

# Spreading processes on networks

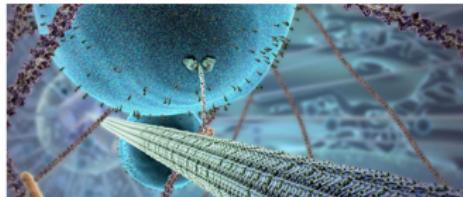
Liubov Tupikina, Marc Santolini

CRI, Bell labs  
**Big data course**

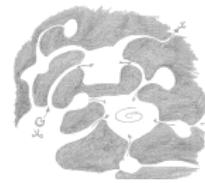
November 27, 2019



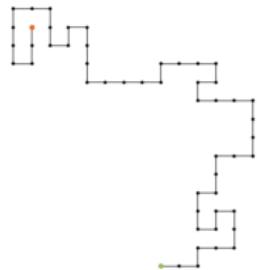
# Spreading processes in nature



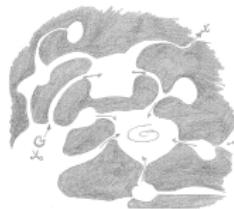
Transport of macromolecules, organelles and vesicles in living cells is a very complicated process that essentially determines and controls many biochemical reactions, growth and functioning of cells.



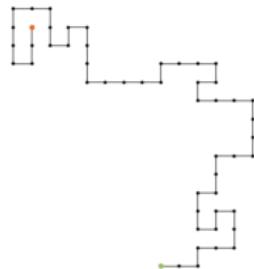
# What we will talk about?



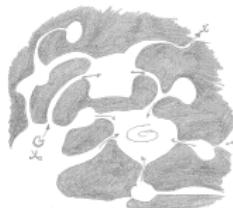
► **Part 1:**  
Spreading processes and diffusion



# What we will talk about?

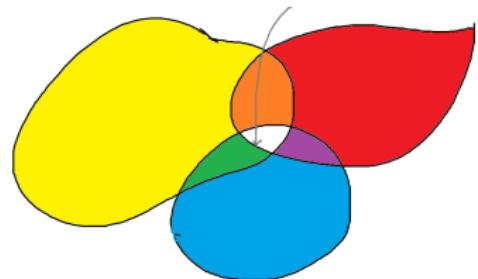


- ▶ **Part 1:**  
Spreading processes and diffusion



- ▶ **Part 2:**  
Spreading processes on networks

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

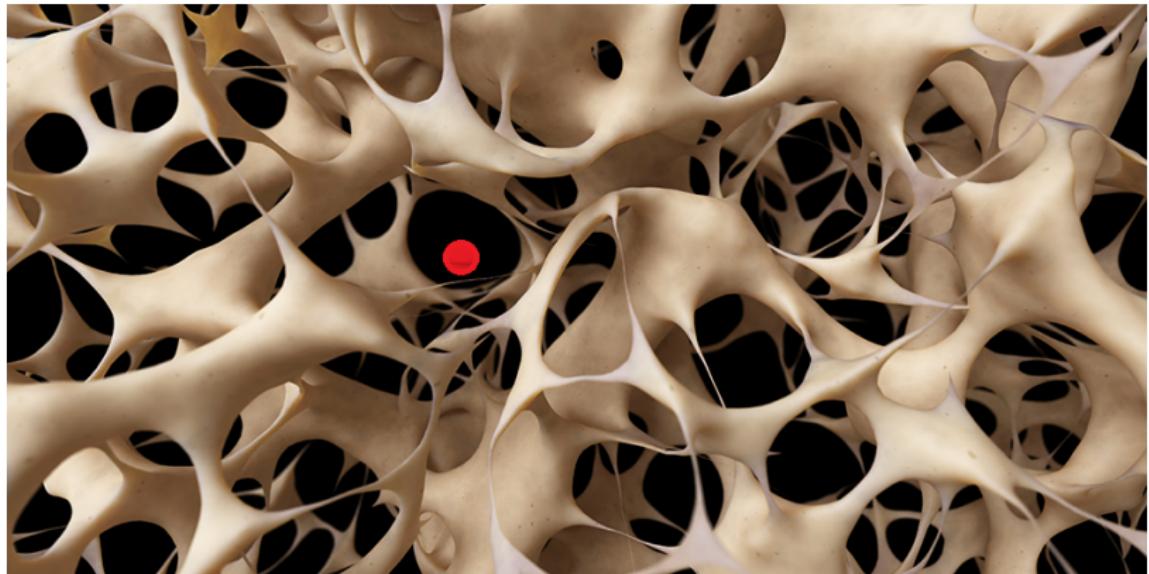


Intersection of Markov chain theory, Stochastic processes, Statistical physics, Disordered systems, Probability theory...

