# Fractional p.d.e and stochastic processes for dispersion: application to porous media

UMR 1114 INRA - UAPV "Environnement Méditerranéen et Modélisation des Agro-Hydrosystèmes"

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ifp

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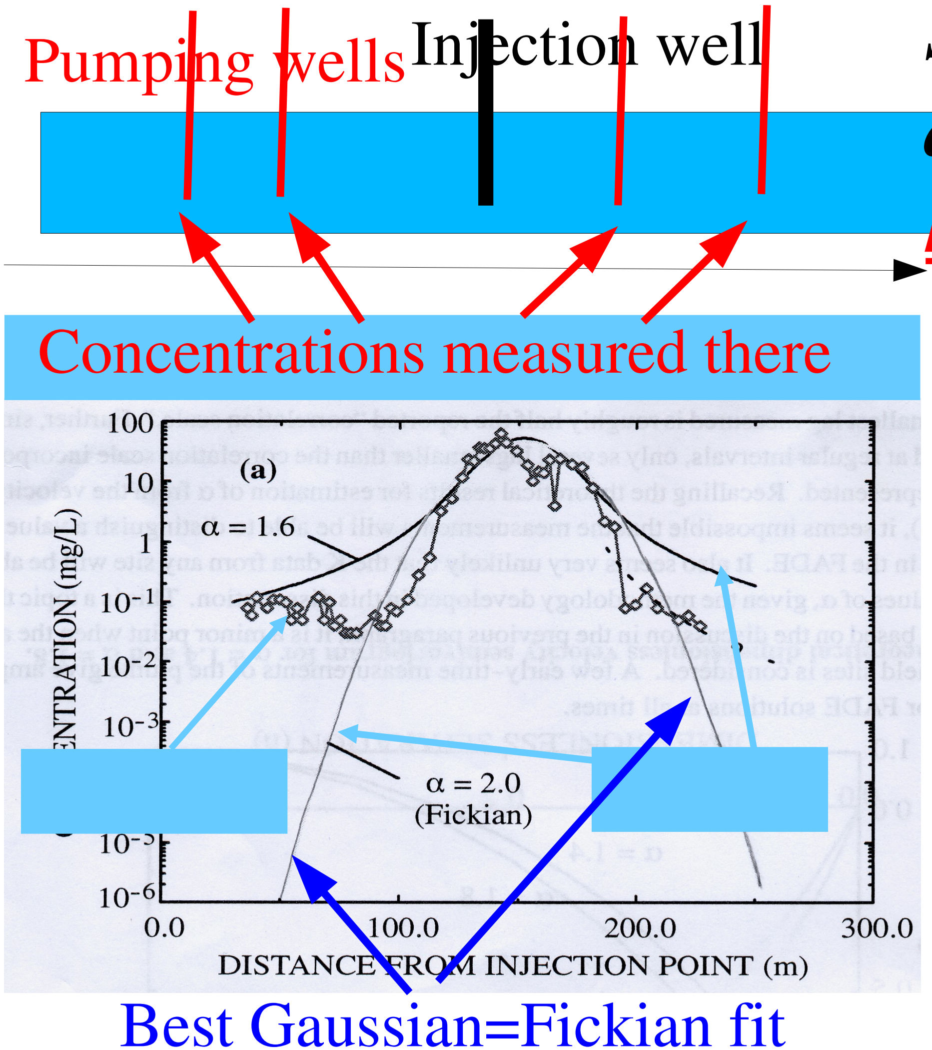
## *Organization*

1. Fractional p.d.e: WHY?
2. Fractional tools
3. Stochastic model and p.d.e for dispersion
4. Space fractional p.d.e
5. The fractal Mobile-Immobile Model
6. Experiments being performed with the help of the fractal MIM

# 1. Motivation:in many natural media, dispersion does not obey Fick's and Fourier's laws

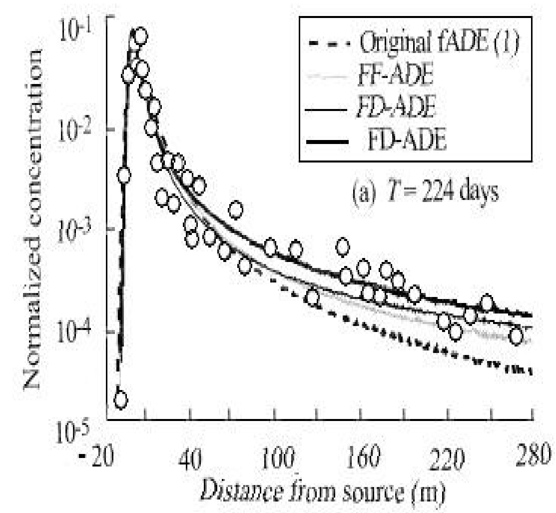
1st example: solutes travel SOMETIMES very fast, very rapidly




*Benson et al. 2000*

***Spreading of a solute in saturated aquifers: profiles # Fourier's law***

***heavy tailed concentration profiles***




***fit/ Space fractional equation Zhang et al. 2007***

## $2^{nd}$ example: memory effects: *heavy tailed Break-Through Curves*

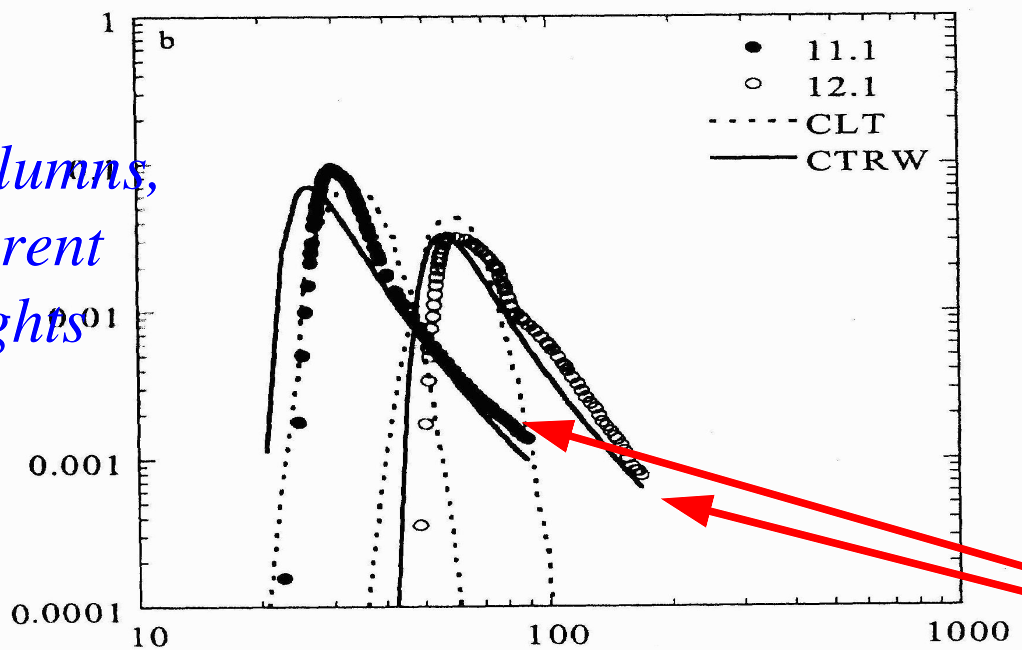
***Experimental data***
***memory effects***

