

# Fractional calculus: basic theory and applications (Part II)

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## 4. Numerical methods

Here we discuss numerical methods for the solutions of partial differential equation of fractional order. We review two methods for the numerical evaluation of fractional derivatives, one based on the direct discretization of the RL integro-differential operator and another based on the Grunwald-Letnikov definition of fractional derivative. For the time evolution we propose an implicit/explicit weighted average method. The stability properties of the method are discussed. Further ideas on the topics discussed here can be found in [Lynch-et al-2003] and [del-Castillo-Negrete-2005c].

## Discretization of fractional derivatives

A key issue in the numerical solution of fractional equations is to develop accurate algorithms for the evaluation of fractional derivatives.

Since we are interested in fractional diffusion equations with physical boundary conditions, we will restrict attention to the Caputo fractional derivative of order  $1 < \alpha < 2$

$${}_a^C D_x^\alpha \phi = \frac{1}{\Gamma(2-\alpha)} \int_a^x \frac{\phi''(u)}{(x-u)^{\alpha-1}} du \quad 1 < \alpha < 2$$

We will discuss two methods: one based on the direct discretization of the RL integral operator and the other based the Grunwald-Letnikov definition of the fractional derivative.

## Direct discretization of integral operator

Consider a grid  $a$  of  $N$  points in the  $x \in (0,1)$  interval with  $\Delta=1/N$  on this grid discretize the integral as

$${}_0^C D_x^\alpha \phi = \frac{1}{\Gamma(2-\alpha)} \int_0^x \frac{\phi''(u)}{(x-u)^{\alpha-1}} du \approx \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{i-1} \int_{x_j}^{x_{j+1}} \frac{\phi''(x-u)}{u^{\alpha-1}} du$$

Each integral in the sum is discretized according to L2 scheme

$$\int_{x_j}^{x_{j+1}} \frac{\phi''(x-u)}{u^{\alpha-1}} du \approx \frac{\phi(x-x_{j+1}) - 2\phi(x-x_j) + \phi(x-x_{j-1}))}{\Delta^2} \int_{x_j}^{x_{j+1}} \frac{du}{u^{\alpha-1}}$$

$$[{}_0^C D_x^\alpha \phi]_i \approx \frac{1}{\Delta^\alpha \Gamma(3-\alpha)} \sum_{j=0}^{i-1} [(j+1)^{2-\alpha} - j^{2-\alpha}] (\phi_{i-j+1} - 2\phi_{i-j} + \phi_{i-j-1})$$

$$\left[ {}^C D_x^\alpha \phi \right] \approx \sum_{j=-1}^i W_j(\alpha) \phi_{i-j}$$

In the limit  $\alpha=2$        $W_{-1} = \Delta^{-2}$        $W_0 = -2\Delta^{-2}$        $W_1 = \Delta^{-2}$

and the method reduces to the standard central difference approximation which is second order accurate

$$\left[ \partial_x^2 \phi \right]_i \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta^2}$$

On the other hand in the limit  $\alpha=1$  the method reduces to a backward two point derivative that is only first order accurate.

$$\left[ \partial_x \phi \right]_i \approx \frac{\phi_{i+1} - \phi_i}{\Delta}$$

The accuracy depends on the value of  $\alpha$ . In particular, for  $\alpha$  close to 2 the above L2 method is good. But as  $\alpha$  approaches 1 it is better to use the following variant known as L2C that is second order for  $\alpha=1$ .

$$\int_{x_j}^{x_{j+1}} \frac{\phi''(x-u)}{u^{\alpha-1}} du \approx \frac{\phi(x-x_{j+2}) - \phi(x-x_{j+1}) + \phi(x-x_{j-1}) - \phi(x-x_j)}{\Delta^2} \int_{x_j}^{x_{j+1}} \frac{du}{u^{\alpha-1}}$$

$$\left[ {}^C D_x^\alpha \phi \right] \approx \sum_{j=-1}^i \hat{W}_j(\alpha) \phi_{i-j}$$

$$\alpha = 1 \quad \left[ \partial_x \phi \right]_i \approx \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta} \quad \text{second order}$$

$$\alpha = 2 \quad \left[ \partial_x^2 \phi \right]_i \approx \frac{\phi_{i+1} + \phi_{i-2} - \phi_i - \phi_{i-1}}{2\Delta^2} \quad \text{first order}$$

