Anomalous diffusion and turbulence

MURI Project Review
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Research Area 1: Theory of non-local operators

- Fractional calculus and hyperdiffusion
- Semi-fractional calculus
- Some new books
- PhD project: Fractional calculus and turbulence
- PhD project: Fractional phase field model of failure

Area 2: Numerical solution of fractional PDEs

- Petrov-Gelerkin spectral methods (update)

- Numerical methods for Zolotarev diffusion

- Fractional Neumann boundary conditions

- Tempered fractional Neumann boundary conditions

Fractional calculus in a nutshell

The nth derivative $\frac{d^n f(x)}{dx^n}$ has FT $(ik)^n \widehat{f}(k)$, using the FT

$$\widehat{f}(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx.$$

The fractional derivative $\frac{d^\alpha f(x)}{dx^\alpha}$ has FT $(ik)^\alpha \widehat{f}(k)$.

The negative frac dvt $\frac{d^\alpha f(x)}{d(-x)^\alpha}$ has FT $(-ik)^\alpha \widehat{f}(k)$.

If $\alpha = n$, an integer, then $\frac{d^n f(x)}{d(-x)^n} = (-1)^n \frac{d^n f(x)}{dx^n}$.

A useful model for power law behavior...

Hyperdiffusion

The simplest hyperdiffusion equation (here $\alpha > 2$):

$$\frac{\partial u(x,t)}{\partial t} = pD\frac{\partial^\alpha u(x,t)}{\partial x^\alpha} + qD\frac{\partial^\alpha u(x,t)}{\partial (-x)^\alpha}$$

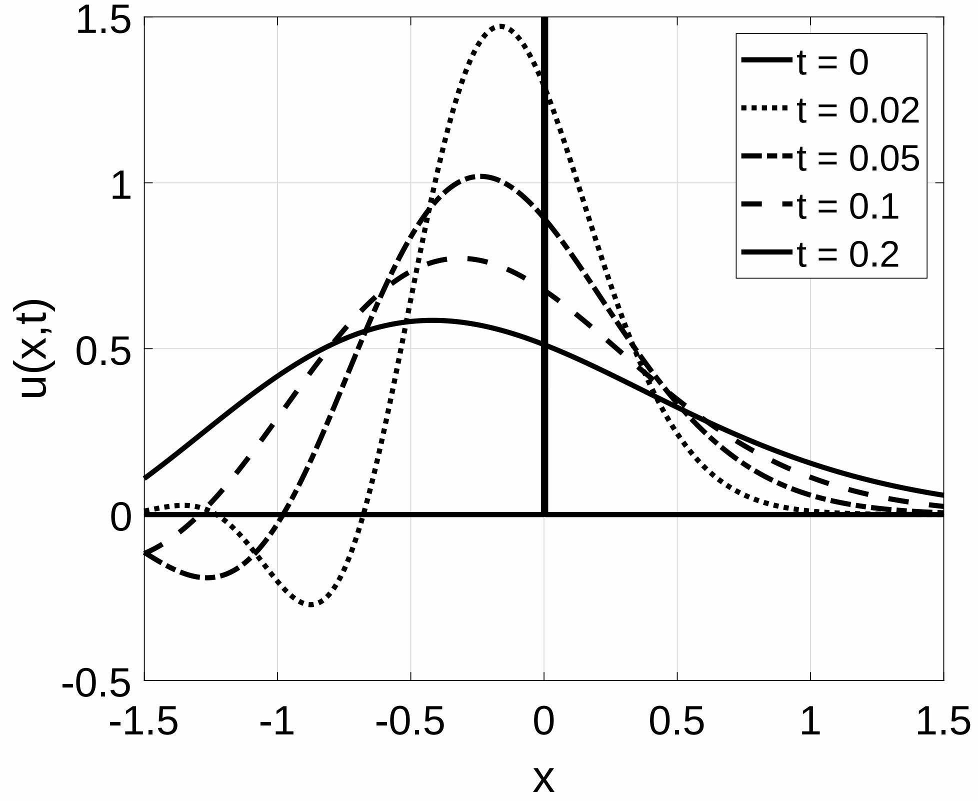
The hyperdiffusion term is useful in CFD, turbulence, image processing, cosmic rays, and calcium sparks.

Fractional diffusion with $0 < \alpha < 2$ is well-understood with many, many applications.

It governs a stochastic process with power law jumps: The chance of jumping further than a distance x falls off like $x^{-\alpha}$

There is no known stochastic model or physical interpretation for hyperdiffusion with $\alpha > 2$.

Hyperdiffusion is not diffusion (here $p = 0$)



Point source solution with $\alpha = 2.5$ and $p = 0$ goes negative for $x < 0$. Same holds for any $\alpha > 2$, except even integers.

A physical understanding

Our hyperdiffusion equation with $2 < \alpha < 3$ is $\partial_t u = A_x^\alpha u$ where

$$A_x^\alpha u(x) = \begin{cases} \frac{\partial^\alpha u(x)}{\partial(-x)^\alpha} & x > 0 \\ \frac{\partial^\alpha u(x)}{\partial x^\alpha} & x < 0 \end{cases}$$

If $\alpha = n$ is even, then $A_x^\alpha u = \frac{\partial^n u(x)}{\partial x^n}$ as usual.

If n is odd, $A_x^\alpha u = -\mathrm{sgn}(x)\frac{\partial^n u(x)}{\partial x^n}$

Now solutions stay positive, model subdiffusion: they spread like $t^{1/\alpha}$ and show a sharp peak at $x = 0$.

Equivalent model uses fractional time derivatives of order $1/\alpha$

Semi-fractional diffusion

Power law scaling at a discrete set of scales appears frequently in physics and finance.

We propose a new model for discrete scale invariance using semi-fractional derivatives.

The simplest semi-fractional derivative has FT $(\pm ik)^{\alpha-ic}\widehat{f}(k)$ where $c > 0$ establishes the discrete scale.

Semi-fractional diffusion equation models power law jumps with log-periodic fluctuations.

A finite difference formula

To estimate a fractional derivative, we use

$$\frac{d^\alpha f(x)}{dx^\alpha} = \lim_{h \to 0} h^{-\alpha} \sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j f(x - jh).$$

which reduces to the usual one-sided difference quotient when $\alpha = n$.

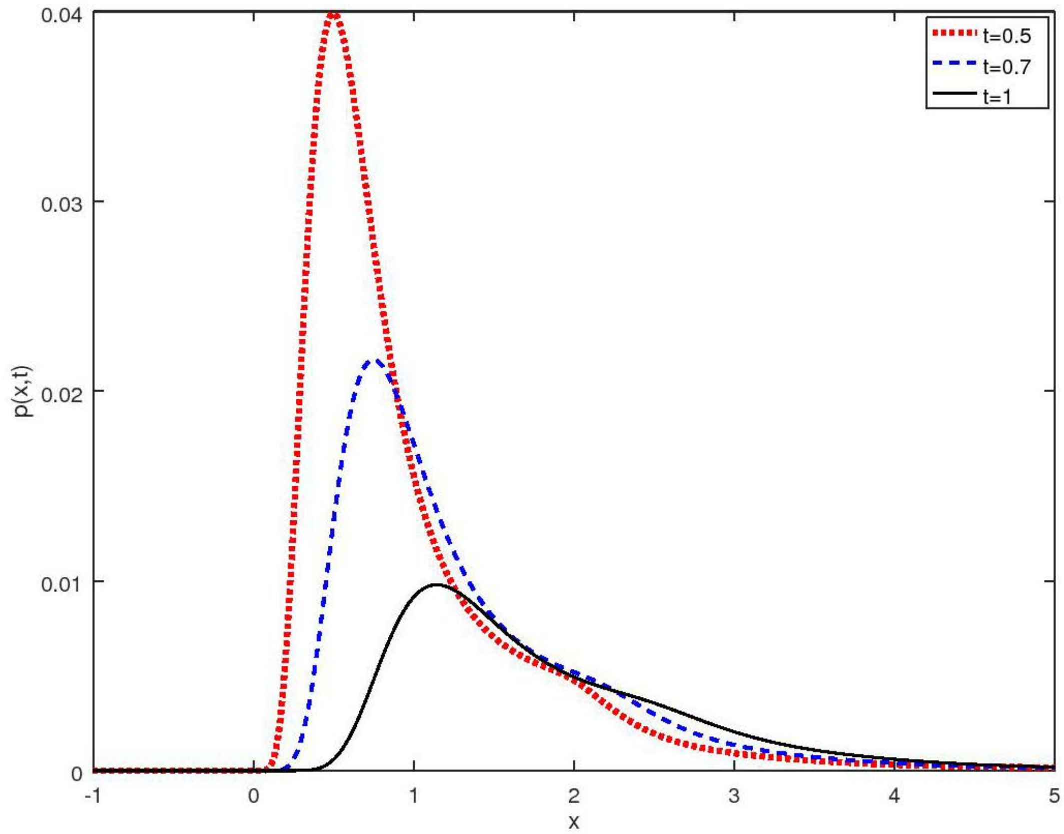
The semi-fractional derivative

$$\mathbb{D}^{\alpha,c} f(x) = \lim_{h \to 0} h^{-\alpha+ic} \sum_{j=0}^{\infty} \binom{\alpha - ic}{j} (-1)^j f(x - jh).$$

A shifted formula with $f(x-(j-p)h)$ yields a useful finite difference code.