*concentration*

+

***Some solutes are trapped in some media***

*2 columns, different lenghts*




*time*

*inlet*

*tracer injected h*

$t^{-\alpha}$

*Non saturated porous medium, in a column*

*outlet*

*flux of tracer measured here*

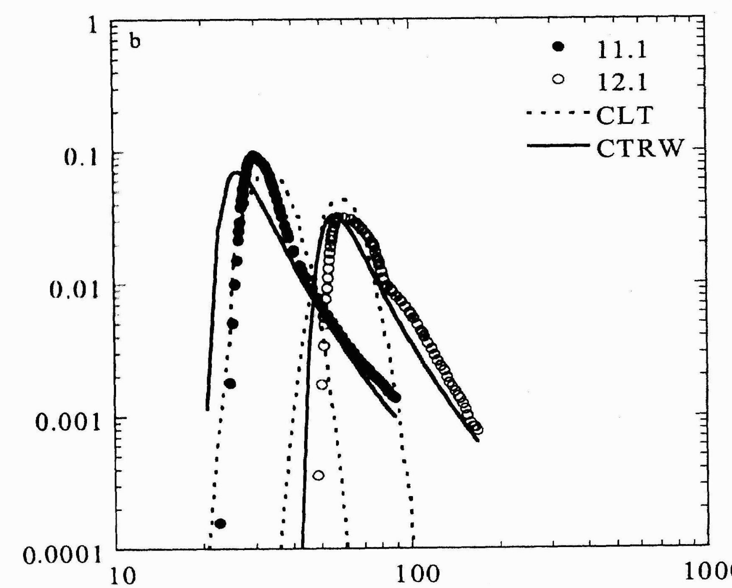
**Bromly M. and Hinz C. (2004) , Water Resour. Res. 40, W0740 .**

*the hallmark of memory effects: the asymptotic behavior*

pb: making sure whether observed memory effects really correspond to the asymptotics of something, or not ?

Some observations in saturated heterogeneous media show that, finally, Gaussian behavior ultimately dominate

To answer: prepare fractional and stochastic tools, that work accurately at finite times



# 2. Fractional tools : in some sense, fractional derivatives are integrals

*integrals*

$$I^{\beta}_{a,+.}f(x)=\frac{1}{\Gamma(\beta)}\int_a^x (x-y)^{\beta-1} f(y)\,dy$$

$$I^{\beta}_{-,b}f(x)=\frac{1}{\Gamma(\beta)}\int_x^b (x+y)^{\beta-1} f(y)\,dy$$

*derivatives: left inverses of integrals: Riemann-Liouville's or Marchaud's or Grünwald-Letnikov's definition*

$$D^{\gamma}_{0,+.}f(t)=\partial_t I^{1-\gamma}_{0,+.}f(t)$$

$$D^{\alpha-1}_{-\infty,+.}f(x)=h^{1-\alpha}\Sigma_{j=0}^{+\infty} w_j(\alpha-1)\,f(x-jh)$$

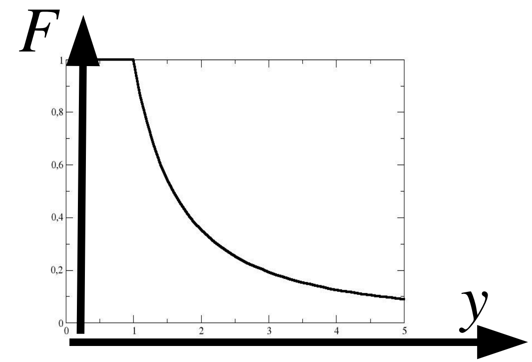
*limit* $h \longrightarrow 0$

$$D^{\alpha-1}_{-,+\infty}f(x)=h^{1-\alpha}\Sigma_{j=0}^{+\infty} w_j(\alpha-1)\,f(x+jh)$$

<u>*Theorem 1*</u> $\alpha > 1$ *not an integer, F integrable, s.t.* $\int_0^{+\infty} y^{\rho} F(y)\,dy = 0$

*for* $\rho$ *any integer between 0 and <* $\alpha$ *with also* $F(y) = F_1(y) + C\,y^{-\alpha}$ *near* $+\infty$

$F_1(y)\,y^{\alpha-1}$ *integrable*




*then:*

$$\lim_{l \to 0} \int_0^{+\infty} \varphi(x+y) \frac{F(y/l)}{l^{\alpha}}\,dy = C\,\Gamma(1-\alpha)\,D^{\alpha-1}_{x,+\infty}\varphi(x)$$

*similar integrals occur when we perform balances, or compute fluxes*

*a version for integer values of* $\alpha$

*Theorem 2* $0<\gamma<1$ *K integrable,* $\Psi(t)=K(t)+\lambda\frac{t^{-\gamma}}{\Gamma(-\gamma)}$

*for t>0 large*

$$\lim_{\tau\to 0}\tau^{-1}\int_0^t \Psi\left(\frac{t'}{\tau^{1/\gamma}}\right)u(t-t')\,dt' \quad = \quad \lambda I_{0,+.}^{1-\gamma}u(t)$$

$=$

$$\lim_{\tau\to}\tau^{-1}\Psi\left(\frac{t}{\tau^{1/\gamma}}\right)*u(t)$$

*similar convolutions occur when we compute fractions of mobile/immobile walkers in random walks with 2 time steps*

# 3. Random walks for normal advection-diffusion

Fick's law,Fourier's law and Gaussian stochastic models for normal diffusion, fractional p.d.e. and heavy-tailed random displacements or trapping durations for heavy tailed profiles or memory effects: this is not new

Fourier's law

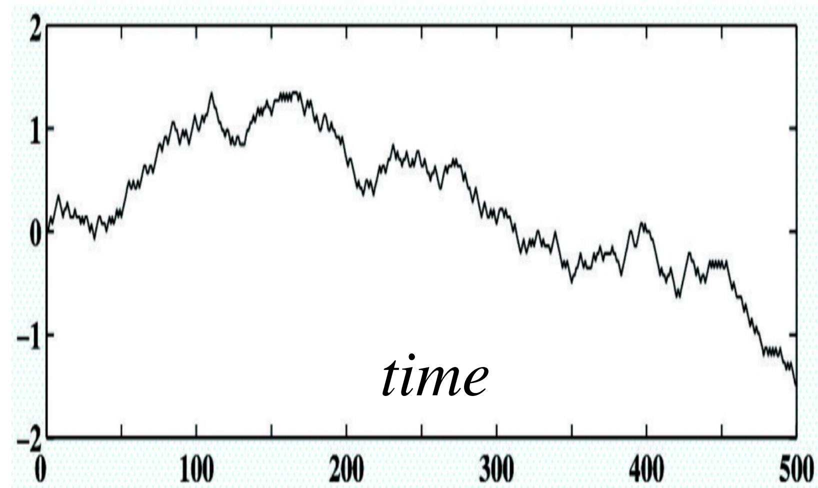
normal diffusion

Brownian motion

$$\partial_t P(x,t) = \Delta D P(x,t) - \nabla v P(x,t)$$

*probability density function*

*space*




*time*

for fluxes of solute: Fick's law

*trajectory of 1 walker*

$$F(x,t) = v P(x,t) - \nabla D P(x,t)$$

*even if D depends on x,t or P*

# random walks approximating Brownian motion with drift

each walker performs random displacements, independent, $J_n$ *distributed as* $l.$ N ← *centered normal law*