## Grunwald-Letnikov definition

The Grunwald-Letnikov definition provides a convenient finite difference discretization of fractional derivative operators

$${}_a D_x^\alpha \phi = \lim_{h \rightarrow 0} \frac{{}_a \Delta_h^\alpha \phi}{h^\alpha} \quad {}_x D_b^\alpha \phi = \lim_{h \rightarrow 0} \frac{{}_x \Delta_h^\alpha \phi}{h^\alpha}$$

$${}^\mp \Delta_h^\alpha \phi = \sum_{j=0}^{K_\mp} w_j^{(\alpha)} \phi(x \mp jh) \quad K_- = \left\lfloor \frac{x-a}{h} \right\rfloor \quad K_+ = \left\lceil \frac{b-x}{h} \right\rceil$$

Where the coefficients are given by the following recursive relation

$$w_0^{(\alpha)} = 1 \quad w_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right) w_{k-1}^{(\alpha)}$$

Which gives a first order discretization of the fractional derivative

## Discretization of Caputo derivative

Consider the Left Caputo fractional derivative of order  $1 < \alpha < 2$

$${}_0^C D_x^\alpha \phi = {}_0 D_x^\alpha [\phi(x) - \phi(0) - \phi'(0)x] = \partial_x \left\{ {}_0 D_x^{\alpha-1} [\phi(x) - \phi(0) - \phi'(0)x] \right\}$$

For the **left** derivative we use a **forward difference** approximation

$$\left[ {}_0^C D_x^\alpha \phi \right] = h^{-1} \left\{ {}_0 D_x^{\alpha-1} [\phi(x) - \phi(0) - \phi'(0)x]_{x+1} - {}_0 D_x^{\alpha-1} [\phi(x) - \phi(0) - \phi'(0)x] \right\}$$

and using the Grunwald-Letnikov definition

$$\left[ {}_0^C D_x^\alpha \phi \right] = h^{-\alpha} \sum_{j=0}^k w_j^{(\alpha)} [\phi_{k-j+1} - \phi_0 - h \phi'_0 (k+1-j)]$$

Up-wind method

$$\alpha = 1 \quad \left[ \partial_x \phi \right]_i \approx \frac{\phi_{i+1} - \phi_i}{\Delta} \quad \alpha = 2 \quad \left[ \partial_x^2 \phi \right]_i \approx \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta^2}$$

In matrix form

$$\left[ {}^C D_x^\alpha \phi \right]_k = h^{-\alpha} \left[ \mathbf{D}^\alpha \phi_k + \phi_N \delta_{k,N-1} - \phi_0 V_k - \phi_0' h W_k \right]$$

$$\mathbf{D}^\alpha = \begin{pmatrix} w_1^{(\alpha)} & w_0^{(\alpha)} & \dots & 0 \\ w_2^{(\alpha)} & w_1^{(\alpha)} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ w_{N-1}^{(\alpha)} & w_{N-2}^{(\alpha)} & \dots & w_1^{(\alpha)} \end{pmatrix}$$

$$\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \dots \\ \phi_{N-1} \end{pmatrix}$$

Boundary vectors

$$V_k = \sum_{j=0}^k w_j^{(\alpha)}$$

$$W_k = \sum_{j=0}^k (k-j+1) w_j^{(\alpha)}$$

For the **right** derivative we use a **backwards difference** approximatuiou

$$\left[ {}^C D_b^\alpha \phi \right] = h^{-1} \left\{ D_b^{\alpha-1} [\phi(x) - \phi(b) - \phi'(b)(x-b)] - {}^C D_b^{\alpha-1} [\phi(x) - \phi(b) - \phi'(b)(x-b)]_{k-1} \right\}$$

In matrix form

$$\left[ {}^C D_1^\alpha \phi \right]_k = h^{-\alpha} \left[ \mathbf{D}^{T\alpha} \phi_k + \phi_0 \delta_{k,1} - \phi_{N0} V_{N-k} - \phi_0' h W_{N-k} \right]$$

