From **random walks** to applications

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CRI, Paris Descrartes University, France, Moscow Institute of Physics and Technology

WWCS 2019, Winter School

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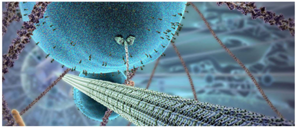
Projects I contributed to



Transport of macromolecules, organelles and vesicles in living cells is a very complicated process that essentially determines and controls many biochemical reactions, growth and functioning of cells.

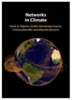
copan – Coevolutionary Pathways in the World-Earth system

A joint project of PIK's Research Domains 1 and 4, dealing with the mid- and long-term coevolution of natural and socio-economic subsystems of the Earth system and its relationship to planetary boundaries

The copan project was featured as a flagship activity of PIK in 2013–2018 and is since continued as a collaboration between the working groups *Co-Evolution of Human-Environment Systems in the Anthropocene* (RD1) and *Social Dynamics in Complex Human-Environment Systems* (RD4), with strong links to PIK's FutureLabs on *Earth Resilience in the Anthropocene* and on *Game Theory and Networks of Interacting Agents*.

copan coevolutionary pathways

Networks in Climate



Get access Coming soon

Henk A. Dijkstra, *Universiteit Utrecht, The Netherlands* , Emilio Hernández-García, *Univers Balears, Spain* , Cristina Masoller, *Universitat Politècnica de Catalunya, Spain* , Marcelo Ba *Universidad de la Republica, Montevideo, Uruguay*

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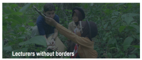
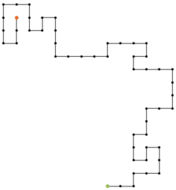
SCIED NETWORK



My main collaborators: E.Hernandez-Garcia C.Masoller I.Sokolov D.Grebenkov J.Kurths H. Bunina H. Dijkstra P.Holme D.Krioukov

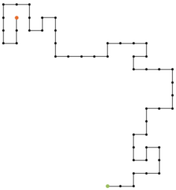
CCEGN 2019 - Les Houches

What we will talk about?



- **Part 1:**
  Random walk theory

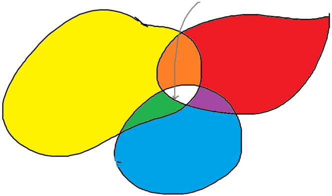
What we will talk about?



- **Part 1:**
  Random walk theory

- **Part 2:**
  Applications of random walk theory

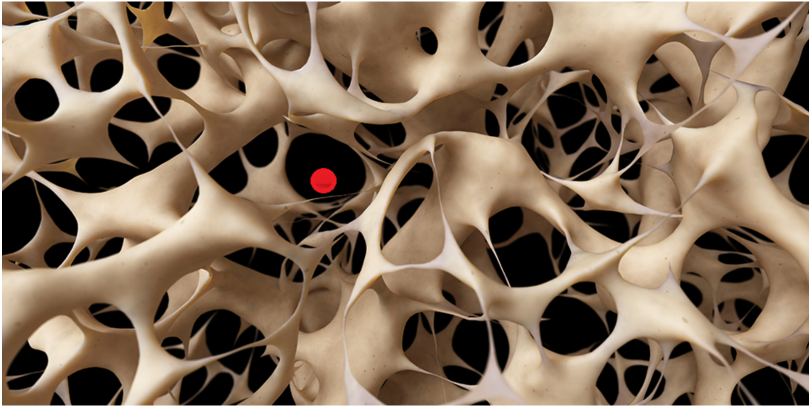
Scientists working on random walk theory: Pearson, Smoluchowski, Langevin, Fermat, Bernoulli, Einstein, Kolmogorov, Pascal, Hughes, Brown, Wiener, Montroll, Weiss...



Intersection of Markov chain theory, Stochastic processes, Statistical physics, Disordered systems, Probability theory...