A special case solves an open problem from last year...

Semi-fractional diffusion α=0.5



Note oscillations on the right tail, characteristic of DSI.

New books coming in 2019…

- **Stochastic and Computational Models for Fractional Calculus**
  - By M.M. Meerschaert, A. Sikorskii, and M. Zayernouri
  - Random walk models for fractional diffusion
  - Vector models
  - Numerical methods and codes
- **Handbook of Fractional Calculus and Applications**
  - Fractional Advection Dispersion Equation
  - Continuous Time Random Walks
  - Inverse Subordinators and Time Fractional Equations
  - Particle Tracking

Kinetic Theory

Derivation of Scalar Transport

Scalar transport equation with the fractional Laplacian:

$$\frac{\partial \boldsymbol{\phi}}{\partial \boldsymbol{t}} + \boldsymbol{V} \,.\, \nabla \boldsymbol{\phi} = \underbrace{\boldsymbol{D}\, \Delta \boldsymbol{\phi}}_{\text{Small displacements of scalar particles}} - \underbrace{\boldsymbol{C_1} (-\Delta)^{\boldsymbol{\beta}} \boldsymbol{\phi} \ - C_2 \Big((-\Delta)^{\beta} (\nabla \phi . \boldsymbol{V}) - \boldsymbol{V} . (-\Delta)^{\beta} (\nabla \phi) \Big)}_{\text{Large displacements of scalar particles}}, \qquad \beta \,\epsilon (0,1)$$

✓ Unit check: $C_1 = -U^{2\beta} t_s{}^{2\beta-1} \Gamma(1-2\beta) \colon \left[\frac{L^{2\beta}}{T}\right], \quad C_2 = 2\Gamma(2+2\beta) U^{2\beta}\, t_s{}^{2\beta} \colon \left[L^{2\beta}\right]$

✓ For $\beta = 1:\ \ (-\Delta)^{\beta}\,(.) = 0,$ $\Longrightarrow$ $\dfrac{\partial \phi}{\partial t} + \boldsymbol{V} \,.\, \nabla \phi = D\, \Delta \phi$

Fractional order (β) inference

Lévy jumps of particles at a specific instant are depending on

- Flow properties (**Re**)
- Scalar diffusion (**Sc**)

Numerical Simulation
Eulerian-Lagrangian Approaches

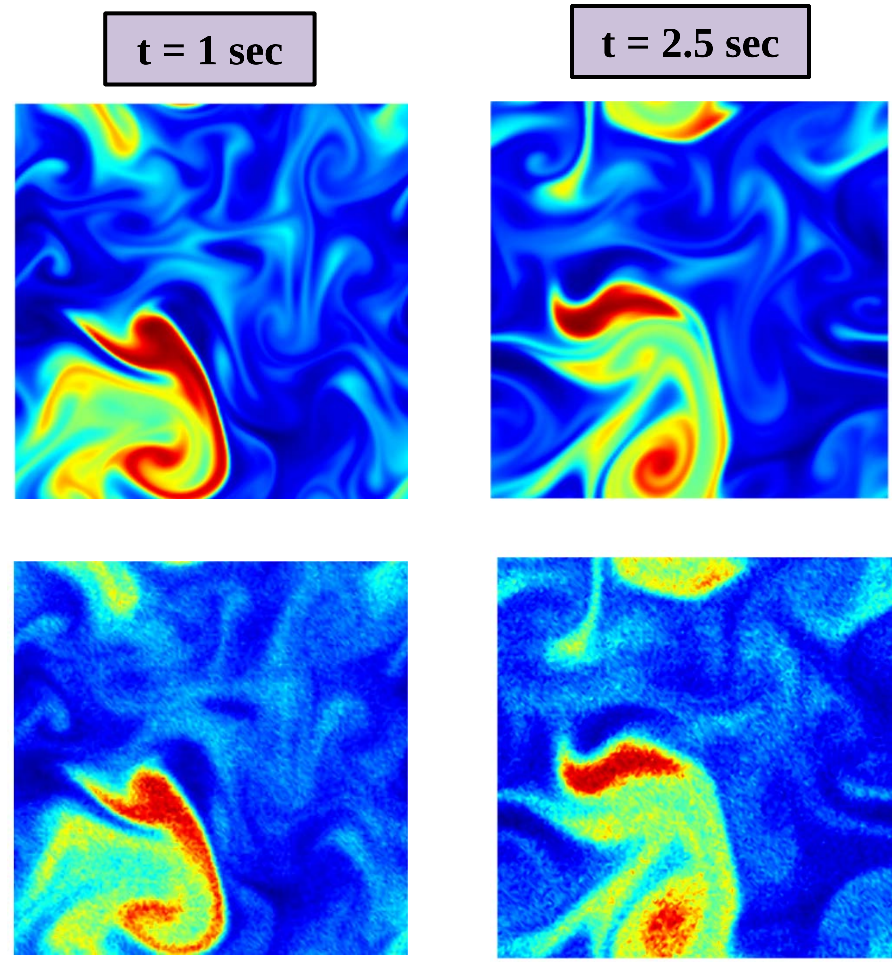
2-D Freely decaying isotropic turbulence

$$Sc = 1, \beta = 0.9$$

Eulerian Approach

$$\frac{\partial \boldsymbol{\phi}}{\partial \boldsymbol{t}} + \boldsymbol{V} \, . \boldsymbol{\nabla \phi} = \boldsymbol{D} \, \Delta \boldsymbol{\phi} - \boldsymbol{C_1} (-\Delta)^{\boldsymbol{\beta}} \boldsymbol{\phi}$$

- ✓ Fourier spectral method
- ✓ Adams-Bashforth scheme
- ✓ Crank-Nicolson for diffusive terms



Lagrangian Approach
(Lévy Walk)

$$d\boldsymbol{X} = \boldsymbol{U_p} \, \delta t + (2D \, \delta t)^{1/2} \, \boldsymbol{\eta}_G(t) \, - (2C_1 \, \delta t)^{1/\beta} \, \boldsymbol{\eta}_\beta(t)$$

$\boldsymbol{U_p}$: Particle velocity ($\boldsymbol{U_p} = \boldsymbol{V}$)

$\boldsymbol{\eta}_G(t)$: Gaussian noise generator

$\boldsymbol{\eta}_\beta(t)$: $Lévy - \beta$ stable noise generator

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Stochastic Phase-Field Modeling of Failure

$(\Omega^s, \mathcal{G}, P)$: probability space $\qquad \xi(\omega) = \{\gamma(\omega), g_c(\omega), a(\omega), b(\omega), c(\omega)\}, \omega \in \Omega^s$