$\mathbf{D}^{T\alpha}$  is the transpose of  $\mathbf{D}^\alpha$

## Time evolution

Having discretized the fractional derivative, the next step is to discretize the time evolution

$$\partial_t \phi = {}^C D_\theta^\alpha \phi \quad D_\theta^\alpha = l {}^C D_x^\alpha + r {}^C D_b^\alpha$$

where  $l$  and  $r$  are parameters determining the asymmetry of the process

$$\frac{\phi_k^{m+1} - \phi_k^m}{\Delta t} = \Lambda \left[ {}^C D_\theta^\alpha \phi \right]_k^{m+1} + (1-\Lambda) \left[ {}^C D_\theta^\alpha \phi \right]_k^m$$

In the case  $\Lambda=1$  the method is fully implicit and in the case  $\Lambda=0$  the method is fully explicit. The case  $\Lambda=1/2$  gives the Crank-Nicholson method.

$$\left[ 1 - \nu \Lambda (\mathbf{D}_\theta^\alpha - \mathbf{B}_\theta) \right] \phi_k^{m+1} = \left[ 1 + \nu (1-\Lambda) (\mathbf{D}_\theta^\alpha - \mathbf{B}_\theta) \right] \phi_k^m + \nu U_k$$

$$\nu = \Delta t / h^\alpha$$

# Von Neuman stability

For simplicity, restrict attention to the left fractional derivative

$$\partial_t \phi = {}^C D_x^\alpha \phi$$

$$\frac{\phi_k^{m+1} - \phi_k^m}{\Delta t} = \Lambda \left[ {}^C D_x^\alpha \phi \right]_k^{m+1} + (1 - \Lambda) \left[ {}^C D_x^\alpha \phi \right]_k^m$$

Given  $\phi_j^m = \lambda^m e^{i\gamma j}$  the method is stable if and only if  $|\lambda| \leq 1$

Using the G-L definition in the limit  $a = -\infty$

$$\left[ {}_{-\infty} D_x^\alpha \phi \right]_k^m = \frac{\lambda^m}{h^\alpha} \sum_{j=0}^{\infty} w_j^{(\alpha)} e^{i\gamma(k-j+1)}$$

Substituting and solving for  $\lambda$  for the special case

$$\Lambda = 2 - \alpha$$

$$\lambda(\alpha, \nu, \gamma) = \frac{e^{-i\gamma} + \nu(2 - \alpha)[1 - e^{-i\gamma}]^\alpha}{e^{-i\gamma} - \nu(\alpha - 1)[1 - e^{-i\gamma}]^\alpha}$$

$$\nu = \Delta t / h^\alpha$$

In the limit  $\alpha=1$   $|\lambda|^2 = 1 - 2\nu(1 - \nu)[1 - \cos \kappa]$

which gives the Courant-Friedrichs-Lewy (CFL) condition  $\nu = \Delta t / h \leq 1$  for conditional stability of the forward difference, time explicit method

In the limit  $\alpha=2$   $\lambda = \frac{1}{1 + 4\nu \sin^2(\kappa/2)}$

$|\lambda| \leq 1$  Unconditional stability of time implicit center difference method

In general, the method is unconditionally stable for  $3/2 \leq \alpha \leq 2$

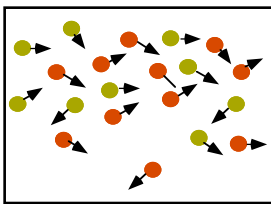
and for  $1 \leq \alpha < 3/2$  the method is stable provided

$$\nu = \frac{\Delta t}{h^\alpha} \leq \frac{1}{2^\alpha(3/2 - \alpha)}$$

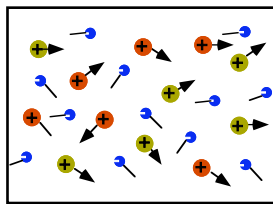
## 4.a) Applications to turbulent transport

Here we discuss the application of fractional calculus to turbulent transport. In particular, we show that transport of tracers in pressure-driven plasma turbulence can be quantitatively described using space-time fractional diffusion equations. The discussion presented here is based on [del-Castillo-Negrete-et al,2004] and [del-Castillo-Negrete-et al,2005] where further details can be found.

