Rare events and scaling in superdiffusive materials and in field-induced anomalous dynamics

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GGI Workshop - Firenze - May 2014

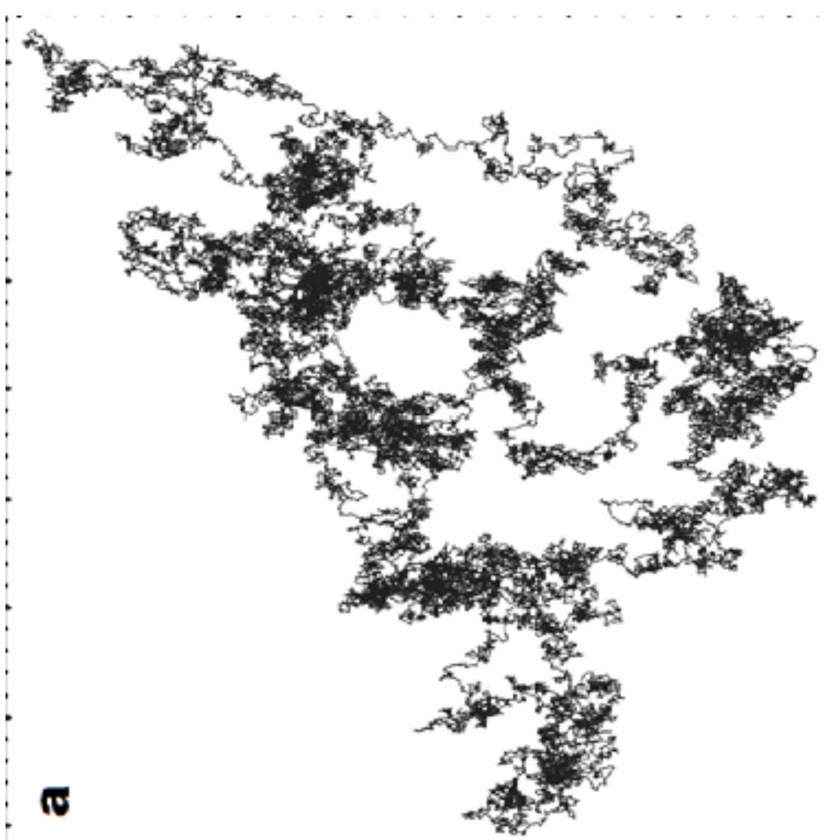
- Standard and anomalous diffusion
- Scaling, scaling violations and strong anomalous diffusion
- Anomalous diffusion from waiting times, traps and broad step length distributions
- Scaling and rare events in an applied field: single out anomalous behavior by studying the effects of an external perturbation in models with waiting times and in Lévy walks.
- Scaling and rare events in superdiffusive materials: transport in Lévy-like materials

Standard Diffusion:

Displacement of a particle generated by the sum of a sequence of independent steps of bounded length and random direction.
At large times

- $\langle x^2(t) \rangle \sim t$ — mean square displacement from the starting position linearly growing in t

- $P(x,t) \sim \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$ — Gaussian probability density function (1d)



Standard Diffusion: scaling properties of the PDF

A powerful method to study the asymptotic behavior at large times of the PDF

- $P(x,t) \sim \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$ has the scaling form

$P\,(x,t) \sim t^{-1/z} F(x/t^{1/z})$ $\ell(t) \sim t^{1/z}$ z=2

$\ell(t)$ is the scaling length of the process

$\langle x^n(t)\rangle \sim \ell^n(t)$ Given the Gaussian form of the scaling function F, the scaling length also rules all the moments

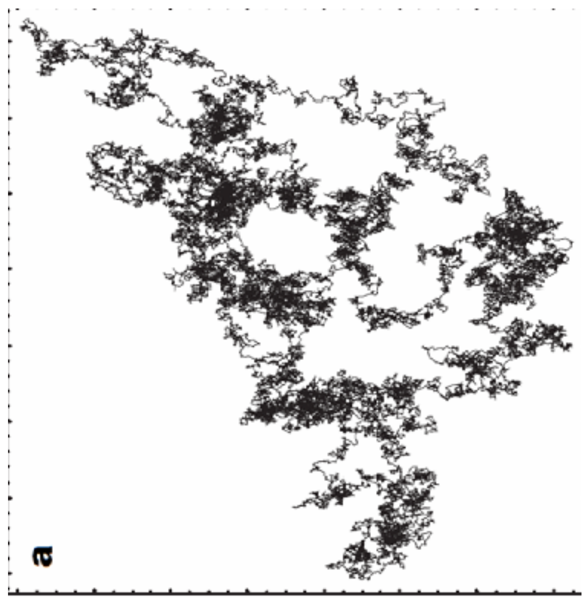
Standard Diffusion: applying a field

- $$P_\epsilon(x,t) \simeq \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x-v_\epsilon t)^2}{4Dt}\right]$$

applying a small field ϵ (unbalancing the probability to make a jump in one direction)

the form of the PDF is still a Gaussian, moving with a finite velocity

$$\langle x(t)\rangle_\epsilon / t \equiv v_\epsilon \neq 0$$



and the typical displacement is $l_T(t) = v_\epsilon t$

$l_T(t)$ is the maximum of the PDF

All this holds if the steps taken by the diffusing particle have bounded length and are uncorrelated, and there are not long waiting times between two jumps.

Often, this is not the case, and anomalous effects arise.

Anomalous diffusion

$$\langle x^2(t)\rangle \sim t^{2/\gamma} \qquad \gamma \neq 2,$$

- $\gamma > 2$ Subdiffusion

- $\gamma < 2$ Superdiffusion

- PDF is non Gaussian, but still can have a scaling form $P_0(x,t) \sim t^{-1/z} F(x/t^{1/z})$

  $\ell(t) \sim t^{1/z}$

- However, scaling can also be violated. Only the central part of the PDF scales with l(t), while for x > l(t) the PDF can develop long tails, leading to "strong anomalous diffusion".

$\langle x^n(t)\rangle \neq \ell^n(t)$ strong anomalous diffusion

$\langle x^n(t)\rangle \sim \ell^n(t)$ is called "weak" anomalous diffusion

Anomalous diffusion

All these anomalous effects occur when diffusion is not standard,
that is some of the previous properties for the step length distribution and time between steps (uncorrelated steps, finite variance, finite waiting time) are not satisfied.

Typical and interesting examples where these properties are naturally violated:

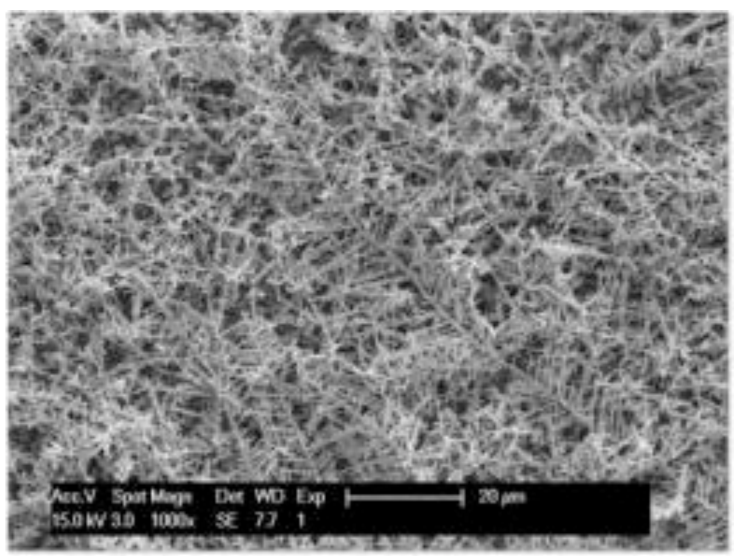
Particles diffusing in a medium where the topology induces correlation between steps, induces traps and broad step length distributions.