Governing Equations

Displacement, Velocity, Damage, Fatigue

$$\begin{cases} \dot{\mathbf{u}} = \mathbf{v}, \\ \dot{\mathbf{v}} = \operatorname{div}\left((1-\varphi)^2 \dfrac{C}{\rho_0}\mathbf{E}\right) + \dfrac{b(\omega)}{\rho_0}\operatorname{div}(\mathbf{D}) - \dfrac{\gamma(\omega)g_c(\omega)}{\rho_0}\operatorname{div}(\nabla\varphi \otimes \nabla\varphi) + \mathbf{f}, \\ \dot{\varphi} = \dfrac{\gamma(\omega)g_c(\omega)}{\lambda}\Delta\varphi + \dfrac{1}{\lambda}(1-\varphi)\mathbf{E}^T C\mathbf{E} - \dfrac{1}{\lambda\gamma(\omega)}[g_c(\omega)\mathcal{H}'(\varphi) + \mathcal{F}\mathcal{H}_f'(\varphi)], \\ \dot{\mathcal{F}} = -\dfrac{\hat{F}}{\gamma(\omega)}\mathcal{H}_f(\varphi), \end{cases}$$

Fatigue potentials

$$\mathcal{H}(\varphi) = \begin{cases} 0.5\varphi^2 & \text{for } 0 \le \varphi \le 1, \\ 0.5 + \delta(\varphi - 1) & \text{for } \varphi > 1, \\ -\delta\varphi & \text{for } \varphi < 0. \end{cases}$$

$$\mathcal{H}_f(\varphi) = \begin{cases} -\varphi & \text{for } 0 \le \varphi \le 1, \\ -1 & \text{for } \varphi > 1, \\ 0 & \text{for } \varphi < 0. \end{cases}$$

Rate of change of damage

$$\frac{1}{\lambda} = \frac{c(\omega)}{(1+\delta-\varphi)^S}$$

Fatigue coefficients

$$\hat{F} = a(\omega)(1-\varphi)\,|(C\mathbf{E} + b\mathbf{D}) : \mathbf{D}|$$

Discretization

- Finite element method
- Semi-implicit time integration scheme

Stochastic damage and fatigue phase-field model

Uncertainty Quantification

Sensitivity Analysis

Assessment and tuning of model form

Operator uncertainty: parameters that multiply them will be more sensitive and influential in total output uncertainty

Single-Edge Notched Tensile Test

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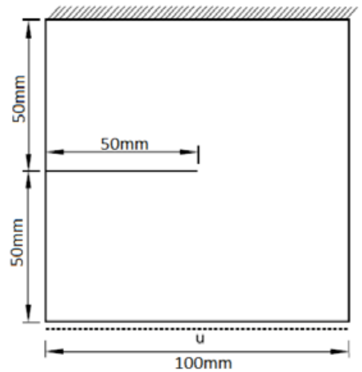
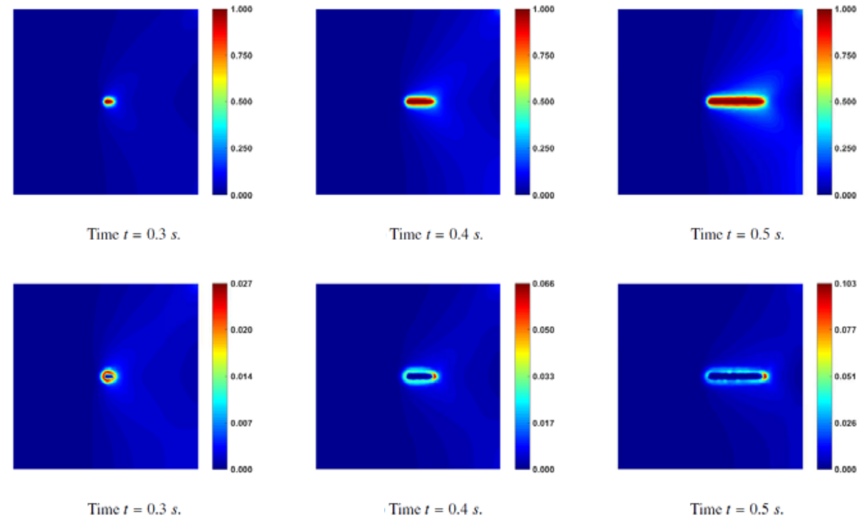


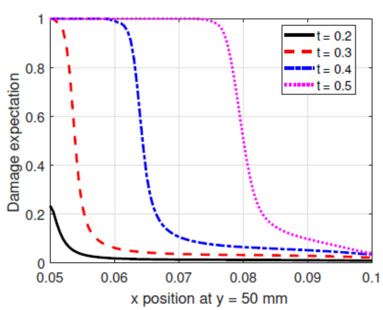
Geometry and BCs

1D PCM of damage field with respect to γ

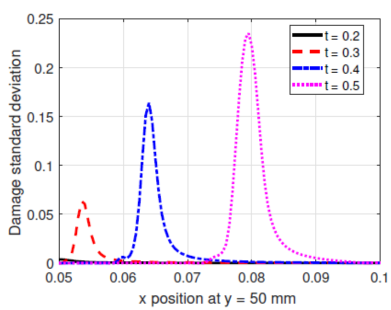
Expectation

Standard deviation





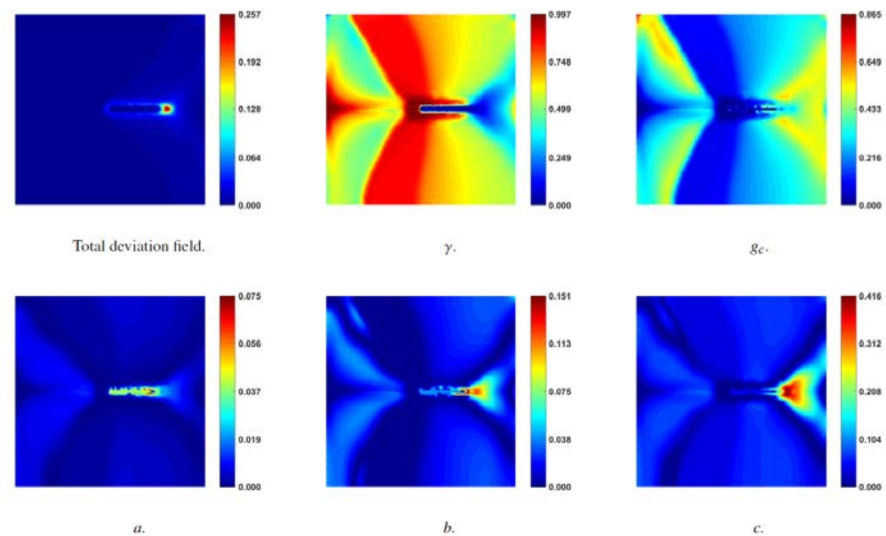
Damage expectation profile.



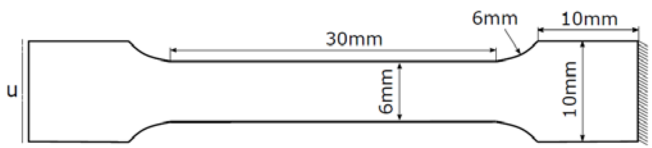
Damage standard deviation profile.

