Backward Probabilities for Contaminants Undergoing Fractional Dispersion

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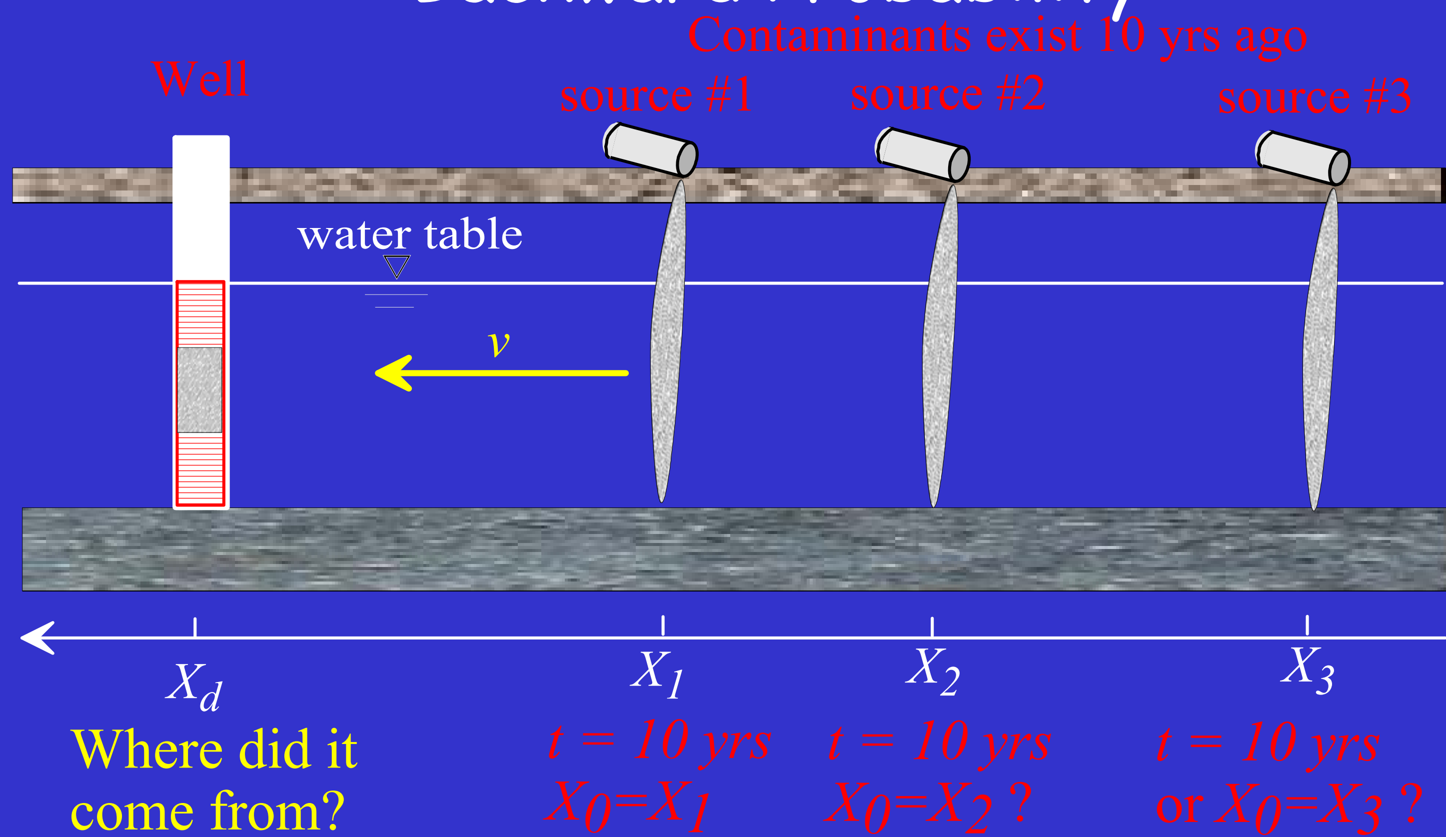
Outline