- correlation + "trapping times" $p_\alpha(\tau) \sim \tau^{-(\alpha+1)}$
- correlation + broad step lengths distributions $p_\alpha(l) \sim l^{-(1+\alpha)}$

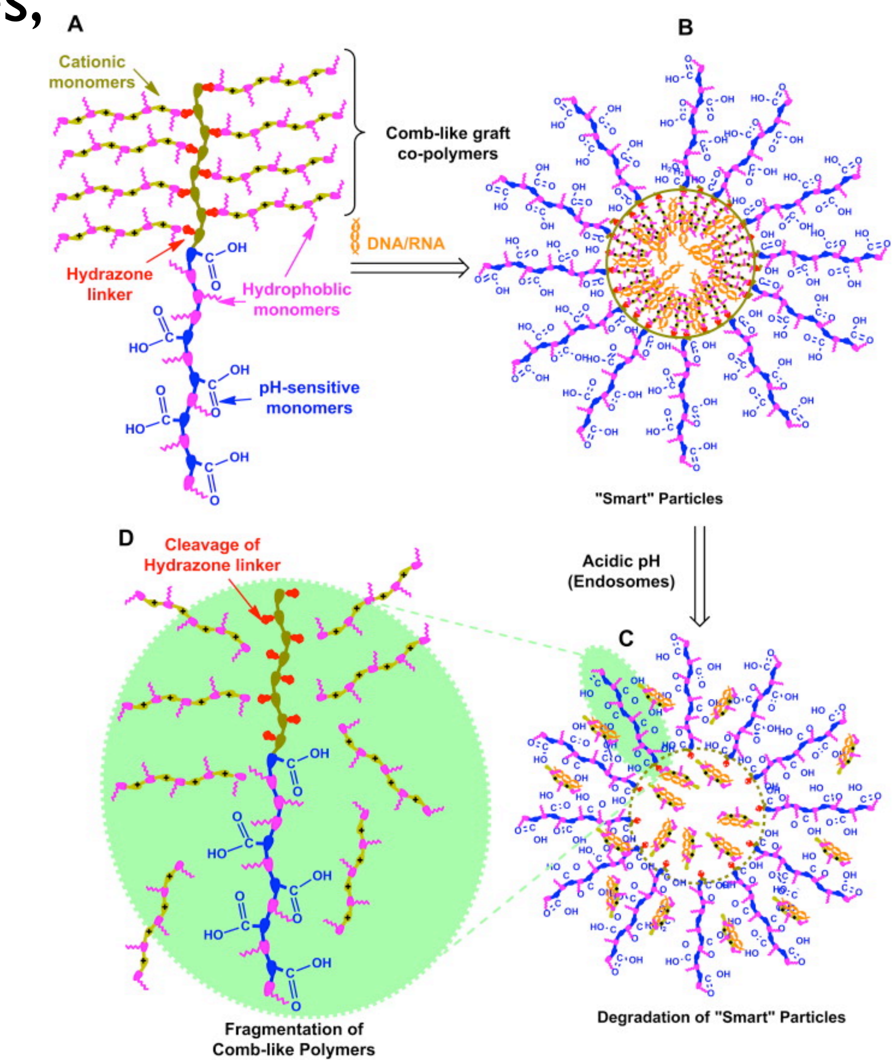
Anomalous diffusion on inhomogeneous substrates:

subdiffusion from “topological” traps, and topological correlation between steps

Fractals trees, percolation clusters, ramified structures, polymer, biological matter



F. Osterloh, UC Davies
Silver fractal trees for solar cells

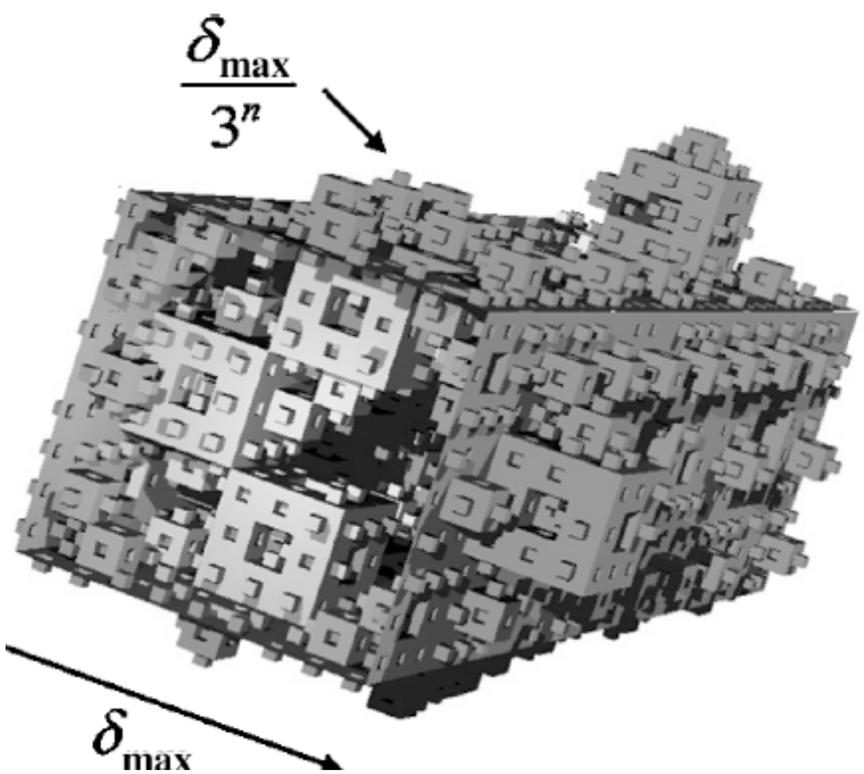


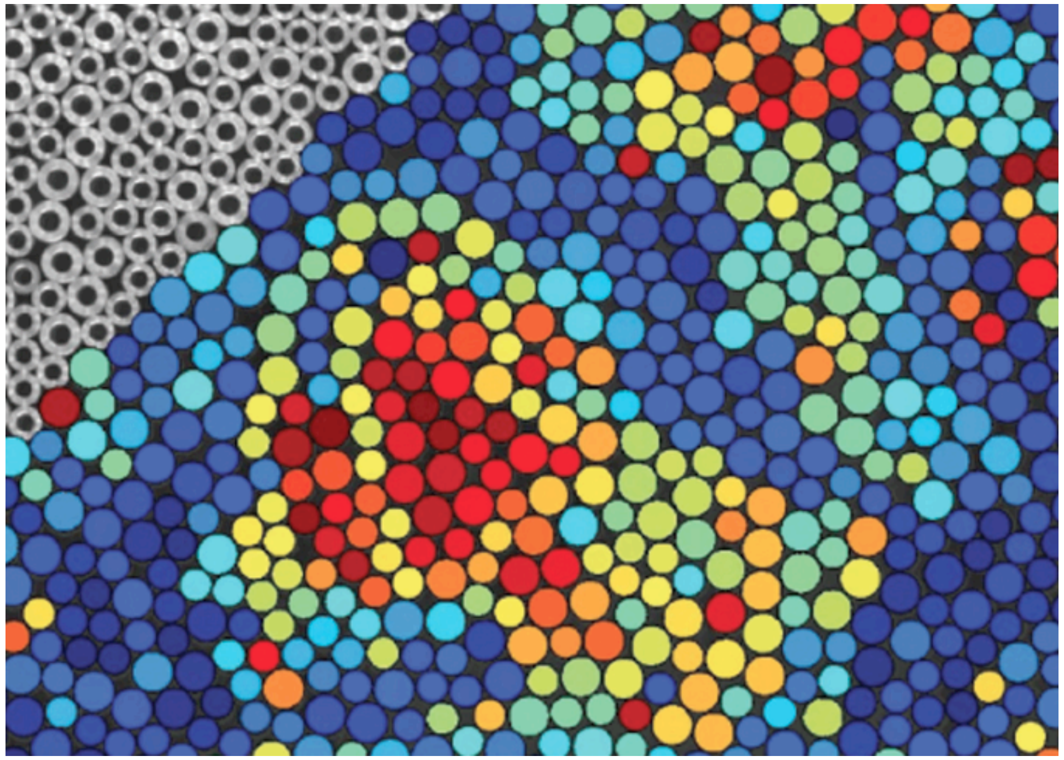
Engineered Comb-like graphs
El- Sayed et al, 2010

$$p_\alpha(\tau) \sim \tau^{-(\alpha+1)}$$ + correlations

Anomalous diffusion on inhomogeneous substrates:

superdiffusion from broad step lengths distribution, and correlation between steps





(P.Levitz EPL 97)
(K. Malek et al PRL 2001)

Molecular diffusion at low pressure (Knudsen diffusion) in porous media

Displacements in vibrating granular materials
(F. Lechenault, R. Candelier, O. Dauchot, J.-P. Bouchaud and G. Biroli Soft Matter 2010)