5D PCM of damage field: expectation and deviation profiles at crack path

5D PCM of damage field: total deviation and global sensitivity indices

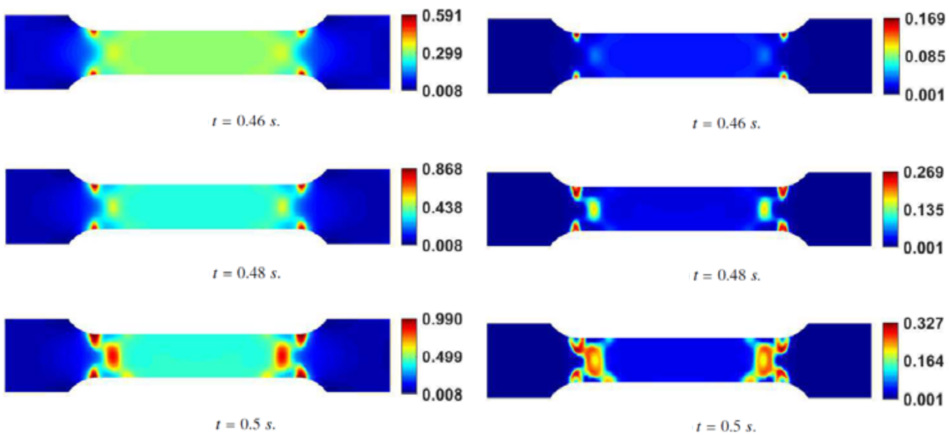


Specimen Tensile Test

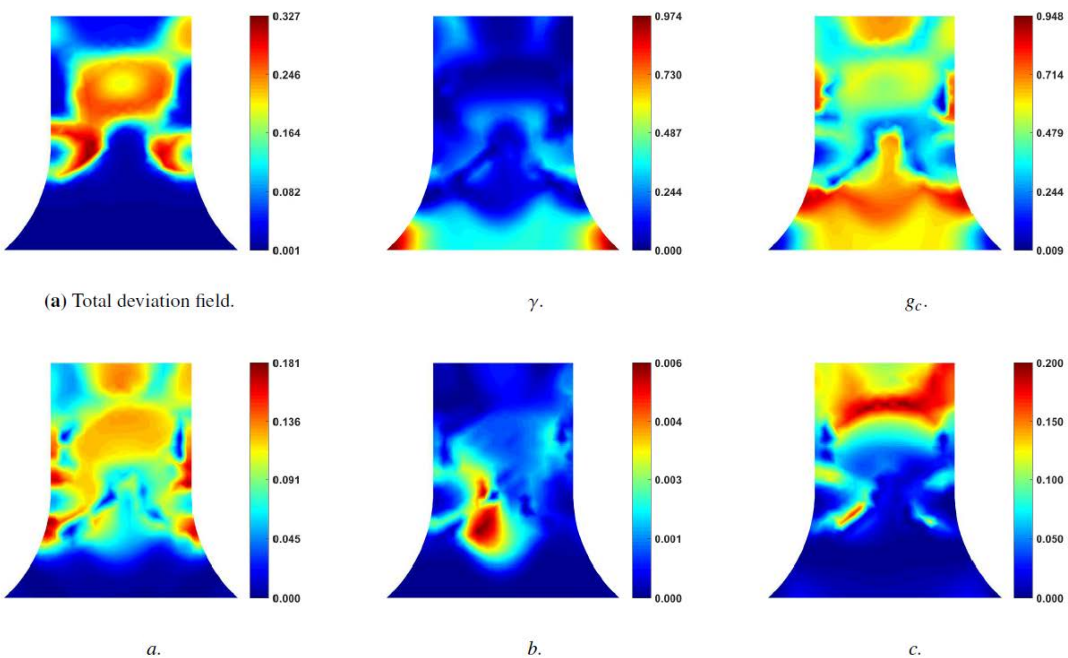


Geometry and BCs

5D PCM of damage field



Expectation **Standard deviation**



5D PCM of damage field: total deviation and global sensitivity indices

Area 2: Numerical solution of fractional PDEs

- Petrov-Gelerkin spectral methods (update)

- Numerical methods for Zolotarev diffusion

- Fractional Neumann boundary conditions

- Tempered fractional Neumann boundary conditions

Petrov-Gelerkin spectral methods (update)

Distributed order space-time diffusion in d dimensions.

Jacobi poly-fractonomials are temporal basis/test functions.

Legendre polynomials are spatial basis/test functions.

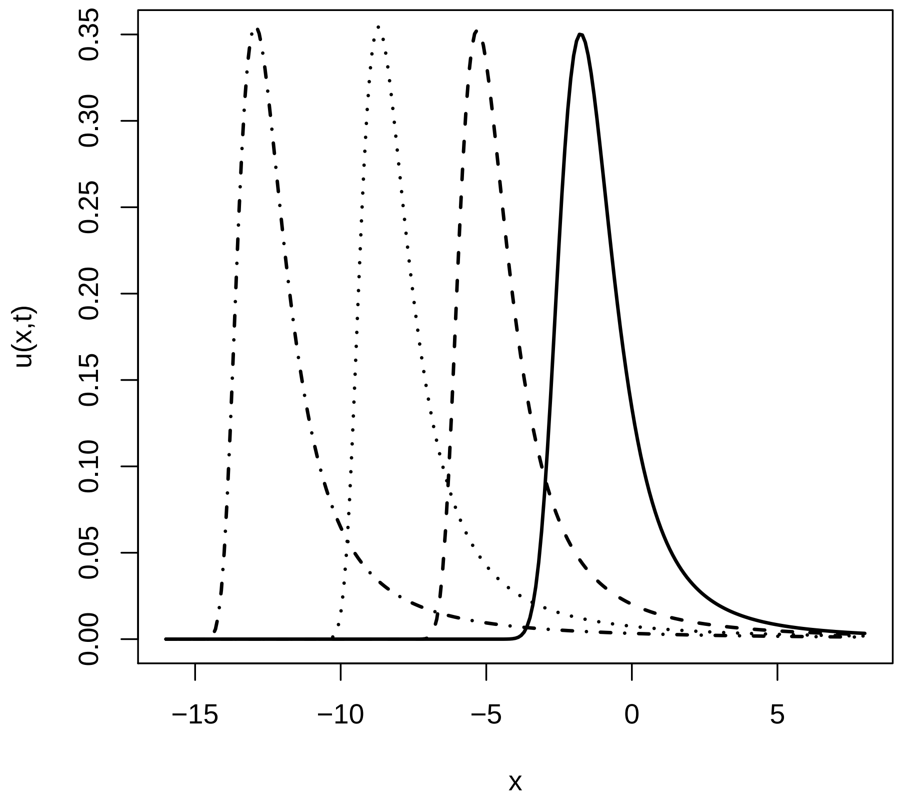
Numerical implementation for fast linear solver.

Well-posedness, stability and error analysis.

Theory based on distributed-order Sobolev spaces.

Now in review at *SIAM Journal on Numerical Analysis*.

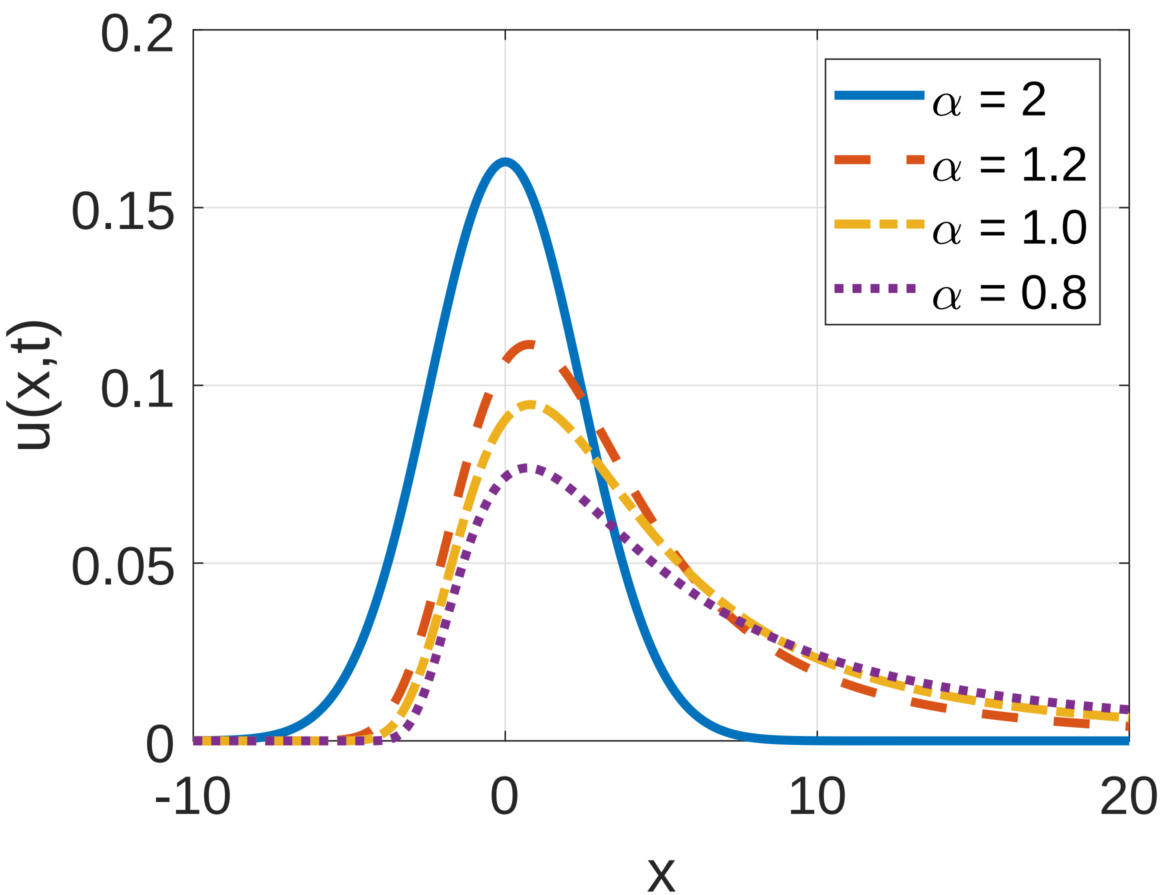
Discontinuity in the fractional diffusion equation



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 $\alpha \downarrow 1$.

