Research Highlights: Michigan State University

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Research Area 1: Theory of non-local operators

- Zolotarev fractional derivative
- Nonlocal Dirichlet boundary conditions
- Duality for tempered fractional diffusion
- PhD project: Fractional calculus and turbulence
- PhD project: Fractional phase field model of failure
Area 2: Numerical solution of fractional PDEs

- Petrov-Galerkin spectral methods (update)

- Fractional Neumann boundary conditions

- Open problem: Fractional Neumann BC in higher dimensions

- Open problem: Numerical methods for Zolotarev derivative
Discontinuity in the fractional diffusion equation

Fractional diffusion equation: \[ \frac{\partial u(x,t)}{\partial t} = \frac{\partial^\alpha u(x,t)}{\partial x^\alpha} \]

Point source solution for \( \alpha = 1.3, 1.1, 1.06, 1.04 \) (right to left) and \( t = 1 \). Solution has mean zero for all \( 1 < \alpha \leq 2 \), but peak drifts to \( -\infty \) as \( \alpha \downarrow 1 \).
The new Zolotarev fractional diffusion equation for $0 < \alpha \leq 2$ is continuous through $\alpha = 1$. 
New Zolotarev fractional derivative

For \( \alpha \neq 1 \) the Zolotarev fractional derivative

\[
D_x^{\alpha,\beta} f(x) = \beta \tan(\theta) \frac{\partial f(x)}{\partial x} - \frac{p}{\cos(\theta)} \frac{\partial^\alpha f(x)}{\partial x^\alpha} - \frac{q}{\cos(\theta)} \frac{\partial^\alpha f(x)}{\partial (-x)^\alpha},
\]

with \( \theta = \frac{\pi \alpha}{2} \), \( \beta = p - q \), Riemann-Liouville FD on the right.

The Zolotarev derivative decomposes the fractional Laplacian:

\[
\Delta^\alpha f(x) = \frac{d^\alpha}{d|x|^\alpha} f(x) = \frac{1}{2} \left[ D_x^{\alpha,1} f(x) + D_x^{\alpha,-1} f(x) \right].
\]

Applications: Groundwater hydrology, Landau (1944) model for ionization losses, power law wave equation for ultrasound.
**Fractional Dirichlet boundary conditions**

The fractional derivative is a nonlocal operator \((n = \lceil \alpha \rceil)\):

\[
\mathbb{D}^\alpha_{[L,x]} f(x) = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_L^x \frac{f(y)}{(x - y)^{\alpha + 1 - n}} dy,
\]

so zero Dirichlet boundary conditions become nonlocal!

Note that \(\mathbb{D}^\alpha_{[L,x]} f(x) = \mathbb{D}^\alpha_{[-\infty,x]} f(x) = \frac{\partial^\alpha f(x)}{\partial x^\alpha}\) applied to the zero extension: \(f(x) = 0\) for \(x < L\).

We show zero Dirichlet BC are absorbing for any nonlocal operator generating a Feller process:

\[
L_x f(x) := -c(x)f(x) + l(x) \cdot \nabla f(x) + \nabla \cdot Q(x)\nabla f(x) \\
+ \int_{y \neq 0} \left( f(x + y) - f(x) - \nabla f(x) \cdot y I_{\{y \leq 1\}} \right) N(x, dy)
\]

We then show fractional Dirichlet problems are well-posed.
Dirichlet boundary conditions (slide 2)

A stable Lévy process $X_t$ has generator

$$L_x f(x) = -a \frac{\partial}{\partial x} f(x) + b \frac{\partial^\alpha}{\partial x^\alpha} f(x) + c \frac{\partial^\alpha}{\partial (-x)^\alpha} f(x).$$

using Riemann-Liouville derivatives on the entire real line.

The process $X_t^D$ absorbed upon exiting $D = [L, R]$ has generator

$$L^D_x f(x) = -a \frac{\partial}{\partial x} f(x) + b \mathbb{D}^\alpha_{[L,x]} f(x) + c \mathbb{D}^\alpha_{[x,R]} f(x).$$

The finite RL derivatives code the zero exterior condition.

Finite domain generator is the same, applied to zero extension.

