Fractional PDEs and Integral Equations Defined by Convolution with the Lévy Measure: Multi-Scaling Diffusions and fBms

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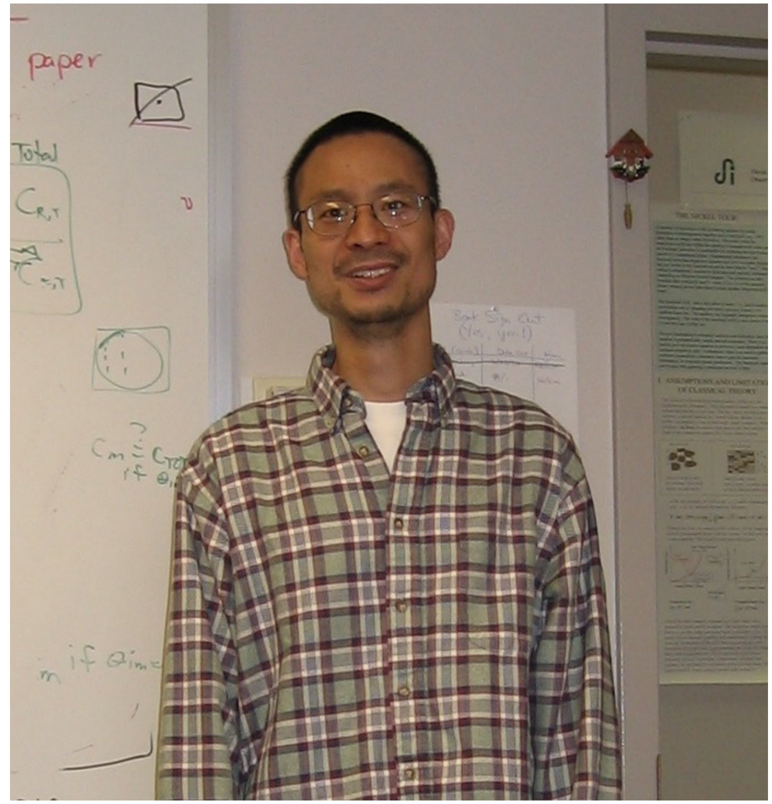
Our esteemed organizer just minutes before his forced introduction to “fractional calculus.”



Some of the original members of the $\sim$ 2001 NSF-sponsored "Fractional Calculus Project."

Outline

- An unabridged history of the science of contaminant hydrology (5 min.)
- Anomalous diffusion, limit theorems, and multi-dimensional fractional differential operators
- Inverses and (matrix) operator-scaling fractional Brownian motion (os-fBm)

Ideal Plume Behavior

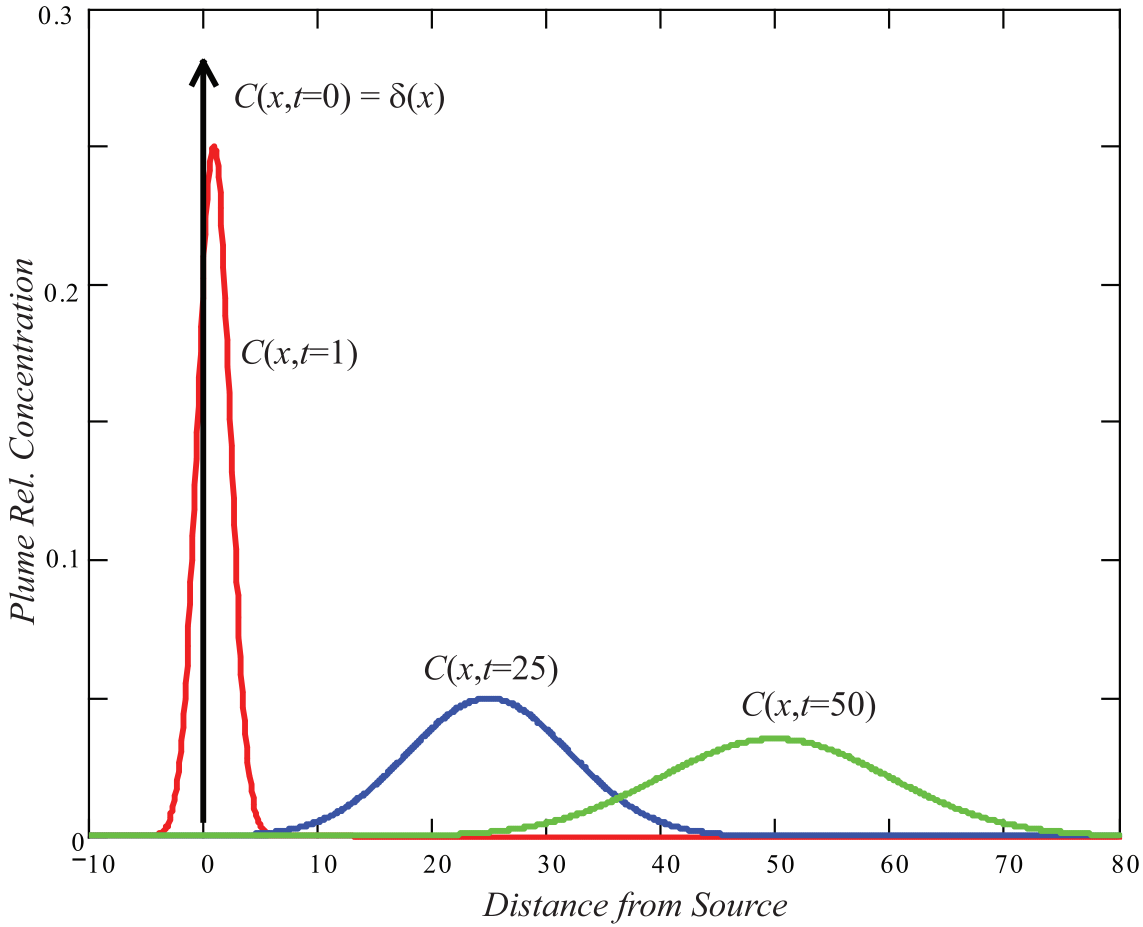
Conservation of mass and an assumption of additive advective and Fickian (Fourier) diffusive flux gives

$$\frac{\partial C}{\partial t} = \nabla \cdot (-vC + D\nabla C)$$

for concentration $C(x,t)$ with variable parameter fields of velocity $v(x)$ and diffusion strength $D(x)$.

- $\sim$ Gaussian Green function - restatement of Central Limit Theorem
- Solute "particles" experience all possible velocities
- Hydrologists love to measure and model $v(x)$
- Dispersion: velocity perturbations sort of a "black box"

Classical ADE profile

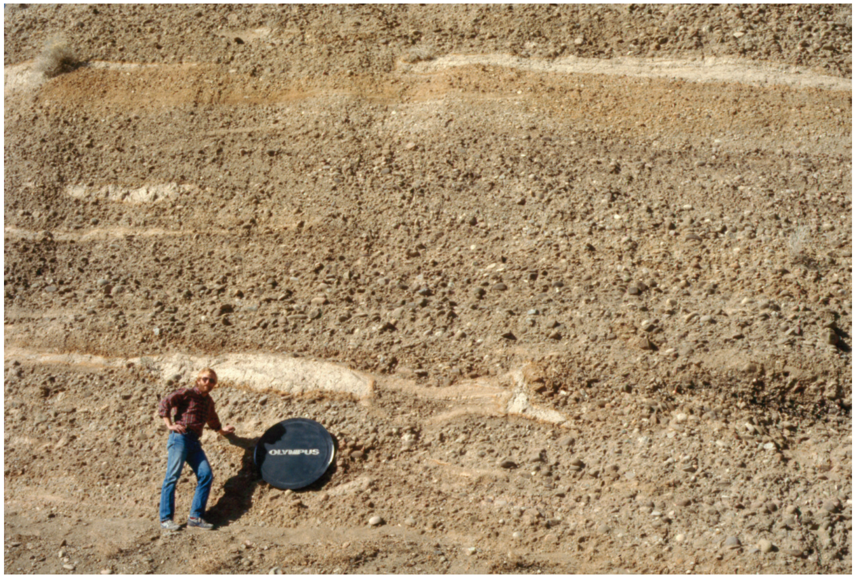


Gaussian density Green function with "variance" that grows linear with time, and tails that drop off like e^{-x^2}.

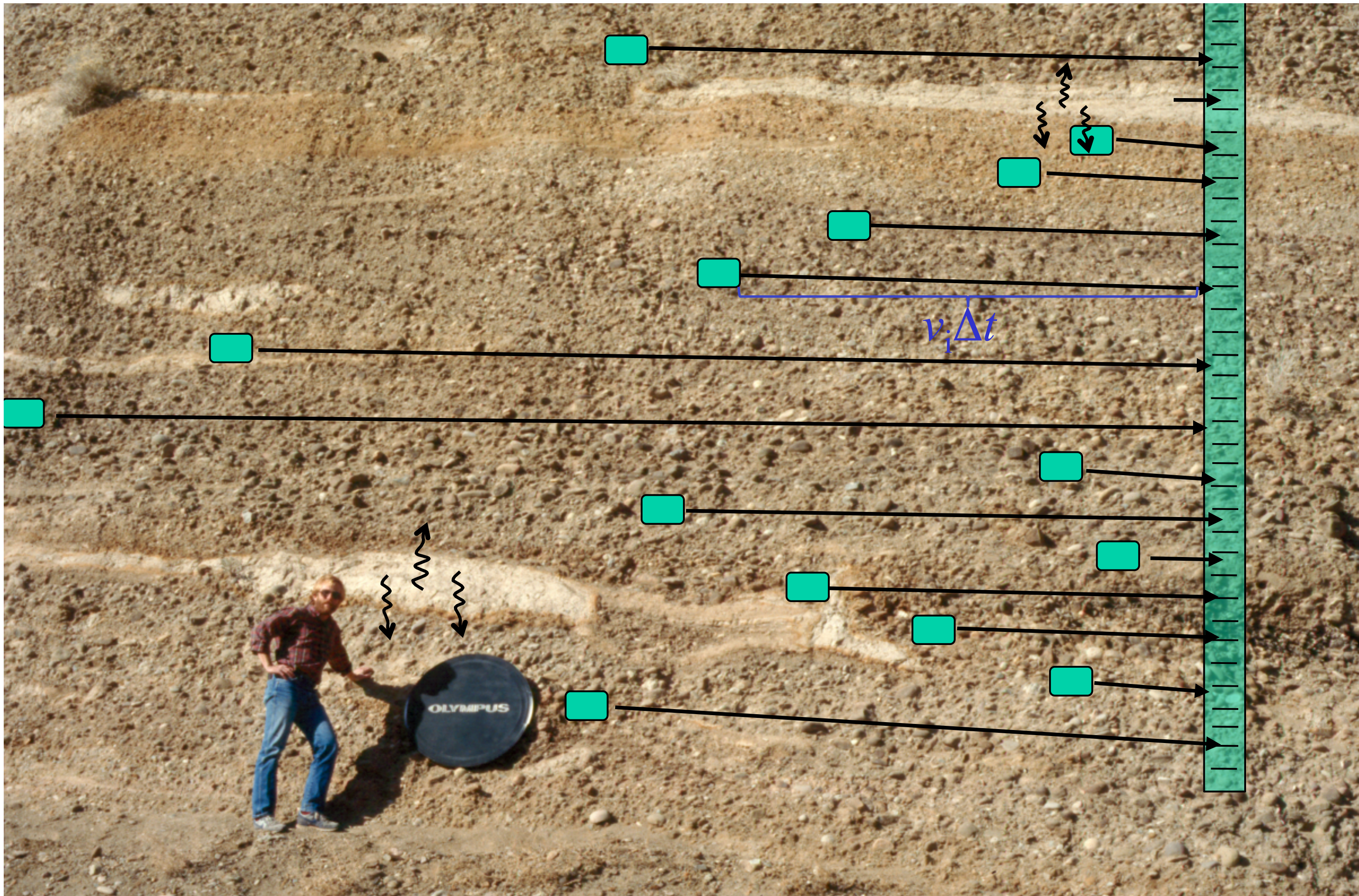
Aquifer material-One of Nature's extreme laboratories

Highly (long-range) autocorrelated,
very high variance (VAR($ln(K) > 20$),
and ...