1. Review of backward probability: the inverse problem of contaminant transport
2. Space fractional advection-dispersion equation (fADE) and its inverse model
3. Eulerian solution
4. Numerical examples
5. Lagrangian solution
6. Future work

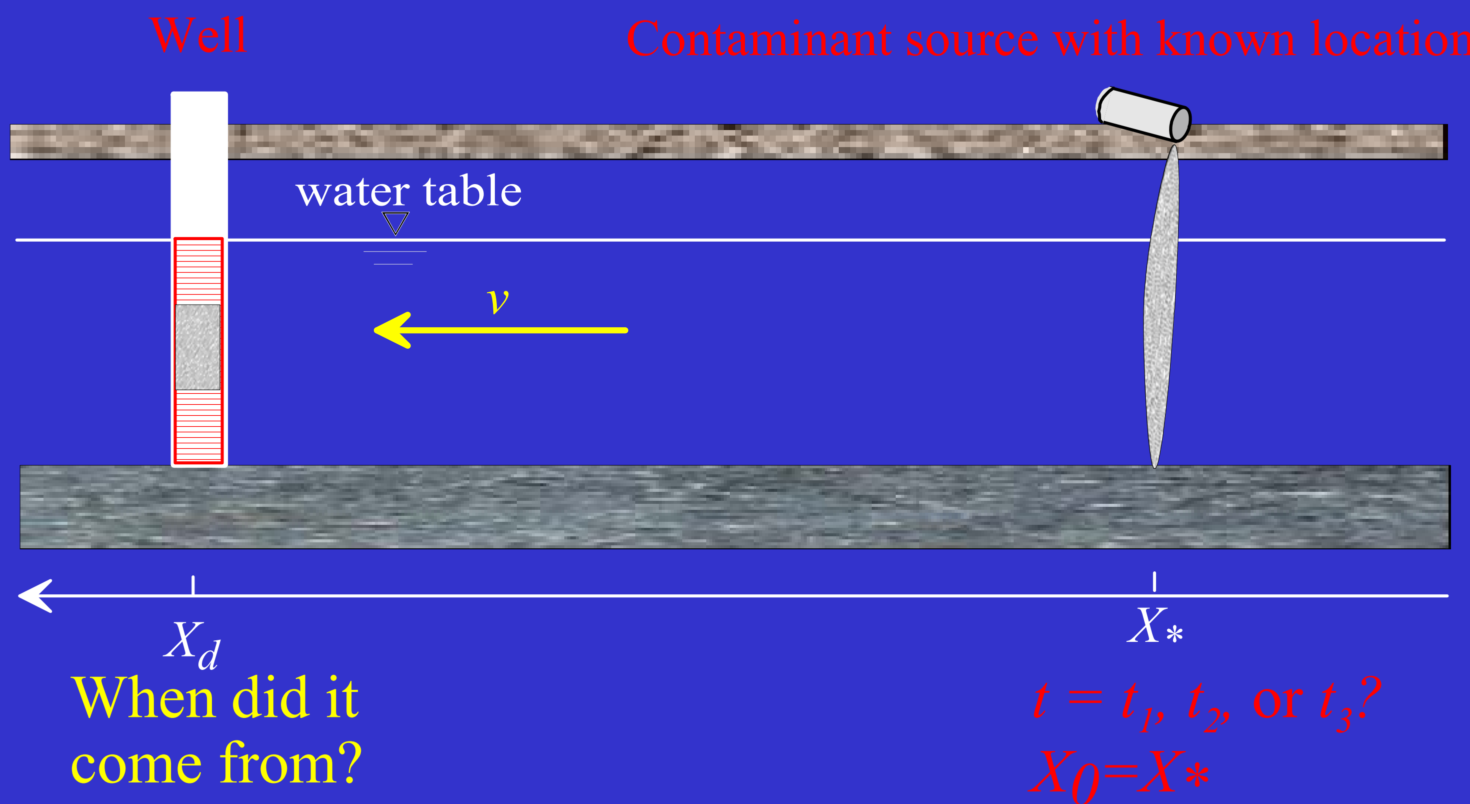
Backward Probability



Backward location PDF – describes the contaminant's former possible location at a specified time in the past.