Extensions: Higher dimensions, variable coefficients, $\alpha = \alpha(x)$. 
Tempered space-time duality

Extends space-time duality to tempered fractional derivatives (see also Jim Kelly poster at this meeting)

Tempered fractional diffusion equation \((1 < \alpha < 2)\):

\[
\partial_t u(x, t) = D_{-x}^{\alpha, \lambda} u(x, t) = e^{\lambda x} D_x^{\alpha} \left[ e^{-\lambda x} u(x, t) \right] - \lambda^\alpha u(x, t).
\]

Dual equation \((\beta = 1/\alpha)\):

\[
-\partial_x h(x, t) = D_t^{\beta, \lambda} h(x, t) = e^{-\lambda \alpha t} D_{[0,t]}^{\beta} \left[ e^{\lambda \alpha t} h(x, t) \right] - \lambda h(x, t).
\]

Objective: Convert fractional BC in space to time operator

Rationale: Easy to handle BC for time-fractional equations
Interpretation: The tempered inverse stable subordinator is the positive part of a tempered fractional diffusion in space.
Velocity spectrum near a wall has a tempered power law correlation, we fit a tempered fractional time series model.
Tempered fractional Navier-Stokes

Replace Laplacian $\Delta$ with fractional Laplacian $\Delta^{\alpha}$

Replace time derivative with (tempered) fractional derivative

Model passive scalar transport

Particle tracking using stable processes

Second part of PhD for Mehdi Samiee
Fractional phase field modeling

Reconsider phase field equations for material failure

Empirical observations of power law Energy spectrum

Investigate fractional phase field modeling

Perform relevant uncertainty quantification

PhD project for Eduardo de Moraes
Area 2: Numerical solution of fractional PDEs

- Petrov-Galerkin spectral methods (update)
- Fractional Neumann boundary conditions
- Open problem: Fractional Neumann BC in higher dimensions
- Open problem: Numerical methods for Zolotarev derivative
Petrov-Gelerkin spectral methods (update)

Space-time diffusion in $d$ dimensions with zero Dirichlet BC.

Jacobi poly-fractonomials are temporal basis/test functions.

Legendre polynomials are spatial basis/test functions.

Numerical implementation for fast linear solver.

Stability and error analysis.

Two papers were revised and resubmitted to the *Journal of Computational Physics*. 


Fractional BC: Mass balance approach

Markov Chain transition model

\[
\begin{align*}
\frac{\partial u(x, t)}{\partial t} &= \frac{\partial^\alpha u(x, t)}{\partial x^\alpha} \\
\Rightarrow u_{k,j+1} &= u_{kj} + h^{-\alpha} \Delta t \sum_{i=0}^{[x/h]+1} g_i^\alpha u_{k-i+1,j}
\end{align*}
\]

\[
g_n = (-1)^n \binom{n}{\alpha}
\]
Absorbing boundary conditions

Numerical solution to fractional diffusion equation with $\alpha = 1.5$ on $0 \leq x \leq 1$ with absorbing BC at time $t = 0$ (solid line), $t = 0.05$ (dashed), $t = 0.1$ (dash dot), $t = 0.5$ (dotted).
Reflecting boundary conditions

Numerical solution to fractional diffusion equation with $\alpha = 1.5$ on $0 < x < 1$ with zero flux BC at time $t = 0$ (solid line), $t = 0.05$ (dashed), $t = 0.1$ (dash dot), $t = 0.5$ (dotted).
Fractional Neumann boundary conditions

The reflecting boundary conditions are written as

\[ \frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}} u(0, t) = 0 \quad \text{and} \quad \frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}} u(1, t) = 0. \]

This is a zero flux BC because

\[ \frac{\partial^\alpha}{\partial x^\alpha} u(x, t) = \frac{\partial}{\partial x} \frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}} u(x, t) = -\frac{\partial}{\partial x} q(x, t) \]

where the flux \( q(x, t) = -\frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}} u(x, t). \)

When \( \alpha = 2 \) this reduces to the usual first derivative condition.

The steady state solution is \( u(x, t) = (\alpha - 1)x^{\alpha-2} \) on \( 0 < x < 1. \)

This solution has zero flux for all \( 0 < x < 1. \)
Reflecting on the left, absorbing on the right

Numerical solution to fractional diffusion equation with $\alpha = 1.5$
on $0 < x < 1$ with Neumann BC at $x = 0$, Dirichlet at $x = 1$, at
time $t = 0$ (solid line), $t = 0.05$ (dashed), $t = 0.1$ (dash dot),
$t = 0.5$ (dotted).
Absorbing on the left, reflecting on the right

Numerical solution to fractional diffusion equation with $\alpha = 1.5$ on $0 < x < 1$ with Dirichlet BC at $x = 0$, Neumann at $x = 1$, at time $t = 0$ (solid line), $t = 0.05$ (dashed), $t = 0.1$ (dash dot), $t = 0.5$ (dotted).
Which fractional derivative?