Fractal (scale invariant)



Zoom in on any part: looks statistically similar to larger picture.



Non-local upscaled transport Eq.

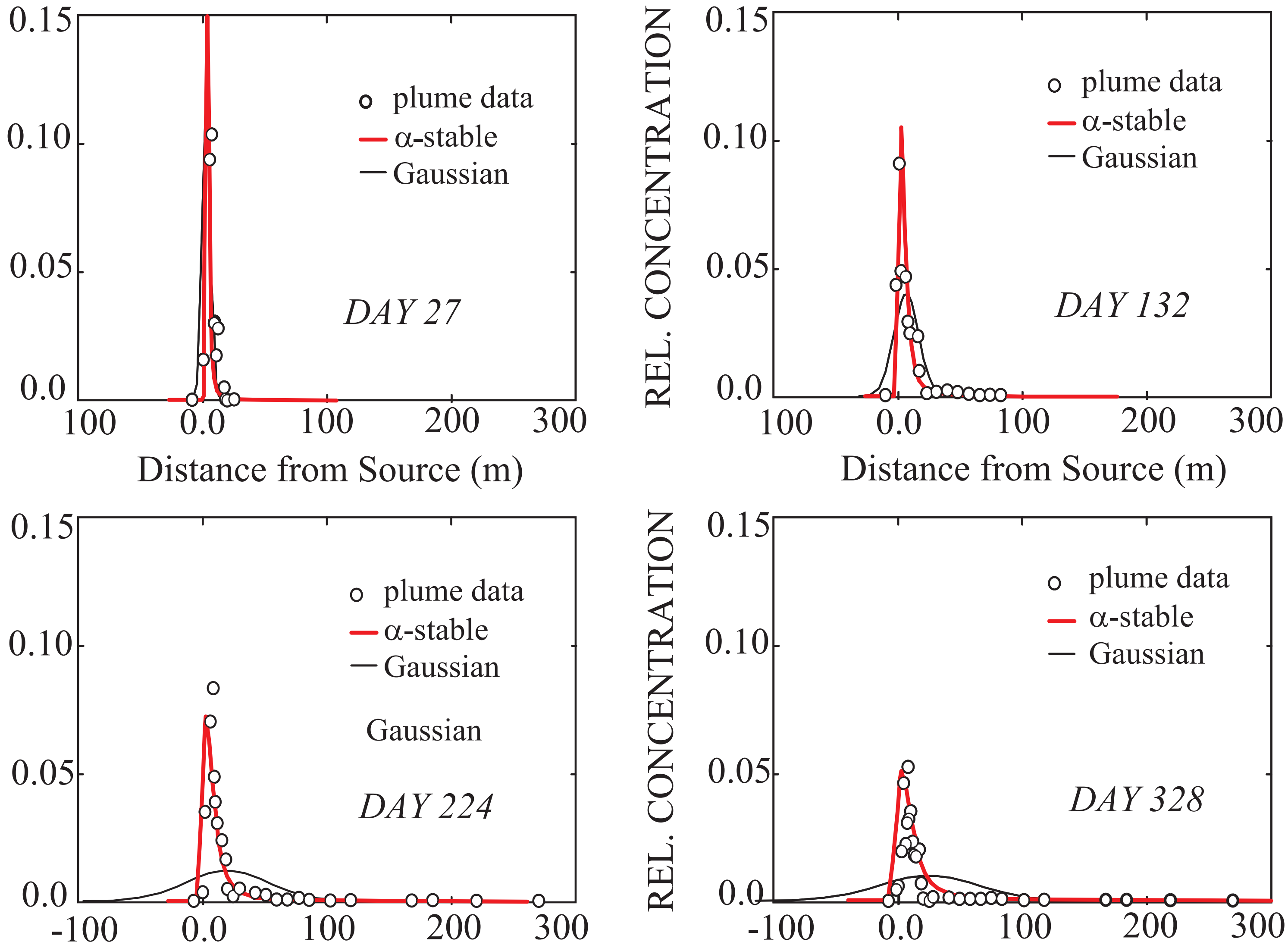
Spatial (dimensional) averaging:

In any small time step Δt, the change in well concentration is due to upstream contributions

$$\frac{\Delta C}{\Delta t} \approx \frac{1}{\Delta x} \sum_{n} \frac{n(v_i)}{n} v_i [C(x - v_i \Delta t) - C(x - v_i \Delta t + \Delta x)]$$

$$\frac{\partial C}{\partial t} \approx \bar{v} \int w(\xi) \frac{dC(x-\xi)}{dx} d\xi$$

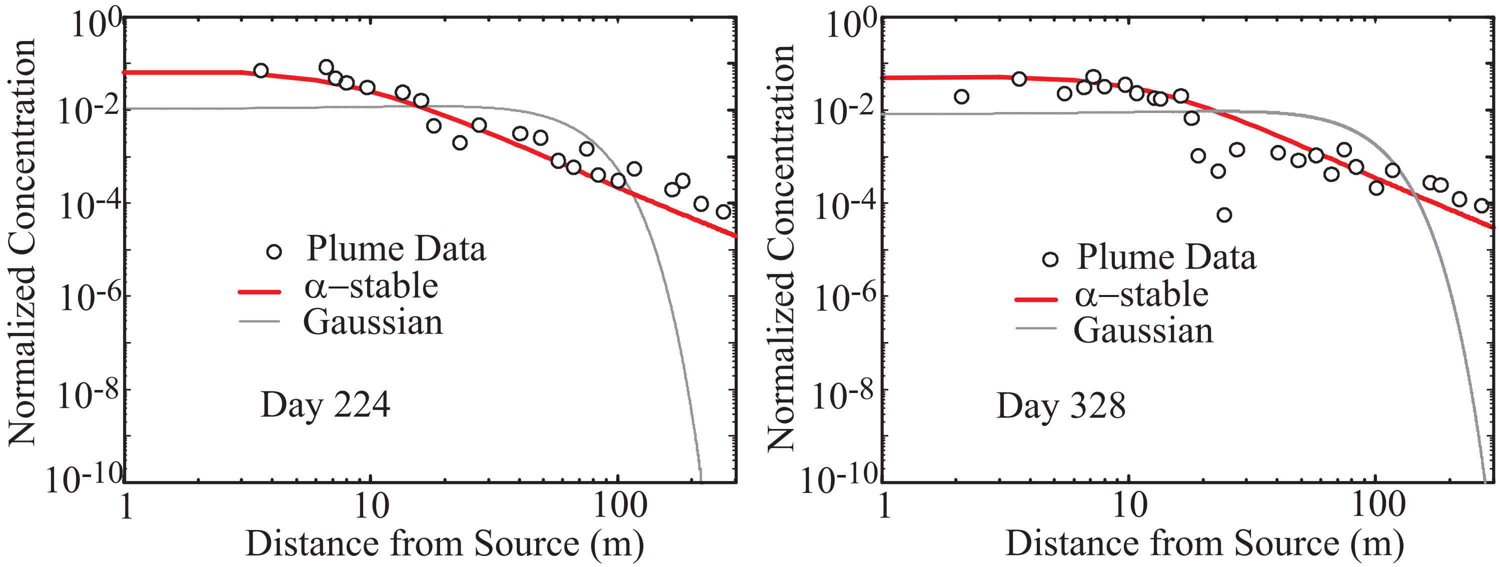
Real Plumes (MADE site)



Follows a space-time nonlocal model at the largest scale.

Power-law leading edge

The Lévy motion's α-stable density $C(x,t)$ with $\alpha = 1.1$ gives a good fit. The Brownian motion's ADE badly underestimates tail concentrations.



Tracer plume has heavy power law tails and spreads like $t^{1/\alpha}$. Let the cat out of the bag:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^\alpha C}{\partial x^\alpha}$$

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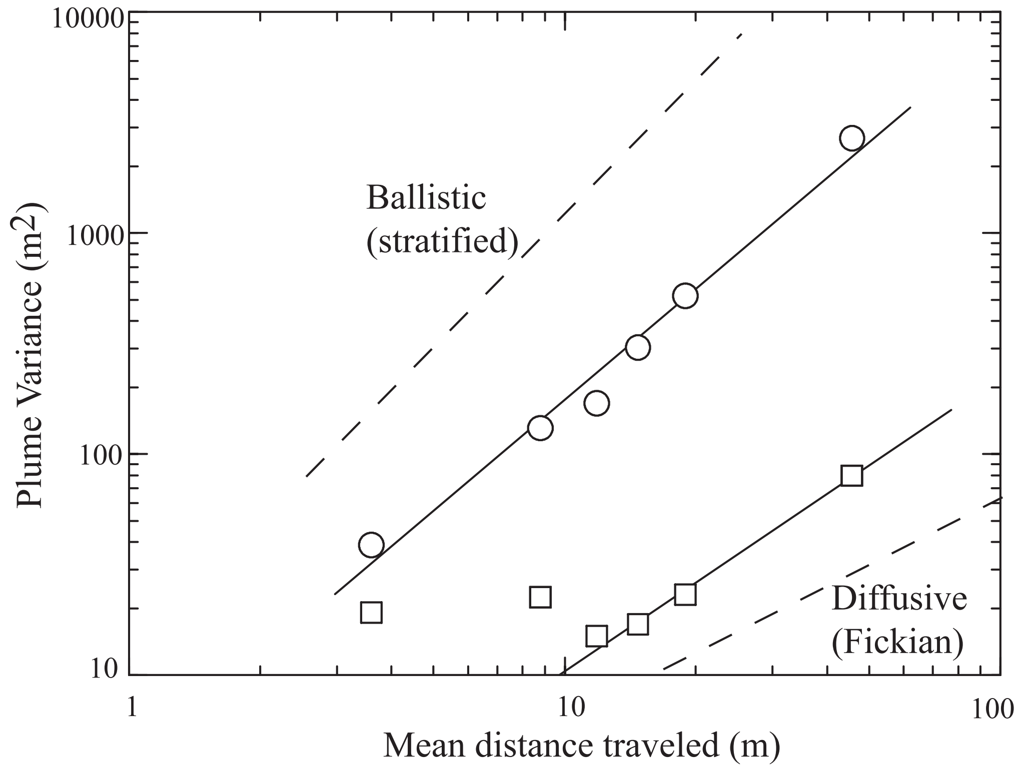
Spreads Faster than Diffusive...