separated by time intervals of duration $\tau$

s.t. $\frac{l^2}{2\tau} = D$ *where they follow the mean flow v*

$\tau, l \to 0$ *( hydrodynamic limit ) location of a walker at time t*

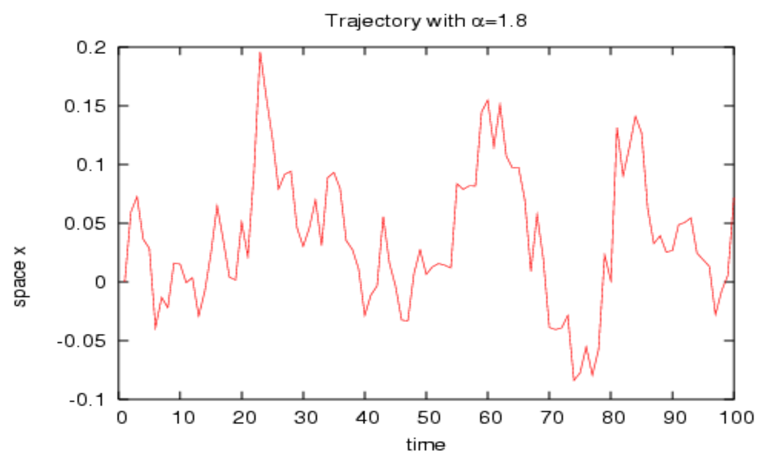
→ $x_0 + vt + \sqrt{2D}B(t)$ ← *Brownian motion*

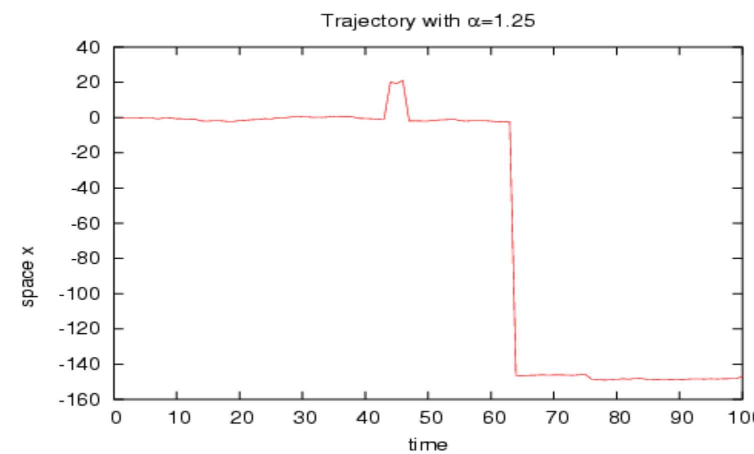
*P density of walkers:* $\partial_t P(x,t) = \Delta D P(x,t) - \nabla vP(x,t)$

# 4. random walk, with more frequent very long jumps, and space-fractional p.d.e

a collection of walkers

trajectory of 1 walker: succession of instantaneous jumps, independent,



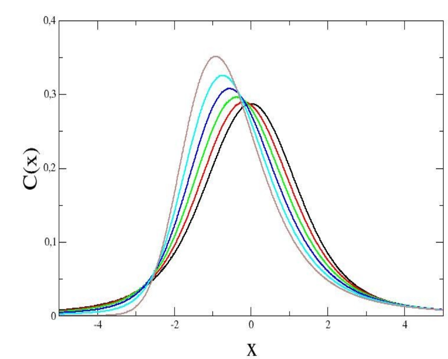




separated by periods of duration $\tau$ : convection

**Amplitude of 1 jump:** $lX$

$\alpha$ Stable Lévy law, p.d.f $p_{\alpha}^{\theta}$

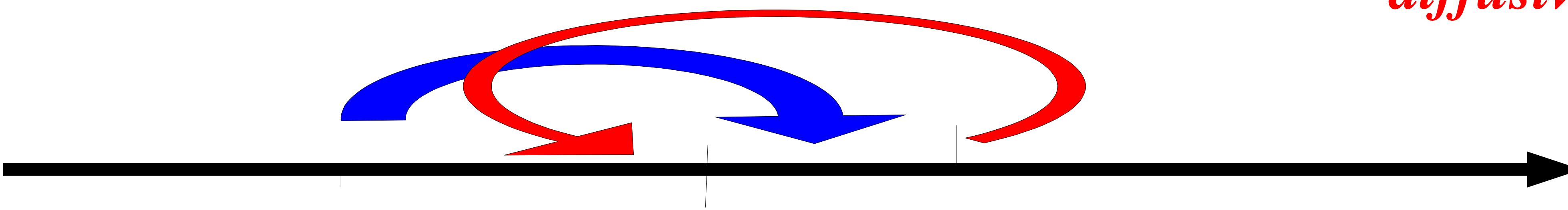
$1 < \alpha < 2$ $\theta$ *: skewness parameter*



<u>**flux of walkers?**</u> ***step 1: compute the flux on the scale of particles***

***step 2: take the diffusive limit*** $l$ ***and*** $\tau$ ***tend to 0***

***while satisfying*** $l^{\alpha}/\tau = D$ ← ***a kind of diffusivity***

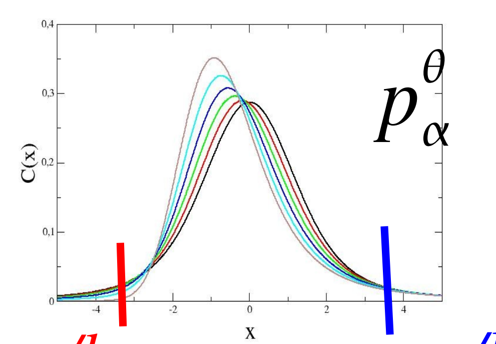



*contribution of random jumps to the right:* $\int_{\cdot}^{+\infty} P(x-y,t) F_{\alpha}^{r,\theta}(y/l) \frac{dt}{\tau} dy$

*contribution of random jumps to the left:* $\int_{\cdot}^{+\infty} P(x+y,t) F_{\alpha}^{l,\theta}(-y/l) \frac{dt}{\tau} dy$

*contribution of convection: vP(x,t)dt*

$$F_{\alpha}^{r,\theta}(y) = \int_{y}^{+\infty} p_{\alpha}^{\theta}(z)\, dz \qquad F_{\alpha}^{l,\theta}(-y) = \int_{-\infty}^{-y} p_{\alpha}^{\theta}(z)\, dz$$