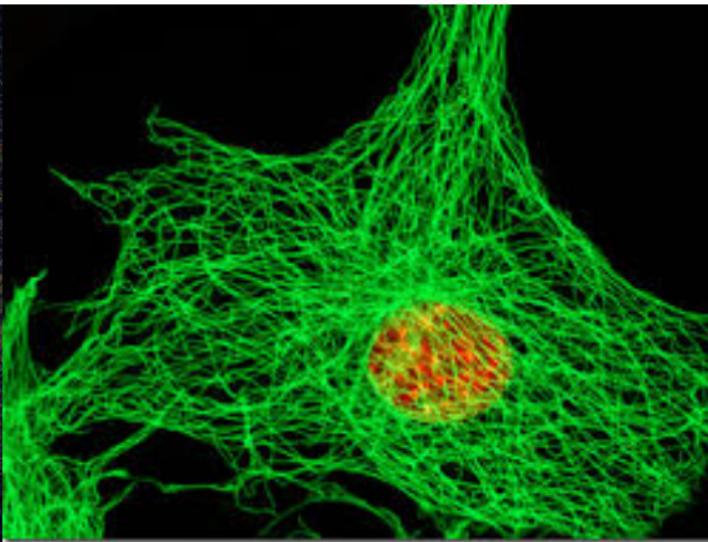
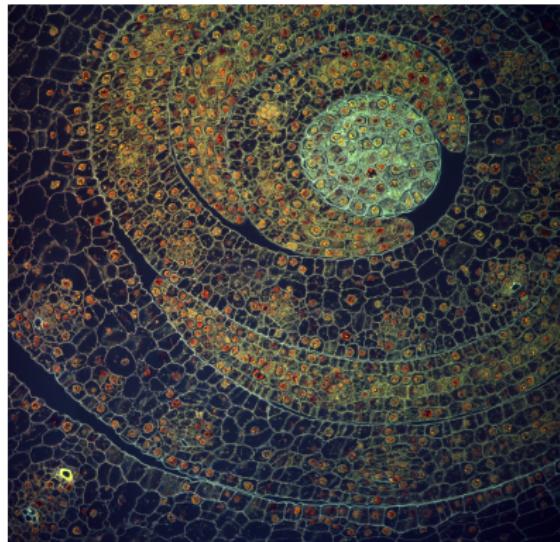
## Real-world examples



## Real-world examples



## Real-world examples



E.Katrukha, microtubules, imaginarycellrepresentation



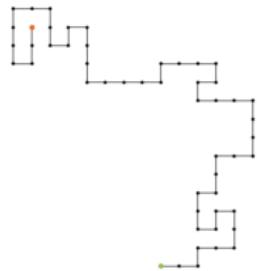
[networkrepository/openflights](https://networkrepository.com/openflights/)



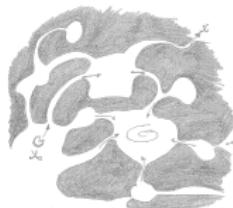


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# Part 1



- ▶ Spreading processes and diffusion history
- random walks
- diffusion models

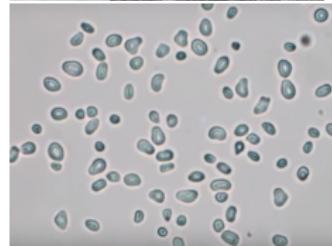


# Spreading processes and diffusion: history

## 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.



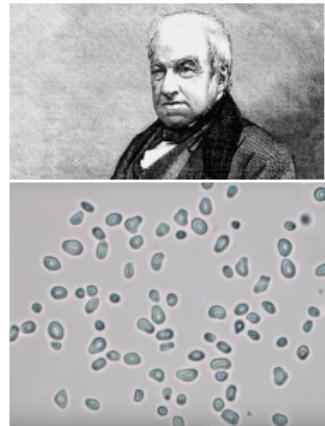
# Spreading processes and diffusion: history

## Experiment:

Brownian motion was discovered in 1785 by Jan Ingenhousz: irregular motion of coal dust particles on the surface.