... but slower than ballistic (constant velocity).

AND different rates in different directions.

Rather than guess at governing equations, look at the limit distributions

For "isotropically scaling" Markovian random walks, take a standard heavy-tailed jump R, with $P(R > r) \sim r^{-1}$ so that $P(R^{1/\alpha} > r) \sim r^{-\alpha}$. Then take independent unit vectors θ with measure on the unit sphere $m(d\theta)$. The random walk converges to Lévy motion $Z(t)$

$$\sum_{i=1}^{[t/dt]} X_i = \sum_{i=1}^{[t/dt]} R_i^{1/\alpha} \cdot \theta_i \Longrightarrow Z(t)$$

with characterisic function (Fourier transform of density function)

$$p(\boldsymbol{k}, t) = \exp\left[-t\langle i\boldsymbol{k}, \boldsymbol{v}\rangle + Dt \int (\langle i\boldsymbol{k}, \theta\rangle)^{\alpha} m(d\theta)\right]$$

(using FT $p(\boldsymbol{k}) = \int e^{i\langle \boldsymbol{k}, \boldsymbol{x}\rangle} p(\boldsymbol{x}) d\boldsymbol{x}$)

From Lévy motion to Fractional Derivatives

The characteristic function of Lévy motion with $0 < \alpha \leq 2$

$$p(\boldsymbol{k}, t) = \text{exp}\left[-t\langle i\boldsymbol{k}, \boldsymbol{v}\rangle + Dt\int (\langle i\boldsymbol{k}, \theta\rangle)^{\alpha} m(d\theta)\right]$$

Solves the Cauchy equation

$$\frac{dp(\boldsymbol{k}, t)}{dt} = \left[-\langle i\boldsymbol{k}, \boldsymbol{v}\rangle + D\int (\langle i\boldsymbol{k}, \theta\rangle)^{\alpha} m(d\theta)\right] p(\boldsymbol{k}, t),$$

which for now we will call the Fourier inverse transform

$$\frac{\partial p(\boldsymbol{x}, t)}{\partial t} = -\boldsymbol{v} \cdot \nabla p(\boldsymbol{x}, t) + D\nabla_m^{\alpha} p(\boldsymbol{x}, t),$$

A Brief Review of Well-Known Cases

$$p(\boldsymbol{k},t) = \exp\left[-t\langle i\boldsymbol{k},\boldsymbol{v}\rangle + Dt\int(\langle i\boldsymbol{k},\theta\rangle)^{\alpha} m(d\theta)\right]$$

1-Dimension: $\theta = \pm 1, m(+1) = p, m(-1) = q$, then

$$p(k,t) = \exp\left[-t(ik)v + Dt(p(ik)^{\alpha} + q(-ik)^{\alpha})\right]$$

$$\frac{\partial p(k,t)}{\partial t} = -v(ik)p(k,t) + D(p(ik)^{\alpha} + q(-ik)^{\alpha})p(k,t)$$

Invert FT:

$$\frac{\partial p(x,t)}{\partial t} = -v\frac{\partial p(x,t)}{\partial x} + \frac{D}{\Gamma(-\alpha)}(p\int_{-\infty}^{x}(x-\xi)^{-1-\alpha}p(\xi,t)d\xi$$

$$+q\int_{x}^{\infty}(\xi-x)^{-1-\alpha}p(\xi,t)d\xi)$$

where convolution with the power law in forward and backward directions define

$$\frac{\partial p(x,t)}{\partial t} = -v\frac{\partial p(x,t)}{\partial x} + D\left(p\frac{\partial^{\alpha}}{\partial x^{\alpha}} + q\frac{\partial^{\alpha}}{\partial(-x)^{\alpha}}\right)p(x,t)$$

A Brief Review of Well-Known Cases, cont.

$$p(\boldsymbol{k},t) = \exp\left[-t\langle i\boldsymbol{k},\boldsymbol{v}\rangle + Dt\int(\langle i\boldsymbol{k},\theta\rangle)^{\alpha}m(d\theta)\right]$$

1-Dimension, add symmetry ($p = q = 1/2$):

$$p(k,t) = \exp\left[-t(ik)v + Dt(p(ik)^{\alpha} + q(-ik)^{\alpha})\right]$$

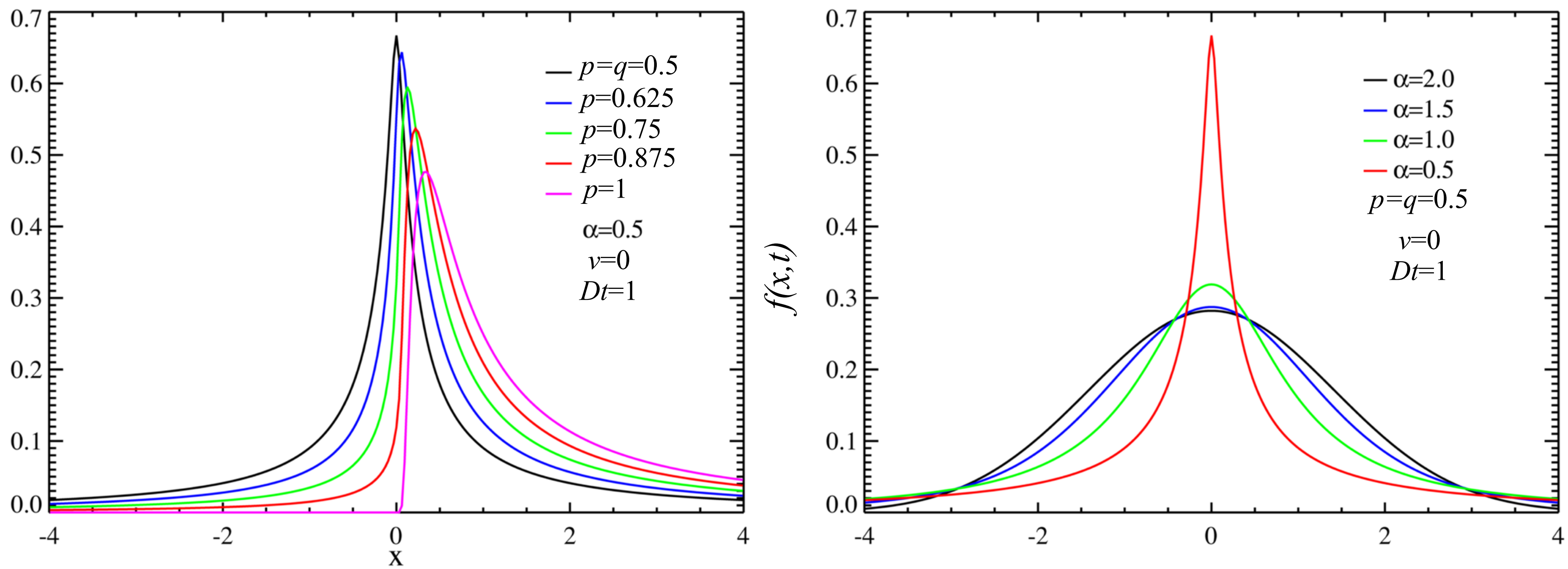
$$p(\boldsymbol{k},t) = \exp\left[-t(ik)v + Dt\cos(\pi\alpha/2)|k|^{\alpha}\right]$$

$$\frac{\partial p(x,t)}{\partial t} = -v\frac{\partial p(x,t)}{\partial x} + D\cos(\pi\alpha/2)\left(\frac{\partial^{\alpha}p(x,t)}{\partial|x|^{\alpha}}\right)$$

(The Riesz fractional derivative)

Note for $\chi = x - vt$ the scaling property $p(\chi,ct) = \frac{1}{c^{1/\alpha}}p(\frac{\chi}{c^{1/\alpha}},t)$

1-D Green Function: Lévy densities



A Brief Review of Well-Known Cases, cont.

$$p(\boldsymbol{k},t)=\exp\left[-t\langle i\boldsymbol{k},\boldsymbol{v}\rangle+Dt\int(\langle i\boldsymbol{k},\theta\rangle)^{\alpha}m(d\theta)\right]$$

$\alpha=2$ (Brownian motion)

$$p(\boldsymbol{k},t)=\exp\left[-t\langle i\boldsymbol{k},\boldsymbol{v}\rangle+Dt\int\sum_{j=1}^{d}(k_j\theta_j)^2m(d\theta)\right]$$

$$p(\boldsymbol{k},t)=\exp\left[-t\langle i\boldsymbol{k},\boldsymbol{v}\rangle+Dt(ik)A(ik)^T\right]$$

where $A_{i,j}=\int\theta_i\theta_j m(d\theta)$. This is a Brownian motion with mean drift $\boldsymbol{v}t$ and covariance matrix $2DtA$. Take the time derivative and invert to get the governing equation for which the pdf of Brownian motion is Green function:

$$\frac{\partial p(\boldsymbol{x},t)}{\partial t}=-\boldsymbol{v}\cdot\nabla p(\boldsymbol{x},t)+\nabla DA\nabla^T p(\boldsymbol{x},t),$$

In General (for scalar order α) ...

The characteristic function of isotropically-scaling Lévy (incl. Brownian) motion can be written

$$p(\boldsymbol{k}, t) = \exp[-t\psi(\boldsymbol{k})]$$

Where $\psi(\boldsymbol{k})$ is the Lévy measure. The motion has Cauchy Eq.

$$\frac{dp(\boldsymbol{k}, t)}{dt} = \psi(\boldsymbol{k})p(\boldsymbol{k}, t)$$

And Inverse transform (propagator)

$$\frac{\partial p(\boldsymbol{x}, t)}{\partial t} = \mathcal{F}^{-1}[\psi(\boldsymbol{k})]p(\boldsymbol{x}, t)$$

In General (isotropic scaling)...