Real-world examples

Real-world examples



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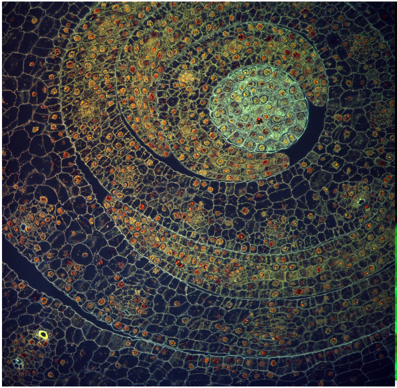

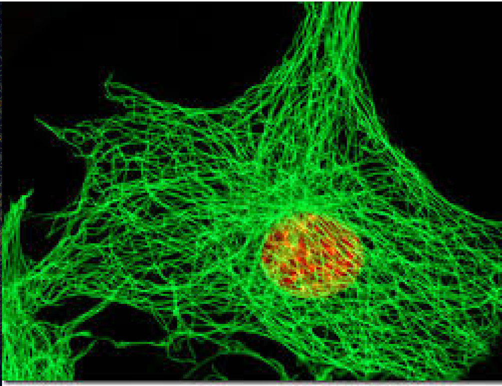

E.Katrukha,microtubules,imaginarycellrepresentation

networkrepository


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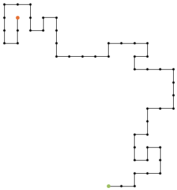
Part 1

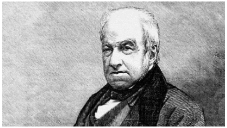


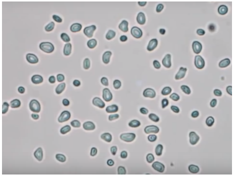
- **Random walk theory**
  history
  types of random walks
  diffusion models

Random walks: history

Experiment:

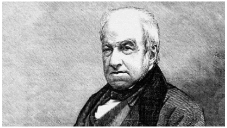
Brownian motion was discovered in 1785 by Jan Ingenhousz: irregular motion of coal dust particles on the surface.
In 1827 Robert Brown, a British botanist, is observing a suspended pollen grain in water.

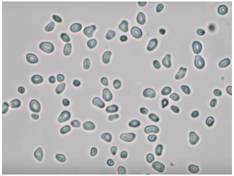




Random walks: history

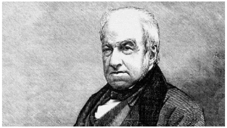
Experiment:
Brownian motion was discovered in 1785 by Jan Ingenhousz: irregular motion of coal dust particles on the surface.
In 1827 Robert Brown, a British botanist, is observing a suspended pollen grain in water. (video)
How to explain the experiment?

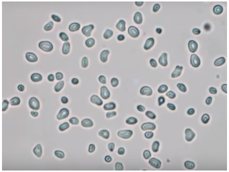




Random walks: How to explain the experiment?

Assumptions:

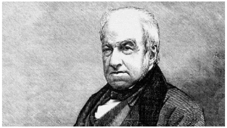


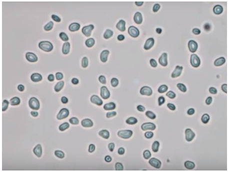


Random walks: How to explain the experiment?

Assumptions:

1. Random walk in 1 dimension
2. Memoryless: random walk forgets what he did last step
3. Symmetry: walk to the left of right with equal probability

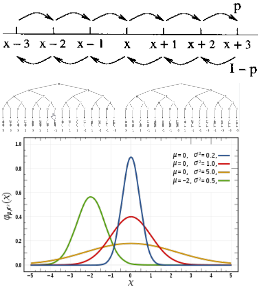




Random walks: building a model

Assumptions:

1. Random walk in 1 dimension
2. Memoryless: random walk forgets what he did last step
3. Symmetry: random walk jumps to the left of right with equal probabilities p, q



Types of random walks

Depending on the walk characteristics:

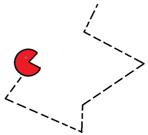
• on continuous or discrete structures (networks) [Redner, 2002]

• time: discrete or continuous [Montroll, Weiss, 1965]

• various probabilities of jumps from each node [Hudges, 2002]

• additional parameters: RW with resetting, self-avoiding random walk, adaptive random walks [Masuda, Lambiotte et al.2017]

• passive vs. active, e.g. node-centric active CTRWs.