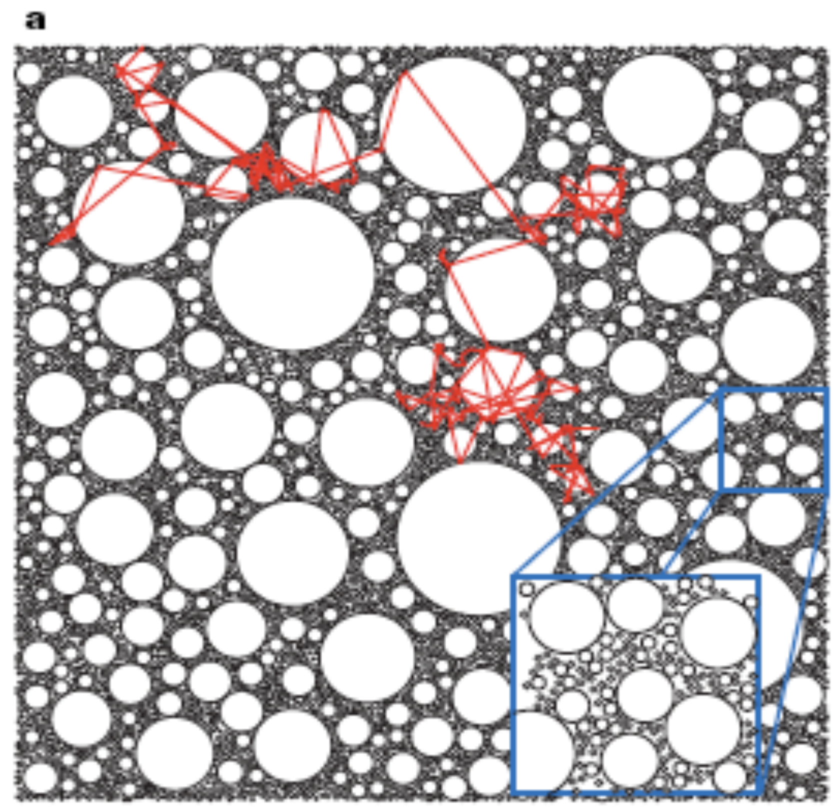
Anomalous superdiffusion

- Random search strategies in complex environments
- Light in disordered media: Image reconstruction, medical imaging
- Enhanced diffusion on DNA molecules and polymer chains
- Active transport in cells
- Atoms in optical lattices, Subrecoil laser cooling

(F. Bardou, J.P.Bouchaud,A. Aspect, C. Cohen Tannoudji "Lévy statistics and laser cooling" 2003)

(O. Benichou, C. Loverdo, Moreau and Voituriez, Rev. Mod. Phys. 2011)

Anomalous diffusion: superdiffusion from broad step lengths distribution and correlations on Lévy Glasses

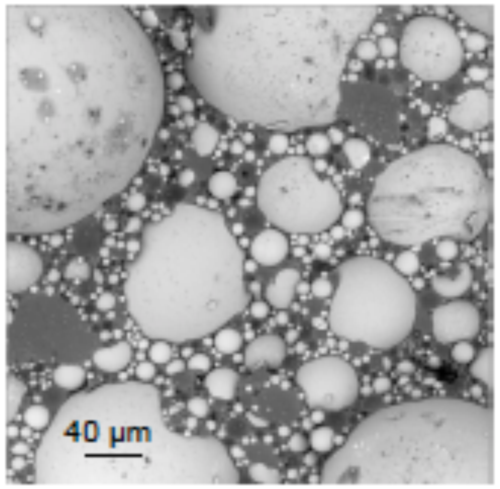


- A glass matrix

•Scattering medium (Ti O2, Strong scatterers)

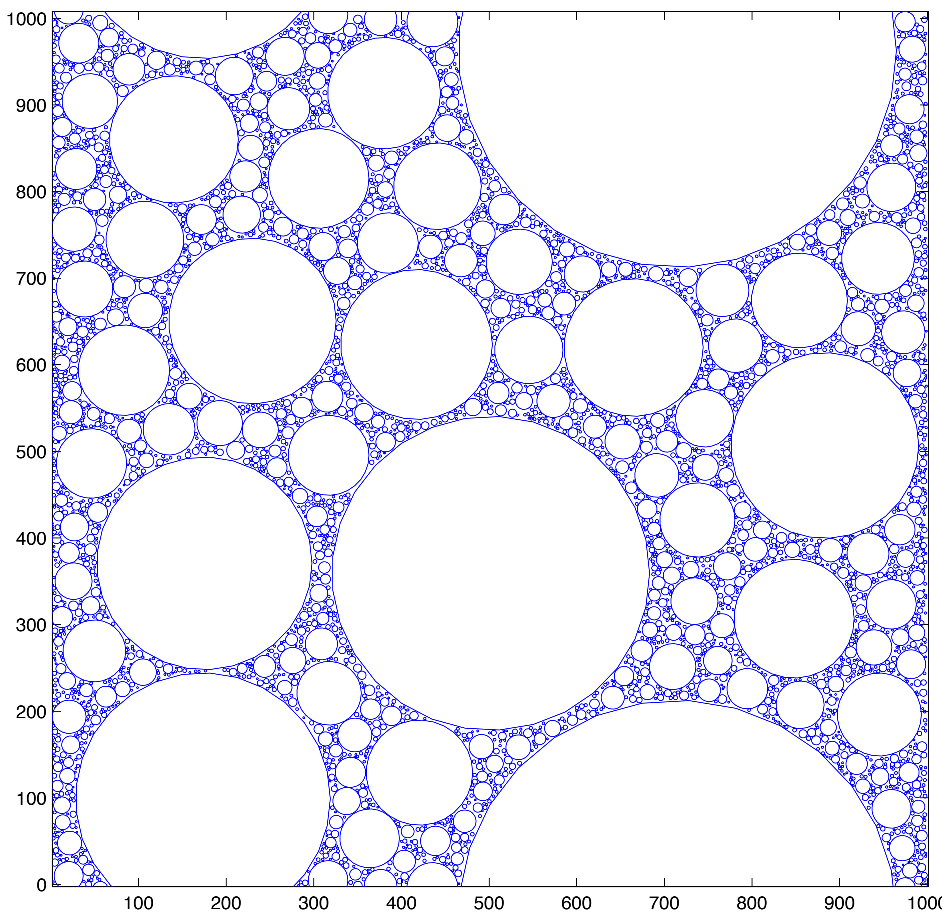
- Glass Spheres, with diameters distributed according to a Lévy tail, that do not scatter light (550-5 μm)

