# Spreading processes on networks

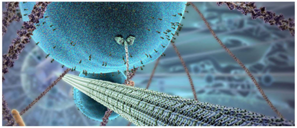
Liubov Tupikina, Marc Santolini

CRI, Bell labs

**Big data course**

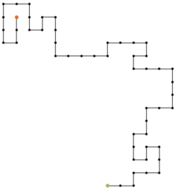
November 26, 2019

# Spreading processes in nature



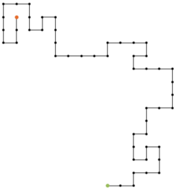
Transport of macromolecules, organelles and vesicles in living cells is a very complicated process that essentially determines and controls many biochemical reactions, growth and functioning of cells.

# What we will talk about?



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

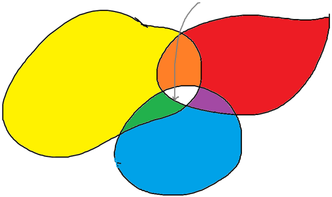
# What we will talk about?



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

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

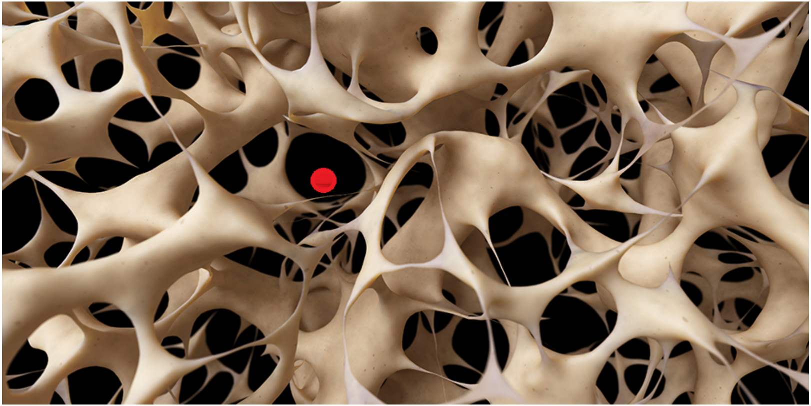
**Scientists working on random walk theory:**
Pearson, Smoluchowski, Langevin, Fermat, Bernoulli, Einstein, Kolmogorov, Pascal, Hughes, Brown, Wiener, Montroll, Weiss...



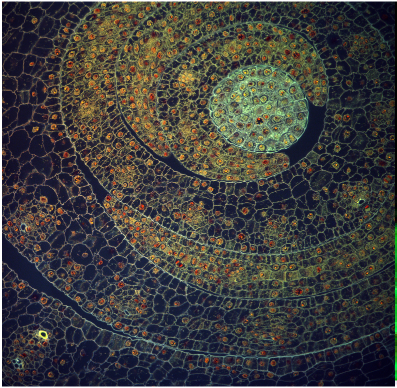
Intersection of Markov chain theory, Stochastic processes, Statistical physics, Disordered systems, Probability theory...

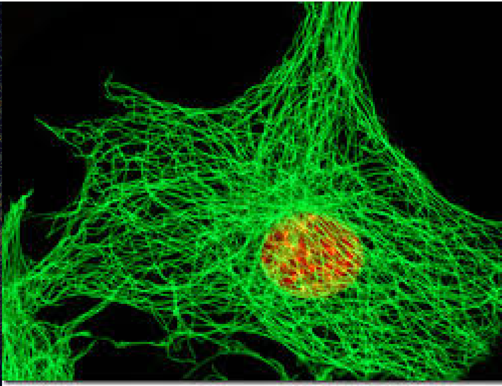
# Real-world examples

# Real-world examples



# Real-world examples



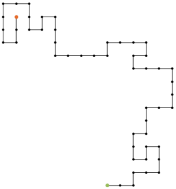


E.Katrukha,microtubules,imaginarycellrepresentation


networkrepository/openflights


©BabyRoutes.co.uk

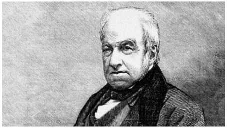
# Part 1

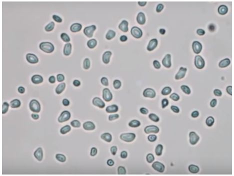


- **Spreading processes and diffusion**
  history
  random walks
  diffusion models