Application: Source identification; Well-head protection zone delineation; Repository location for waste storage; etc.

Backward Probability (Continued)



Backward travel time PDF – describes the previous possible time for the contaminant to reach the sampling location from a known upgradient location.

Application: Release history recovery; Groundwater age calculation; Vulnerability assessment; etc.

Classical ADE model and its inverse problem

[*Neupauer & Wilson*, 2001]

Forward ADE

$$\frac{\partial}{\partial t}(\theta C) = -\frac{\partial}{\partial x}(\theta v C) + \frac{\partial}{\partial x}\left[\theta D \frac{\partial C}{\partial x}\right] + q_I C_I - q_O C$$

$$C(x, t=0) = C_i(x),$$

$$C(x,t)\big|_{x=+\infty} = 0,$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=-\infty} = 0.$$

Backward ADE

($s = T\text{-}t$)

$$\frac{\partial}{\partial s}(\theta \varphi) = \frac{\partial}{\partial x}(\theta v \varphi) + \frac{\partial}{\partial x}\left[\theta D \frac{\partial \varphi}{\partial x}\right] - q_I \varphi + \frac{\partial h}{\partial C}$$

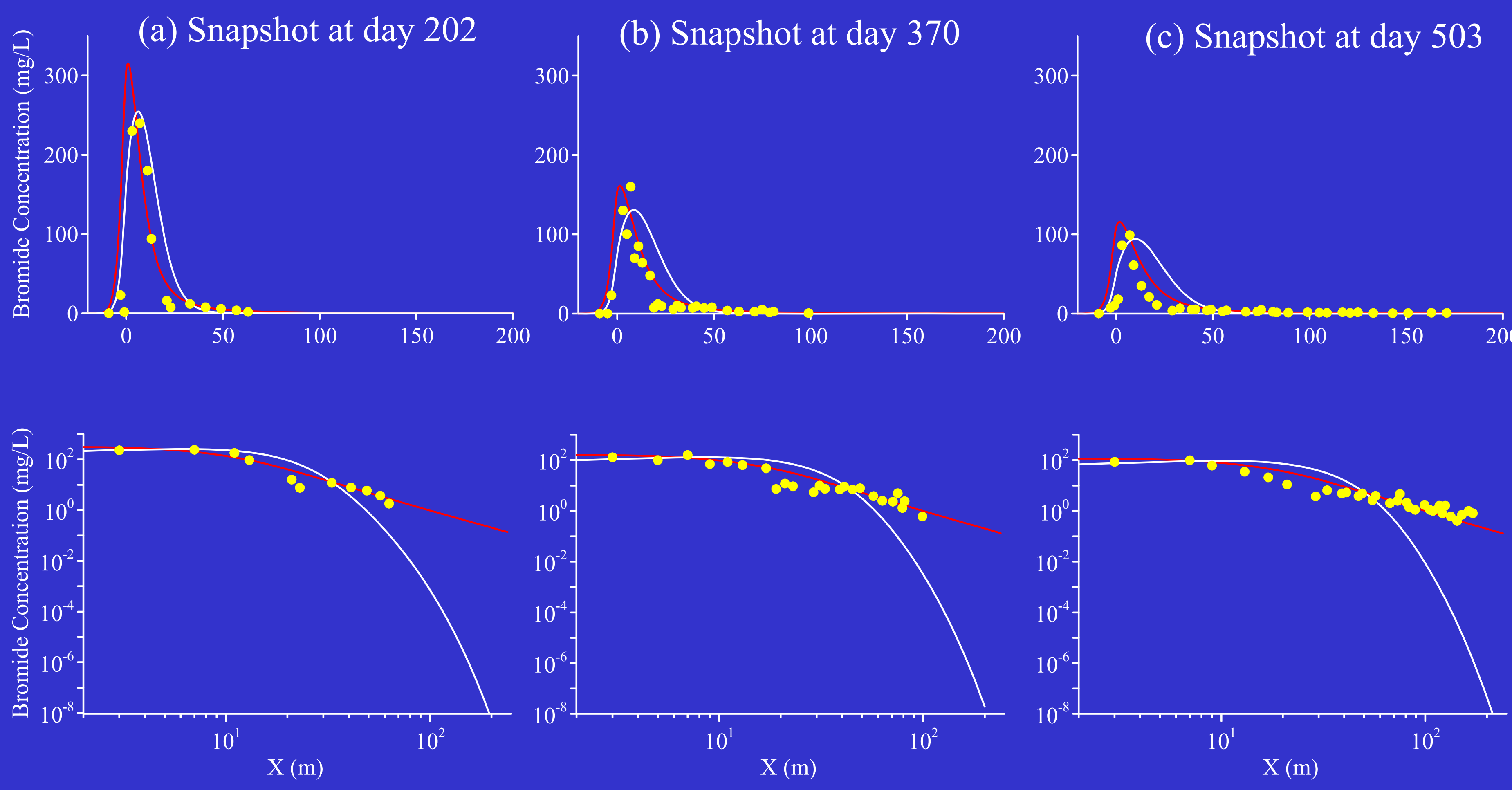
$$\varphi(x, s=0) = 0,$$

$$\varphi(x,s)\big|_{x=+\infty} = 0,$$

$$\left.\left[D \frac{\partial}{\partial x}\varphi(x,s) + v\varphi(x,s)\right]\right|_{x=-\infty} = 0.$$

Why the space fADE?

Example: The MADE-site Bromide snapshots



Forward Transport Models

Scaling limit of CTRW

Jump Size Variance	Waiting Time Moments: Infinite	Waiting Time Moments: Finite
Finite	Sub-diffusion (Time fADE)	Brownian Motions (ADE)
Infinite	Sub/Super-diffusion (Space+Time fADE)	Super-diffusion (Space fADE)

TLM

Space fractional advection-dispersion equation