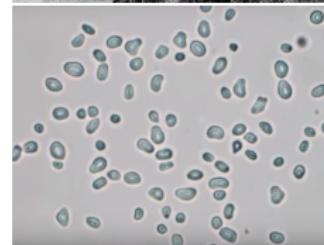
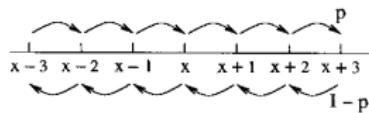
In 1827 Robert Brown, a British botanist, is observing a suspended pollen grain in water.  
(video)

How to explain the experiment?



# Random walks: How to explain the experiment?

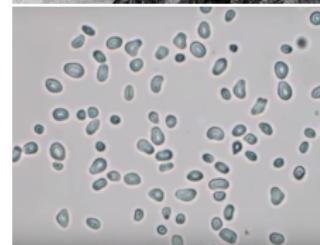
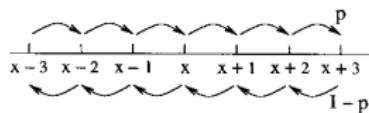
## Assumptions:



## Random walks: How to explain the experiment?

### Assumptions:

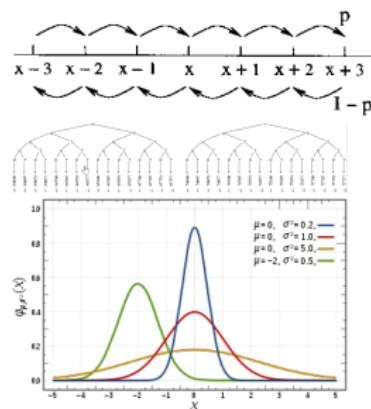
1. Random walk in 1 dimension
2. Memoryless: random walk forgets what he did last step
3. Symmetry: walk to the left of right with equal probability



## Diffusion: 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 or right with equal probabilities  $p, q$

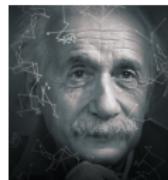


## Examples of diffusion

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

Diffusion equations:

$$\frac{dT}{dt} = D \frac{d^2 T}{dx^2} \rightarrow D(x, t) \frac{d^2 T}{dx^2}$$



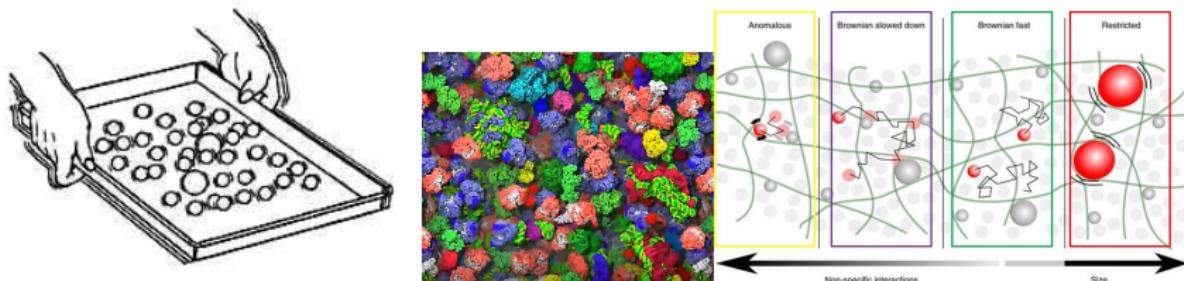
INVESTIGATIONS ON  
THE THEORY OF THE  
BROWNIAN MOVEMENT  
BY  
ALBERT EINSTEIN, PH.D.

This new Dover edition, first published in 1956, is an unabridged and unaltered reprint of the translation first published in 1926. It is published through special arrangement with Methuen and Co., London, and with the estate of Albert Einstein.

Manufactured in the United States  
of America.