# Spreading processes and diffusion: history

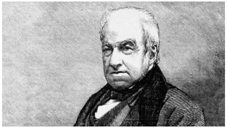
**Experiment:**
Brownian motion was discovered in 1785 by Jan Ingenhousz: irregular motion of coal dust particles on the surface.
In 1827 Robert Brown, a British botanist, is observing a suspended pollen grain in water.

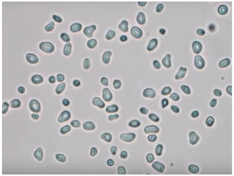




# Spreading processes and diffusion: history

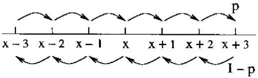
**Experiment:**
Brownian motion was discovered in 1785 by Jan Ingenhousz: irregular motion of coal dust particles on the surface.
In 1827 Robert Brown, a British botanist, is observing a suspended pollen grain in water. (video)
How to explain the experiment?

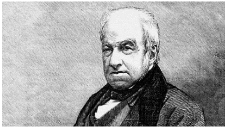


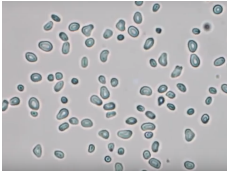


# Random walks: How to explain the experiment?

**Assumptions:**



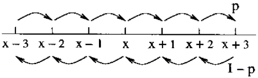



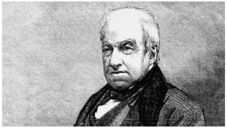


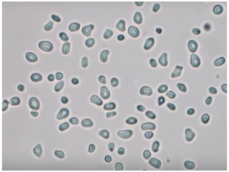
# Random walks: How to explain the experiment?

**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



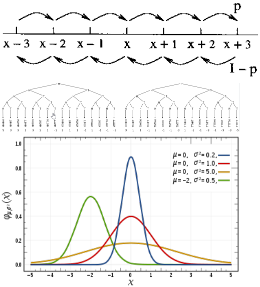





# Diffusion: building a model

**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 of right with equal probabilities $p, q$

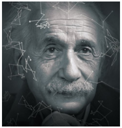


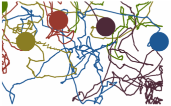
# Examples of diffusion

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

Diffusion equations:

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





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

Manufactured in the United States of America.

INVESTIGATIONS ON THE THEORY OF ,THE BROWNIAN MOVEMENT

BY

ALBERT EINSTEIN, PH.D.

EDITED WITH NOTES BY

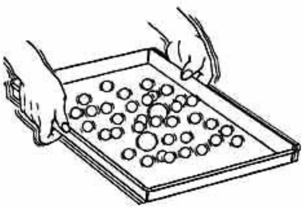
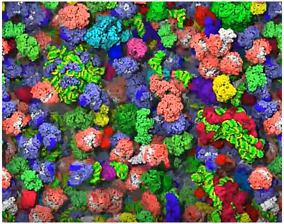
R. FÜRTH