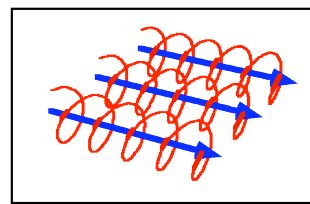
## Magnetic confinement of fusion plasmas



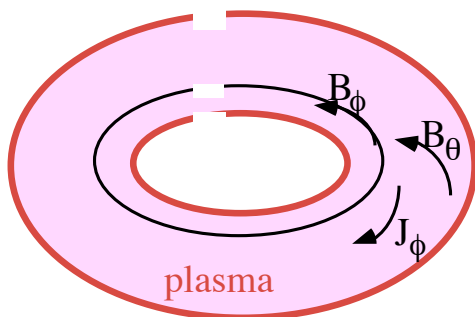
Gas



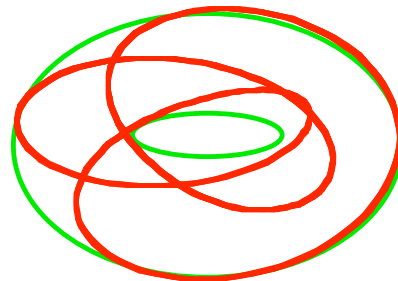
Plasma



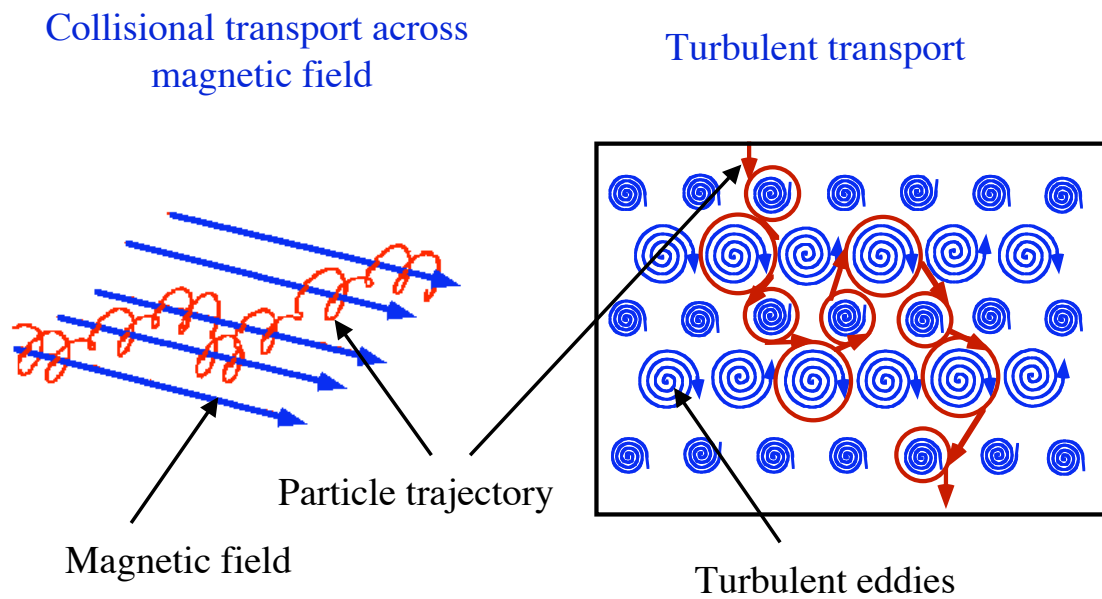
Magnetic confinement



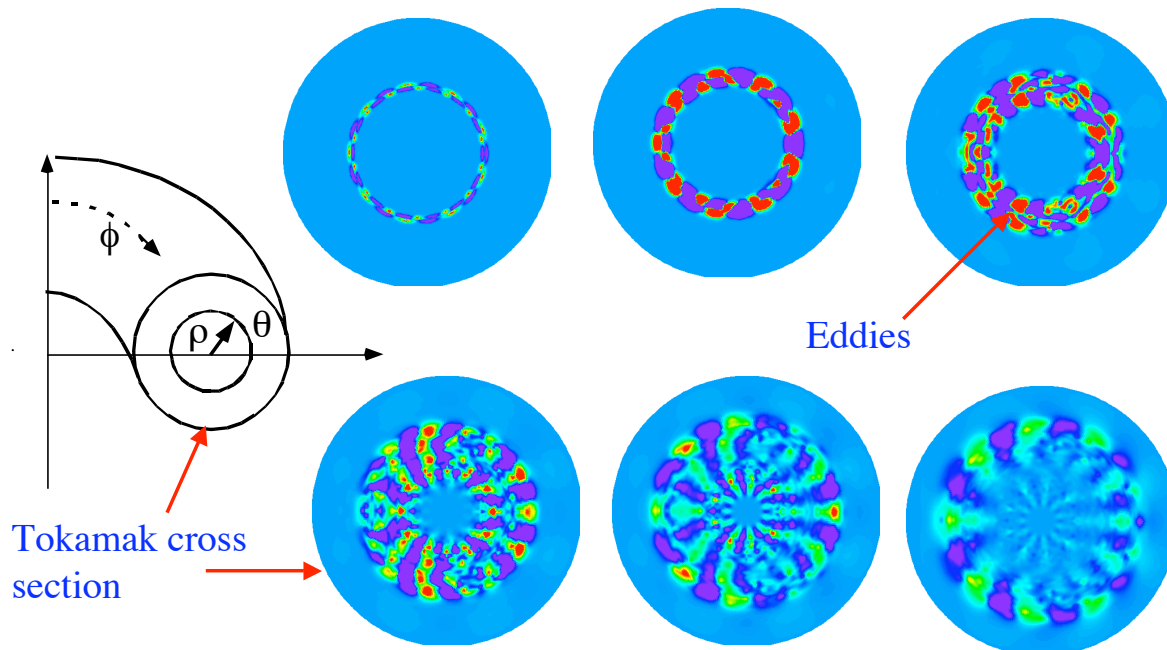
Tokamak



# Transport in magnetically confined plasmas

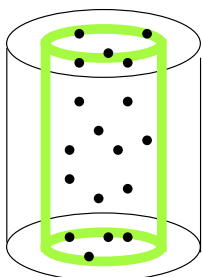