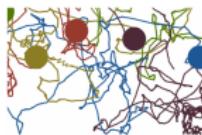
EDITED WITH NOTES BY  
R. FÜRTH  
TRANSLATED BY  
A. D. COWPER

WITH 3 DIAGRAMS

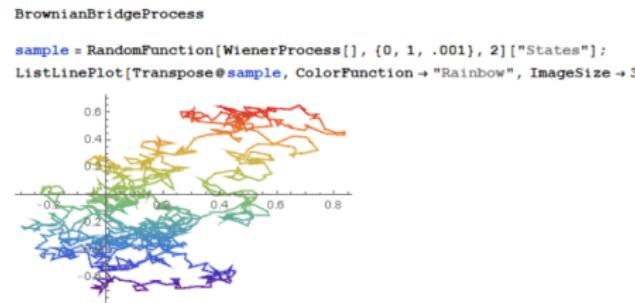


- Simulations of the crowded cell environment [McGuffee, Elcock, 2010] (video)
- Estimation of the properties for biological cells (first passage times distribution for the medical substance, etc.) [Klafter, Sokolov, 2010]

## Numerical simulations



One can validate your hypothesis using numerical simulations.



Wolfram Mathematica random walks

## Random walks properties

**Probability density**  $P(x, t)$  is probability that we will find random walk in  $x$  at time  $t$

**First-passage time**  $F(x, t)$  is probability that at time  $t$  random walk is at  $x$  for the first time  
[Metzler et al., Redner, 2002]

Network measures based on random walks

Check reversed classroom topics (something, which is NOT in wikipedia)



## Random walks: discrete space and time

**Master equation** describing probability

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

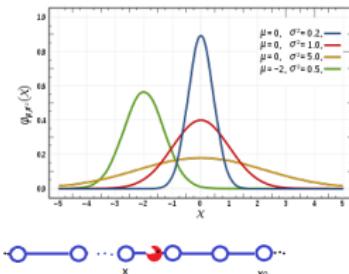
using the generating function and Fourier transformation

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

$$\text{We get } P(k, z) = 1 / (1 - z(pe^{ik} + qe^{-ik}))$$

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

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

# Why do we need numerical simulations?

## Continuous time random walk in 1D

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

Probability that no event occurred till time  $t$ :

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

Probability that one event occurred till time  $t$ :

$$P^1(t) = \int_t^\infty \psi(t')p(0, t - t')dt'$$

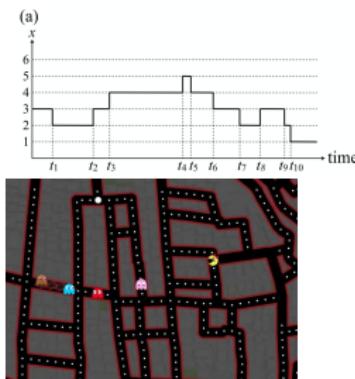
Apply trick to time:  $t \rightarrow s$

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

...

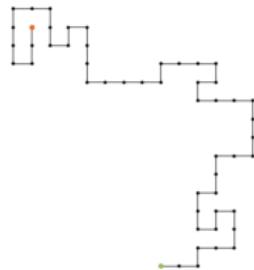
Probability that  $n$  events occurred till time  $t$ :

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



[N.Masuda et al.  
2017]

# What we will talk about?



- ▶ **Part 1:**  
Spreading processes



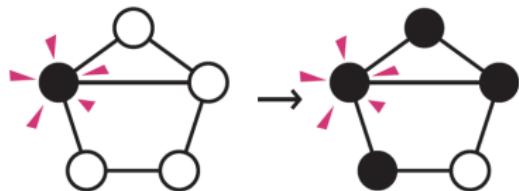
- ▶ **Part 2::**  
Spreading processes on networks

# Where can we find spreading processes?

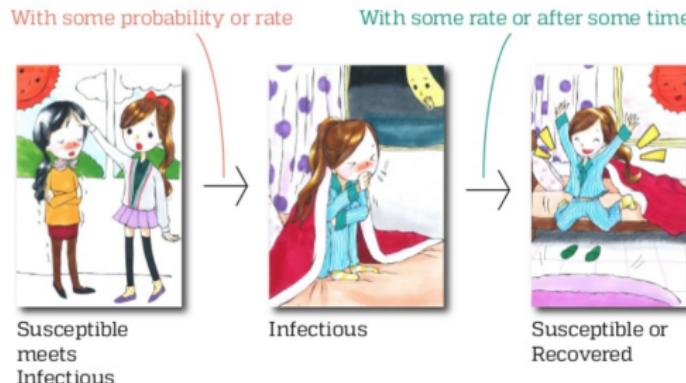
# Spreading everywhere



P.Holme petterhol.me



P.Holme, LT, NJP (2018)