TRANSLATED BY

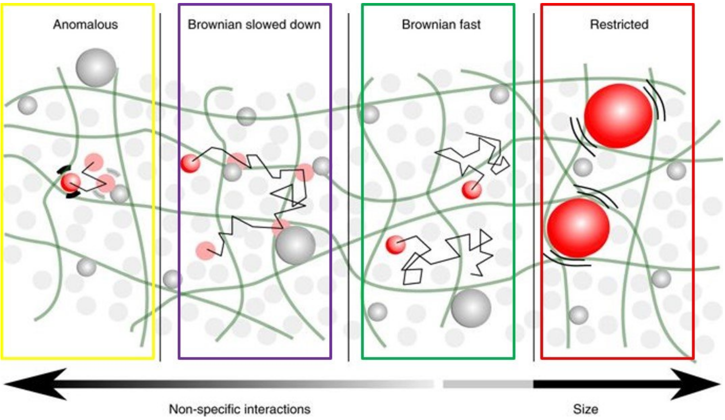
A. D. COWPER

WITH 3 DIAGRAMS

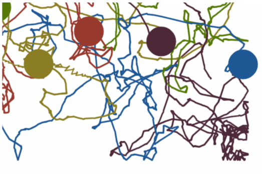
# Applications of diffusion theory

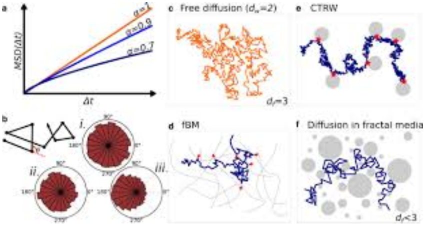



- Simulations of the crowded cell environment [McGuffee, Elcock, 2010] (video)
- Estimation of the properties for biological cells (first passage times distribution for the medical substance, etc.) [Klafter, Sokolov, 2010], [Metzler, Chechkin et al.]


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

# Applications of random walk theory

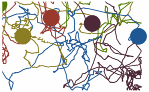





Modelling of the intracellular environment (R.Metzler, A.Cherstvyj, D.Grebenkov, A.Chechkin)

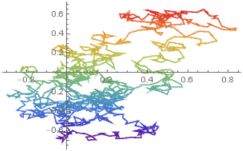
# Random walks: What did we learn?

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



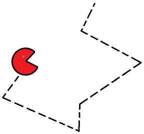
BrownianBridgeProcess

```
sample = RandomFunction[WienerProcess[], {0, 1, .001}, 2]["States"];
ListLinePlot[Transpose@sample, ColorFunction → "Rainbow", ImageSize → 3
```



# 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 [Hudges, 2002]
- Random walks with resetting, self-avoiding random walk, adaptive random walks... [Masuda, Lambiotte et al.2017]

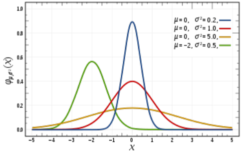


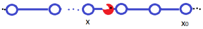
# Random walks properties

**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**
$P(k,z) = \sum_{n=0}^{\infty} z^n \sum_{x=-\infty}^{\infty} e^{ikx} P(x,n)$
We get $P(k,z) = 1/(1 - z(pe^{ik} + qe^{ik}))$
Then the final probability distribution for DTRW
$P(x,n) = \frac{N!}{(N+x)/2!(N-x)/2!} p^{(N+x)/2}(1-p)^{(N-x)/2}$



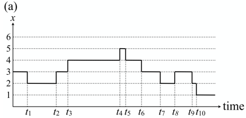




Gaussian in the long-time limit
$P(x,n) \rightarrow \frac{1}{\sqrt{2\pi npq}} e^{-(x-np)^2/2npq}$

# Random walks: discrete space, continuous time

**Continuous time random walk in 1D**

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




[N.Masuda et al. 2017]

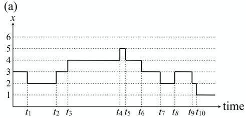
# Random walks: discrete space, continuous time

**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 $t$:

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




[N.Masuda et al. 2017]

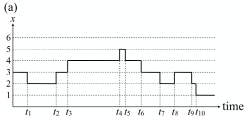
# Random walks: discrete space, continuous time

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




[N.Masuda et al. 2017]

# Random walks: discrete space, continuous time

**Continuous time random walk in 1D**

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

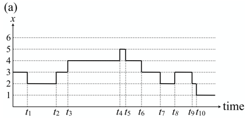
Probability that no event occurred till time $t$:
$P^0(t) = \int_t^\infty \psi(t')dt'$

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: $t \to s$

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

...