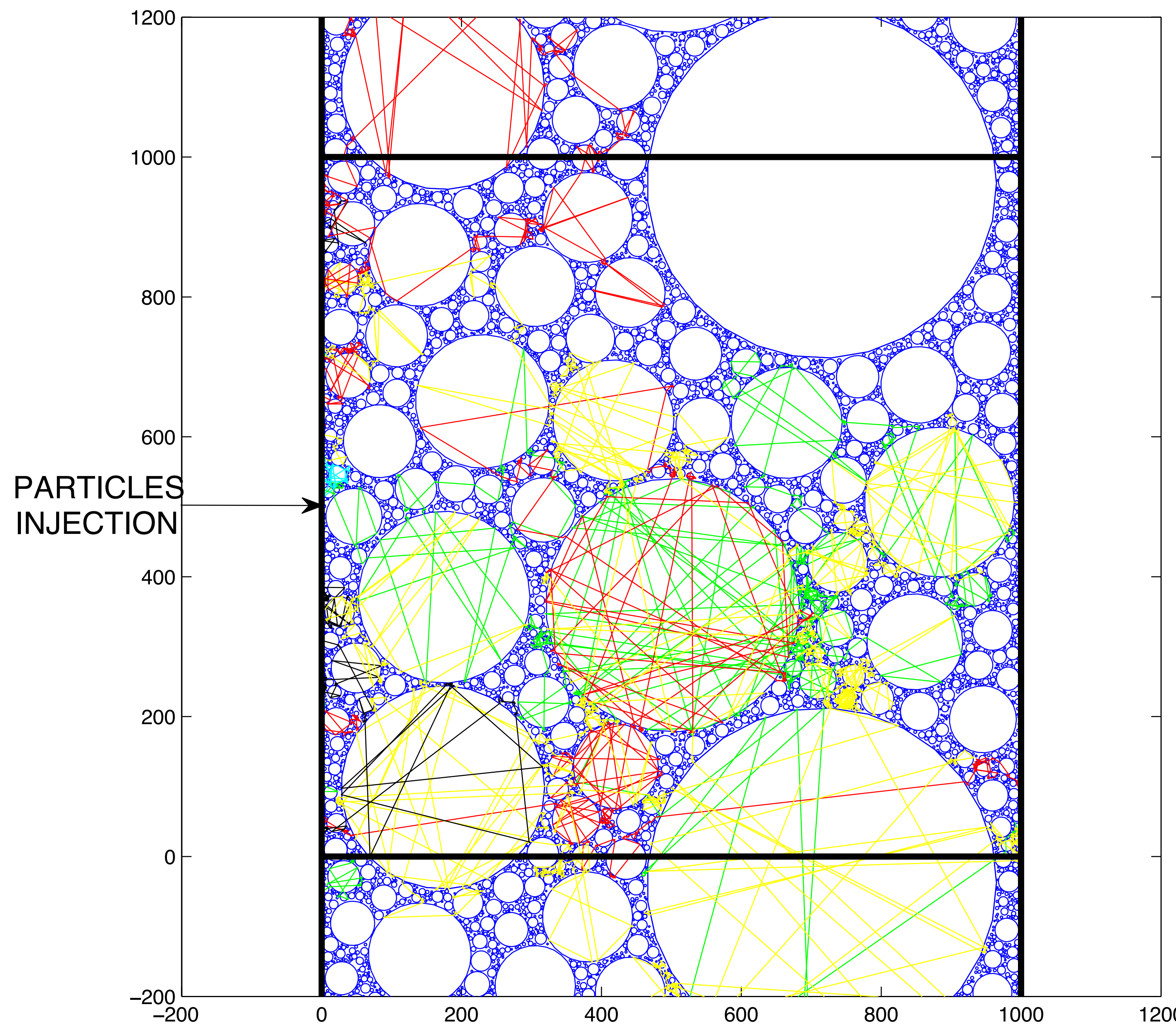
$$p_\alpha(l) \sim l^{-(1+\alpha)}$$ + correlations



D.Wiersma, J. Bertolotti and P. Barthelemy, Nature 2008
J. Bertolotti, K.Vynck, et al Adv Material 2010

- Superdiffusion in Lévy like structures:





Diffusion in a packing of spheres with Lévy distributed radii (here disks)

(R. Burioni, E. Ubaldi, A Vezzani PRE 2014)

Anomalous diffusion:

What would be interesting to calculate:

- the exponents for the mean square displacement, and other moments
- the form of the PDF : does it have a scaling form?
- the effects of a field

as a function of the quenched structure.

As long tails and correlations induced by the geometry are present,
we expect large fluctuations and rare events to influence the dynamics.

I will discuss here the estimate of rare events effects in two cases:

- a simpler case with no correlations: Continuous Time Random Walks in a field

- no field, and correlations: Superdiffusion in Lévy like quenched random structures

Anomalous diffusion

- correlation + "trapping times" $p_\alpha(\tau) \sim \tau^{-(\alpha+1)}$
- correlation + broad step lengths distributions $p_\alpha(l) \sim l^{-(1+\alpha)}$
- ~~correlation~~ + "trapping times"
- ~~correlation~~ + broad step lengths distributions

+ field

Ansatz: Single Long Jump to estimate the largest contribution of rare events

Anomalous diffusion: no correlations

The continuous time random walk

Random motion defined by assigning each jump a jump length x and a waiting time t elapsing between two successive jumps, drawn from the two probability densities $\varphi(t)$ and $\lambda(x)$, typically with slow (Lévy like) decays at large x and t.
The two densities $\varphi(t)$ and $\lambda(x)$ fully specify the probability density of moving to a distance x in a time t in a single motion event, $\psi(x,t)$, and the probability density function $P(x, t)$, describing the random process.

The two prob. densities can be decoupled:

$$\psi(x,t) = \phi(t)\lambda(x)$$

or coupled. A physical coupling, with finite velocity: the Lévy walk
The steps are Lévy distributed and they take a time proportional to their length.

$$\psi(x,t) = p(x|t)\lambda(x)$$

$$p(x|t) = \delta(|x| - vt)$$

cond prob. to make a step
of length x in time t

Traps and broad step lengths: the model

Traps: the particle moves with prob. 1/2 to x to $x \pm \delta_0$, with δ_0 constant (same results if it is extracted from a symmetric distribution with finite variance).

Between two steps, the particle waits for a time τ extracted from

$$p_\alpha(\tau) \sim \tau^{-(\alpha+1)}$$

Lévy walks: time intervals extracted from the previous distribution but now the particle, during this time lag, moves at constant velocity v, chosen from a symmetric distribution with finite variance, and performs displacement l = vt. Here we choose $v = \pm v_0$

$$p_\alpha(l) \sim l^{-(1+\alpha)}$$

Traps and broad step lengths: the model

Do these models always show anomalous diffusion? No, it depends on α .
At large times

Traps: $0 < \alpha < 1$ Subdiffusive scaling length, Non Gaussian P $\ell(t) \sim t^{\alpha/2}$

$\alpha > 1$ Standard diffusion, Gaussian P

(see i.e. Klafter, Sokolov "First steps in Random walks", 2001)

Lévy walks:

$\alpha > 2$ Standard diffusion, Gaussian P

$1 < \alpha < 2$ Non Gaussian P, Superdiffusive scaling length
Strong anomalous $\ell(t) \sim t^{1/\alpha}$

$0 < \alpha < 1$ Non Gaussian P, Ballistic scaling length $\ell(t) \sim t$

(see i.e. Klafter, Zumofen 1993)

The Model: applying a field

Traps: unbalance the jumping probability $(1 \pm \epsilon)/2$

Lévy Walks: acceleration during the flight $\delta = v\tau + \epsilon\tau^2$

Question: what are the scaling properties of the probability distributions with an applied field, as a function of the parameter ruling the tails of the waiting time and step length distribution?

Main steps:

- Write the master equation of the process in a field

- Fourier transform, k ω

- Derive the leading behavior for the P(k,ω) at $k \to 0 \quad \omega \to 0$

- Extract the scaling length and

- the scaling form of the PDF, and its tails

Applying a field: how to single out anomalous behavior by studying the response to an external perturbation

- As expected, in the anomalous regimes, the PDF are very sensitive to the presence of a field. A superdiffusive scaling length arises in the trap model.

- More surprisingly, the systems is very sensitive also when the form of the distribution is a Gaussian at "equilibrium".

The field induces a non Gaussian behavior with strong anomalous diffusion in the trap and Lévy walk model, in a particular range of the parameter where these systems are diffusive without a field. Contributions from rare events.

$$P_\epsilon(x,t) \sim t^{-1/z} F[(x - v_\epsilon t)/t^{1/z}]\ \Theta\left(\epsilon t^2 - x\right)$$ Lévy walks

$$P_\epsilon(x,t) \sim t^{-1/z} F[(x - v_\epsilon t)/t^{1/z}]\ \Theta(x)$$ Traps

Traps: $\epsilon \neq 0$

$$\tilde{P}_\epsilon(k,\omega) \approx \begin{cases} \frac{C_1\omega^{\alpha-1}}{i\epsilon\delta_0 k + C_2\omega^\alpha} & \text{if} \quad 0<\alpha<1 \\ \frac{\langle t\rangle}{i(\epsilon\delta_0 k + \langle t\rangle\omega) + C_3\omega^\alpha} & \text{if} \quad 1<\alpha<2 \\ \frac{\langle t\rangle}{(\delta_0 k)^2/2 + i(\epsilon\delta_0 k + \langle t\rangle\omega)} & \text{if} \quad \alpha>2. \end{cases}$$

$\langle t^p\rangle = \int t^p p_\alpha(t)dt$

$C_i \in C$

but Im C changes sign with ω so that P is real

$\boxed{P_\epsilon(x,t)}$

- $\alpha > 2$ Standard diffusion, F Gaussian moving at constant speed $v_\epsilon = \epsilon\delta_0/\langle t\rangle$
- $0<\alpha<1$ Scaling length $\ell(t) \sim t^\alpha$ $v_\epsilon = 0$

$1/2 < \alpha < 1$

Superdiffusive scaling length

(see i.e. Bouchaud, Georges, Phys. Rep. 1990)