$$\frac{\partial}{\partial t}(\theta C) = -\frac{\partial}{\partial x}(\theta v C) + \frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}}\left[\theta D \frac{\partial C}{\partial x}\right] + q_I C_I - q_O C$$

$$C(x, t=0) = C_i(x),$$

$$C(x,t)\Big|_{x=+\infty} = 0,$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=-\infty} = 0.$$

The adjoint probability method [*Neupauer & Wilson*, 2001; *Zhang et al.*, 2006]

1. Differentiate each term with respective to a system parameter M_0, where $\partial C/\partial M_0 = \psi$ denotes the state sensitivity.
2. Take the inner product of each term with the adjoint state φ.
3. Eliminate the state sensitivity ψ from the equation. The resultant governing equation and boundary/initial conditions for φ is the inverse/adjoint model.

Inverse model

Forward fADE

$$\frac{\partial}{\partial t}(\theta C) = -\frac{\partial}{\partial x}(\theta v C) + \frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}}\left[\theta D \frac{\partial C}{\partial x}\right] + q_I C_I - q_O C$$

$$C(x, t=0) = C_i(x),$$

$$C(x,t)\big|_{x=+\infty} = 0,$$

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=-\infty} = 0.$$

Backward fADE

($s = T\text{-}t$)

$$\frac{\partial}{\partial s}(\theta \varphi) = \frac{\partial}{\partial x}(\theta v \varphi) - \frac{\partial}{\partial x}\left[\theta D \frac{\partial^{\alpha-1}\varphi}{\partial(-x)^{\alpha-1}}\right] - q_I \varphi + \frac{\partial h}{\partial C}$$

$$\varphi(x, s=0) = 0,$$

$$\varphi(x,s)\big|_{x=+\infty} = 0,$$

$$\left.\left[D\frac{\partial^{\alpha-1}}{\partial(-x)^{\alpha-1}}\varphi(x,s) - v\,\varphi(x,s)\right]\right|_{x=-\infty} = 0.$$