[N.Masuda et al. 2017]

# Random walks: discrete space, continuous time

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

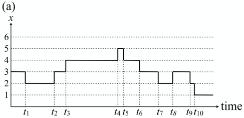
Probability that one event occurred till time $t$:
$P^1(t) = \int_t^\infty \psi(t')p(0, t - t')dt'$

Apply trick to time: $t \to s$

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

...

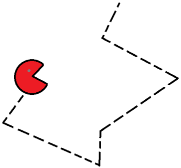
Probability that $n$ **events** occurred till time $t$:
$\tilde{P}^n(s) = \tilde{\psi}^n(s)\tilde{P}^{n-1}(s) = \tilde{\psi}^n(s)\frac{1-\tilde{\psi}(s)}{s}$




[N.Masuda et al. 2017]

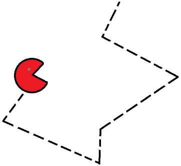
# Random walks: continuous space and time

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

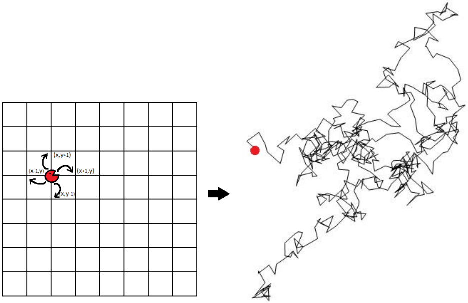


# Random walks: continuous space and time

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



# Generalization of random Walk framework



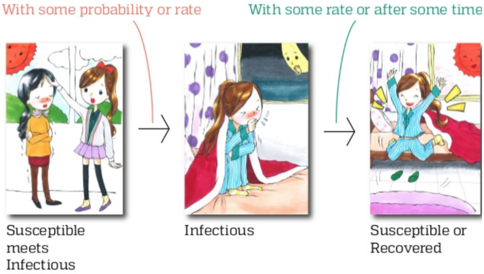

**Homogeneous random walk** (RW) on a discrete lattice in discrete time

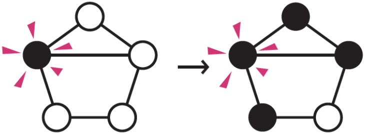
**Homogeneous continuous time random walk** (CTRW) in continuous space

R.Metzler, J.Klafter, Phys.Rep. [2000]


P.Holme petterhol.me

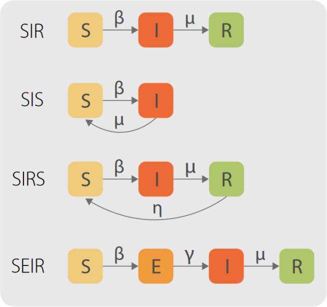

BUS
network



P.Holme, LT, NJP (2018)

SI (viral spreading see notebook), SIS, SIR model

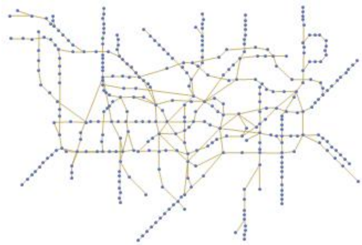


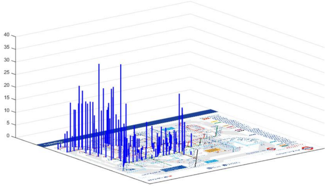

$$\frac{dS}{dt} = -\frac{\beta IS}{N},$$

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

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

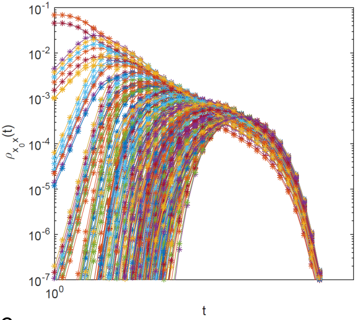
# Applications: random walks or spreading on networks



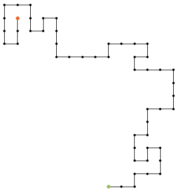



Londontube

Random walks properties $\rho_{x_0 x}(t)$ on a network of London metro. Dependence on the initial node $x_0$.