Random walks properties

It is interesting to look at:

Probability density $P(x, t)$ [Klafter, Sokolov, 2010]

First-passage time $F(x, t)$ [Metzler et al., Redner, 2002]

Network measures based on RWs [Winter School Scientists ;)]

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Looking forward to tutorial from Alexandre

Main trick

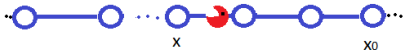
$$P(x,t) = \frac{e^{-(x-vt)^2/4Dt}}{\sqrt{4\pi D t}} \qquad\qquad P(k,t) = e^{-(ikv + Dk^2)t}$$

$$\begin{tikzcd}
(x,t) \arrow[r, leftrightarrow, "\text{Fourier}"] \arrow[d, leftrightarrow] & (k,t) \arrow[d, leftrightarrow, "\text{Laplace}"] \\
(x,s) \arrow[r, leftrightarrow] & (k,s)
\end{tikzcd}$$

$$P(x,s) = \frac{e^{-(v \mp \sqrt{v^2+4Ds})\,|x|/2D}}{\sqrt{v^2+4Ds}} \qquad\qquad P(k,s) = \frac{1}{s + ikv + Dk^2}$$

Random walks: discrete space and time

$P(x, t)$ is probability to find RW at x coordinate at time t.



Random walks: discrete space and time

$P(x,t)$ is probability to find RW at x coordinate at time t.

Master equation describing probability

$P(x,n) = pP(x-1,n-1) + qP(x+1,n-1)$

using the generating function and Fourier **transformation**

$P(k,z) = \sum_{n=0}^{\infty} z^n \sum_{x=-\infty}^{\infty} e^{ikx} P(x,n)$

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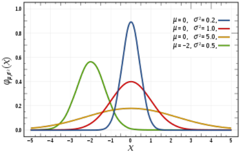
Then the final probability distribution for DTRW

$P(x,n) = \frac{N!}{(N+x)/2!(N-x)/2!} p^{(N+x)/2}(1-p)^{(N-x)/2}$



Gaussian in the long-time limit

$P(x,n) \to \frac{1}{\sqrt{2\pi npq}} e^{-(x-np)^2/2npq}$

Random walks: discrete space and time

Will we get Gaussian for any hopping process, where $\langle x^2 \rangle$ is finite?

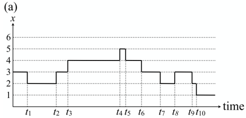
Random walks: discrete space and time

Will we get Gaussian for any hopping process, where $\langle x^2 \rangle$ is finite?
Yes! Probability distribution is independent from details of single-step hopping [Gnedenko, Kolmogorov 1954]

Random walks: discrete space, continuous time

Continuous time random walk in 1D

At each x, where CTRW jumps, RW waits for τ distributed with $\psi(t)$.



[N.Masuda et al. 2017]

Random walks: discrete space, continuous time

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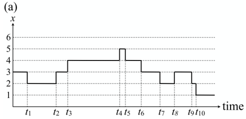
Probability that no event occurred till time t:

$P^0(t) = \int_t^\infty \psi(t')dt'$



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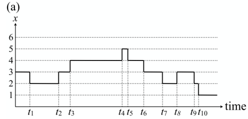

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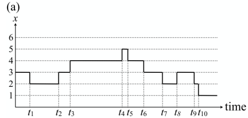
Apply trick to time: $t \to s$

$\tilde{P^1}(s) = \tilde{\psi}(s)\tilde{P^0}(s)$

...



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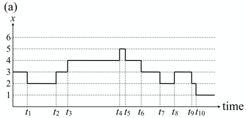
Apply trick to time: $t \to s$

$\tilde{P^1}(s) = \tilde{\psi}(s)\tilde{P^0}(s)$

...

Probability that n **events** occurred till time t:

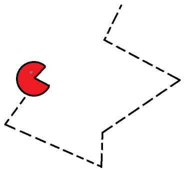
$\tilde{P^n}(s) = \tilde{\psi}^n(s)\tilde{P}^{n-1}(s) = \tilde{\psi}^n(s)\frac{1-\tilde{\psi}(s)}{s}$



[N.Masuda et al. 2017]

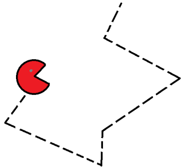
Random walks: continuous space and time

Continuous time random walk model (CTRW): CTRW waits at each x, where CTRW jumps, it waits time step for τ distributed with $\psi(t)$. The length of the steps are distributed with $f(x)$ function.



Random walks: continuous space and time

Continuous time random walk model (CTRW) $P(x, t)$ is probability to find RW at x coordinate at time t.