## Pressure driven plasma turbulence





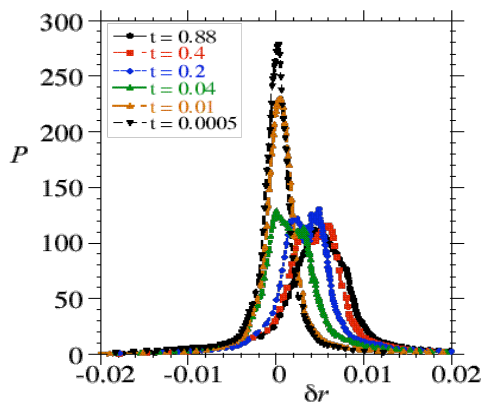
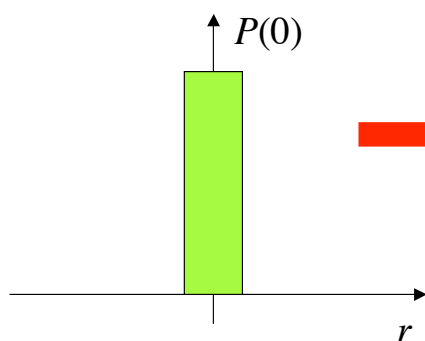
# Tracer transport



Focus on tracers following the flow velocity

$$\frac{d\mathbf{r}}{dt} = \mathbf{V}(\mathbf{r}, t)$$

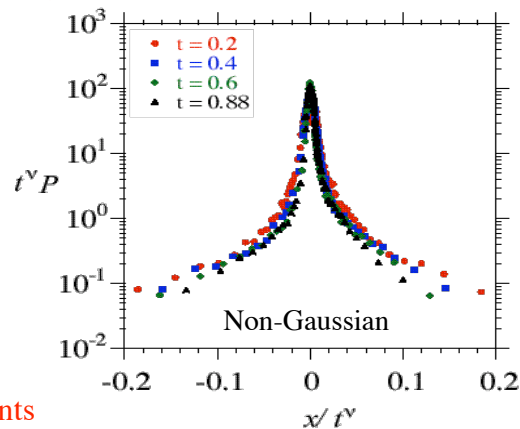
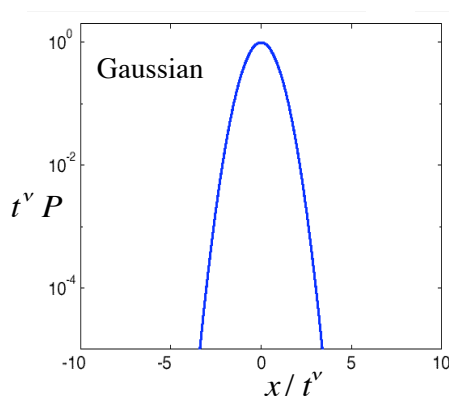
Initial condition: localized in radius, uniformly distributed in  $z$  and  $\theta$