Benichou, Illen, Mejia-Monasterio, Oshanin Jstat (2013,2014)

F decays fast, weak anomalous regime $\langle x^n(t)\rangle_\epsilon \sim \ell^n(t)$

- F changes shape and becomes asymmetric as soon as the field is switched on

Traps: the most intriguing case

- $1 < \alpha < 2$ (Remember that without the field this is Gaussian regime)

F non Gaussian, moving at constant speed, $v_\epsilon = \epsilon\delta_0/\langle t \rangle$ $x_p(t) \sim \langle x(t) \rangle_\epsilon \sim t$ Peak

$l(t) \sim t^{1/z}$ $z = \alpha < 2$ Superdiffusive spreading

F power tail, strong anomalous regime driven by rare events of long waiting times:

Prob. of finding a particle at a distance $\xi = x - x_p(t)$ from the peak of the distribution = prob for the particle to experience a stop of duration τ

$v_\epsilon \tau = \xi$

single event $p_\alpha(\tau)d\tau = p_\alpha(\tau(\xi))\frac{d\tau}{d\xi}d\xi \sim \frac{1}{\xi^{1+\alpha}}d\xi,$ $P_\epsilon(\xi, t) \sim \frac{N(t)}{\xi^{1+\alpha}} \sim \frac{t}{\xi^{1+\alpha}}$ N(t) n. of scattering events

so that $P_\epsilon(\xi, t) = \frac{1}{t^{1/\alpha}}F\left(\frac{\xi}{t^{1/\alpha}}\right) = \frac{1}{t^{1/\alpha}}F\left(\frac{|x - vt|}{t^{1/\alpha}}\right)$

$$\boxed{\langle \xi^2(t) \rangle_\epsilon \sim t^{3-\alpha} \neq \ell^2(t) \sim t^{2/\alpha}}$$

mean square displacement around the peak of the PDF

Traps:

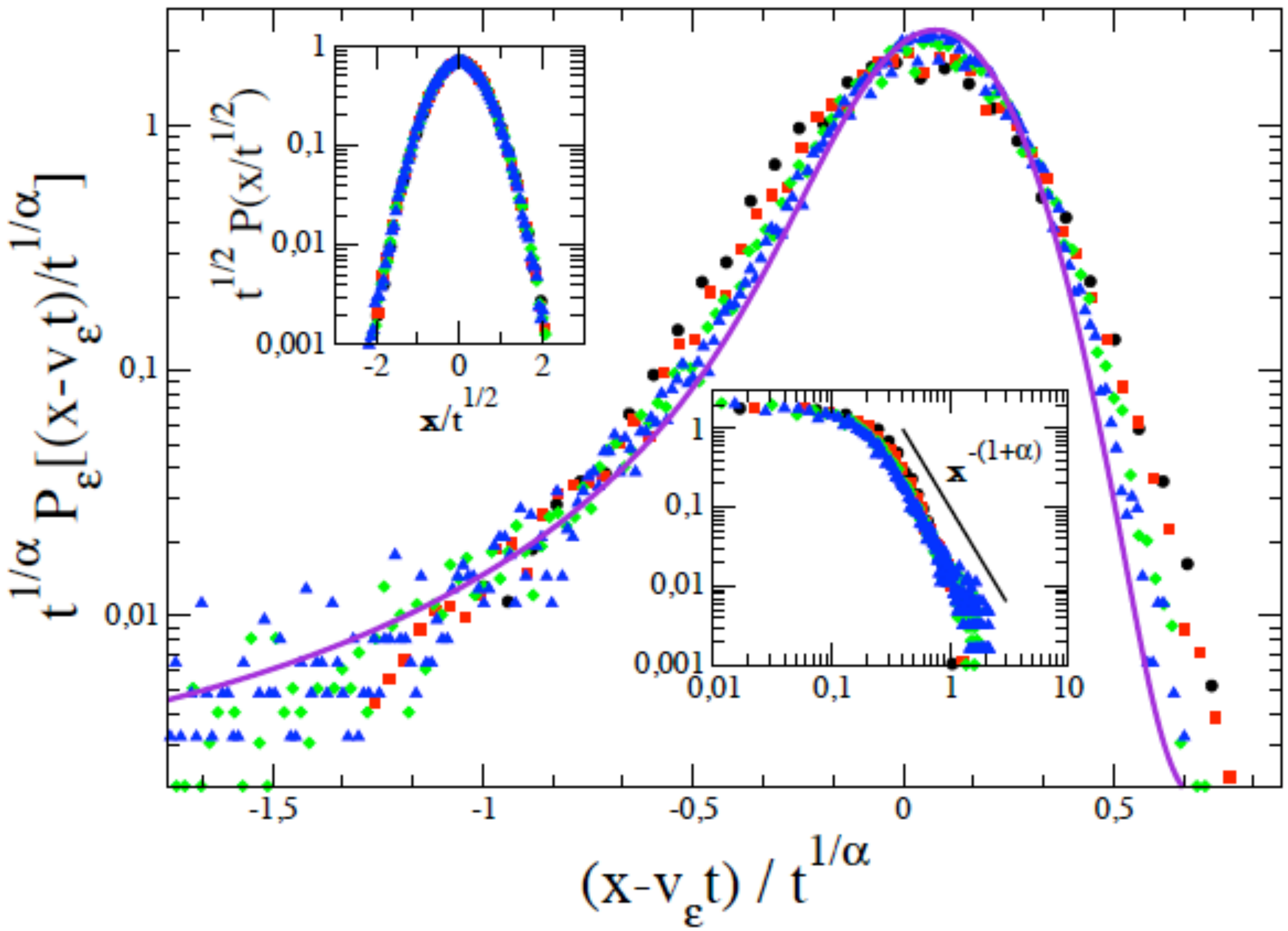


Figure 1. (color online) Collapse of the PDFs of the CTRW, for $\alpha = 1.5$ and field $\epsilon = 0.15$ according to Eq. (3) with velocity $v_\epsilon = 0.1$. Symbols correspond to different times: $t = 10^3$ (●), $t = 2 \cdot 10^3$ (■), $t = 5 \cdot 10^3$ (♦), and $t = 10^4$ (▲). The continuous line represents the numerical inverse Fourier transform of Eq. (8). Central inset: same data of the main figure in log-log scale, as function of $|x - v_\epsilon t|$. Notice the power law behavior $P_\epsilon(x,t) \sim x^{-(1+\alpha)}$. Top left inset: collapse of the PDF for $\alpha = 1.5$ with zero drift, $\epsilon = 0$. Notice the simple Gaussian behavior, $\ell(t) \sim t^{1/2}$,

Lévy Walks $\epsilon \neq 0$

$$\tilde{P}_\epsilon(k,\omega) \approx \begin{cases} \frac{\omega^{\alpha-1} g(k^{1/2}/\omega)}{C_5 \epsilon^{\alpha/2} k^{\alpha/2} + C_2 \omega^\alpha} & \text{if} \quad 0<\alpha<1 \\ \frac{\langle t \rangle}{C_5 \epsilon^{\alpha/2} k^{\alpha/2} + i\langle t \rangle \omega} & \text{if} \quad 1<\alpha<2 \\ \frac{\langle t \rangle}{C_5 \epsilon^{\alpha/2} k^{\alpha/2} + i(\epsilon \langle t^2 \rangle k + \langle t \rangle \omega)} & \text{if} \quad 2<\alpha<4 \\ \frac{\langle t \rangle}{\langle t^2 \rangle v_0^2 k^2/2 + i(\epsilon \langle t^2 \rangle k + \langle t \rangle \omega)} & \text{if} \quad \alpha>4 \end{cases}$$

$g(x)$ regular complex function with $g(0) = C_1$

$g(x) \sim x^{\alpha-1}$ for $x \to \infty$

$\boxed{P_\epsilon(x,t)}$

- $\alpha > 4$ Standard diffusion, F Gaussian moving at constant speed $v_\epsilon = \epsilon\langle t^2\rangle/\langle t\rangle$
- $\alpha < 2$ The rigid translation is subdominant, asymmetry $(v_\epsilon t \ll t^{2/\alpha})$