The Lévy measure $\psi(dr, d\theta)$ is best described by a mixture of directional fractional derivatives. The first derivative of $f(x)$ in the θ direction is $df(x+s\theta)/ds = dg(s)/ds$ and the scalar fractional derivative is then

$$D_{+}^{\alpha} g(r) = \frac{1}{\Gamma(-\alpha)} \int_0^\infty r^{-1-\alpha} g(s-r)dr$$

A mixture of these according to the measure $m(d\theta)$ gives the (single-order) multi-dimensional fractional derivative

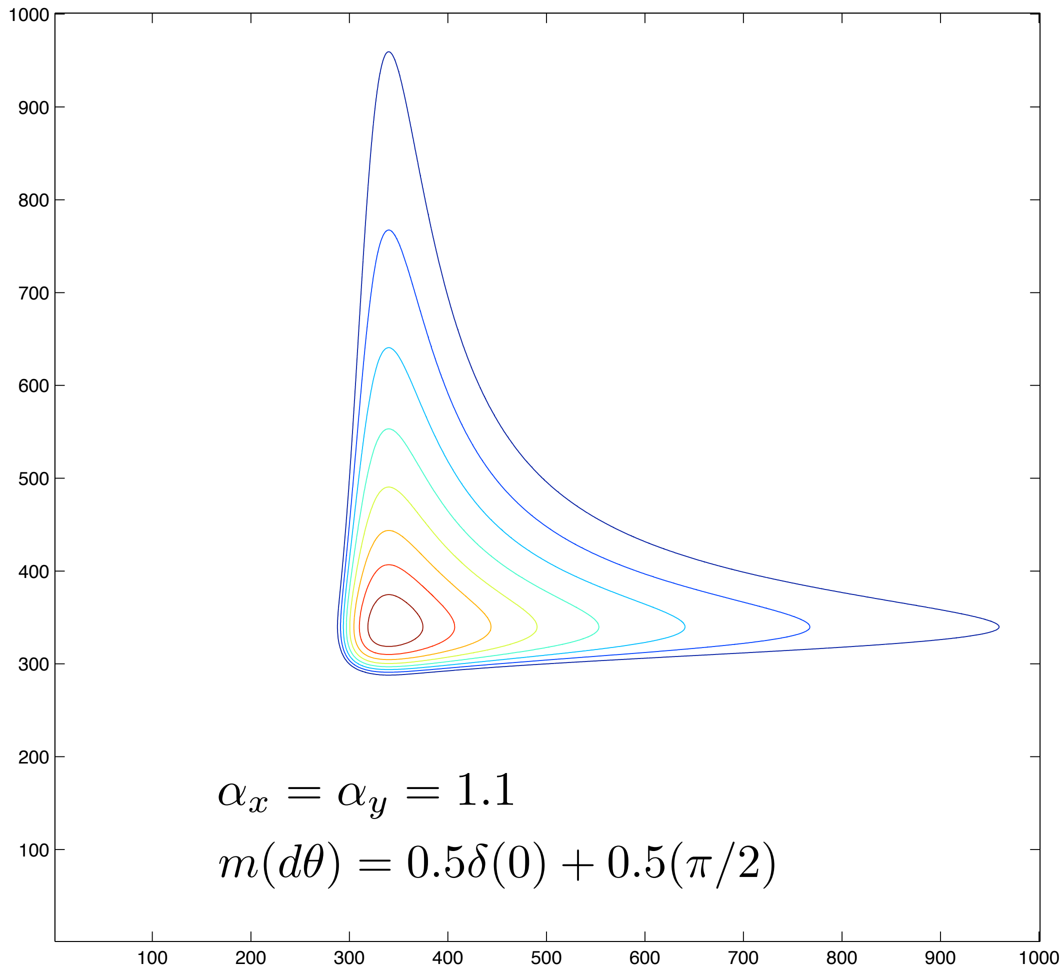
$$\nabla_m^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \int_{|\theta|=1} \int_0^\infty r^{-1-\alpha} f(x - r\theta)dr\, m(d\theta)$$

Which is a (radial) convolution with the Lévy measure

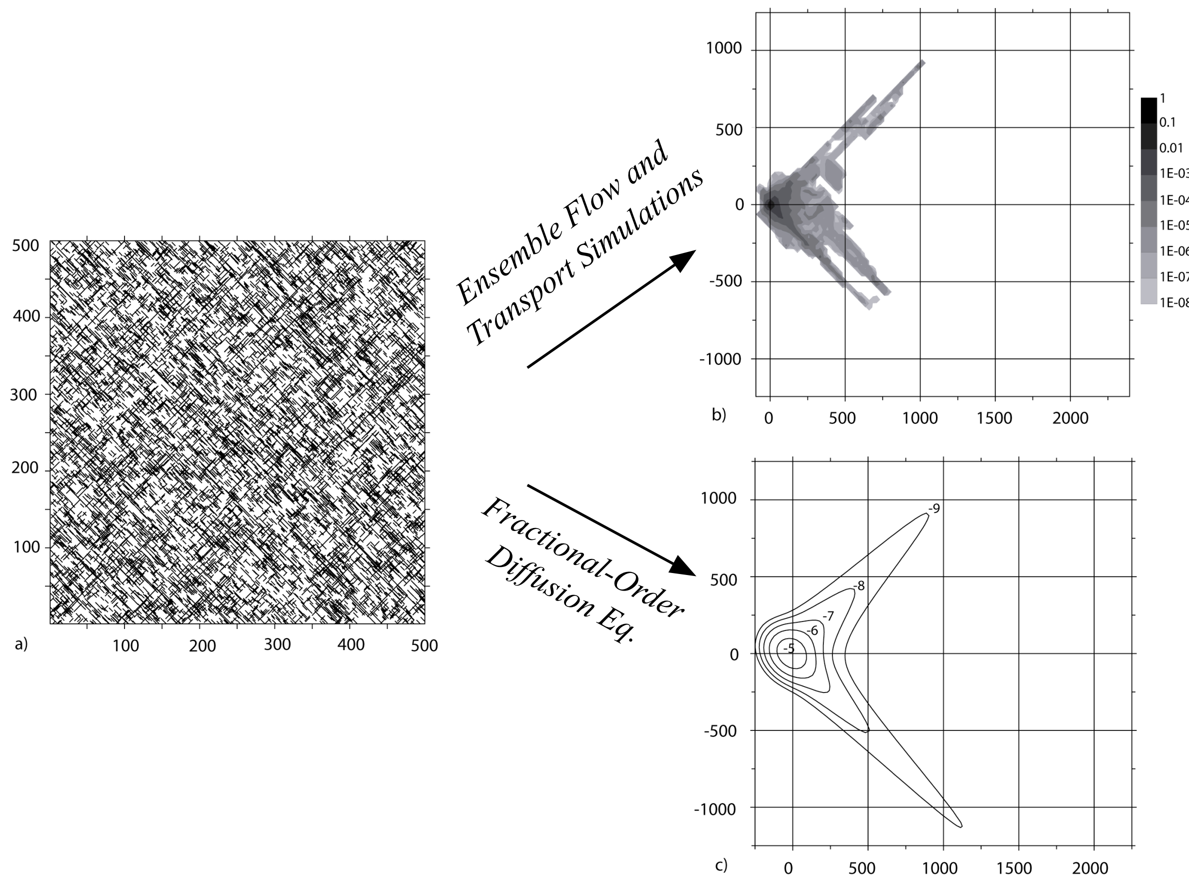
$$\psi(dr, d\theta) = \alpha r^{-1-\alpha} m(d\theta)/\Gamma(-\alpha)$$

.

Example 2-D Green Function: multi-stable densities



Motivation: Transport in Fractured Rock



Reeves et al., Transport of conservative solutes in simulated fracture networks: 2. Ensemble solute transport and the correspondence to operator-stable limit distributions, Water Resour. Res., 2008.

But I lied. Big jumps can be different in different directions (i.e. fracture sets).

For "anisotropically scaling" Markovian random walks, take a standard heavy-tailed jump R, with $P(R > r) \sim r^{-1}$. Rescale jumps by growth rate matrix $\boldsymbol{H}$ so the jump size matrix $R^{\boldsymbol{H}}$ has probabilities that fall off like $r^{-\alpha_i}$ in the ith eigendirection. Also take independent unit vectors θ with measure on the unit sphere $m(d\theta)$. The random walk converges to *operator-scaling* Lévy motion $Z(t)$

$$\sum_{i=1}^{[t/dt]} X_i = \sum_{i=1}^{[t/dt]} R_i^{\boldsymbol{H}} \cdot \theta_i \Longrightarrow Z(t)$$

with characteristic function (Fourier transform of density function)

$$p(\boldsymbol{k}, t) = \exp\left[-t\langle i\boldsymbol{k}, \boldsymbol{v}\rangle + t\boldsymbol{k} \cdot A\boldsymbol{k} + Dt\psi(\boldsymbol{k})\right]$$

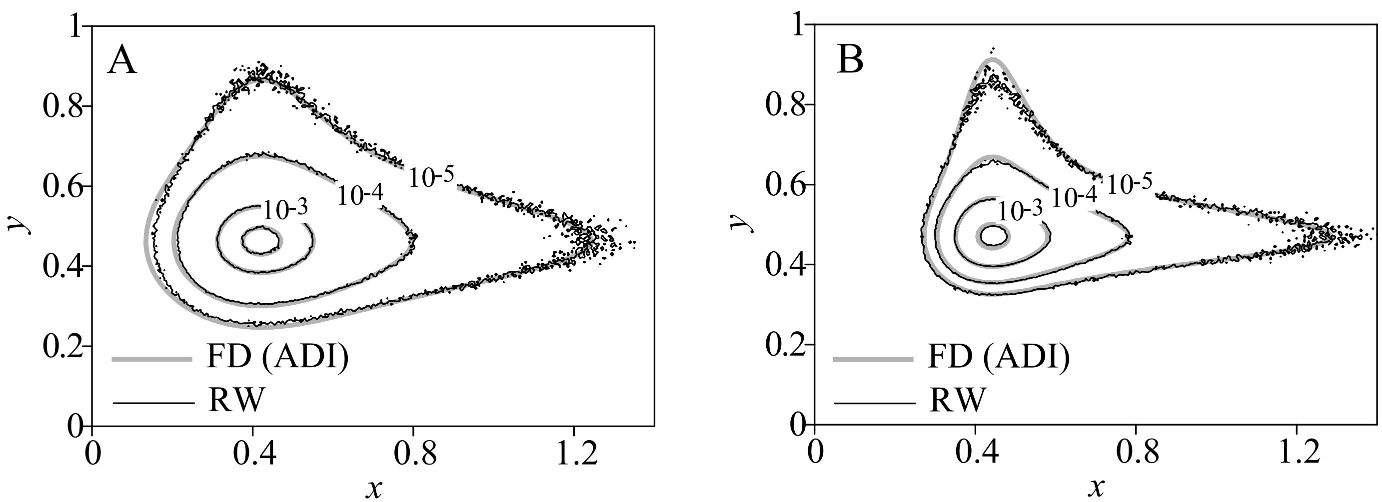
where the operator-scaling Lévy measure now is primarily defined by its matrix scale-invariance $\psi(c^{\boldsymbol{H}}\boldsymbol{k}) = c\psi(\boldsymbol{k})$ (different power laws in different directions).