*proba for a random jump to be >y* <-y /

# By Theorem 1:fractional Fick's law :

***Flux=D times the sum of*** $(L D^{\alpha-1}_{-\infty,+.} - R D^{\alpha-1}_{-.,+\infty}) P(x,t) + vP(x,t)$

**+ local correction, where C is singular**

**if there are no boundaries or absorbing boundaries**

**+ Mass conservation** $\partial_t P(x,t) = K \nabla^{\alpha}_{\theta} P(x,t) - \nabla vP(x,t)$

***C.L. of derivatives of the order of α*** $(L D^{\alpha}_{-\infty,+.} + R D^{\alpha}_{-.,+\infty}) P(x,t)$

***in Fourier variables :*** $-|k|^{\alpha} e^{i sgn(k)\theta\frac{\pi}{2}} P(k,t)$

$\Delta P(x,t)$ *for* $\alpha = 2$

# Domain, limited by an absorbing wall, v=0

Fractional Fick's law **+** $\partial_t P(x,t) = -\partial_x Flux(x,t)$

$$\partial_t P(x,t) = K \nabla_\theta^\alpha P(x,t)$$

***Numerical Simulation***

***+ computation of the Flux/***

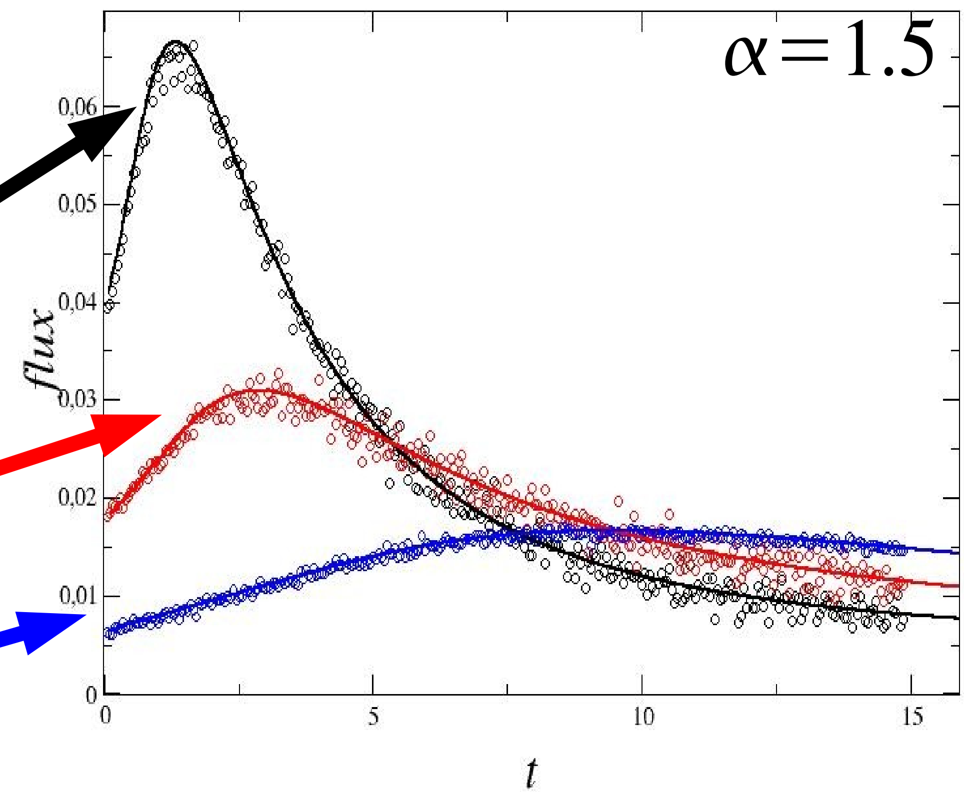
***Direct simulation of the CTRW***

***Flux at***

***x=3***

***x=5***

***x=10 (wall)***



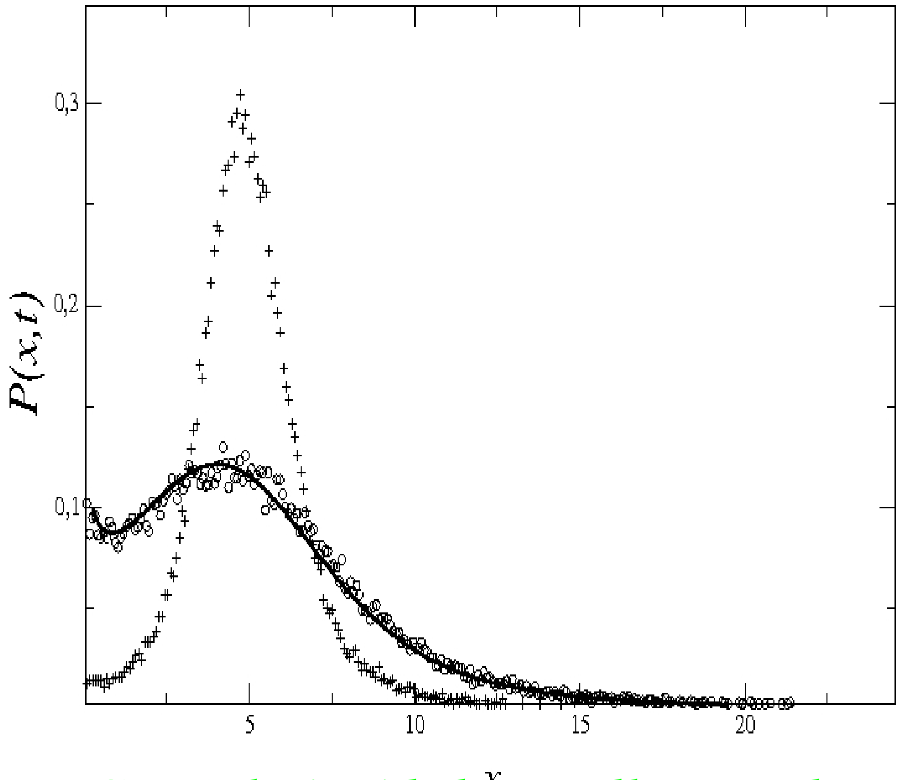
In domains, limited by reflecting boundary conditions: an additional item in the flux, accounting for particles, bouncing on a reflecting wall.

Consequence: also a complementary item in the fractional pde for P

For α <2 the item does not disappear in the hydrodynamic limit

For α =2, it does because regular derivatives are local operators

***Simulation of the fractional p.d.e (with the supplementary item), comparison / direct simulation of the CTRW***




***Initial data: Dirac impulse et x=5, reflecting wall at x=0***

$\alpha = 1.5 \qquad \theta = 0.2$

*M.C.Néel, A. Abdennadher and M. Joelson, 2007, J. Math. Phys. A*

# 5. Model for advection-dispersion with memory effects

walkers accumulating successive steps, made of

1-convective displacement due to mean flow v, during a time interval, duration $\tau$

2- just at the end: random displacement $J_n$ distributed as

$l.\ N$ ← *centered normal law*

*ending, say, at x*

s.t. $\frac{l^2}{2\tau} = D$

*3- the walker stops with probability h(x)*

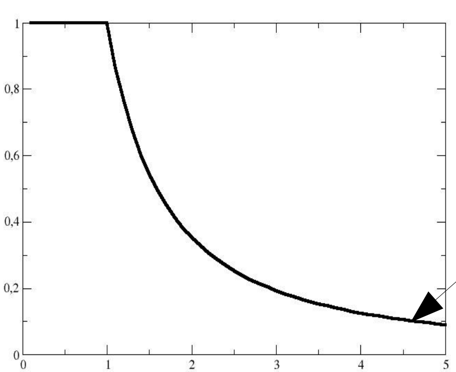
*for a duration of* $\tau^{1/\gamma} W_n$ *independent of the past*

*maximally skewed Lévy*

*law of stability exponent γ<1*

*Laplace transform of the p.d.f:* $e^{-\lambda s^\gamma}$

*p.d.f*




*t*

$-\lambda \frac{t^{-\gamma-1}}{\Gamma(-\gamma)}$

*the probability for an immobile stay to be larger than t satisfies the hypotheses of Th2*