P.Holme [petterhol.me](http://petterhol.me)

**Nodes states:** S (susceptible),  
I (infected),  
R (recovered)

**Types of models:** SI (viral spreading), SIS, SIR model [see notebook](#)

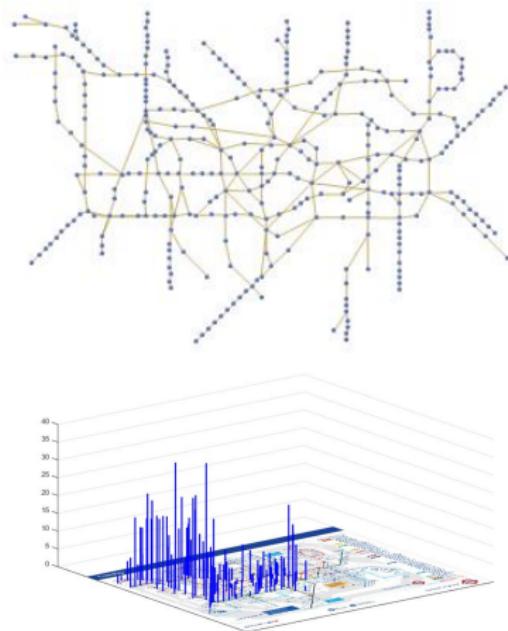


$$\frac{dS}{dt} = -\frac{\beta IS}{N},$$

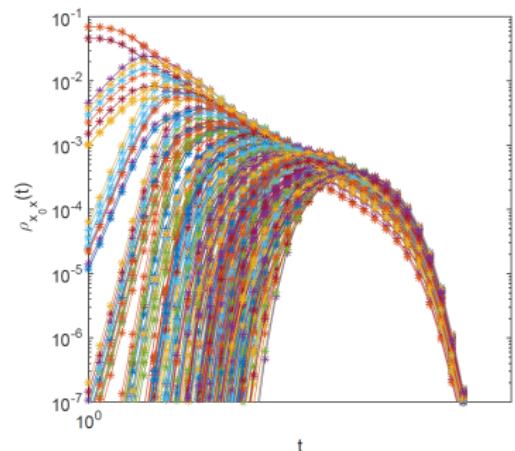
$$\frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I,$$

$$\frac{dR}{dt} = \gamma I.$$

## Applications: spreading on networks



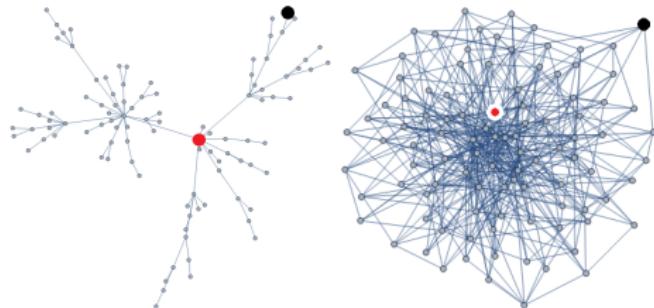
Random walks properties  $\rho_{x_0 x}(t)$   
on a network of London metro.  
Topics for your network projects



- PageRank and other network measures
- Community detection algorithms
- Spreading processes on networks

## Hands-on part

Looking at notebooks



For notebooks go to:

<https://github.com/Big-data-course-CRI/>

Slide after all the maths

You did it!

Programs and articles on random walks, networks:  
<https://github.com/Big-data-course-CRI/>