Riemann-Liouville fractional derivative of order $1 < \alpha < 2$ :

$$
\mathbb{D}^\alpha_{[L,x]} f(x) = \frac{1}{\Gamma(2 - \alpha)} \frac{d^2}{dx^2} \int_L^x \frac{f(y)}{(x - y)^{\alpha - 1}} dy.
$$

Caputo fractional derivative of order $1 < \alpha < 2$ :

$$
\partial^\alpha_{[L,x]} f(x) = \frac{1}{\Gamma(2 - \alpha)} \int_L^x \frac{f'''(y)}{(x - y)^{\alpha - 1}} dy.
$$

Caputo flux (the middle path):

$$
\mathbb{D}^\alpha_{[L,x]} f(x) = \frac{1}{\Gamma(n - \alpha)} \frac{d}{dx} \int_L^x \frac{f'(y)}{(x - y)^{\alpha - 1}} dy.
$$

We will show that Caputo is inappropriate for diffusion modeling!

The Caputo flux model is promising…
Caputo fractional diffusion not mass preserving!

Numerical solution to Caputo fractional diffusion equation with \( \alpha = 1.5 \) on \( 0 < x < 1 \) with zero Dirichlet BC at time \( t = 0 \) (solid line), \( t = 0.01 \) (dashed), \( t = 0.04 \) (dash dot), \( t = 0.2 \) (dotted).
Absorbing boundary conditions (Caputo flux)

Since $D_{[0,x]}^{\alpha}u(x,t) = \mathcal{D}_{[0,x]}^{\alpha}u(x,t) - u(0,t)x^{-\alpha}/\Gamma(1-\alpha)$, solution is the same as Riemann-Liouville for left Dirichlet BC $u(0,t) = 0$. 
Reflecting boundary conditions (Caputo flux)

Now the steady state solution is $u(x, t) = 1$ for all $0 < x < 1$ (zero Caputo flux).
Reflect left, absorb right (Caputo flux)

Numerical solution to fractional diffusion equation Caputo flux on \(0 < x < 1\) with Neumann BC at \(x = 0\), Dirichlet at \(x = 1\), for \(\alpha = 1.5\), at time \(t = 0\) (solid line), \(t = 0.05\) (dashed), \(t = 0.1\) (dash dot), \(t = 0.5\) (dotted).
Absorb left, reflect right (Caputo flux)

Same as Riemann-Liouville due to left Dirichlet BC.
Idea: Zero flux BC for the fractional Laplacian

The fractional Laplacian $\Delta^{\alpha}f(x)$ has FT $-\|k\|^{\alpha}\hat{f}(k)$.

Then $\Delta^{\alpha} = -(-\Delta)^{\alpha/2}$ using operator fractional powers.

Then we can write

$$-(-\Delta)^{\alpha/2}u = -(-\Delta)(-\Delta)^{\alpha/2-1}u = \nabla \cdot \nabla (\Delta^{\alpha/2-1}u) = -\nabla \cdot q$$

where the flux $q = -\nabla (-\Delta)^{\alpha/2-1}u$ using the Riesz fractional integral (Riesz potential) $(-\Delta)^{\alpha/2-1}u$.

Setting $n \cdot \nabla (-\Delta)^{\alpha/2-1}u = 0$ gives a zero-flux BC.
Idea: Neumann BC for Convolution flux model

Cushman and Ginn (1993) convolution flux model

\[
\frac{\partial u(x, t)}{\partial t} = \nabla \cdot \int K(x - y, t) \nabla u(y, t) \, dy.
\]

Take \( K(y, t) \) power law for a fractional diffusion.

Traditional conservation of mass:

\[
\frac{\partial u(x, t)}{\partial t} = -\nabla \cdot q(x, t)
\]

where \( q(x, t) = -\int K(x - y, t) \nabla u(y, t) \, dy \) is the convolution flux.

Set \( n \cdot q = 0 \) on the boundary for zero flux BC.

Neumann BC for a general nonlocal diffusion model!
Open problem: Numerical methods for Zolotarev dvt

Grünwald-Letnikov approximation for $\alpha \neq 1$:

$$\frac{d^\alpha f(x)}{dx^\alpha} \approx h^{-\alpha} \sum_{i=0}^{\infty} g_i^\alpha f(x - (i - 1)h)$$

using the Grünwald weights

$$g_i^\alpha = (-1)^i \binom{\alpha}{i} = -\alpha(1 - \alpha) \cdots (i - 1 - \alpha) \frac{i!}{i!}.$$ 

When $\alpha = 1$ this is the first derivative!