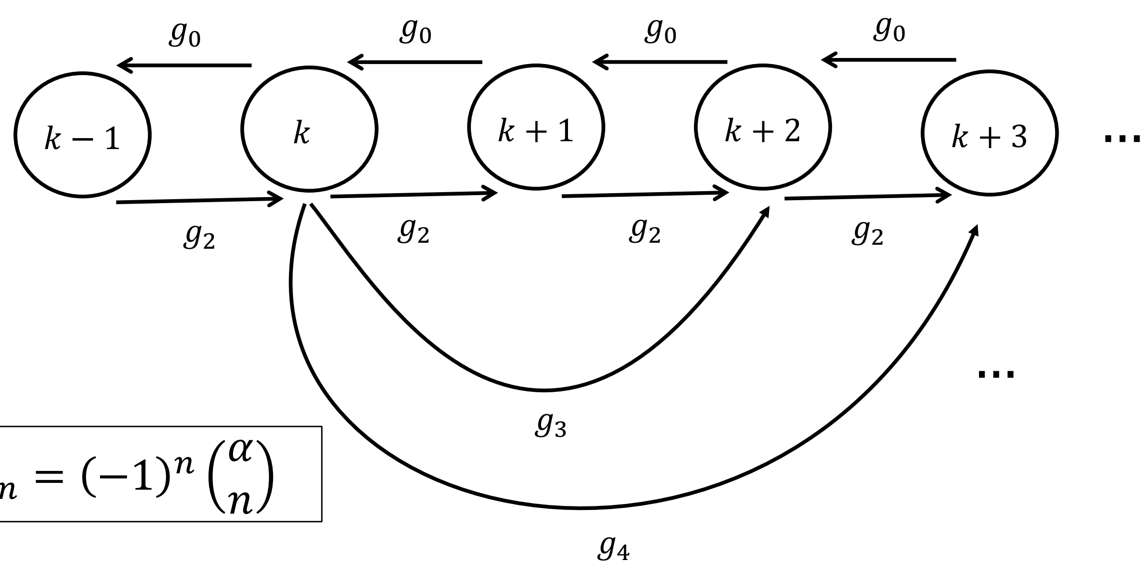
New Zolotarev fractional diffusion equation



The new Zolotarev fractional diffusion equation for $0 < \alpha \leq 2$ is continuous through $\alpha = 1$. Semi-fractional diffusion theory yields a stable numerical method.

Fractional BC: Mass balance approach

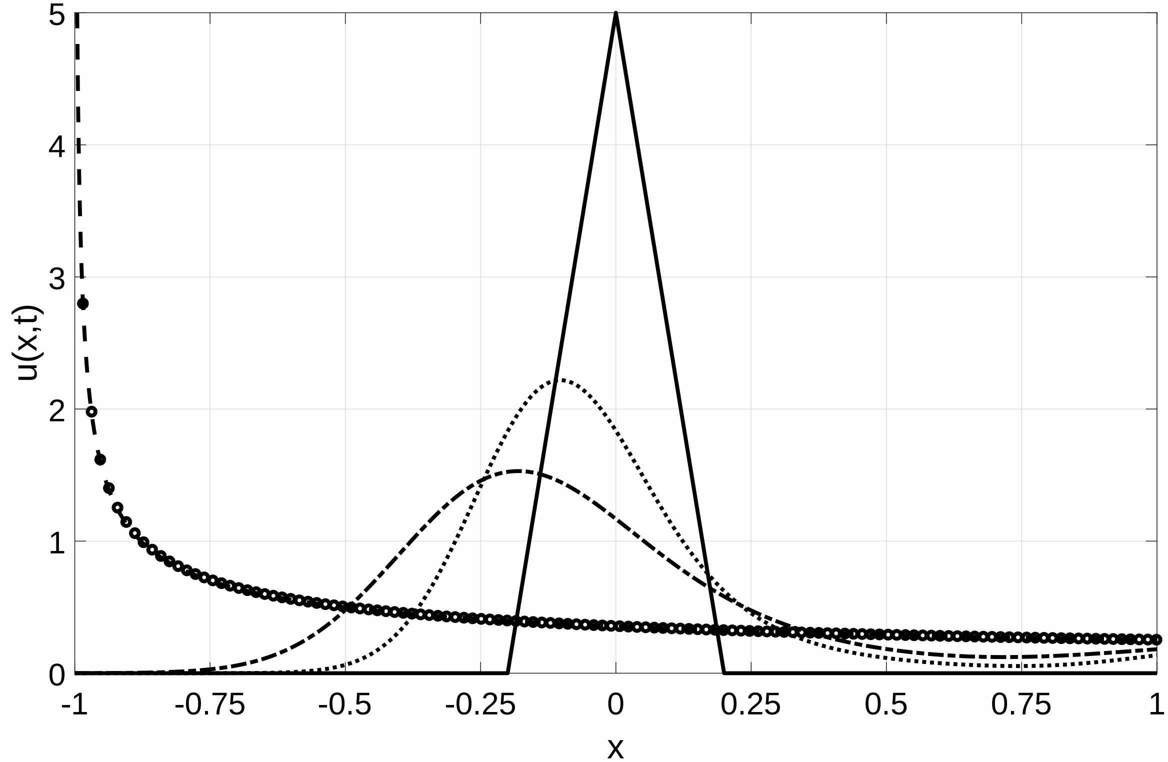
Markov Chain transition model



$$\boxed{g_n = (-1)^n \binom{\alpha}{n}}$$

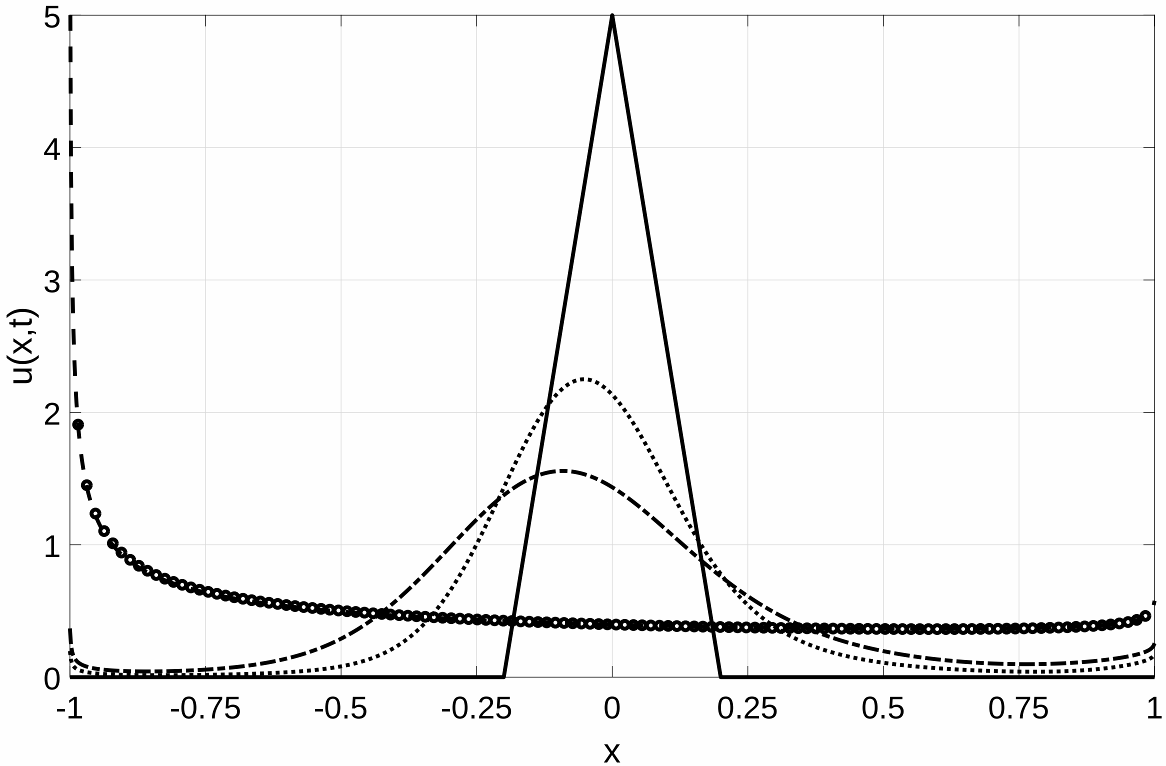
$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^\alpha u(x,t)}{\partial x^\alpha} \quad \Rightarrow \quad u_{k,j+1} = u_{kj} + h^{-\alpha} \Delta t \sum_{i=0}^{[x/h]+1} g_i^\alpha u_{k-i+1,j}$$