Random walks: continuous space and time

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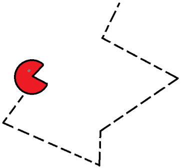
We can use the probability $P(x,n)$ from discrete time random walk
$P(x,t) = \sum_{n=0}^{\infty} P(x,n)p(n,t)$
Then using **renewal theory, Green function**



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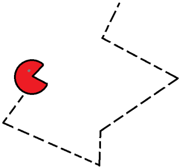
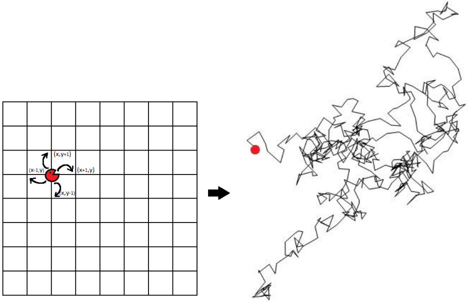
Then using **renewal theory, Green function** we get the final equation
$P(k,s) = \frac{1-\tilde{\psi}(s)}{s}\frac{1}{1-f(k)\tilde{\psi}(s)}$



Generalization of random Walk framework

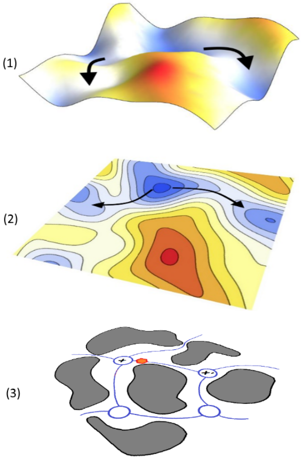


Homogeneous random walk (RW) on a discrete lattice in discrete time

Homogeneous continuous time random walk (CTRW) in continuous space

R.Metzler, J.Klafter, Phys.Rep. (2000], M.Jaume et al., EPJ [2017]

What about heterogeneous motion?


(1)
(2)
(3)

Heterogeneous Continuous Time Random Walk model

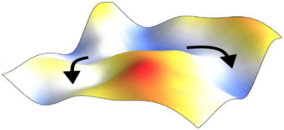
on a graph:

- graph with transition **matrix** Q,
- heterogeneous **travel time distributions** $\psi_{xx'}(t)$ between nodes x, x'.

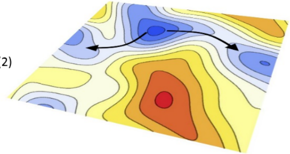
The generalized transition matrix

$$Q_{xx'}(t) = Q_{xx'}\psi_{xx'}(t)$$

(1)



(2)



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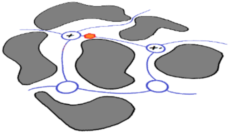
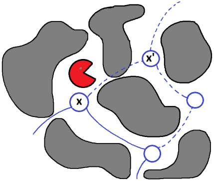


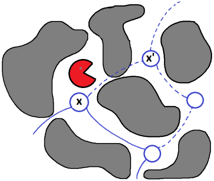
HCTRW is a formalism for studying diffusion in heterogeneous structures (1),(2).

Analytical results for HCTRW model



HCTRW on a graph:
1. graph with transition matrix Q,
2. travel times $\psi_{xx'}(t)$ between nodes x, x'

Analytical results for HCTRW model



HCTRW on a graph:

1. graph with transition matrix Q,
2. travel times $\psi_{xx'}(t)$ between nodes x, x'

Analytic formula for HCTRW propagator $\tilde{P}_{x_0 x}(s)$:

$$\boxed{\tilde{P}_{x_0 x}(s) = \frac{1 - \sum_{x'} \tilde{Q}(s)_{xx'}}{s} [(I - \tilde{Q}(s))^{-1}]_{x_0 x}}, \qquad (1)$$

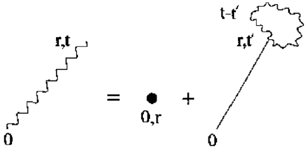
where $\tilde{Q}_{xx'}(s) = Q_{xx'} \tilde{\psi}_{xx'}(s)$.

Long-time behaviour for HCTRW propagator $P_{x_0 x}(t)$:

$$\boxed{\tilde{P}_{x_0 x}(s) \simeq \underbrace{p_{st}(x)}_{stat.dist.} + t(x) \sum_{k>0} \frac{u_{0k}^{\dagger}(x)\, v_{0k}(x_0)}{\lambda_{0k} + s\lambda_{1k}}} \qquad (2)$$

λ_{0k} are eigenvalues, u_{0k}, v_{0k} eigenvectors of $I - Q$.
$\lambda_{0k} + s\lambda_{1k}$ is the 1^{st} order correction for $I - Q + sT$,
$T_{xx'} = Q_{xx'} \langle \mathcal{T}_{xx'} \rangle$, $t(x) = \sum_{x'} T_{xx'}$.