Eulerian approximations of the fADE

$$\frac{\partial}{\partial t}\left[\theta(x)C(x,t)\right]=-\frac{\partial}{\partial x}\left[\theta(x)v(x)\,C(x,t)\right]+\frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}}\left[\theta(x)D(x)\frac{\partial C(x,t)}{\partial x}\right]$$

Grünwald finite difference approximation

$$\frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}}w(x,t)\approx\frac{1}{h^{\alpha-1}}\sum_{j=0}^{i}f_j\,w_{i-j}^{n+1}$$

Implicit Euler scheme

Unconditionally stable (Greschgorin theorem).

Numerical Example 1 – Backward Location pdf

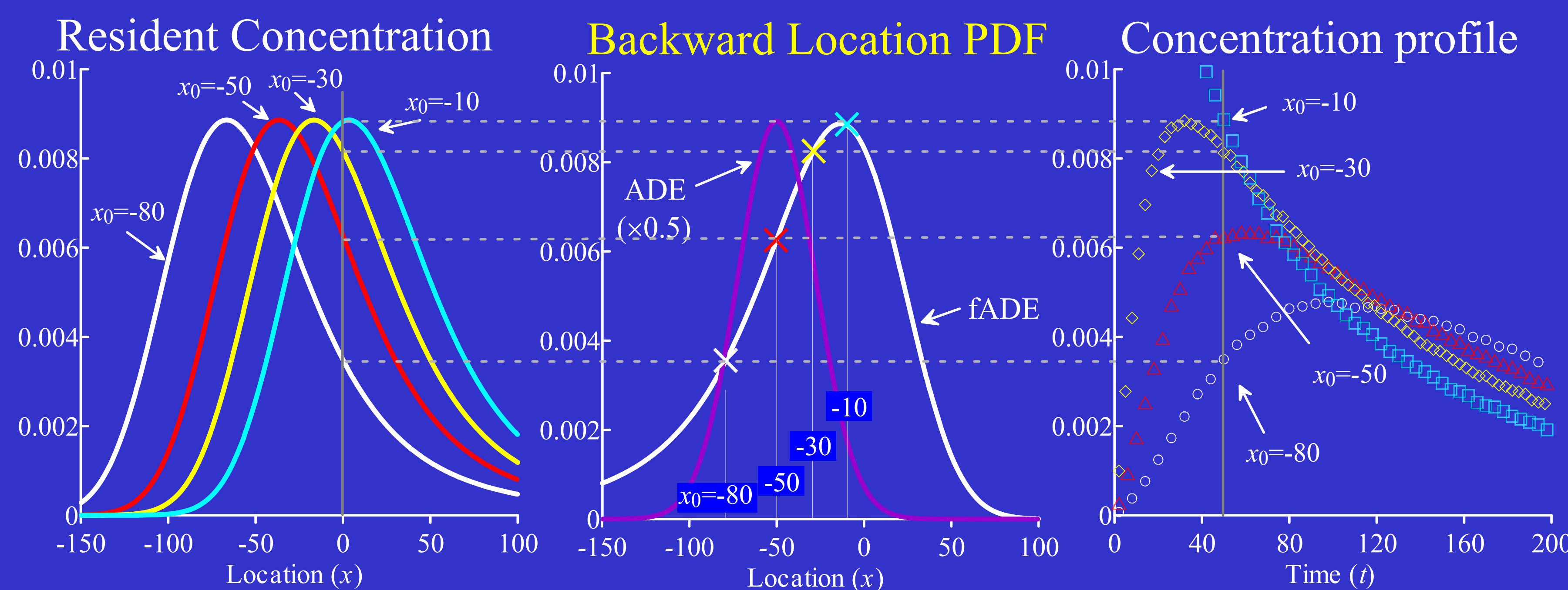
$$\frac{\partial C}{\partial t} = \left(-v\frac{\partial}{\partial x} + D\frac{\partial^\alpha}{\partial x^\alpha} \right) C \qquad \frac{\partial \varphi_L}{\partial s} = \left[v\frac{\partial}{\partial x} + D\frac{\partial^\alpha}{\partial (-x)^\alpha} \right] \varphi_L + \delta(x - x_d)\,\delta(s)$$