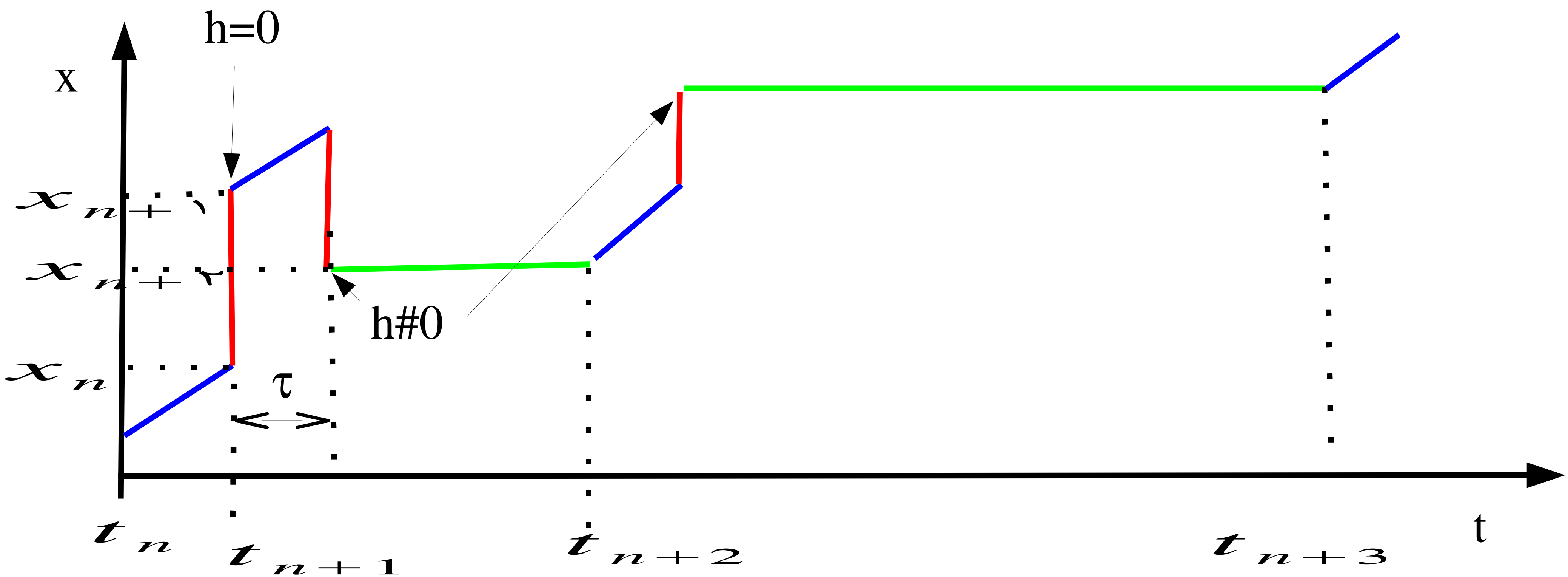
Trajectories: join points $(x_n, t_n)$

$$x_{n+1} = x_n + \int_{t_n}^{t_n+\tau} v(t')\,dt' + J_n$$

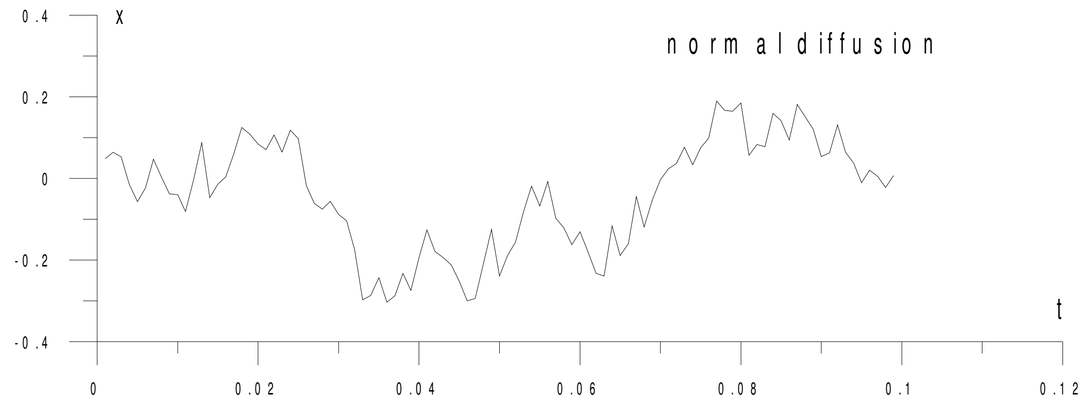
*mobile walkers*
*+*
*immobile walkers*

$t_{n+1} = t_n + \tau$ with probability $1 - h(x_{n+1})$

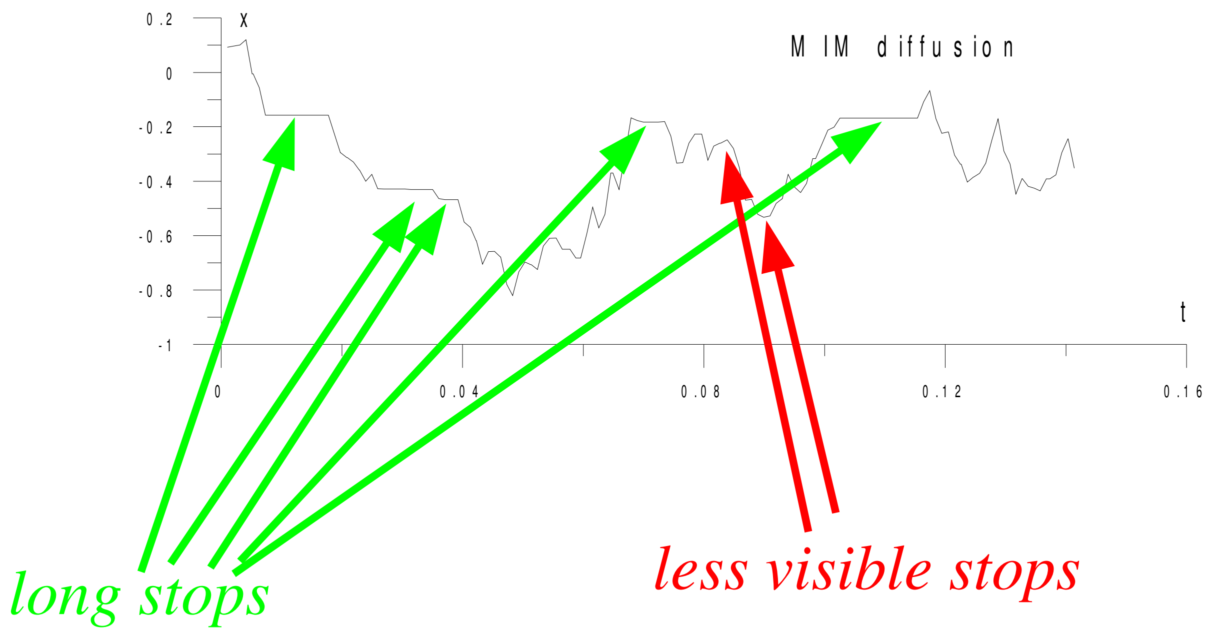
$t_{n+1} = t_n + \tau + \tau^{1/\gamma} W_n$ with probability $h(x_{n+1})$