First passage time



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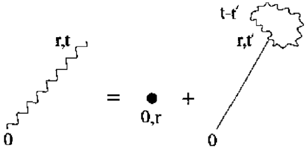
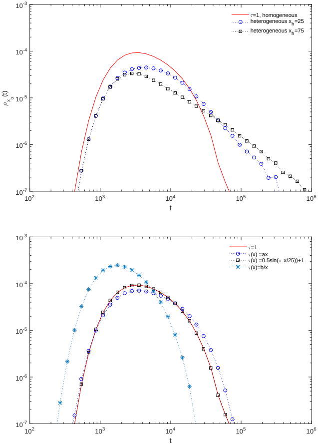


$F(x,t)$ - first passage time probability, then using renewal approach, [Redner, 2002]:
$P(x,t) = \delta_{x,0}\delta_{t_0} + \sum_{t' \neq t} F(r,t')P(0,t-t')$

Results for Heterogeneous random walks



The FPT density of HCTRW on an interval, absorbing $x = 100$: (top) hetero-nodes $x_h = 25, 75$ with heavy-t.distr. $\alpha = 0.5$; (bottom) $\tau_{\pm} = 1$; $\tau_{xx\pm\mathbf{1}} = ax$; $\tau_{xx\pm\mathbf{1}} = 0.5\sin(\pi x/25) + 1$; $\tau_{xx\pm\mathbf{1}} = b/x$.

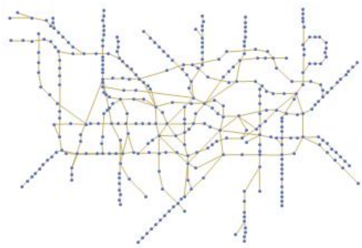
Analytic formula for HCTRW propagator $P_{x_{\mathbf{0}}x}(t)$ on a graph is derived.

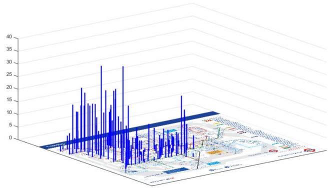
Analytic framework of HCTRW links structural graph properties and dynamical RW properties

HCTRW framework allows of study asymptotic solutions, FPT for processes on graphs.

- Grebenkov, Tupikina, "Heterogeneous continuous time random walks", PRE 012148 (2018)

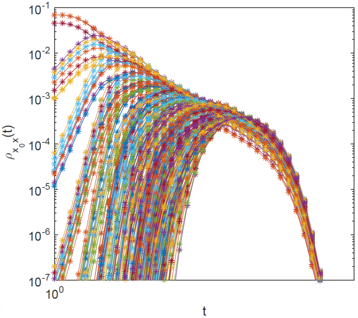
Applications: HCTRW model



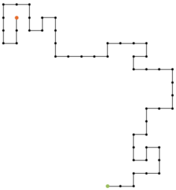


Londontub

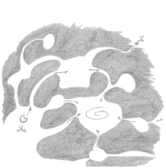
First passage time distributions $\rho_{x_0x}(t)$ for a graph of London metro. Dependence on the initial node x_0.



What we will talk about?



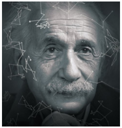
- **Part 1:**
  Random walk theory

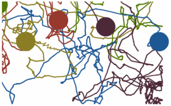


- **Part 2:**:
  Applications of random walk theory

Random walks applications: diffusion

Physics view:
In 1905 the paper "About particles suspended in the liquid(...)" appeared. Molecular motion was suggested the explanation.





INVESTIGATIONS ON THE THEORY OF ,THE BROWNIAN MOVEMENT

BY

ALBERT EINSTEIN, PH.D.

EDITED WITH NOTES BY

R. FÜRTH

TRANSLATED BY

A. D. COWPER

WITH 3 DIAGRAMS

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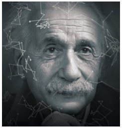
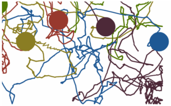
Manufactured in the United'States of America.