$0<\alpha<1$ $z = 1/2$ $\ell(t) \sim t^2$ accelerated motion

$1<\alpha<2$ $z = \alpha/2$ $\ell(t) \sim t^{2/\alpha}$ super-ballistic

Lévy Walks $\epsilon \neq 0$

- $2 < \alpha < 4$ F non Gaussian with drift speed ← (Gradenigo,Sarracino Villamaina,Vulpiani 2012)

$$\ell(t) \sim t^{2/\alpha}$$

F power tail, strong anomalous regime

$\xi = x - x_p(t)$ $\xi = v\tau + \epsilon/2\tau^2$ due to acceleration

$$p(\tau)d\tau = p(\tau(\xi))\frac{d\tau}{d\xi}d\xi \sim \frac{1}{\xi^{1+\alpha/2}}d\xi$$

$$P_\epsilon(x,t) \sim \frac{N(t)}{(x - x_p(t))^{1+\alpha/2}}$$

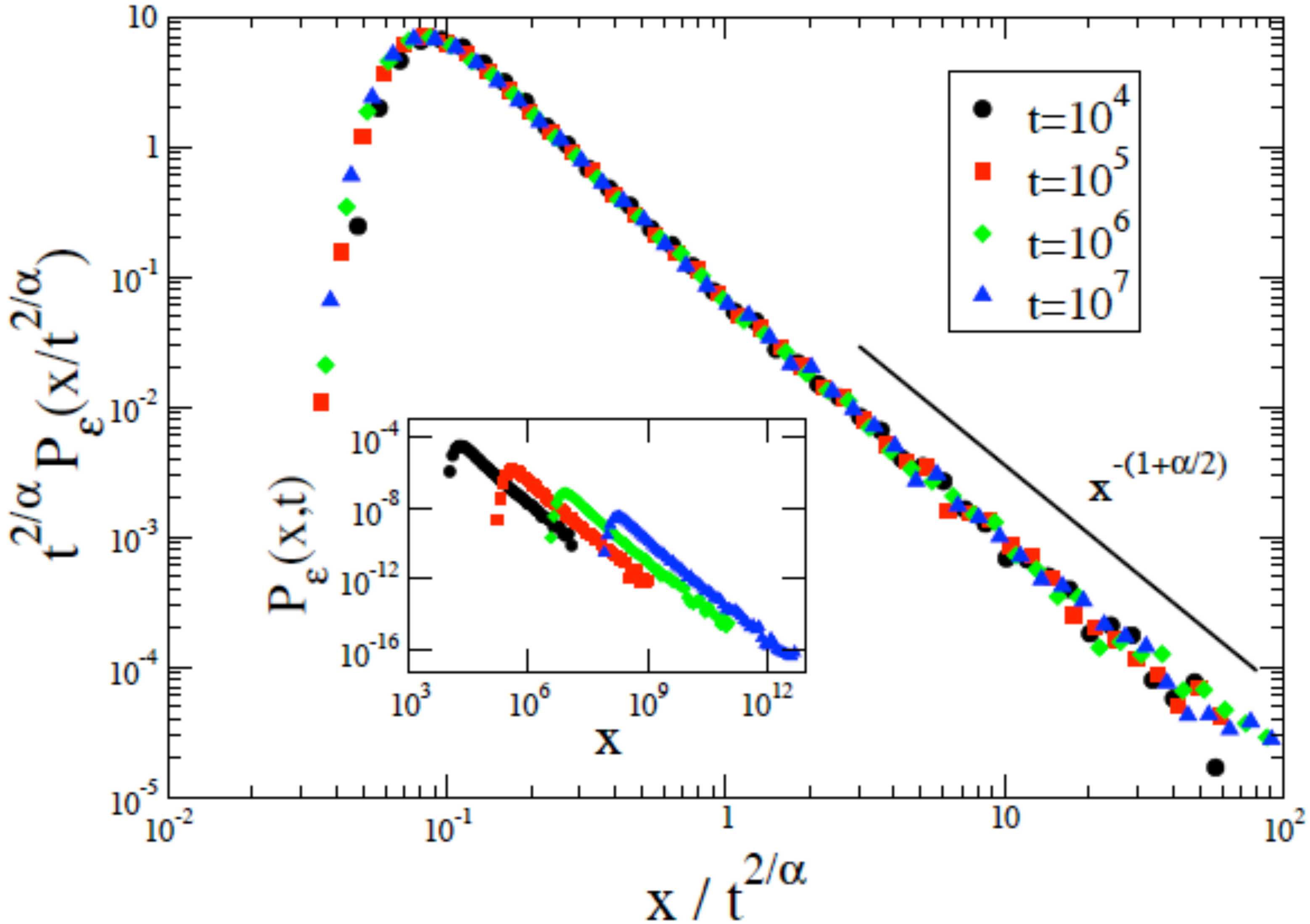
$$P_\epsilon(x,t) \sim x^{-(1+\alpha/2)}$$

$$\boxed{\langle[\delta x(t)]^2\rangle_\epsilon = \langle x^2(t)\rangle_\epsilon - \langle x(t)\rangle_\epsilon^2 \sim t^{5-\alpha} \neq \ell(t)^2 \sim t^{4/\alpha}}$$

A way to single out the underlying anomalous dynamics?

Rebenshtok, Denisov, Hanggi, Barkai PRL 2014

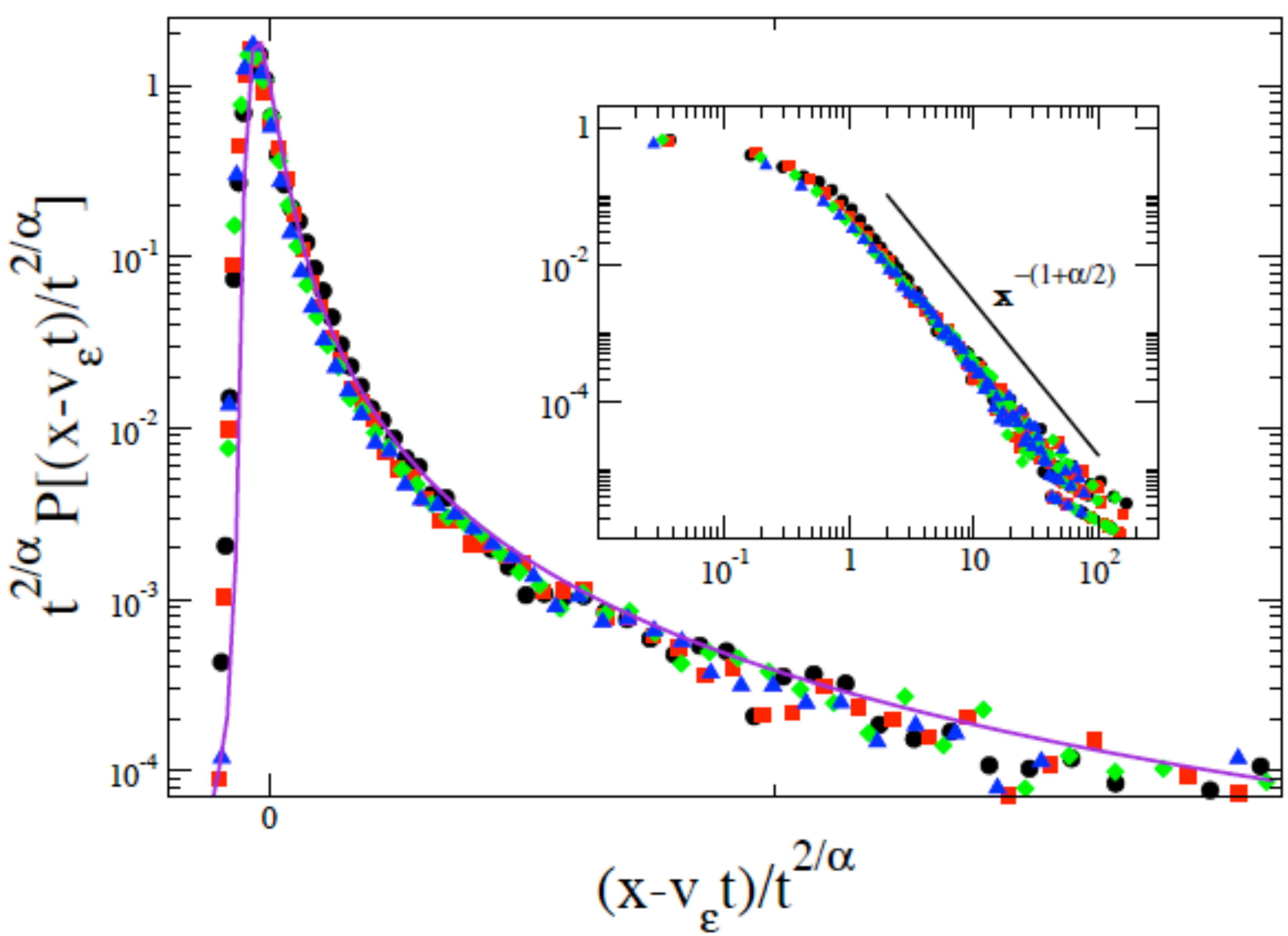
Lévy Walks



Collapse of PDFs with the scaling $t^{2/\alpha}P_\epsilon(x/t^{2/\alpha})$, for the Lévy walk with exponent $\alpha = 1.5$ and field $\epsilon = 0.25$. Inset: $P_\epsilon(x,t)$ at different times. Notice that the approximation $(x - v_\epsilon t)/t^{2/\alpha} \sim x/t^{2/\alpha}$ works very well asymptotically.