For $\alpha = 1$ we can write

$$D_{x,1}^\alpha f(x) = \frac{2}{\pi} \int_0^\infty \left( f(x - y) - f(x) + f'(x) \sin y \right) y^{-2} dy$$

How can we approximate the Zolotarev derivative?


7. Anomalous Diffusion with Ballistic Scaling: A New Fractional Derivative, Journal of Computational and Applied Mathematics, to appear the Special Issue on Modern fractional dynamic systems and applications (with James F. Kelly, Department of Statistics and Probability, Michigan State University; and Cheng-Gang Li, Department of Mathematics, Southwest Jiaotong University, Chengdu, China).
8. Boundary Conditions for Fractional Diffusion, revised for the Journal of Computational and Applied Mathematics (with Boris Baeumer, Department of Mathematics and Statistics, University of Otago, Dunedin, New Zealand; Mihály Kovács, Department of Mathematics, Chalmers University of Technology, Sweden; and Harish Sankaranarayanan, Department of Statistics and Probability, Michigan State University).

9. Space-time fractional Dirichlet problems, revised for Mathematische Nachrichten (with Boris Baeumer, Department of Mathematics and Statistics, University of Otago, Dunedin, New Zealand; and Tomasz Luks, Institut für Mathematik, Universität Paderborn, Germany).


12. Asymptotic behavior of semistable Lévy exponents and applications to fractal path properties, Journal of Theoretical Probability, to appear (with Peter Kern, Mathematisches Institut, Heinrich-Heine-Universität Düsseldorf, Germany; and Yimin Xiao, Department of Statistics and Probability, Michigan State University).

13. Relaxation patterns and semi-Markov dynamics, under review at Stochastic Processes and Their Applications (with Bruno Toaldo, Department of Statistical Sciences, Sapienza University of Rome).

14. Parameter Estimation for Tempered Fractional Time Series, in revision (with Farzad Sabzikar, Department of Statistics, Iowa State University; and A. Ian McLeod, Department of Statistical and Actuarial Sciences, University of Western Ontario).
Fractional Modeling of Scalar Turbulence: Eulerian and Lagrangian

Governing Equations:
- **Continuity Eq.**:
  \[ \nabla \cdot \mathbf{U} = 0 \]
  \( \nu \): kinematic viscosity
- **Momentum Eq.**:
  \[ \mathbf{U}_t + \mathbf{U} \cdot \nabla \mathbf{U} = -\nabla \mathbf{P} + \nu \Delta \mathbf{U} + \mathbf{F} \]
  \( \mathbf{U} \): Velocity Field
  \( \mathbf{P} \): Pressure
  \( \mathbf{F} \): Force
  \( \nu \): kinematic viscosity
  \( \Delta \): Laplacian operator
- **Passive Scalar Transport Eq.**:
  \[ \frac{\partial \bar{C}}{\partial t} + \mathbf{U} \cdot \nabla \bar{C} = D \Delta \bar{C} + F_C \]
  \( \bar{C} \): mean Passive scalar
  \( C = \bar{C} + c \)

Stochastic modeling of particle dispersion in turbulence

**Eulerian Stochastic Equation**

\[ \frac{\partial p(x,t)}{\partial t} + \mathbf{U} \cdot \nabla p(x,t) = D \Delta^\beta p(x,t) + F_p \]

\[ \int_{||s||=1} w(s) \partial_s^\beta p(x,t) \, ds; \]
\( \partial_s^\beta \): RL fractional derivative with \( \beta \in (1,2] \)

\( p(x,t) \): PDF of \( c \)

**Particle Tracking Method: Lagrangian Approach**

\[ dX = U_p \, dt + D \, d\eta(t) \]

\( U_p \): Particle velocity
\( D \): diffusion coefficient
\( \eta(t) \): Levy noise representing anomalous dispersion
Fourier Fast Transform for 2D Decaying Turbulence

Anomalous Transport due to highly intermittent vorticity field

**Method**
- FFT
- Time-Integrator scheme: AB for nonlinear terms and CN for diffusion term.

**Resolution**
- 164*164

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**Vorticity**
- t = 0
- t = 6
- t = 12
- t = 18