A simple example

Let $\boldsymbol{H} = \begin{bmatrix} 1/\alpha_1 & 0 \\ 0 & 1/\alpha_2 \end{bmatrix}$, and $m([1 \quad 0]) = m([0 \quad 1]) = 0.5$, then

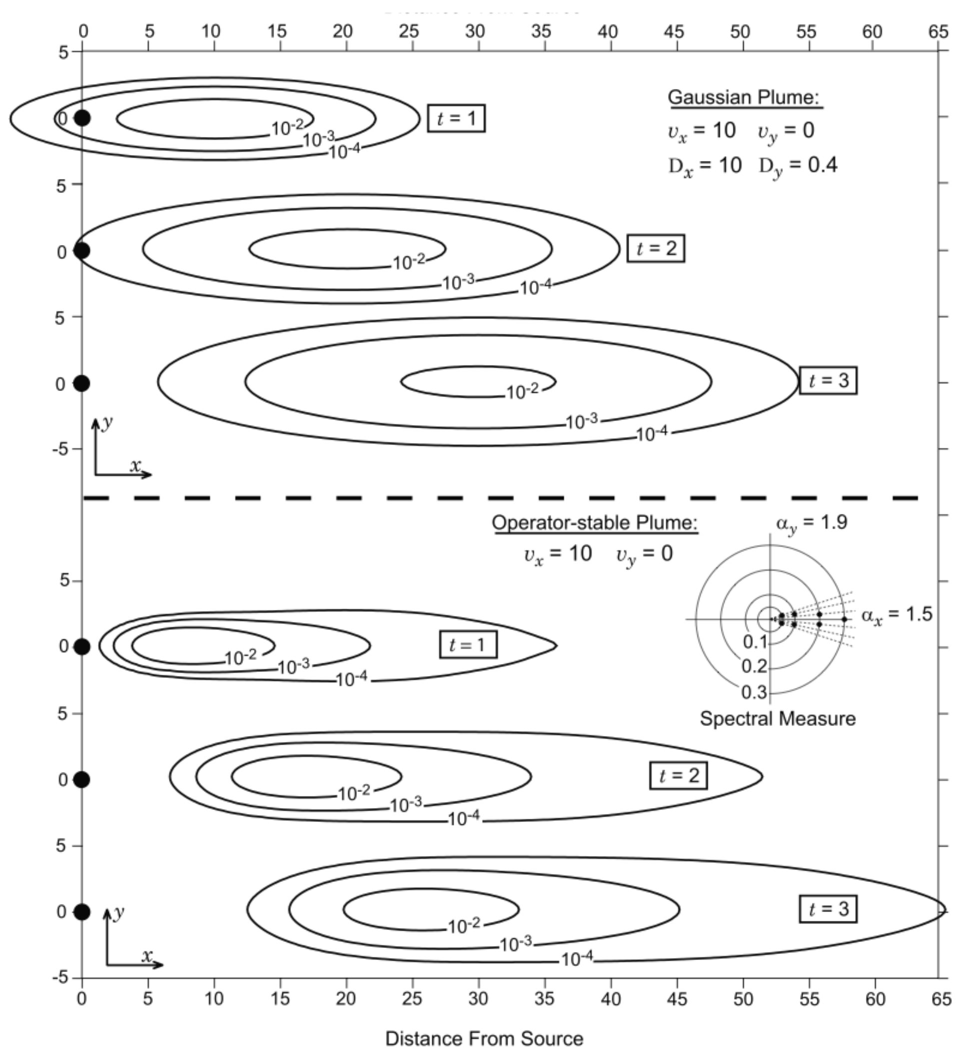
$$\psi(\boldsymbol{k}) = 0.5(ik_1)^{\alpha_1} + 0.5(ik_2)^{\alpha_2}$$

$$\frac{\partial p(\boldsymbol{x},t)}{\partial t} = 0.5\left(p\frac{\partial^{\alpha_1}}{\partial x^{\alpha_1}} + q\frac{\partial^{\alpha_2}}{\partial y^{\alpha_2}}\right)p(\boldsymbol{x},t)$$



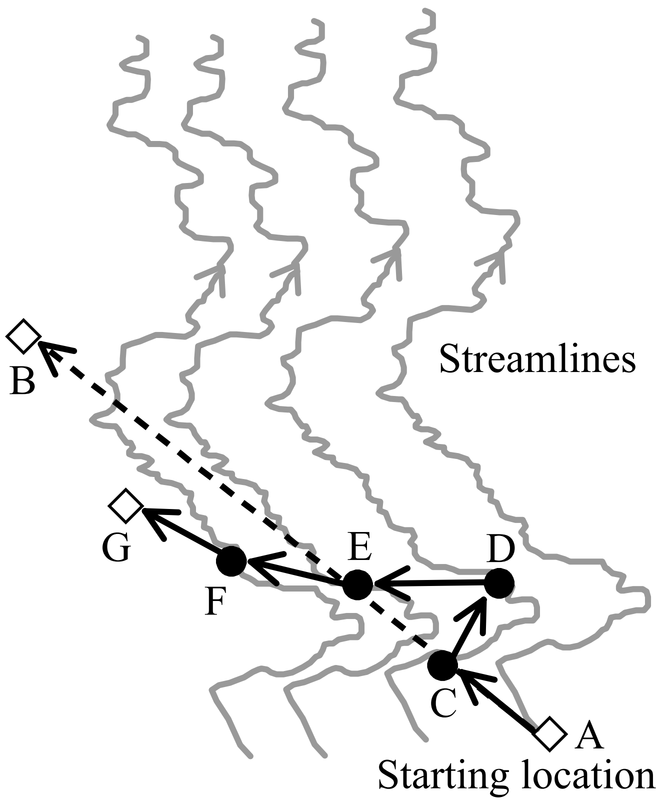
$\alpha_x = 1.6, \alpha_y = 1.8$ (Finite-difference and RW)

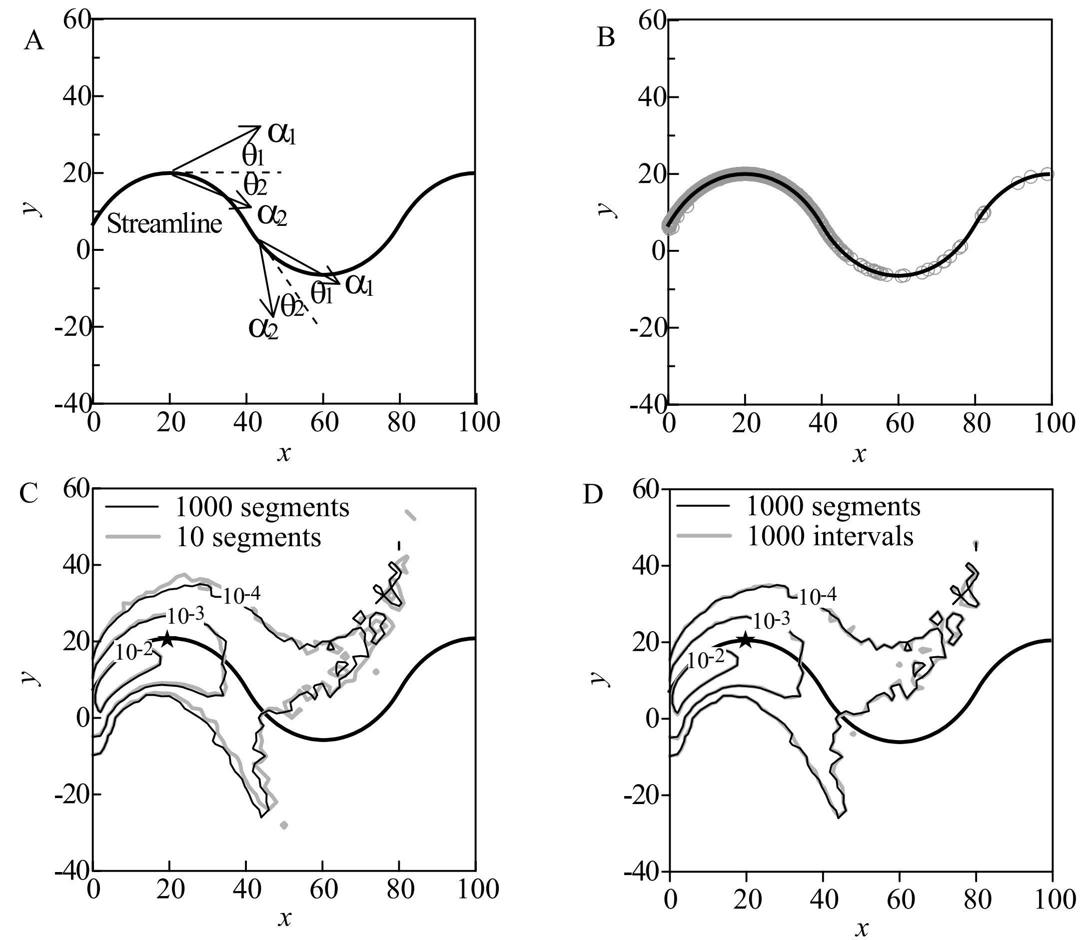
Example operator-scaling Lévy densities (bottom)



Schumer et al., Multiscaling fractional advection-dispersion equations and their solutions, Water Resour. Res., 2003

But what about the part that hydrologists love to measure and simulate - $v(x)$?





Probably can only be done via random walks (see great paper by Yong Zhang et al.)

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Random walk approximation of fractional-order multiscaling anomalous diffusion

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Random walks are developed to approximate the solutions of multiscaling, fractional-order, anomalous diffusion equations. The essential elements of the diffusion are described by the matrix-order scaling indexes and the mixing measure, which describes the diffusion coefficient in every direction. Two forms of the governing equation (also called the multiscaling fractional diffusion equation), based on fractional flux and fractional divergence, are considered, where the diffusion coefficient and the drift vary in space. The particle-tracking algorithm is also extended to approximate anomalous diffusion with a streamline-dependent mixing measure, using a streamline-projection technique. In this and other general cases, the random walk method is the only known way to solve the nonhomogeneous equations. Five numerical examples demonstrate the flexibility, simplicity, and efficiency of the random walk method.