Reflecting boundary conditions ($p = 1$)



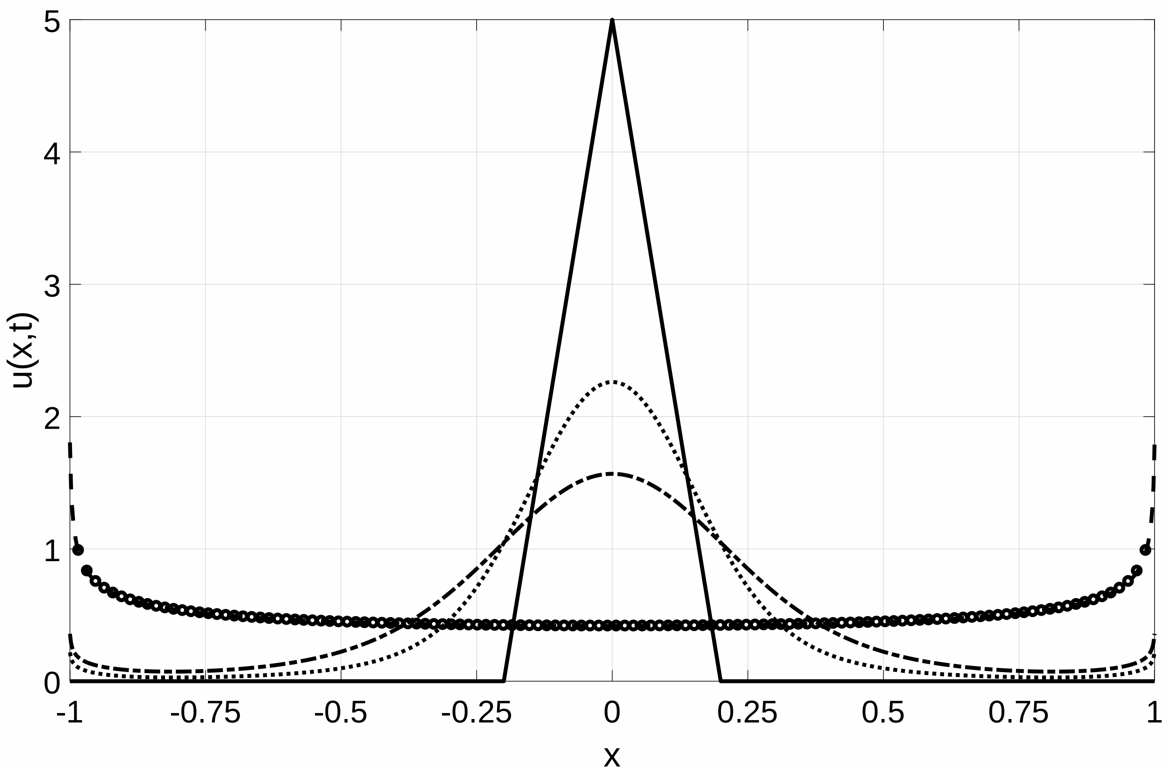
Numerical solution to fractional diffusion equation with $\alpha = 1.5$ on $0 < x < 1$ with zero flux BC at time $t = 0$ (solid), $t = 0.05$ (dashed), $t = 0.1$ (dash dot), $t = 0.5$ (dotted).

Reflecting boundary conditions ($p = 0.75$)



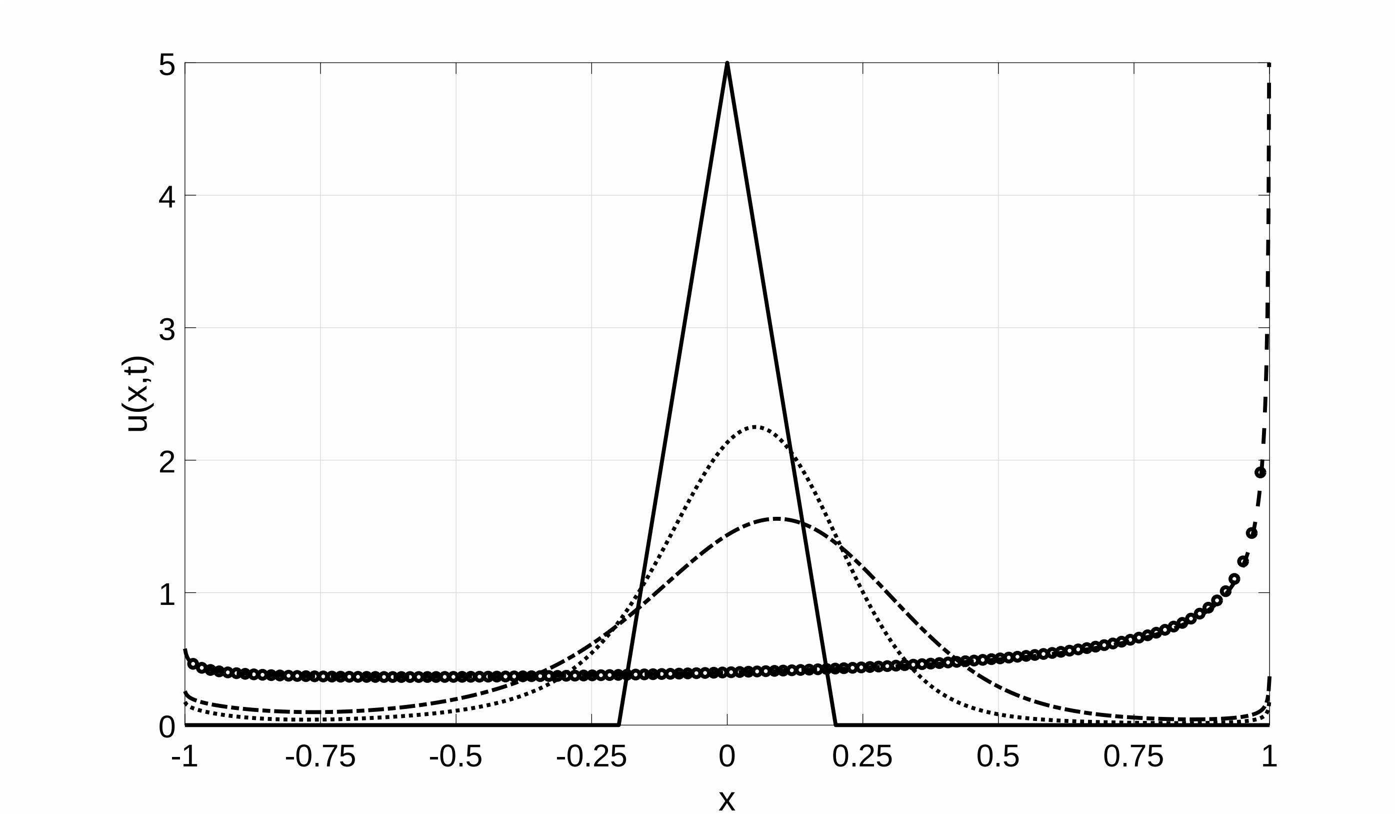
Numerical solution to fractional diffusion equation with $\alpha = 1.5$ on $0 < x < 1$ with zero flux BC at time $t = 0$ (solid), $t = 0.05$ (dashed), $t = 0.1$ (dash dot), $t = 0.5$ (dotted).