$$C(x, t=0) = \delta(x - x_0) \quad \Longrightarrow \quad \varphi_L(x, s=0) = 0$$

$$C(x,t)\big|_{x=-\infty} = 0 \qquad \varphi_L(x,s)\big|_{x=-\infty} = 0$$

$$C(x,t)\big|_{x=+\infty} = 0 \qquad \varphi_L(x,s)\big|_{x=+\infty} = 0$$

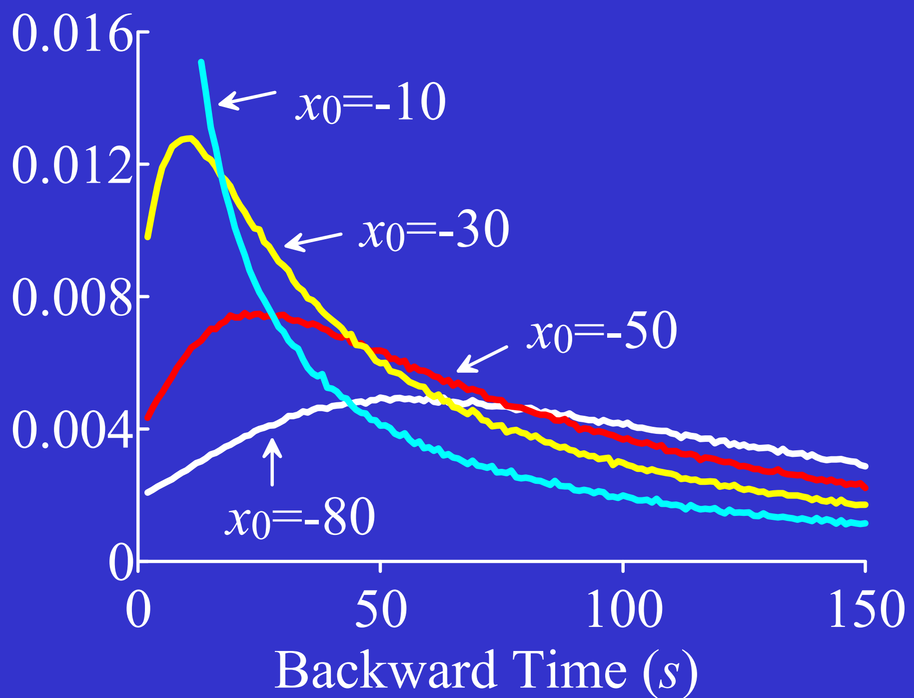
Parameters: α=1.5, v=1, D=5, x_d=0, at time s = 50.