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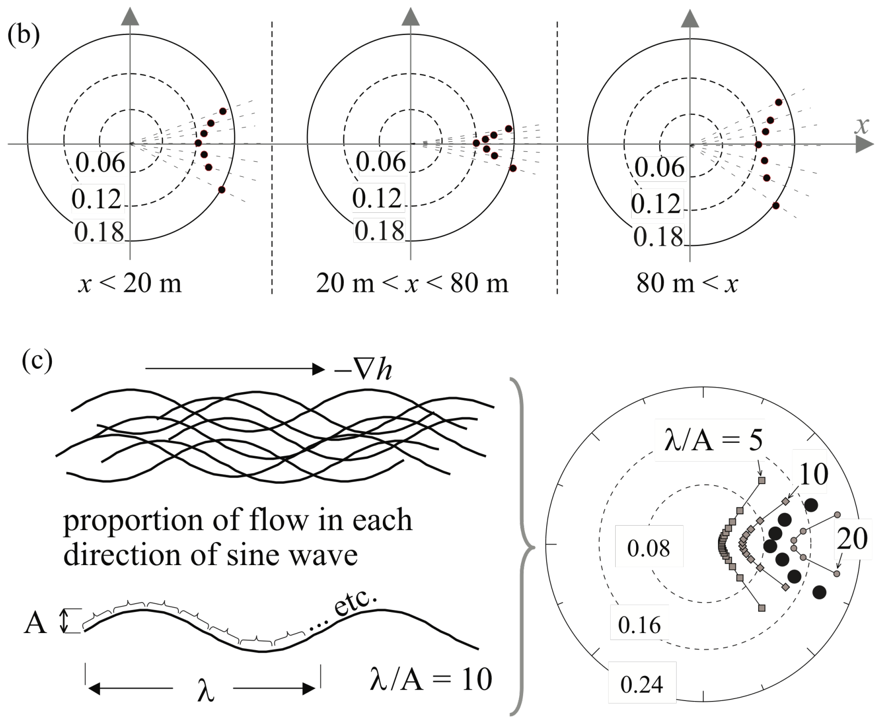
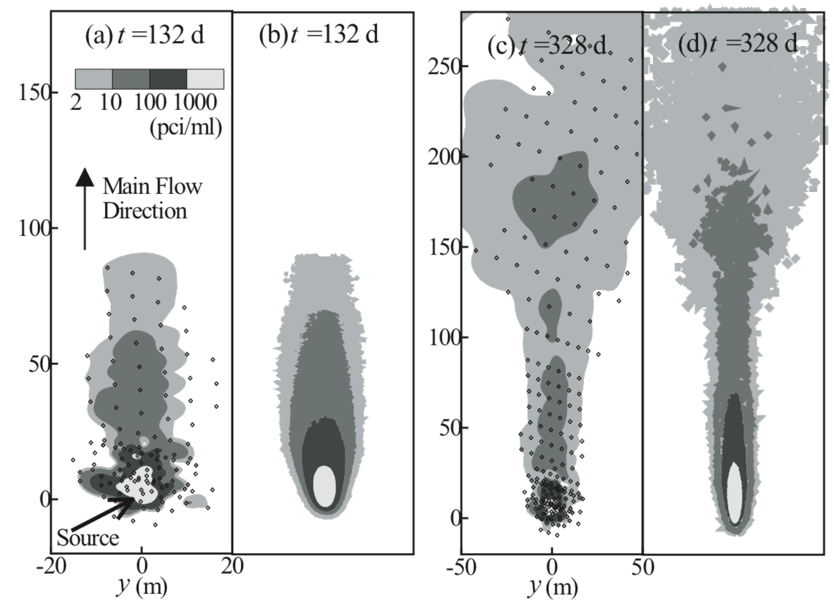
Plume Simulation at the MADE site

Estimation of mixing measure m



Particle tracking simulation of os-stable plume



Zhang, Y., and D.A.Benson, Lagrangian simulation of multidimensional anomalous transport at the MADE site, Geophys. Res. Lett., 2008.

The Inverse Operator (Fractional Integration)

If the most general fractional derivative operator (for eigenvalues $0 < \alpha_i \leq 2$) can be denoted by the diffusion equation for operator-scaling Lévy motion

$$\frac{dp(\boldsymbol{x},t)}{dt} = D\nabla_m^{\boldsymbol{A}} p(\boldsymbol{x},t)$$

with FT

$$\frac{dp(\boldsymbol{k},t)}{dt} = D\psi(\boldsymbol{k})p(\boldsymbol{k},t),$$

where ψ is defined only by its scale invariance $\psi(c^{\boldsymbol{A}^{-1}}\boldsymbol{k}) = (1/c)\psi(\boldsymbol{k})$, then there *must* be one or more inverse operator defined by $\phi(\boldsymbol{k}) = [\psi(\boldsymbol{k})]^{-1}$, so that

$$p(\boldsymbol{k}) = \psi(\boldsymbol{k})\phi(\boldsymbol{k})p(\boldsymbol{k})$$

Generalized Fractional Integration

Similar to the derivative model, an integral equation may take the matrix-order form

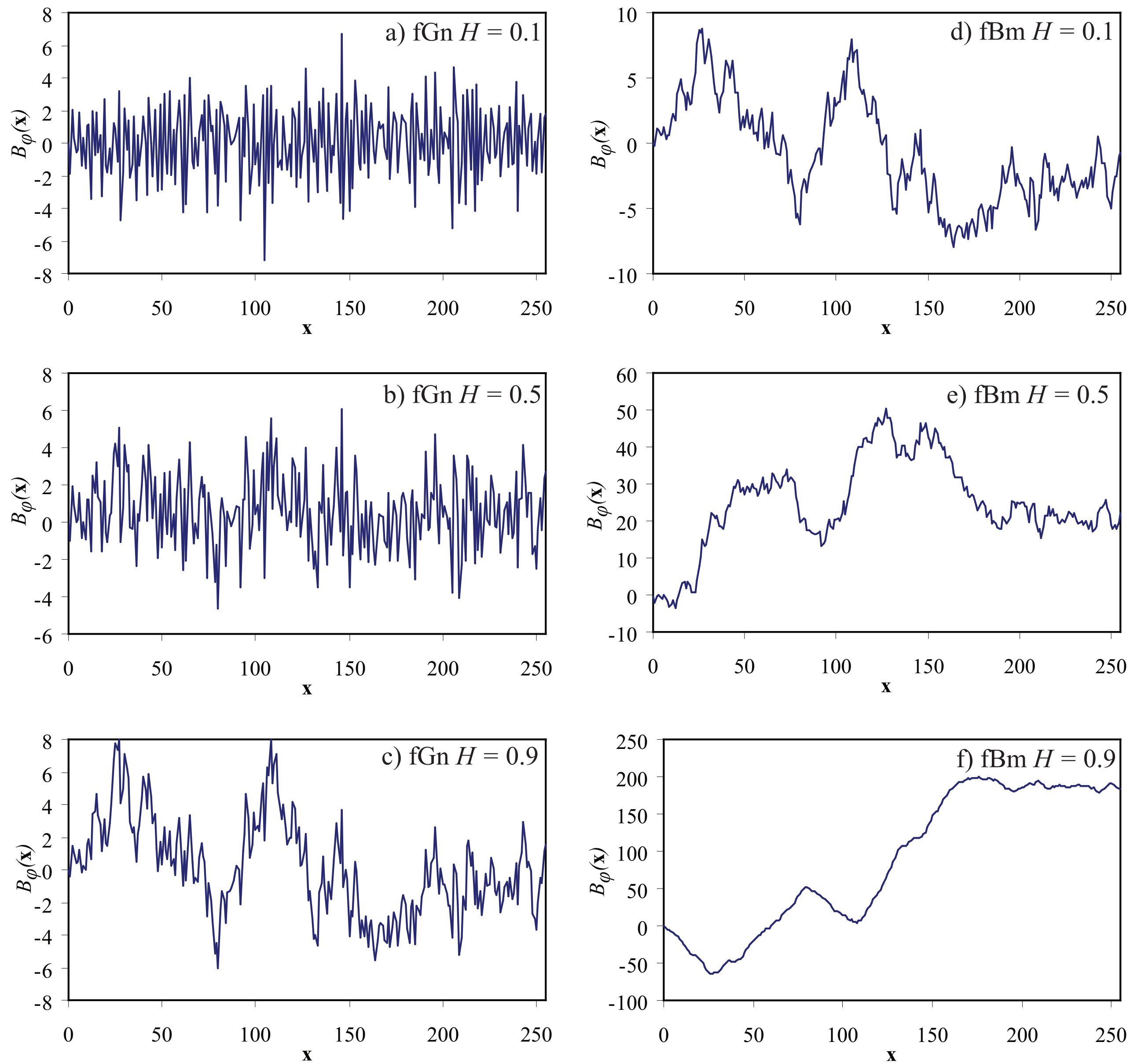
$$g(\boldsymbol{x}) = I_m^{\boldsymbol{A}} f(\boldsymbol{x}) \quad \text{with orders } 0 < \alpha_i \le 2$$

defined by the convolution $g(\boldsymbol{k}) = \phi(\boldsymbol{k}) f(\boldsymbol{k})$

Example: Classical 1-D fractional Brownian motion *USES* $A = H + 1/2, m(+1) = 1$

$$B_H(x) = \int_{-\infty}^{x} (x-y)^{H-1/2} B(dy)$$

where $B(dy)$ is white noise. Now $\phi(k) = (ik)^{-H-1/2} = (ik)^{-A}$, and $\phi(c^{1/A}k) = (1/c)\phi(\boldsymbol{k})$


a) fGn H = 0.1
b) fGn H = 0.5
c) fGn H = 0.9
d) fBm H = 0.1
e) fBm H = 0.5
f) fBm H = 0.9
$B_\varphi(\mathbf{x})$
$\mathbf{x}$

Constructing an isotropic d-dimensional fBm

$$B_H(\boldsymbol{x}) = \int \left[\|\boldsymbol{x} - \boldsymbol{y}\|^{H-d/2} - \|\boldsymbol{y}\|^{H-d/2} \right] B(d\boldsymbol{y}) \tag{1}$$

with $B(d\boldsymbol{y})$ the increment of a Brownian field (a Wiener process) and Hurst index $0 < H < 1$. Numerically, we start with the (divergent) convolution

$$B_H(\boldsymbol{x}) = \int \|\boldsymbol{x} - \boldsymbol{y}\|^{H-d/2} B(d\boldsymbol{y})$$