Reflecting boundary conditions ($p = 0.5$)



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

Reflecting boundary conditions ($p = 0.25$)



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

Fractional Neumann boundary conditions

The reflecting boundary conditions are written as

$$F(x) = -pD\frac{\partial^{\alpha-1}u(x,t)}{\partial x^{\alpha-1}} + qD\frac{\partial^{\alpha-1}u(x,t)}{\partial(-x)^{\alpha-1}} = 0$$

at the boundary points $x = 0, 1$. This is a zero flux BC because

$$pD\frac{\partial^{\alpha}u(x,t)}{\partial x^{\alpha}} + qD\frac{\partial^{\alpha}u(x,t)}{\partial(-x)^{\alpha}} = -\frac{\partial}{\partial x}F(x,t).$$

When $\alpha = 2$ this reduces to the usual first derivative condition

$$F(x) = -D\frac{\partial u(x,t)}{\partial x} = 0,$$

since $p + q = 1$ and

$$\frac{\partial u(x,t)}{\partial(-x)} = -\frac{\partial u(x,t)}{\partial x}$$

The resulting solutions are mass-preserving.

Steady state solutions

The two-sided fractional diffusion equation with Neumann BC has steady state solution

$$u_\infty(x) = C(1-x)^\mu(1+x)^\nu$$

where $\mu + \nu = \alpha - 2$ and

$$p - q = \cot\left(\pi\left(\frac{\alpha-1}{2} - \mu\right)\right)\tan\left(\frac{\alpha-1}{2}\pi\right).$$

If $p = q = 0.5$ (symmetric) this reduces to

$$u_\infty(x) = C(1-x^2)^{\alpha/2-1}$$

If $p = 1$ (positive skew) we get $Cx^{\alpha-2}$

If $q = 1$ (negative skew) we get $C(1-x)^{\alpha-2}$

Tempered fractional diffusion

Fractional diffusion profiles have power law tails, so some moments are divergent.

Tempering $u(x,t) \mapsto e^{-\lambda x} u(x,t)$ cools the largest jumps, all moments exist.

Many applications in turbulence, geophysics, astronomy, and finance exhibit a tempered power law profile.

The tempered fractional derivative has FT $[(\lambda + ik)^\alpha - \lambda^\alpha]\widehat{f}(k)$.

Reflecting BC and stable numerical schemes are developed.

Steady state solutions

The tempered fractional diffusion equation with Neumann BC has steady state solution

$$u_\infty(x) = Ce^{-\lambda x}\left[(\lambda x)^{\alpha-2}E_{\alpha,\alpha-1}((\lambda x)^\alpha) - (\lambda x)^{\alpha-1}E_{\alpha,\alpha}((\lambda x)^\alpha)\right]$$

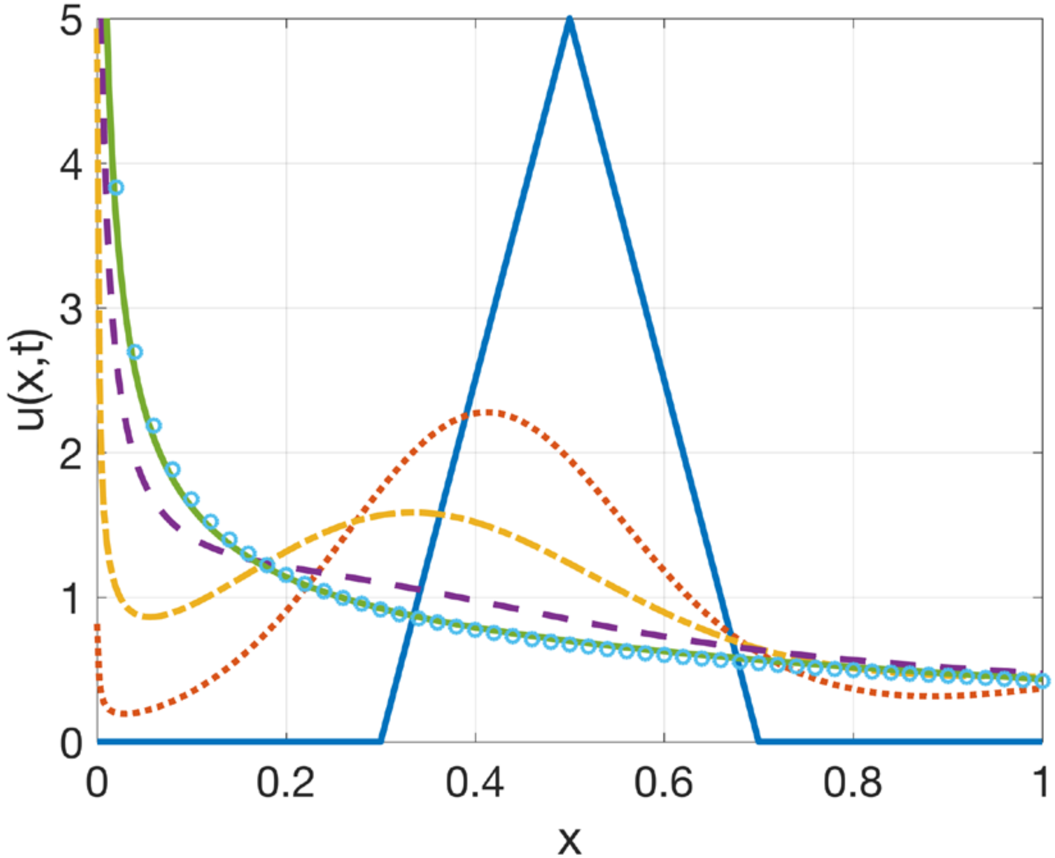
where the two-parameter Mittag-Leffler function

$$E_{\alpha,\beta}(x) = \sum_{k=0}^{\infty} \frac{x^k}{\Gamma(\alpha k + \beta)}$$

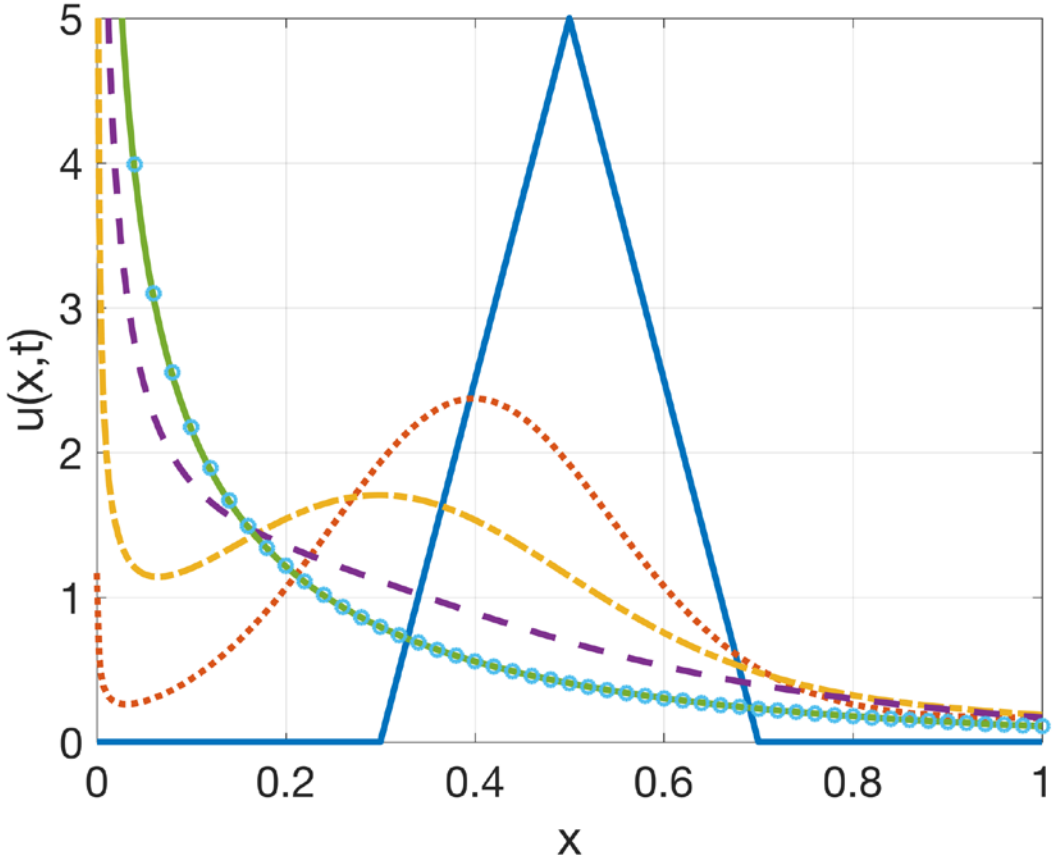
for any $\alpha > 0$ and $\beta \in \mathbb{C}$.