*Random walk approximating Brownian motion*




*fter convective displacement*
*- random displacement : the walker*
*ay stop*



On the small scale, i.e. for the random walk:

$$P_i(x,t)=(h\,P_m)*(\frac{1}{\tau}\Psi(\frac{t}{\tau^{1/\gamma}}))(x,t)+error$$

*proba for a trapping duration to be >t*

$\Psi(t)$ *: survival probibility= proba for* $W_n$ *to take a value>t*

☆ <u>Theorem 2:</u> *when* $l, \tau \to 0$ *with* $D = l^2/(2\tau)$

*the densities of mobile* $P_m(x,t)$ *and immobile* $P_i(x,t)$ *walkers satisfy*

$$P_i(x,t) = \lambda I^{1-\gamma}(h P_m)(x,t)$$

*scaling parameter*

*probability of becoming immobile when arriving at x*

$$I^{\beta} f(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t-t')^{\beta-1} f(t')\, dt'$$

*fractional integral order 1–γ*

*γ<1*

☆ ***Probability current:*** $v(t) P_m(x,t) - \partial_x D P_m(x,t)$

☆ $P = P_m + P_i \rightarrow P = (Id + h\lambda I^{1-\gamma}) P_m \rightarrow P_m(x,t) = (Id + \lambda I^{1-\gamma} h)^{-1} P(x,t)$

☆ *mass conservation:* $\partial_t P(x,t) = -\nabla.(\nabla D - v)(Id + \lambda I^{1-\gamma} h)^{-1} P(x,t) + r(x,t)$

## the density of tracer

*fractal MIM, R. Schumer et al. WRR 2003*

$$\partial_t P(x,t)+\lambda h I^{1-\gamma}\partial_t P(x,t)=-\nabla.(\nabla D-v)P(x,t) + \text{ initial data}$$

Caputo

fractional derivatives

$$\partial_t P(x,t)=-\nabla.(\nabla D-v)(Id+\lambda I^{1-\gamma}h)^{-1}P(x,t)+r(x,t)$$

flux — source

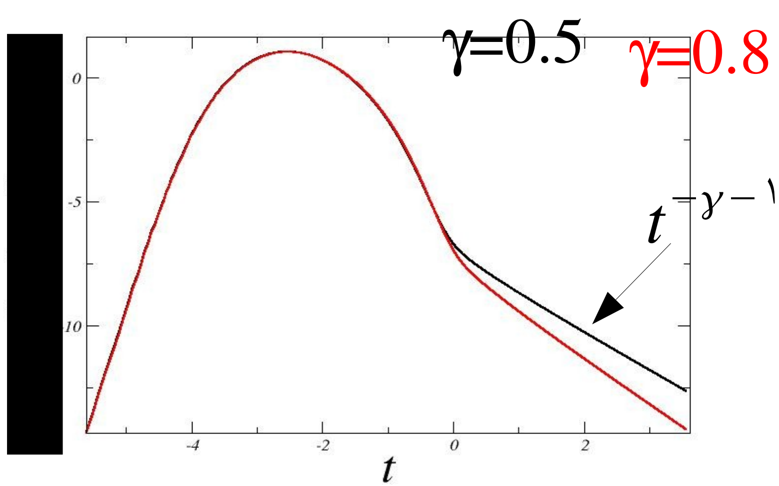
$$\partial_t P_m(x,t)+\partial_t\lambda I^{1-\gamma}h P_m(x,t)=-\nabla.(\nabla D-v)P_m(x,t)+r(x,t)$$

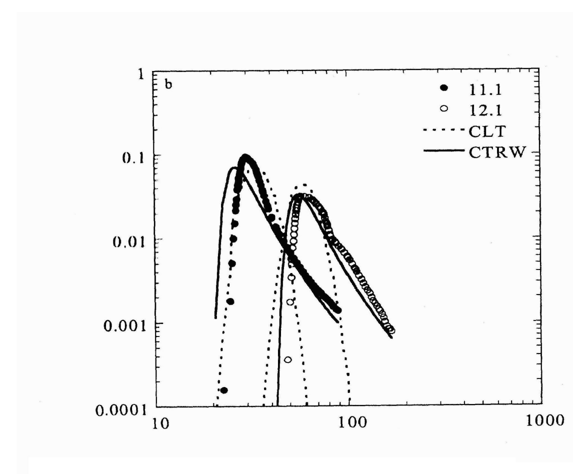
Riemann-Liouville

$$P_m(x,t)=(Id+\lambda I^{1-\gamma}h)^{-1}P(x,t)$$

$$P(x,t)=(Id+\lambda I^{1-\gamma}h)P_m(x,t)$$

$P(x,t)$



*Proved, even if v depends on t, or if D depends on x and t, or if h depends on x. if h depends on t, also OK provided we put h inside the fractional integral*

*provided D does not vary too rapidly*

*M.C.Néel, A. Zoia and M. Joelson, Phys.Rev. E 80 (2009)*

*Proved numerically by comparing histograms/ solutions of the p.d.e even if D and v depend on the density of walkers*

*A. Zoia, M.C.Néel, and A. Cortis, Phys.Rev. E 81 (2010)*

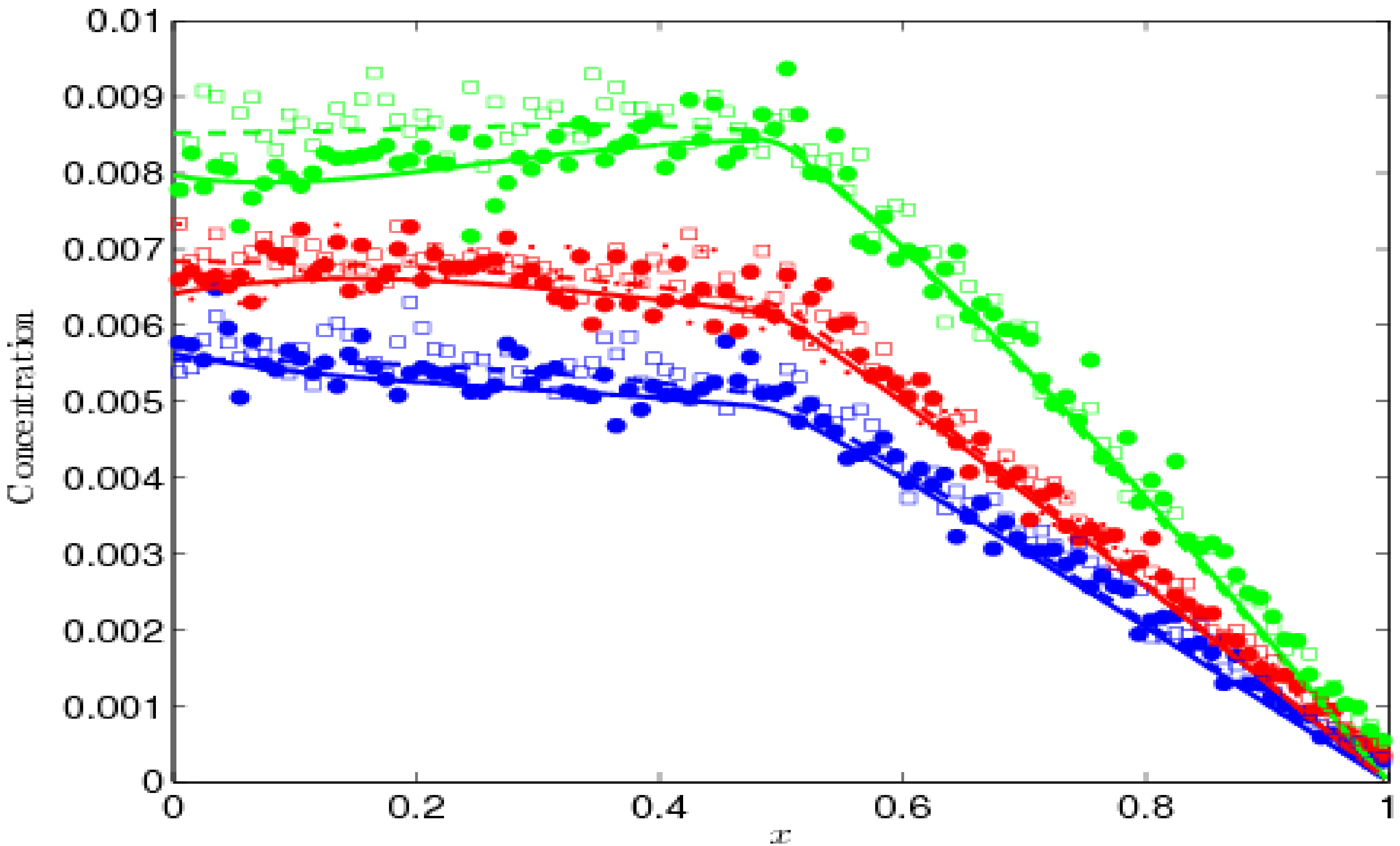
Solution of $\partial_t P(x,t) = -\nabla.(\nabla D - v)(Id + \lambda I^{1-\gamma} h)^{-1} P(x,t) + r(x,t)$