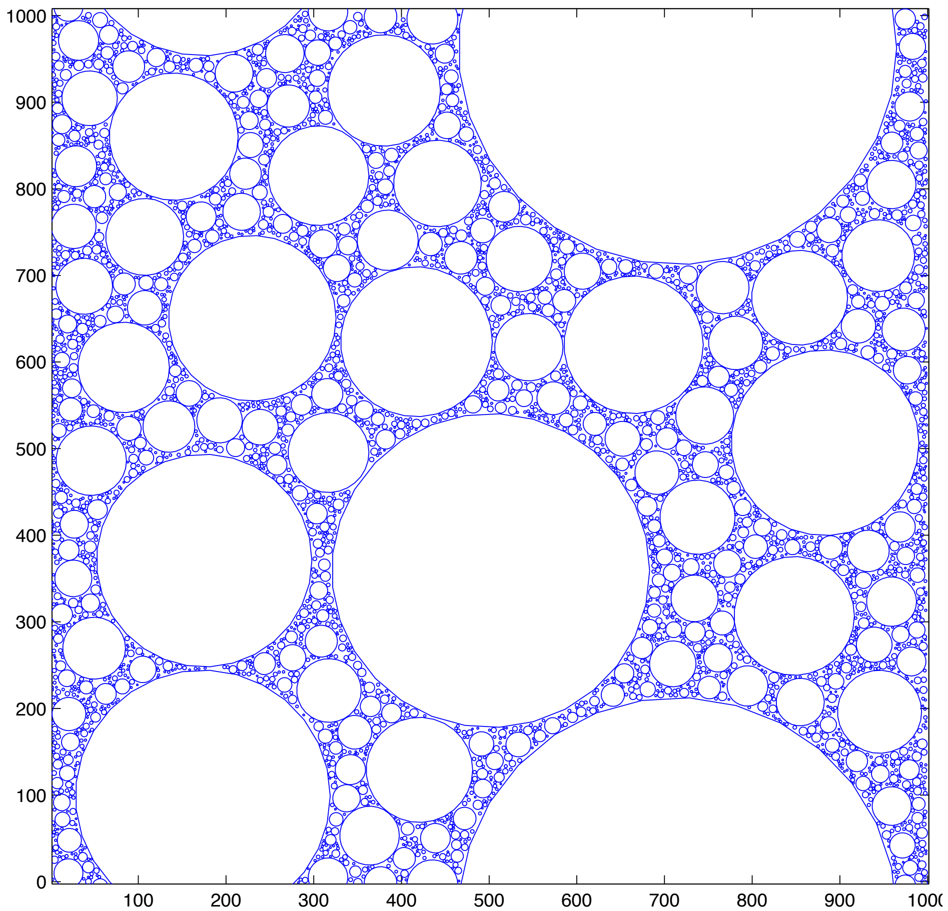
Lévy Walks

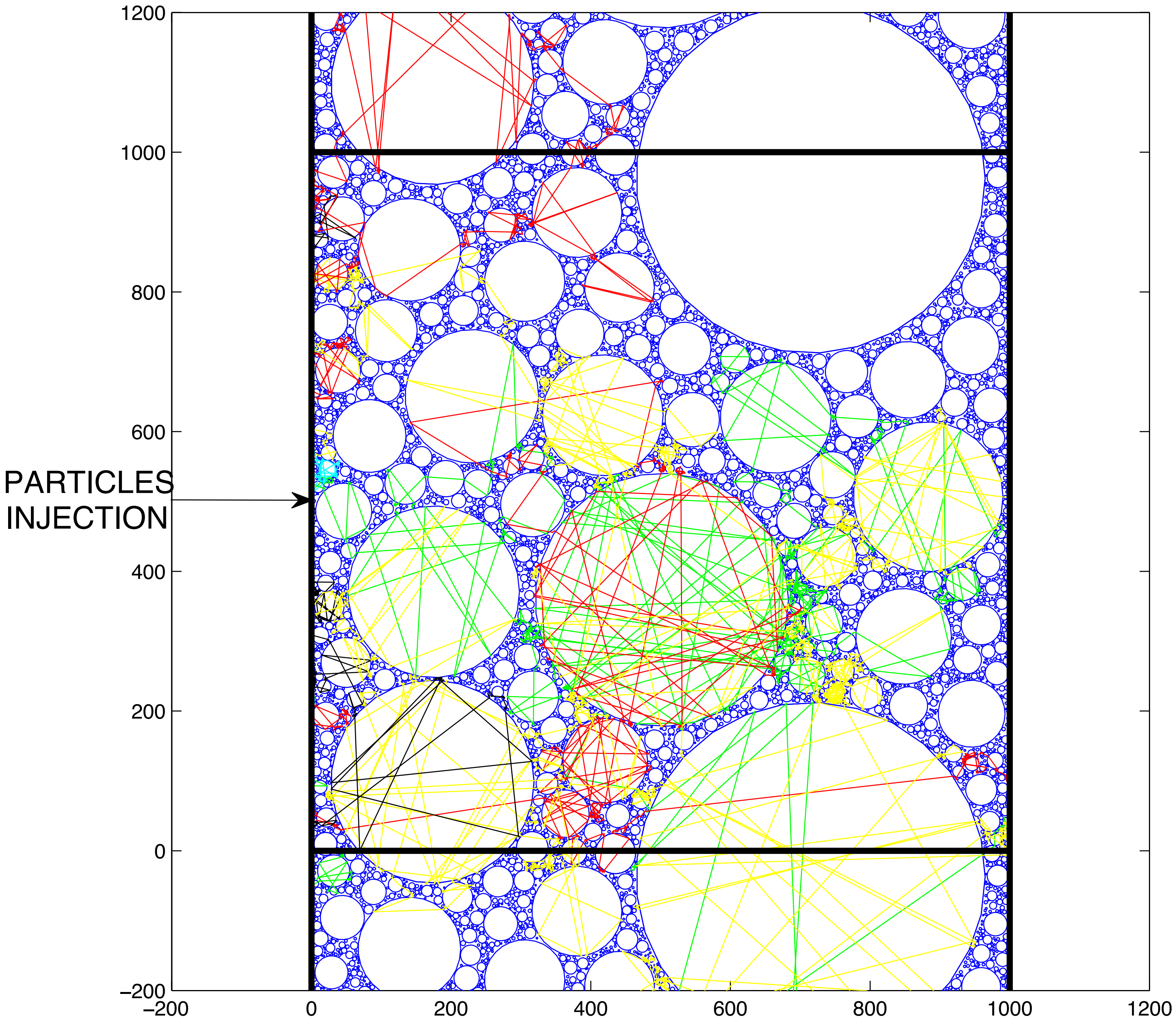
R.B., G. Gradenigo, A. Sarracino, A.Vezzani, A.Vulpiani 2013



Collapse of the PDFs with the scaling $t^{2/\alpha}P_\epsilon[(x-v_\epsilon t)/t^{2/\alpha}]$, for the Lévy walk with exponent $\alpha = 2.5$ and field $\epsilon = 0.25$, with $v_\epsilon = 0.38$. Symbols correspond to different times: $t = 1.6 \cdot 10^4$ (●), $t = 3.2 \cdot 10^4$ (■), $t = 6.4 \cdot 10^4$ (♦), and $t = 1.28 \cdot 10^5$ (▲). The line represents the numerical inverse Fourier transform of Eq. (12). Inset: same data of the main figure in log-log scale.