(Formally a fractional-order integral)

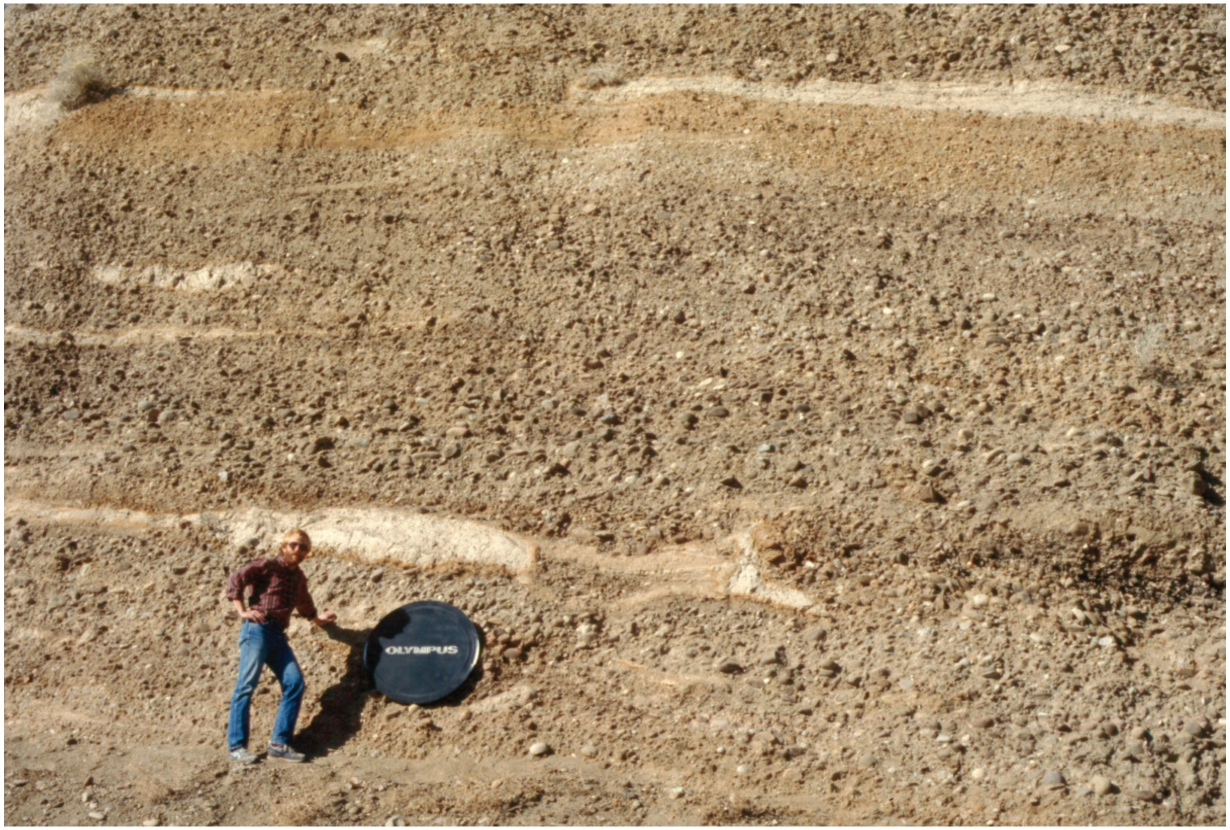
$$B_H(\boldsymbol{x}) \approx \sum \phi(\boldsymbol{x} - \boldsymbol{y}) B(\Delta \boldsymbol{y})$$

$$\phi(x) = \frac{\Gamma(H + 1 - d/2 + \|\boldsymbol{x}\|)}{\Gamma(\|\boldsymbol{x}\| + 1)\Gamma(H + 1 - d/2)} \sim \frac{\|\boldsymbol{x}\|^{H-d/2}}{\Gamma(H + 1 - d/2)}$$

Solve using FFT:

$$B_H(\boldsymbol{x}) \propto \mathsf{FFT}^{-1} \|\boldsymbol{k}\|^{-H-d/2} B(\Delta \boldsymbol{k})$$

Problem: It's obvious which way is vertical versus horizontal



Solution: Different H in different directions

Operator-Scaling fBm

Now require different scaling (zooming) in different directions:

$$B_\varphi(c^{\boldsymbol{Q}}\boldsymbol{x}) \stackrel{d}{=} c^H B_\varphi(\boldsymbol{x})$$

where $\boldsymbol{Q}$ is a scaling matrix (can also contain rotations). Also require that $Tr(\boldsymbol{Q}) = d$. A simple example is $\boldsymbol{Q} = diag(q_1, q_2)$ and

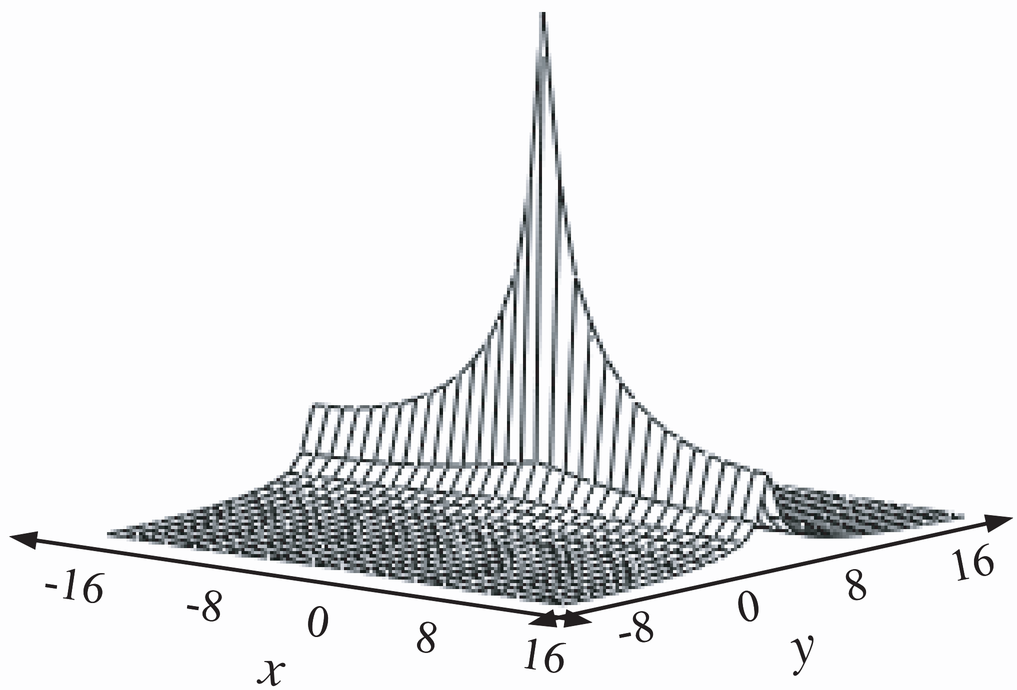
$$c^{\boldsymbol{Q}} = \begin{bmatrix} c^{q_1} & 0 \\ 0 & c^{q_2} \end{bmatrix}$$

Now the only requirement of the convolution function $\varphi(\boldsymbol{x})$ is that

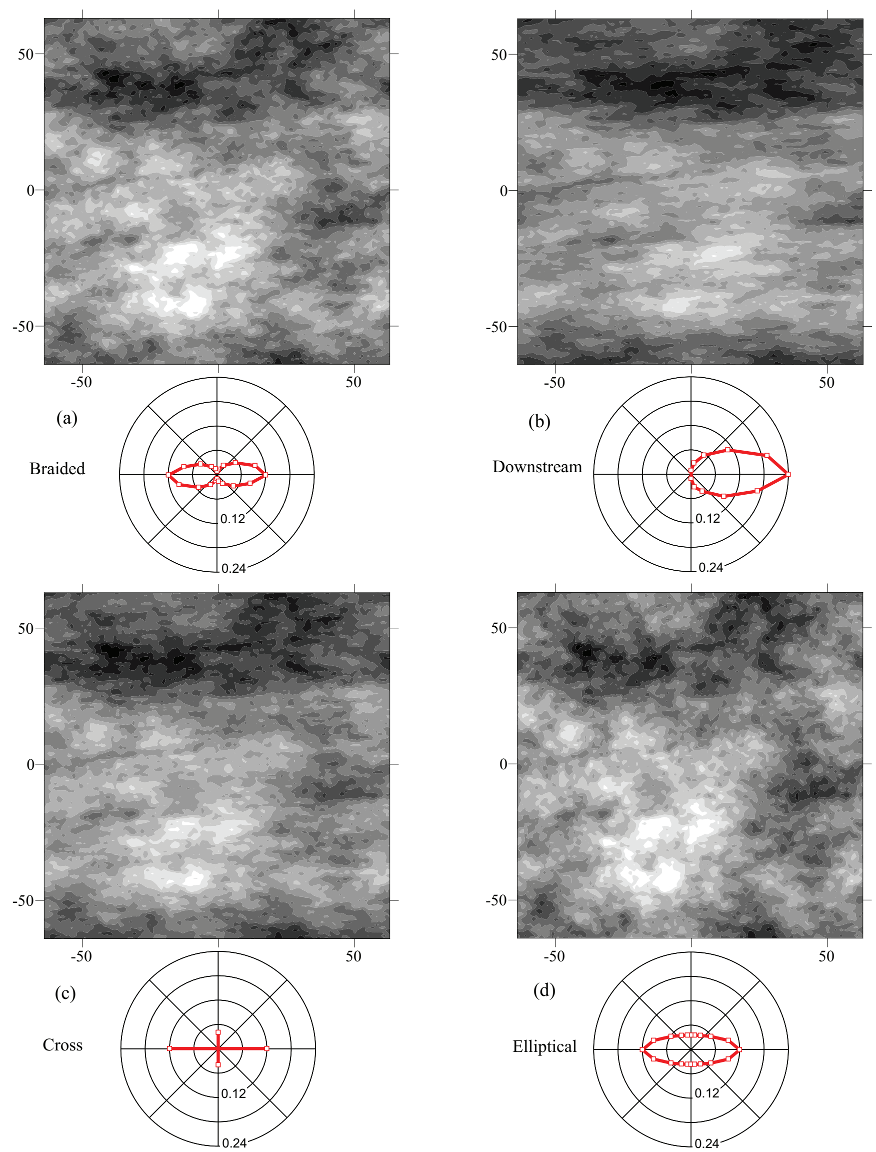
$$\varphi(c^{\boldsymbol{Q}}\boldsymbol{x}) = c^{H-d/2}\varphi(\boldsymbol{x})$$