*Flux=0 at x=0, P=0 at x=1, r(x,t)=δ(x-0.5)δ(t)*

$t_1 < t_2 < t_3$

*lines: pde*

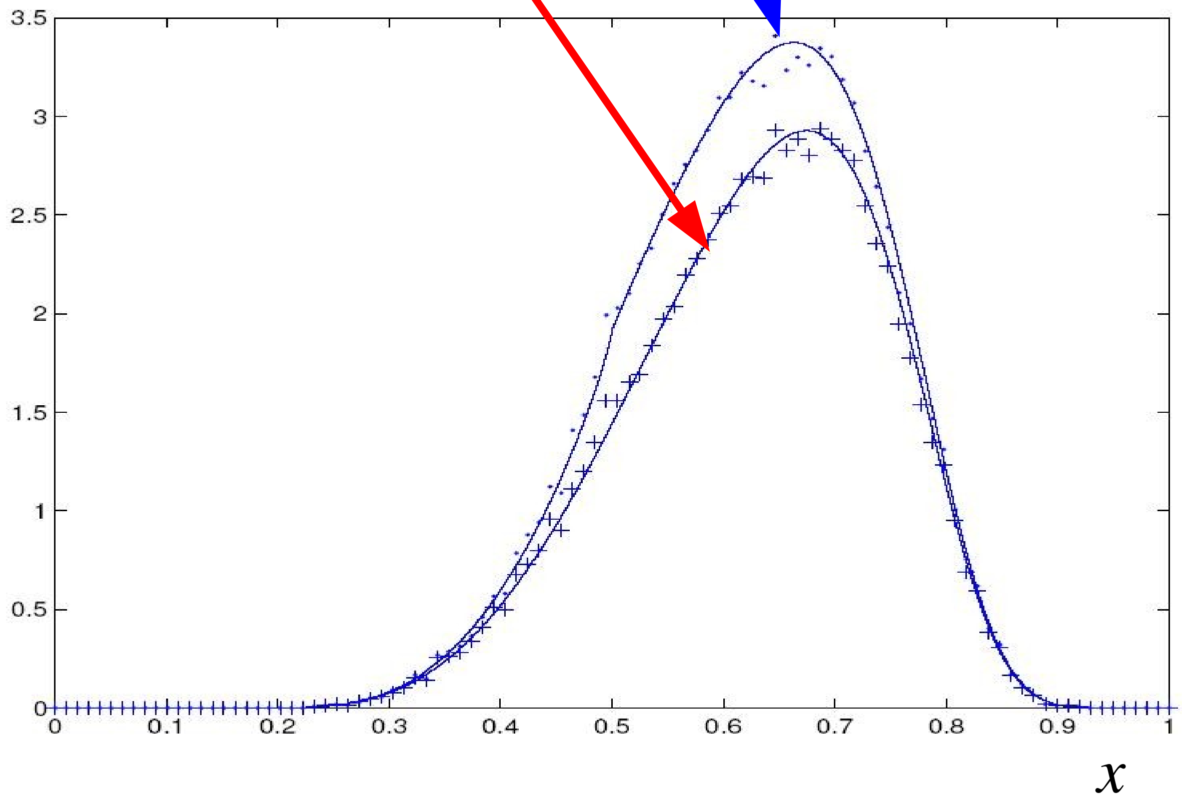
*circles: histograms of the random walk*



*Density of mobile particles , and total density*
*P=0 at both ends*

*D and v: powers of P*

*lines: pde*
*symbols: histograms*




*compactly supported initial data → compactly supported density later*

## 6. check whether memory effects really are observed

### 1. tracing experiment

*Bromly and Hinz observed heavy tailed Break-Through Curves, but in general making sure that the asymptotic regime has been reached is not so easy*

$$\partial_t P(x,t) = -\nabla.(\nabla D - v)(Id + \lambda I^{1-\gamma} h)^{-1} P(x,t) + r(x,t)$$

*Christelle Latrille and Alain Caratalade CEA Saclay (Labo de Mesure et Modélisation de la Migration des Radionucléides, et Département de Modélisation des Systèmes et Structures), TRAM project*

$x$

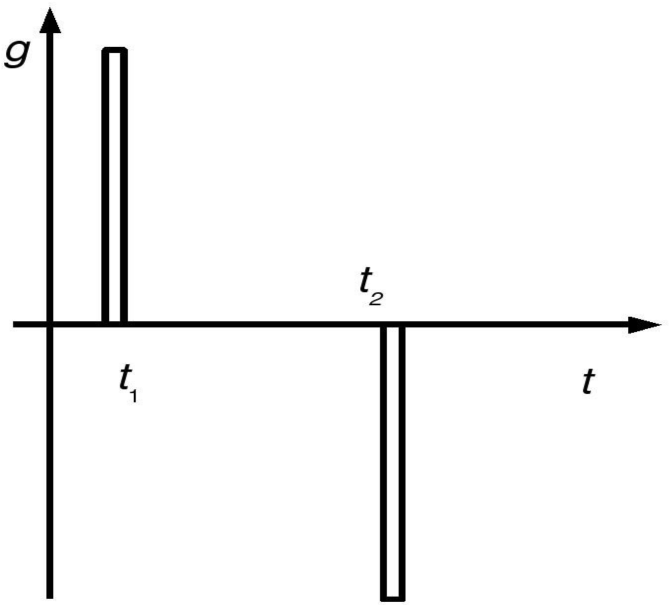
# 2. Nuclear Magnetic resonance velocimetry ( M. Fleury, IFP, TRAM project)