## Appendix: 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 or right with different probabilities
4. New one??

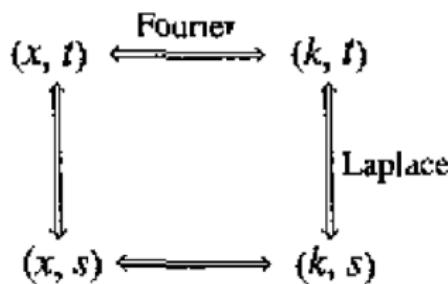


Fractal trajectories of random walk in  $2D$

## Main trick

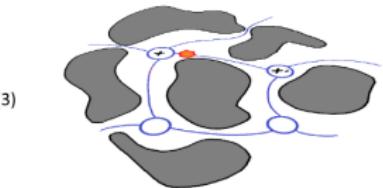
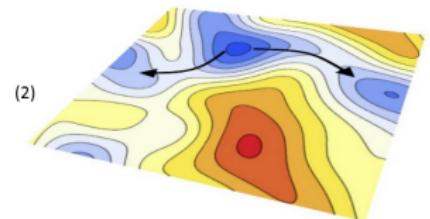
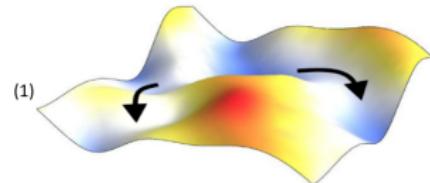
$$P(x, t) = \frac{e^{-(x-vt)^2/4Dt}}{\sqrt{4\pi Dt}}$$

$$P(k, t) = e^{-(ikv + Dk^2 t)}$$



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

$$P(k, s) = \frac{1}{s + ikv + Dk^2}$$

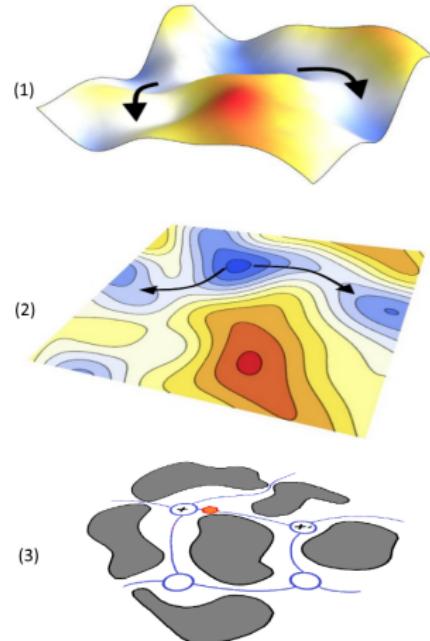


## Heterogeneous Continuous Time Random Walk model on a graph:

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

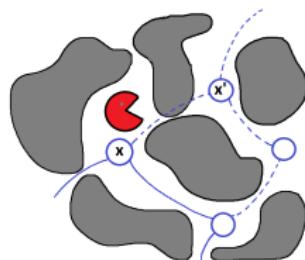
The generalized transition matrix

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



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

## Analytical results for HCTRW model



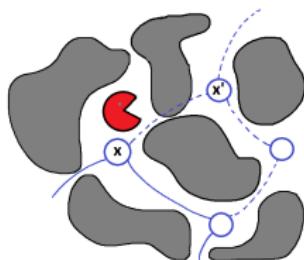
**HCTRW** on a  
graph:

1. graph with  
transition **matrix  $Q$** ,

2. travel times

$\psi_{xx'}(t)$  between  
nodes  $x, x'$

## Analytical results for HCTRW model

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

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

where  $\tilde{Q}_{xx'}(s) = Q_{xx'} \tilde{\psi}_{xx'}(s)$ .Long-time behaviour for HCTRW propagator  $P_{x_0 x}(t)$ :**HCTRW** on a graph:

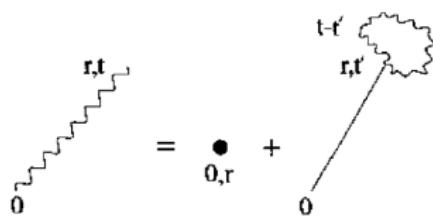
- graph with transition matrix  $Q$ ,
- travel times

$\psi_{xx'}(t)$  between nodes  $x, x'$

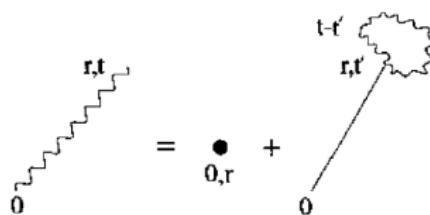
$$\tilde{P}_{x_0 x}(s) \simeq \underbrace{p_{st}(x)}_{\text{stat. dist.}} + t(x) \sum_{k>0} \frac{u_{0k}^\dagger(x) v_{0k}(x_0)}{\lambda_{0k} + s \lambda_{1k}} \quad (2)$$