Standard diffusion

Plasma turbulence

Probability density function



Moments

Diffusive scaling  $\nu = 1/2$

$$\langle x^n \rangle \sim t^{n\nu}$$

Anomalous scaling super-diffusion  $\nu \sim 2/3$

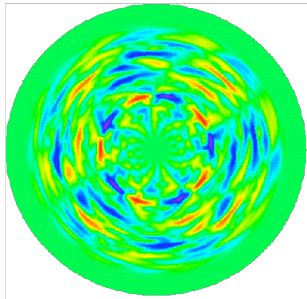
$$\partial_t P = \partial_x [\chi \partial_x P]$$

Model

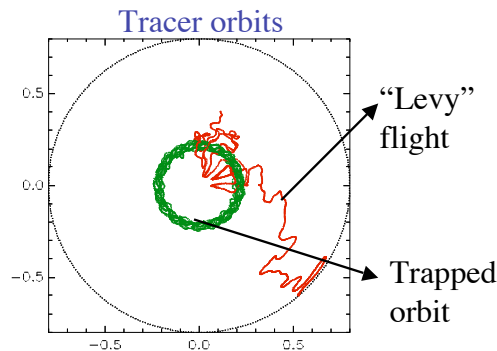
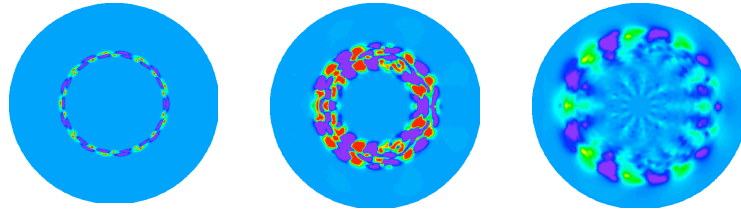
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## What causes this non-diffusive transport?

$E \times B$  flow velocity eddies induce large tracer trapping that leads to temporal non-locality

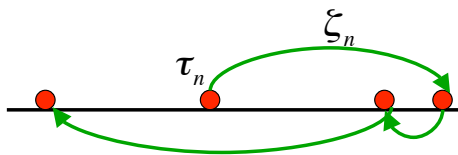


“Avalanche like” phenomena induce large tracer displacements that lead to spatial non-locality



The combination of tracer trapping and flights leads to anomalous diffusion

## Continuous time random walk model



$\tau_n$  = waiting time     $\psi(\tau)$  = waiting time pdf

$\xi_n$  = jump     $\lambda(\xi)$  = jump size pdf

**Master Equation**

(Montroll-Weiss 1965)

$$P(x, t) = \underbrace{\delta(x) \int_t^\infty \psi(t') dt'}_{\text{Contribution from particles that have not moved during } (0, t)} + \underbrace{\int_0^t \psi(t - t') \left[ \int_{-\infty}^\infty \lambda(x - x') P(x', t') dx' \right] dt'}_{\text{Contribution from particles located at } x' \text{ and jumping to } x \text{ during } (0, t)}$$

Contribution from particles that have not moved during  $(0, t)$

Contribution from particles located at  $x'$  and jumping to  $x$  during  $(0, t)$

No memory

$$\psi(\tau) \sim e^{-\mu\tau}$$

No long displacements

$$\lambda(\xi) \sim e^{-\xi^2 / 2\sigma^2}$$

$$\partial_t P = \partial_x [\chi \partial_x P] + S$$

Standard diffusion model

## Fractional transport model

Long waiting times  $\psi(\tau) \sim \tau^{-(\beta+1)}$   
 Long displacements (Levy flights)  $\lambda(\xi) \sim \xi^{-(\alpha+1)}$

$$\partial_t^\beta \phi = \chi \partial_{|x|}^\alpha \phi$$

$$[\partial_{|x|}^\alpha \phi](k) = -|k|^\alpha \phi(k)$$

$$[\partial_t^\beta \phi](s) = s^\beta \phi(s) - s^{\beta-1} \phi(0)$$

$$\phi(k, s) = \frac{s^{\beta-1}}{s^\beta + \chi |k|^\alpha} \phi(k, t=0)$$

$$[E_\beta(-c t^\beta)](s) = \frac{s^{\beta-1}}{s^\beta + c} \quad E_\beta(z) = \sum_n \frac{z^n}{\Gamma(\beta n + 1)} \quad \text{Mittag-Leffler function}$$

$$\phi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} E_\beta(-\chi |k|^\alpha t^\beta) dk$$