- Superdiffusion in Lévy like structures:

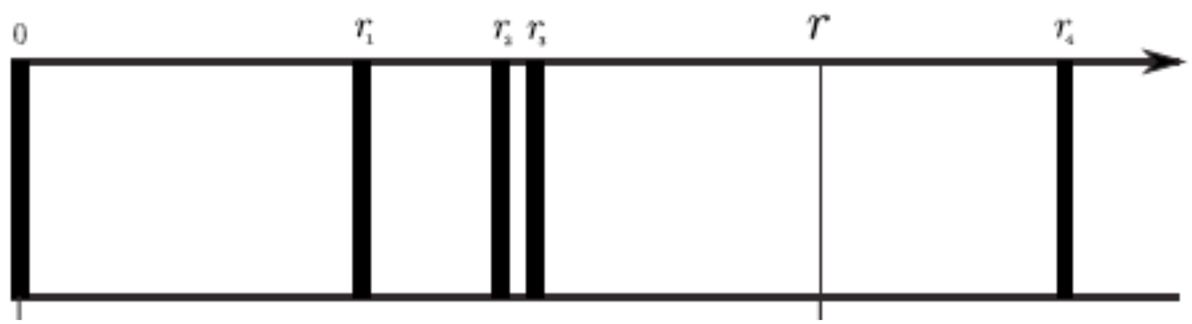




Diffusion in a packing of spheres with Lévy distributed radii (here disks)

- quenched (correlations?)
- $p_\alpha(l) \sim l^{-(1+\alpha)}$

The 1d version: 1d Lévy-Lorentz gas



$$p(r_{i+1} - r_i) = \frac{\alpha r_0^\alpha}{|r_{i+1} - r_i|^{1+\alpha}} \qquad |r_{i+1} - r_i| > r_0$$

$$p(r_{i+1} - r_i) = 0 \qquad \text{otherwise}$$

Scatterers are placed in the positions r_i, spaced according to a Lévy distribution with parameter α , with r_0 setting the space scale

Lévy walk model: the walker moves at constant velocity between two scatterers, hits a scatterer and it is transmitted or reflected with equal probability (Lévy-Lorenz gas) (Barkai, Fleurov, Klafter 2000)

- Generalized scaling relations holds: in the process, there is a growing scaling length, characterized by an exponent. This rules the scaling properties of physical quantities for $r \ll l(t)$. However, rare events can give access to $r \gg l(t)$

- Now we cannot estimate the large fluctuations from the master equation. Then the "single long jump" ansatz, estimating the largest fluctuation contributing to the process, is used to establish the contribution coming from $r \gg l(t)$ to all main physical quantities (fluctuations, transmissions etc), in terms of z and α. Need N(t)!

- In 1d models, exact results using the mapping with the equivalent electric network problem, which gives the exact value for the scaling length l(t) and for N(t) and z, as a function of the Lévy parameter.

- In other cases, the scaling length must be determined experimentally, and then the scaling behavior of other quantities is known. Interestingly, the scaling length can be measured from time resolved transmission measurements in experiments.

The importance of long tails: how to estimate the anomalous effects. The "single long jump hypothesis"

Anomalous effects appears when r>> l(t). We can suppose that the walker reaches the distance r>> l(t) with a single long jump of length r, and the other scattering processes contribute until a distance l(t).
Then:

$$P(r,t) \sim N(t)/r^{1+\alpha}$$

$N(t)$ Number of scatterers seen by the walker in a time t

Prob. that a scatterer is followed by a jump of length r>>l(t)

$N(t)$ - has to be calculated (as a function of l(t), recalling that before the long jump the walker has travelled a distance of order l(t))

The importance of long tails: how to estimate the anomalous effects. The "single long jump hypotesis" in the 1d Lévy Lorentz gas: exact expression for the

$$\langle r^2(t)\rangle \sim \begin{cases} t^{(2+2\alpha-\alpha^2)/(1+\alpha)} & \text{if } 0<\alpha<1 \\ t^{5/2-\alpha} & \text{if } 1\le\alpha\le 3/2 \\ t & \text{if } 3/2<\alpha. \end{cases}$$

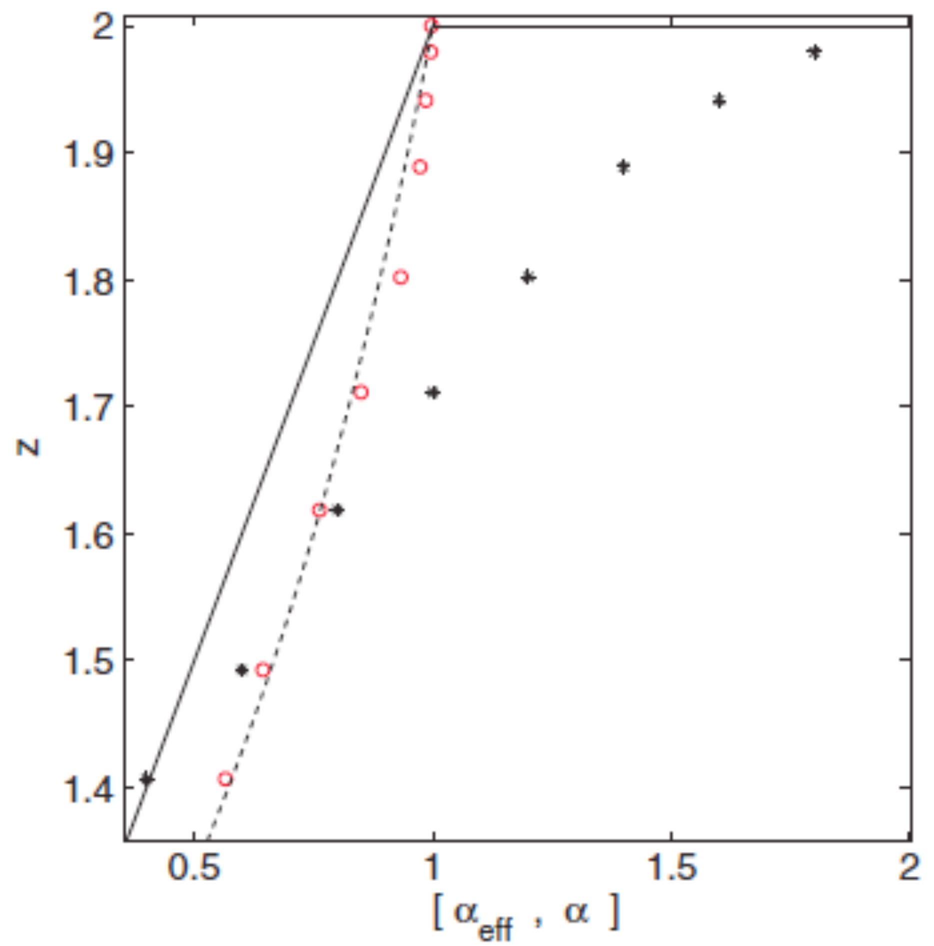
$$\langle r^p(t)\rangle \sim \begin{cases} t^{\frac{p}{1+\alpha}} \sim \ell(t)^p & \text{if } \alpha<1,\ p<\alpha \\ t^{\frac{p(1+\alpha)-\alpha^2}{1+\alpha}} & \text{if } \alpha<1,\ p>\alpha \\ t^{\frac{p}{2}} \sim \ell(t)^p & \text{if } \alpha>1,\ p<2\alpha-1 \\ t^{\frac{1}{2}+p-\alpha} & \text{if } \alpha>1,\ p>2\alpha-1 \end{cases}$$

Extremely well verified numerically: a rigorous proof?

R.B, L.Caniparoli, A.Vezzani 2010
R.B., S. di Santo, S Lepri, A.Vezzani 2012

Beenakker, Groth, Akhmerov 2009, 2011

The scaling length in a self similar packing and in random disks packings:



Ansatz $z(\alpha) = \frac{2}{2-\alpha}$

P. Buonsante, R.B., A. Vezzani P2011

R.B., A Vezzani, E. Ubaldi 2014

- Effects of rare events in systems with broad distributions
- In CTRW in a field: an external perturbation induces strong anomalous diffusion on a process that showed standard diffusion without a field, caused by rare events.
- a way to detect experimentally the subtle presence of anomalous behavior?
- Lévy random packings: estimate of effects of large fluctuations in transport in random inhomogeneous media