Random walks applications: diffusion

Physics view:
In 1905 the paper "About particles suspended in the liquid(...)" appeared. Molecular motion was suggested the explanation.
Diffusion equations:
$\frac{dT}{dt} = D\frac{d^2T}{dx^2} \rightarrow D(x,t)\frac{d^2T}{dx^2}$





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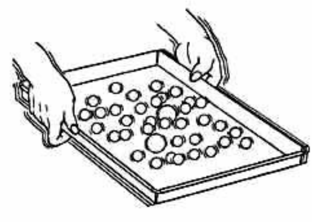
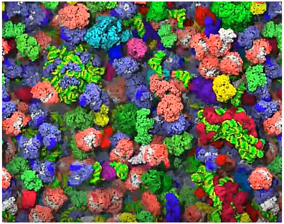
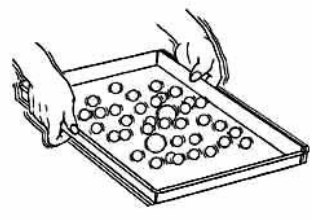
Applications of random walk theory

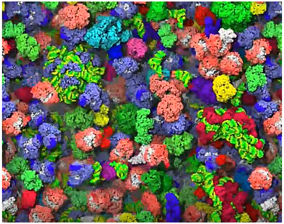




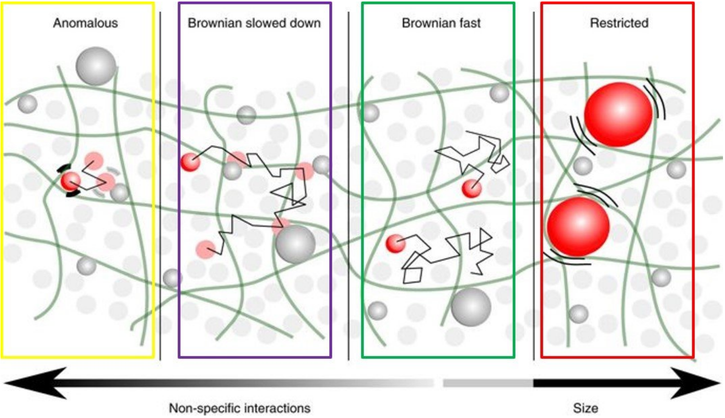
Applications of the random walks theory:

Applications of random walk theory

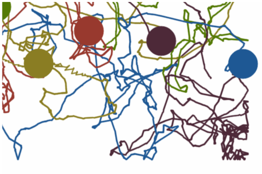


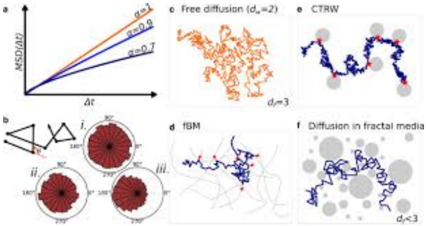


Applications of the random walks theory:
simulations of the crowded cell environment [McGuffee, Elcock, 2010] (video)
estimation of the properties for biological cells (first passage times distribution for the medical substance, etc.) [Klafter, Sokolov, 2010], [Metzler, Chechkin et al.]


Anomalous
Brownian slowed down
Brownian fast
Restricted
Non-specific interactions
Size

Applications of random walk theory

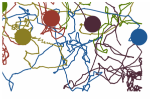


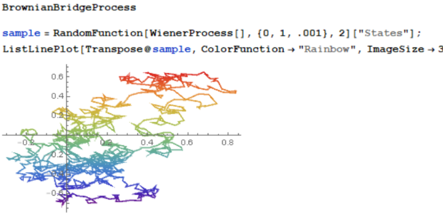


Modelling of the intracellular environment (R.Metzler, A.Cherstvyj, D.Grebenkov, A.Chechkin)

Random walks: What did we learn?

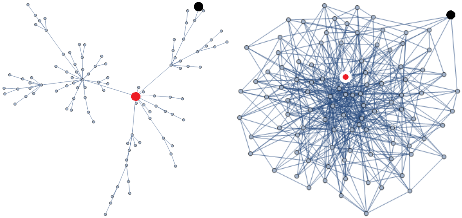
How to analyze motion inside the heterogeneous media? What is the full distribution of the first passage time probability?





Various open problems

Looking forward to tutorial from Alexandre



Applications of random walk theory

What happens if we violate the assumptions?

1. Random walk in $R \rightarrow$ in dimension R^N
2. Memoryless $\rightarrow$ with memory: random walk remembers what he did last step
3. Non-Symmetry: random walk jumps to the left of right with different probabilities
4. New one??

Fractal trajectories of random walk in $2D$

Applications of random walk theory

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Fractal trajectories of random walk in $2D$

"Thank you for your attention"-slide

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Programs and articles on random walks, flow networks:
https://liubovkmatematike.wordpress.com
https://scied.network

Some references

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