Mass-preserving solutions converge to steady state for any IC.

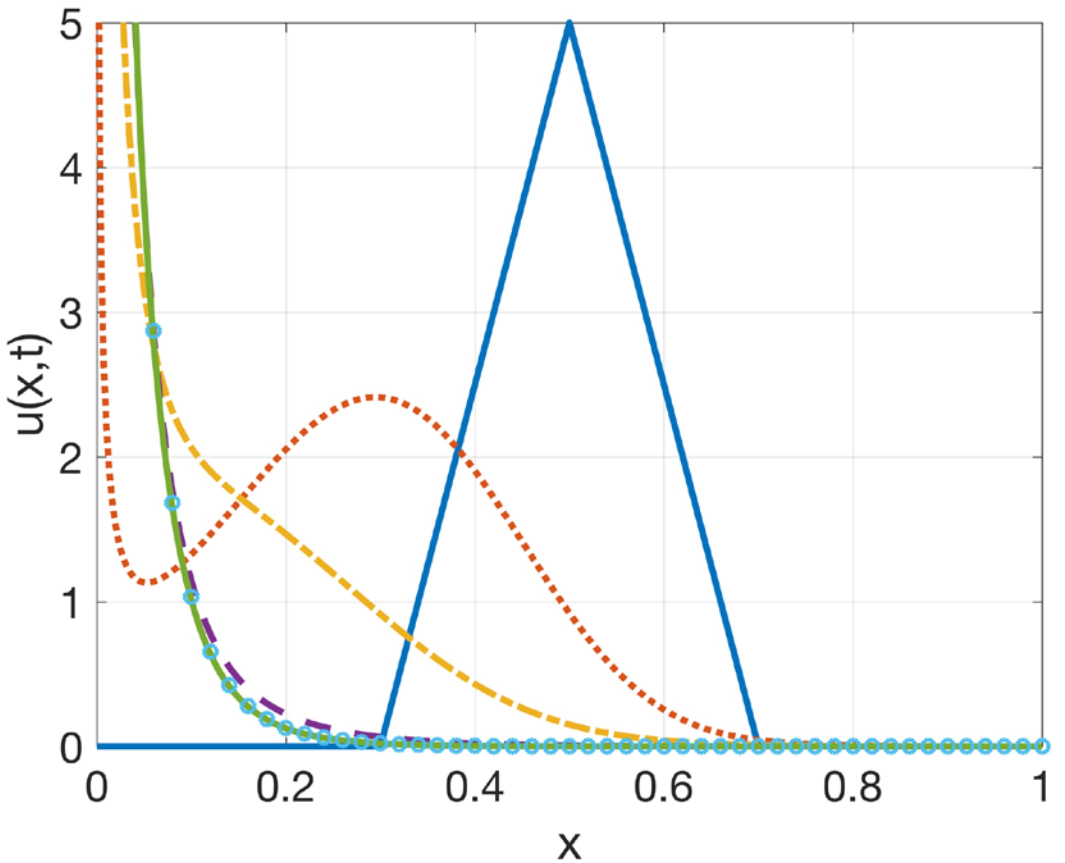
Tempered fractional diffusion
(α=1.5, λ=0.1)



Tempered fractional diffusion
(α=1.5, λ=1.0)



Tempered fractional diffusion
(α=1.5, λ=10)



Products

1. J.F. Kelly, H.Sankaranarayanan and M.M. Meerschaert, Boundary conditions for two-sided fractional diffusion, *Journal of Computational Physics*, Vol. 376 (2019), pp. 1089–1107.
2. J.F. Kelly, C.G. Li and M.M. Meerschaert, Anomalous Diffusion with Ballistic Scaling: A New Fractional Derivative, *Journal of Computational and Applied Mathematics*, Vol. 339 (2018), pp. 161–178. Special Issue on Modern fractional dynamic systems and applications.
3. P. Kern, M.M. Meerschaert, and Y. Xiao, Asymptotic behavior of semistable Lévy exponents and applications to fractal path properties, *Journal of Theoretical Probability*, Vol. 31 (2018), No. 1, pp. 598–617.
4. B. Baeumer, M. Kovács, M.M. Meerschaert, and H. Sankaranarayanan, Boundary Conditions for Fractional Diffusion, *Journal of Computational and Applied Mathematics*, Vol. 336 (2018), pp. 408–424. Click here to download the R codes for this paper.
5. G. Didier, M.M. Meerschaert, and V. Pipiras, Domain and range symmetries of operator fractional Brownian fields, *Stochastic Processes and their Applications*, Vol. 128 (2018), No. 1, pp. 39–78.
6. A unified spectral method for FPDEs with two-sided derivatives; part I: A fast solver, *Journal of Computational Physics*, to appear (with Mohsen Zayernouri and Mehdi Samiee, Department of Computational Mathematics, Science and Engineering, Michigan State University).
7. The fractional advection-dispersion equation for contaminant transport, *Handbook of Fractional Calculus with Applications*, to appear (with James F. Kelly, Department of Statistics and Probability, Michigan State University).
8. Inverse subordinators and time fractional equations, *Handbook of Fractional Calculus with Applications*, to appear (with Erkan Nane, Department of Mathematics and Statistics, Auburn University: and P. Vellaisamy, Department of Mathematics, Indian Institute of Technology Bombay).

9. Continuous time random walks and space-time fractional differential equations, *Handbook of Fractional Calculus with Applications*, to appear (with Hans-Peter Scheffler, Fachbereich Mathematik, University of Siegen, Germany).

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

11. A Unified Spectral Method for FPDEs with Two-sided Derivatives; Part II: Stability and Error Analysis, *Journal of Computational Physics*, to appear (with Mohsen Zayernouri and Mehdi Samiee, Department of Computational Mathematics, Science and Engineering, Michigan State University).

12. Relaxation patterns and semi-Markov dynamics, *Stochastic Processes and their Applications*, to appear (with Bruno Toaldo, Department of Statistical Sciences, Sapienza - University of Rome).

13. Lagrangian approximation of vector fractional differential equations, *Handbook of Fractional Calculus with Applications*, to appear (with Yong Zhang, Department of Geological Sciences, University of Alabama).

14. What Is the Fractional Laplacian? (with Anna Lischke, Guofei Pang, Mamikon Gulian, Fangying Song, Xiaoning Zheng, Zhiping Mao, Mark Ainsworth, and George Em Karniadakis, Division of Applied Mathematics, Brown University; Christian Glusa, Center for Computing Research, Sandia National Laboratory; and Wei Cai, Department of Mathematics, Southern Methodist University, Dallas, TX).

15. Parameter estimation for ARTFIMA time series, (with A. Ian McLeod, Department of Statistical and Actuarial Sciences, University of Western Ontario; and Farzad Sabzikar, Department of Statistics, Iowa State University).

16. Petrov-Galerkin Method for Fully Distributed-Order Fractional Partial Differential Equations (with Mohsen Zayernouri, Mehdi Samiee, and Ehsan Kharazmi, Department of Computational Mathematics, Science and Engineering, Michigan State University).

17. Semi-fractional diffusion equations (with Svenja Lage and Peter Kern, Mathematical Institute, Heinrich-Heine-University Düsseldorf, Germany).

18. Space-Time Duality and Fractional Hyperdiffusion (with James F. Kelly, Department of Statistics and Probability, Michigan State University).