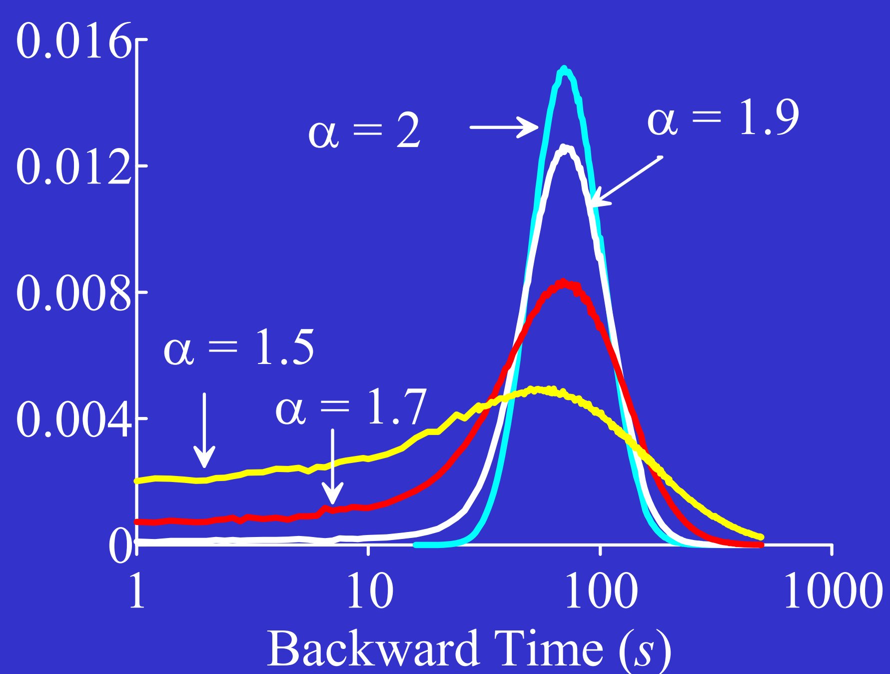
Numerical Example 2 – Backward travel time pdf

$$\frac{\partial \varphi_T}{\partial s} = \left[v\frac{\partial}{\partial x} + D\frac{\partial^\alpha}{\partial(-x)^\alpha} \right]\varphi_T + \delta(x - x_d)\,\delta(s) + \frac{D}{v}\,\frac{d\delta(x - x_d)}{dx}\,\delta(s)$$

Case 1: α=1.5, v=1, D=5. The monitoring well is located at $x_d=0$. The upgradient location is x_0 = -10, -30, -50, and -80.



Case 2: α=1.5~2, v=1, D=5. The monitoring well is located at $x_d=0$, and the upgradient location is fixed at x_0 = -80.



Lagrangian approximations of the fADE

Forward Model

fADE
$$\frac{\partial}{\partial t}\left[\theta(x)C(x,t)\right]=-\frac{\partial}{\partial x}\left[\theta(x)v(x)\,C(x,t)\right]+\frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}}\left[\theta(x)D(x)\frac{\partial C(x,t)}{\partial x}\right]$$

Langevin equation
$$dX(t)=v(x)\,dt+B_1(x)\,dL_\alpha^{+}+B_2(x)\left(dL_{\alpha-1}^{+}\right)_1+B_3(x)\left(dL_{\alpha-1}^{+}\right)_2$$

$$\left|B_1(x)\right|\propto\left|D(x)\right|^{1/\alpha};\quad \left|B_2(x)\right|\propto\left|\frac{\partial D}{\partial x}\right|^{1/(\alpha-1)};\quad \left|B_3(x)\right|\propto\left|D\frac{\partial \ln n}{\partial x}\right|^{1/(\alpha-1)}.$$

Backward Model

Backward fADE
$$\frac{\partial}{\partial s}\left[\theta(x)\,\varphi(x,s)\right]=\frac{\partial}{\partial x}\left[\theta(x)v(x)\,\varphi(x,s)\right]-\frac{\partial^{\alpha-1}}{\partial(-x)^{\alpha-1}}\left[\theta(x)D(x)\frac{\partial\varphi(x,s)}{\partial x}\right]$$
$$+\delta(x-x_d)\,\delta(s)$$

Langevin equation
$$dX(s)=-v(x)\,ds+B_1^{*}(x)\,dL_\alpha^{-}+B_2^{*}(x)\left(dL_{\alpha-1}^{-}\right)_1+B_3^{*}(x)\left(dL_{\alpha-1}^{-}\right)_2$$

Future works

- Time fADE and its inverse model
- Realistic boundary and initial conditions
- Chemical reactions
- Measurement uncertainty
- TLM model
- Coupled CTRW

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