Example 2-D Convolution Kernel

$$H_x = 0.9; H_y = 0.3; m(0) = 0.8; m(\pi/2) = 0.2$$

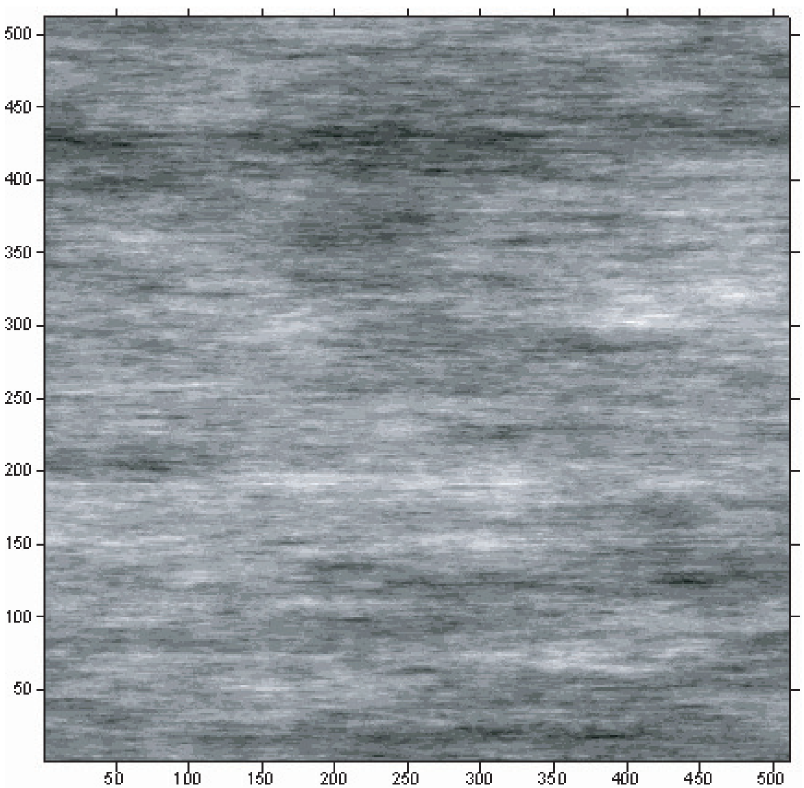


Effect of weights $m(\theta)$: Hold scaling H isotropic

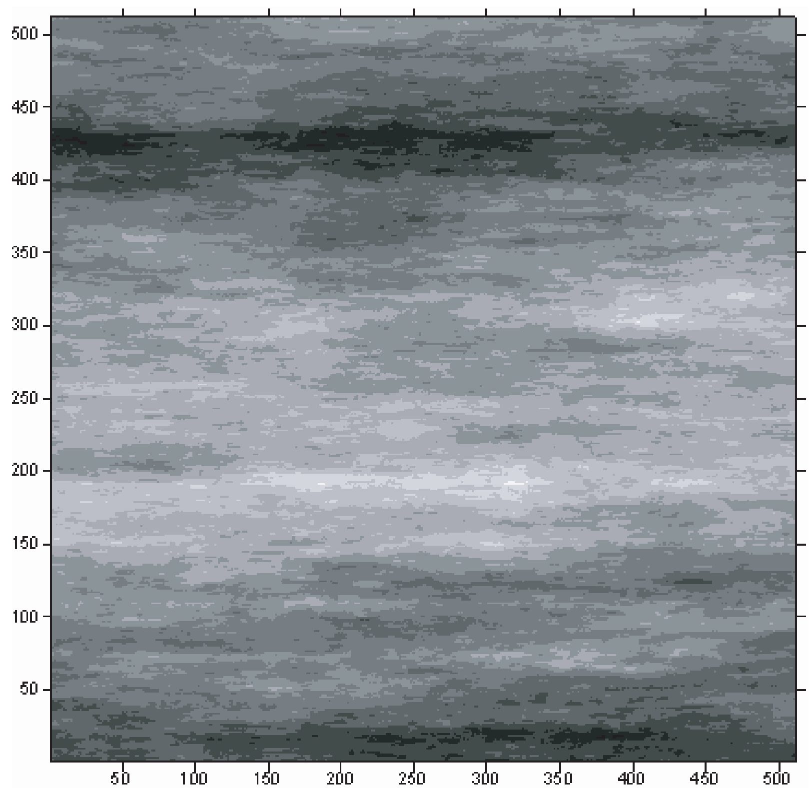


Example: Effect of changing scaling H in one direction

$H_{vert} = 0.4$



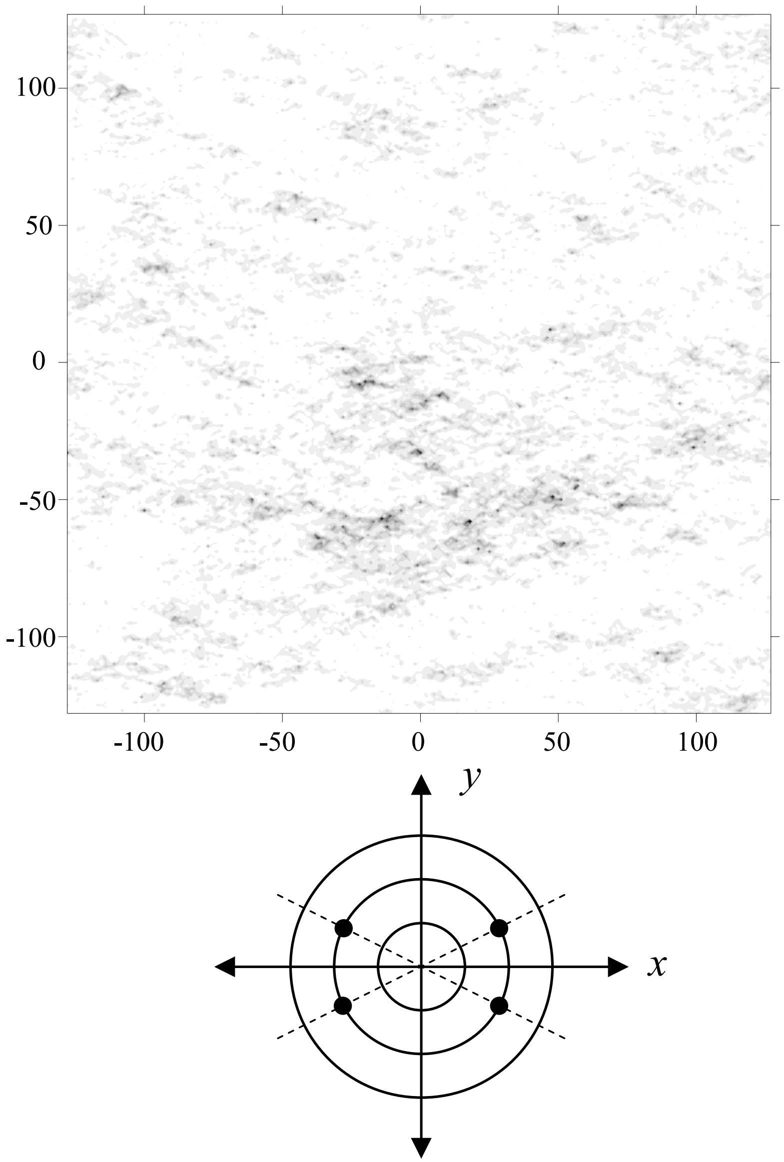
$H_{vert} = 0.7$

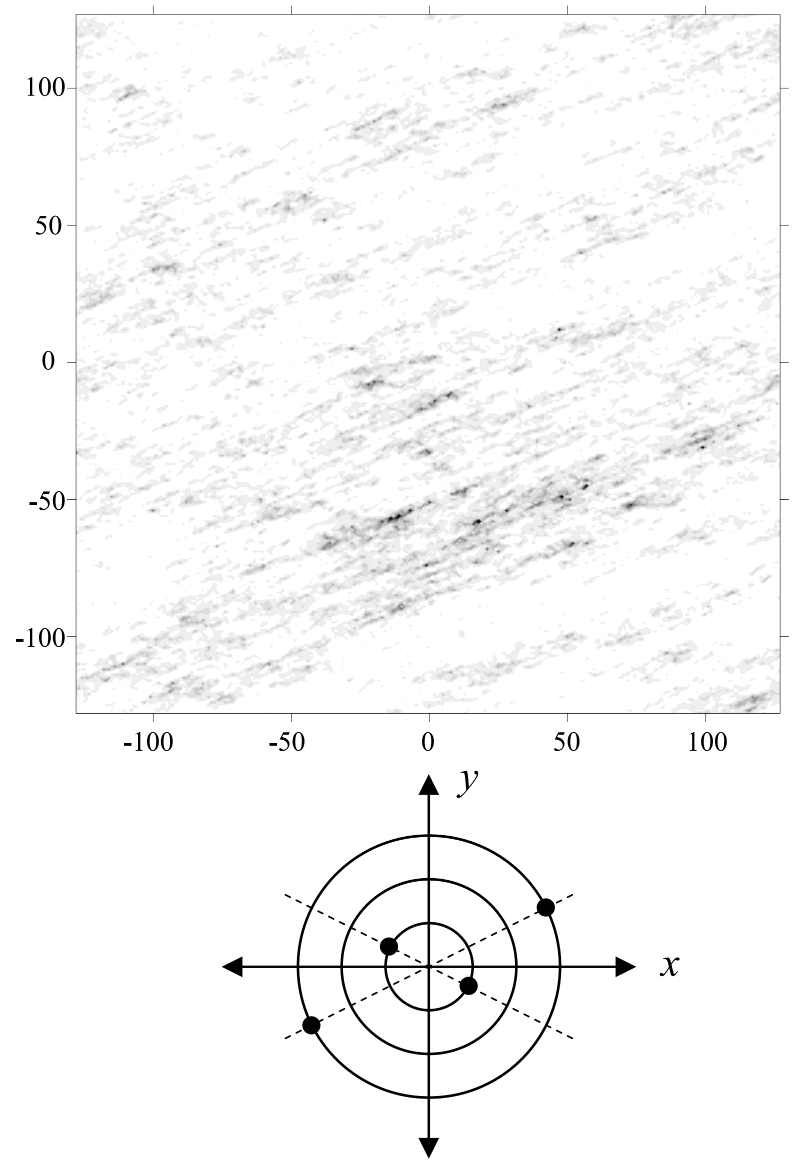


$H_{horiz} = 0.7$

Plumes mix and slow down when $H_{transverse}$ *in smaller ...*

Examples (atomistic $m(\theta)$)





Conclusions (Future Directions?)

- Particle methods rock!

- Applied mathematicians hate them: nothing to prove!

- Almost always a Langevin equation to your goofy fractional PDE.

- Hydrologists need easy-to-use plug-and-play fractional simulator. Nothing else will do.