**Passive scalar**
- t = 0
- t = 6
- t = 12
- t = 18

**Energy Spectrum**
- t = 0
- t = 6
- t = 12
- t = 18

**Enstrophy Spectrum**
- t = 0
- t = 6
- t = 12
- t = 18

**Spectrum of a Passive Scalar**
- t = 0
- t = 6
- t = 12
- t = 18
Multifractal Modeling of Scalar Turbulence

Future Plan

• Simulation of anomalous dispersion employing stochastic Lagrangian and Eulerian methods with fractional Laplacian: mixing layer, jet flow, and boundary layers

• Developing new spectral methods for fully-distributed fractional PDEs

\[
\int_{\alpha_{\text{min}}}^{\alpha_{\text{max}}} \phi(\alpha) R_0 D_\xi^{\alpha} u(t, x_j) d\alpha - \sum_{j=1}^{d} \int_{\beta_{j_{\text{min}}}^{\text{max}}}^{} \psi_j(\beta_j) \left[ \kappa_{l_j} R L_{x_j}^{\beta_j} + \kappa_{r_j} R L_{b_j}^{\beta_j} \right] u(t, x_j) d\beta_j + \gamma u(t, x_j) = f(t, x_j),
\]

where \( \alpha \in (0, 1), \beta_j \in (1, 2), \) and \( \kappa_{l_j}, \kappa_{r_j}, \gamma \) are constant.

• Local and nonlocal boundary conditions
**Integer-to-Fractional Phase-Field Modeling of Failure**

**Governing equations**

\[
\dot{u} = \mathbf{v}, \\
\dot{\mathbf{v}} = \text{div} \left( (1 - \varphi)^2 \frac{C}{\rho_0} \mathbf{E} \right) + \frac{1}{\rho_0} \text{div} \left( \mathbf{D} - \frac{g_c}{\rho_0} \text{div} (\nabla \varphi \otimes \nabla \varphi) \right) + \mathbf{f}, \\
\dot{\varphi} = \frac{g_c}{\lambda} \Delta \varphi + \frac{1}{\lambda} (1 - \varphi) \mathbf{E}^T \mathbf{CE} - \frac{1}{\lambda \gamma} [g_c \mathcal{H}'(\varphi) + \mathcal{F} \mathcal{H}_f(\varphi)], \\
\dot{\mathcal{F}} = -\frac{\mathcal{F}}{\gamma} \mathcal{H}_f(\varphi), \\
\frac{1}{\hat{\lambda}} = \frac{\hat{c}}{1 + \delta - \varphi}, \quad \hat{\mathcal{F}} = \hat{a} (1 - \varphi) \left( \mathbf{CE} + \hat{b} \mathbf{D} \right) : \mathbf{D}
\]

**Fatigue potentials**

\[
\mathcal{H}(\varphi) = \begin{cases} 
\frac{1}{2} \varphi^2 & \text{for } 0 \leq \varphi \leq 1, \\
\frac{1}{2} + \delta (\varphi - 1) & \text{for } \varphi > 1, \\
-\delta \varphi & \text{for } \varphi < 0,
\end{cases}
\]

\[
\mathcal{H}_f(\varphi) = \begin{cases} 
-\varphi & \text{for } 0 \leq \varphi \leq 1, \\
-1 & \text{for } \varphi > 1, \\
0 & \text{for } \varphi < 0,
\end{cases}
\]

**Fields**

- $\mathbf{u}$ - Displacement
- $\mathbf{v}$ - Velocity
- $\varphi$ - Damage
- $\mathcal{F}$ - Fatigue

**Mode I crack propagation**

(Chiarelli et.al. 2017, CAMWA)

**Other parameters**

- $b$ - Viscous damping
- $\gamma$ - Phase field width
- $g_c$ - Griffith fracture energy
- $\rho_0$ - Density

\[
\mathbf{E} = \nabla^S \mathbf{u}, \quad \mathbf{D} = \nabla^S \mathbf{v}
\]
Future Plan

Fractional Modeling of Failure

- Phase field model
  - Allen-Cahn equation for damage
  - Cracks are diffuse interfaces
  - Fatigue is an internal variable

- Acoustic energy bursts distribution
  - (Miguel et al. 2001, Nature)

- Crack path for different width parameters
  - (Chiarelli et al. 2017, CAMWA)

- Experimental evidence of power-law behavior
- Uncertainty quantification
  - Global/local sensitivity
  - Sources of uncertainty
  - Probabilistic collocation method

Dislocation dynamics
Acoustic emission