$\alpha$  determines the asymptotic scaling in space

$$\phi(x, t) = t^{-\beta/\alpha} K(\eta)$$

$$\eta = t^{-\beta/\alpha} x$$

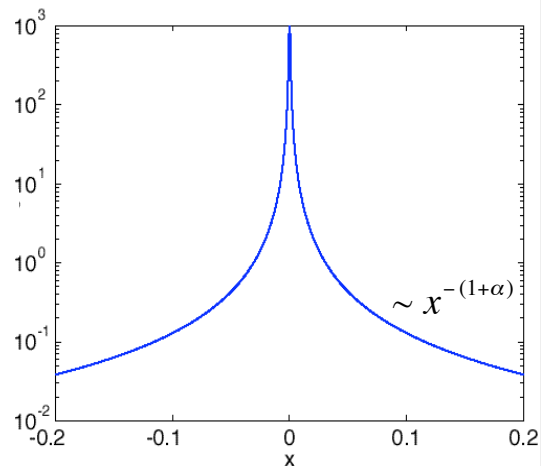
Space similarity variable

$$K(\eta) = \frac{1}{\pi} \int_0^\infty \cos(\eta z) E_\beta(-\chi z^\alpha) dz$$

$$\eta \rightarrow \infty \quad K(\eta) \sim \eta^{-(1+\alpha)}$$

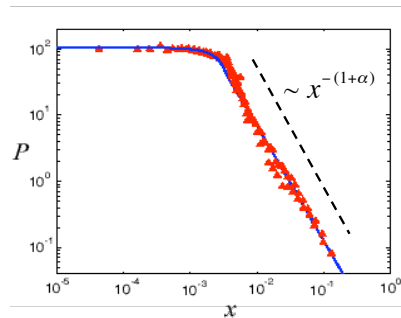
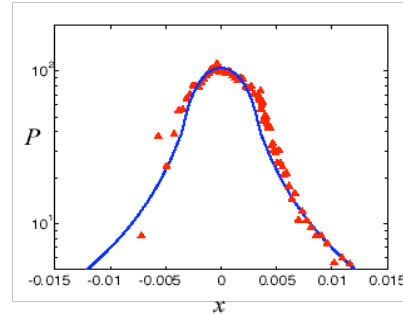
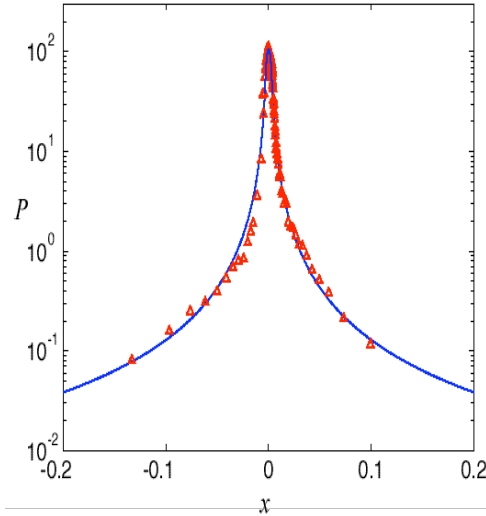
For fixed  $t$  and large  $x$

