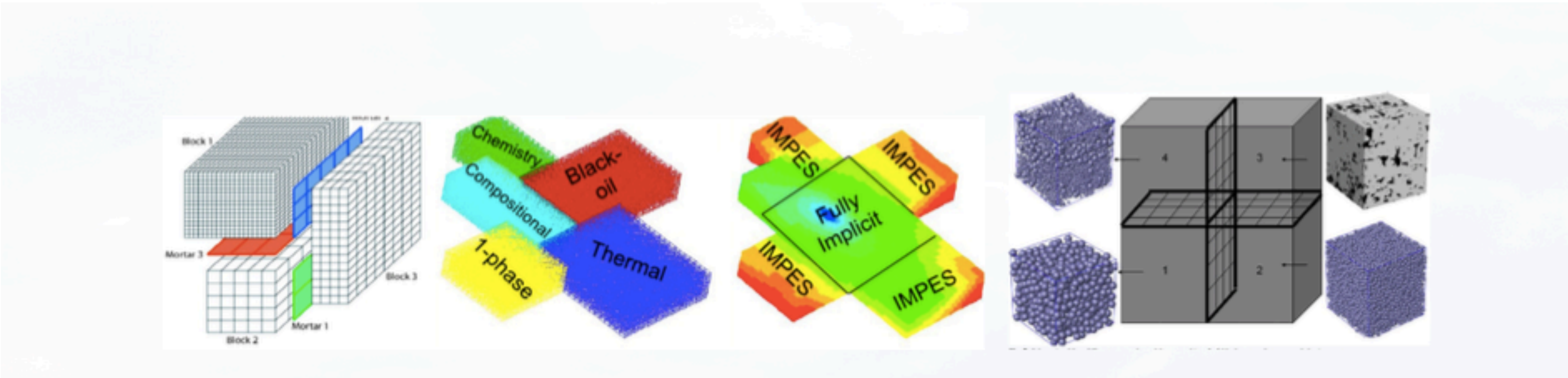
```
Res=rho(k)*cp(k)*udot*v+diff(k)*dTdx*dvdx –f*v
```

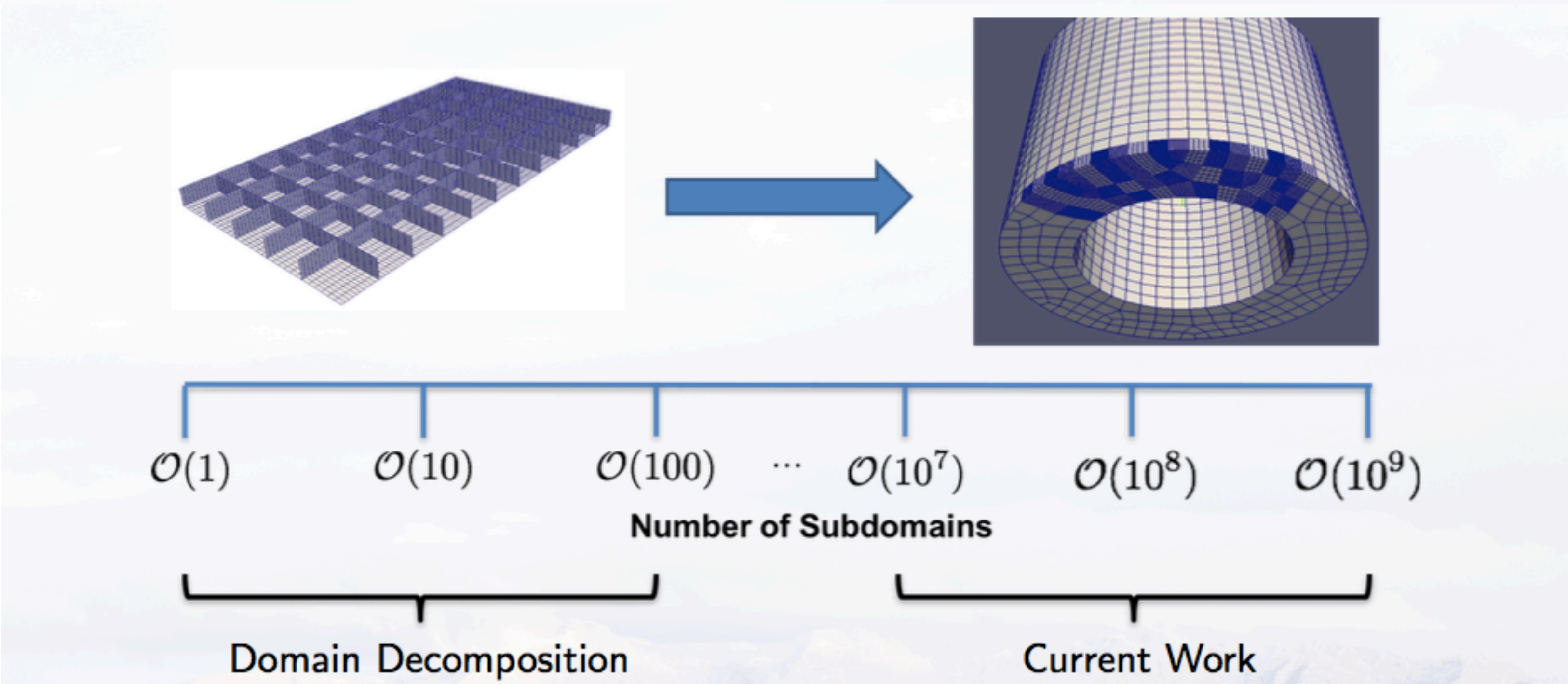
Automates:

- 3D Parallel
- Adjoints
- Opt under uncertainty
- Unstructured
- Multiscale
- Multiphysics



Novel Development of Multiscale Capability using Mortar Methods





Summary

- Implemented fractional Helmholtz with adjoint and gradients
- Demonstrated simple inversion capability
- Software infrastructure enables automatic interface to optimization

Future work :

- *Implement multiple frequency inversion*
- *Implement solution to space-time cylinder problem*
- *Extend to Maxwell's*

Thank you!