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

## First passage time



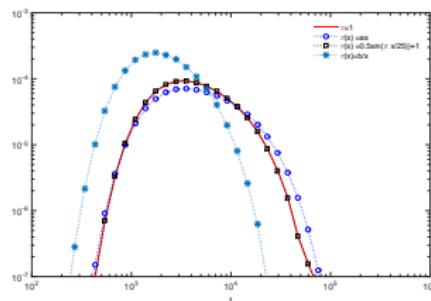
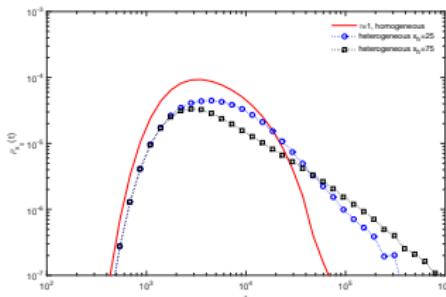
## First passage time



$F(x, t)$  - 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)  $\tau_{\pm} = 1$ ;  $\tau_{xx \pm 1} = ax$ ;  
 $\tau_{xx \pm 1} = 0.5 \sin(\pi x/25) + 1$ ;  $\tau_{xx \pm 1} = b/x$ .

## Analytic formula for HCTRW

propagator  $P_{x_0 x}(t)$  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)

## 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

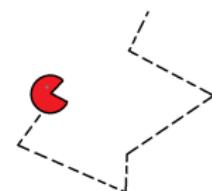
Will we get Gaussian for any hopping process, where  $\langle x^2 \rangle$  is finite?

Yes! Probability distribution is independent from details of single-step hopping [Gnedenko, Kolmogorov 1954]



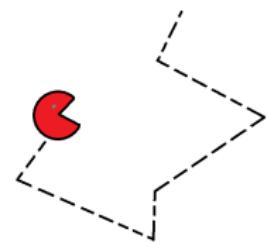
## Types of random walks

- Continuous or discrete (networks) underlying system [Redner, 2002]
- Discrete or continuous time [Montroll, Weiss, 1965]
- Probability distributions of jumps from each node [Hedges, 2002]
- Random walks with resetting, self-avoiding random walk, adaptive random walks... [Masuda, Lambiotte 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  $\tau$   
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**

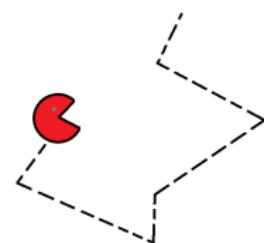
(CTRW)  $P(x, t)$  is probability to find RW at  $x$  coordinate at time  $t$ .

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**  
we get **the final equation**

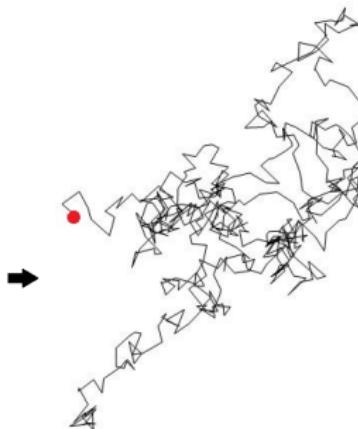
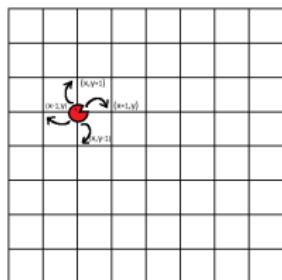
$$P(k, s) = \frac{1 - \tilde{\psi}(s)}{s} \frac{1}{1 - f(k)\tilde{\psi}(s)}$$



## Some references

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3. N. Molkenthin, K. Rehfeld V. Stolbova L. Tupikina and J. Kurths, "On the influence of spatial sampling on climate networks", *Nonlin. Processes Geophys.*, 21, 651-657 (2014)
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## Random walks on other systems



**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]



# Main Collaborators



*Nora Molkenthin,  
Jonathan Donges  
Cristóbal López,  
Emilio Hernández-García,  
Henk Dijkstra,  
Norbert Marwan, Jobst Heitzig,  
Jürgen Kurths, Petter Holme  
Denis Grebenkov*