$$\phi(x, t_0) \sim x^{-(1+\alpha)}$$



## Comparison with fractional model Probability density function of tracers

$$\alpha=3/4, \quad \beta=1/2, \quad \chi=0.09$$



$\beta$  determines the asymptotic scaling in time

$$\phi(x, t) = |x|^{-1} \xi^{-\beta/\alpha} K(\xi^{-\beta/\alpha})$$

$$\xi = t |x|^{-\alpha/\beta} \quad \text{Time similarity variable}$$

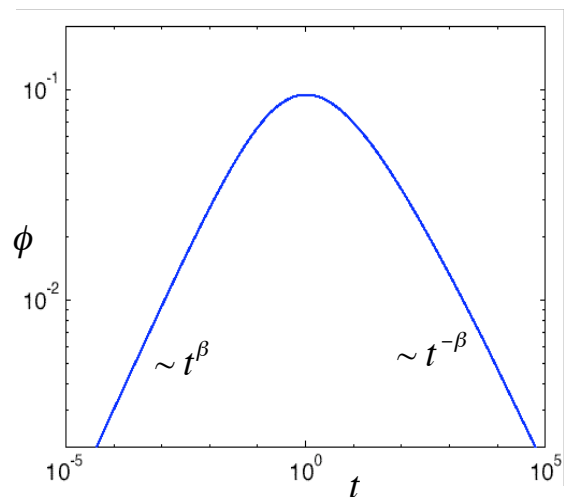
$$K(\eta) = \frac{1}{\pi} \int_0^\infty \cos(\eta z) E_\beta(-\chi z^\alpha) dz$$

$$\eta \rightarrow \infty \quad K(\eta) \sim \eta^{-(1+\alpha)}$$

$$\eta \rightarrow 0 \quad K(\eta) \sim 1 + \eta^{-(1-\alpha)}$$

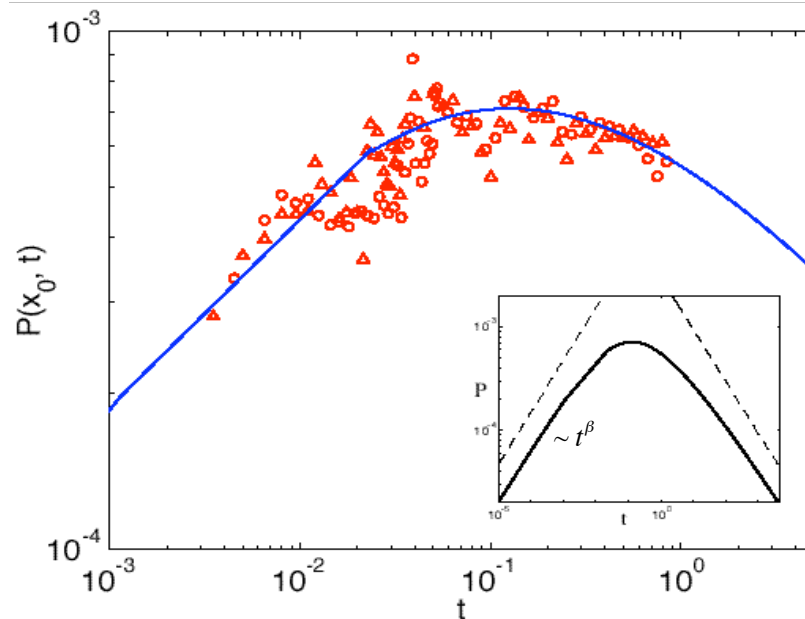
For fixed  $x$ :

$$\phi(x_0, t) \sim \begin{cases} t^\beta & \text{for } t \sim 0 \\ t^{-\beta} & \text{for } t \rightarrow \infty \end{cases}$$



## Comparison with fractional model Probability density function of tracers

$$\alpha=3/4, \quad \beta=1/2, \quad \chi=0.09$$



## Self-similarity and non-diffusive scaling

$$\partial_t^\beta P = \chi \partial_{|x|}^\alpha P$$

Similarity  
variable

$$\eta = t^{-\beta/\alpha} x$$

Fundamental  
solution

$$P(x, t) = t^{-\beta/\alpha} K(\eta)$$

$$P(x, \lambda t) = \frac{1}{\lambda^{\beta/\alpha}} P\left(\frac{x}{\lambda^{\beta/\alpha}}, t\right)$$

Self-similar scaling

Moments

$$\langle x^n \rangle = \int x^n \phi(x, t) dx = t^{n\beta/\alpha} \int \eta^n K(\eta) d\eta$$

$$\langle x^n \rangle \sim t^{n\beta/\alpha}$$

$$\frac{2\beta}{\alpha} \begin{cases} > 1 & \text{Super-diffusion} \\ < 1 & \text{Sub-diffusion} \end{cases}$$

# Comparison with turbulence model

Scaling of moments

$$\langle x^n \rangle \sim t^{n\mu}$$