A magnetic field is imposed,  some manipulations of the field are applied, and a time-dependent gradient influences the phase of spin bearers= water molecules

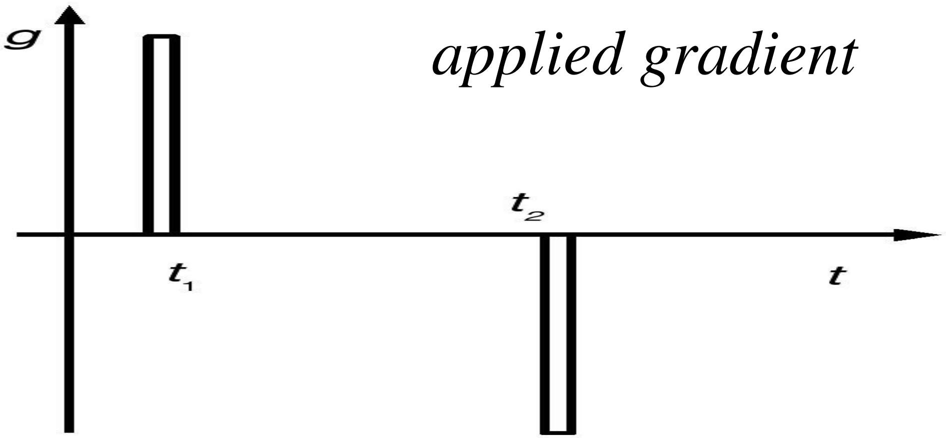
*Let us follow 1 spin bearing particle: x(t)*  *phase=* $\int_0^t g(t')x(t')dt$

*contribution to the measured signal:* $e^{i\int_0^t g(t')x(t')dt}$

signal: $.<e^{i\int_0^t g(t')x(t')dt}>.$




*when such a gradient is applied:  the signal is dominated by first moment and multi-time correlations of* $x(t_1)-x(t_2)$




*applied gradient*

$$t_1 = t_2 + T$$

$$.< e^{i\int_0^t g(t')x(t')dt} >. \approx 1 + .$$

$$i < x(t_1) - x(t_2) >. - \frac{1}{2} < (x(t_1) - x(t_2))^2 >. + \ldots$$

---

*without immobile periods:* $x(t) = x_0 + vt + \sqrt{2D}\,B(t)$ ← *Brownian motion*

$$.< x(t_1) - x(t_1 + T) >. = vT$$ *and* $$.< (x(t_1) - x(t_1 + T))^2 >. = v^2 T^2 + 2DT$$

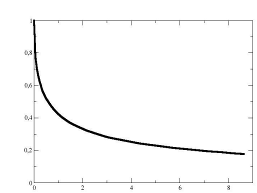
---

*Immobile periods of infinite mean: the operational time=time that a tagged walker spent moving up to t= stochastic process Z(t)=inverse stable subordinator*

$x(t) = x_0 + vZ(t) + \sqrt{2D}\,B(Z(t))$ ← *subordinated Brownian motion*

$.< -x(t_1) + x(t_1 + T) >. = v \int_{t_1}^{t_1+T} E_{1-\gamma}(-\lambda t^{1-\gamma})$ ← *Mittag -Leffler function*

$$.< (x(t_1) - x(t_1 + T))^2 >. = v^2 A(t_{1,} T) + 2DF(t_{1,} T)$$




*Memory effects , h=1*

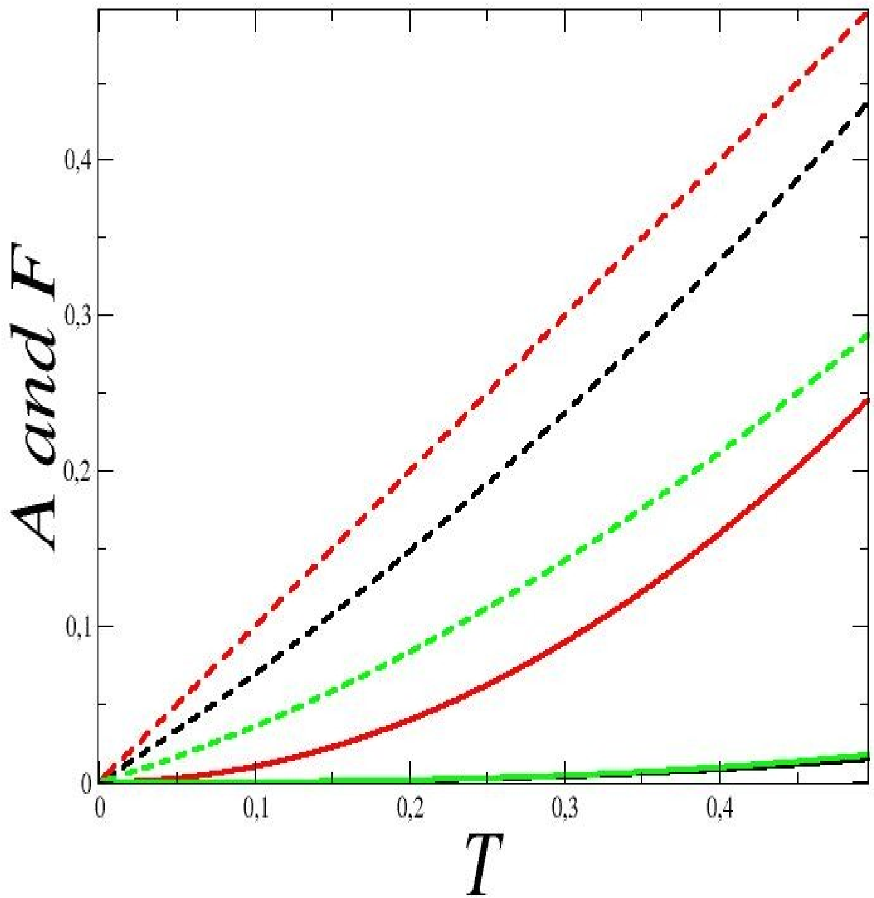
*expectation of the square of the displacement/$t_1$,$t_1$+T*

$$.<(x(t_1)-x(t_1+T))^2>.=v^2 A(t_1,T)+2\mathrm{DF}(t_1,T)$$

$$A(t_1,T)=E_{1-\gamma}(-\lambda(t_1+y)^{1-\gamma})*(\int_0^y E_{1-\gamma}(-\lambda z^{1-\gamma})dz)$$

$$F(t_1,T)=\int_{t_1}^{t_1+T} E_{1-\gamma}(-\lambda(z)^{1-\gamma})\,dz$$

*this function, its integral and many connected functions are easily computed by using the mapping $(Id+\lambda I^{1-\gamma}h)^{-1}$ that links mobile/immobile densities*




*Black, green: two values of $t_1$, for the fractal MIM*

*red: all values of $t_1$ for Brownian motion with drift*

*full lines: A, dotted lines: F*

Memory effects: the signal also depends on $t_1$ , and not only on T

# *Conclusions*

*. Apparently, some natural processes are ruled by fractional pde*
*. Proving this is not always easy, even when classical models are definitively unsatisfactory*
*. Dispersion: Fractional versions of Fick's law correspond to specific classes of stochastic models*
*. pde: connected with densities- for a tracer, injected not everywhere*
*. for other experiments, the stochastic process may provide more information*
*. both may be combined*