# What we will talk about?



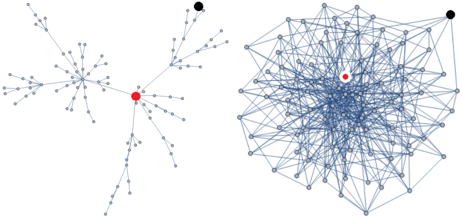
- **Part 1:**
  Spreading processes

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

- 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/`

# 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 $2D$

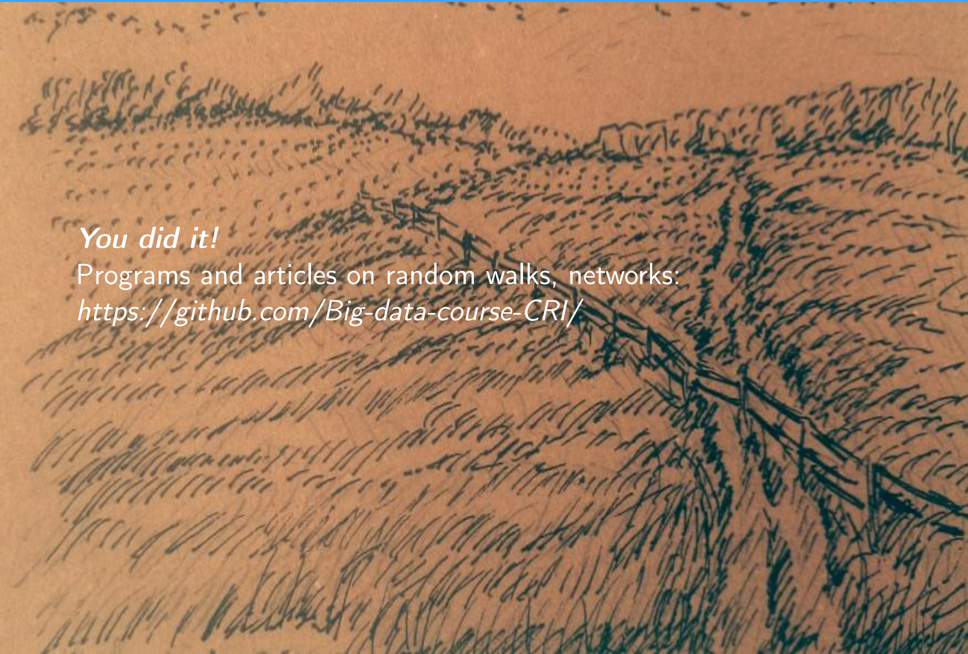
# Applications of random walk theory

**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 $2D$

# Slide after all the maths



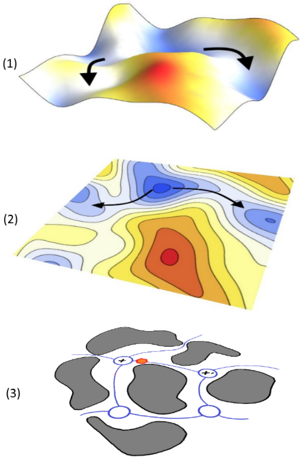
***You did it!***
Programs and articles on random walks, networks:
*https://github.com/Big-data-course-CRI/*

# Main trick

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

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

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


(1)
(2)
(3)

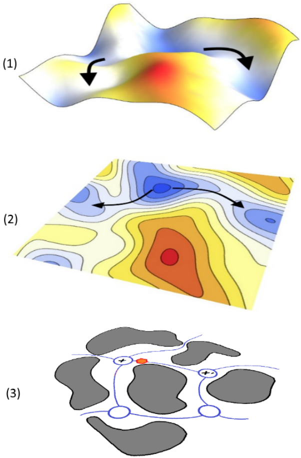
## Heterogeneous Continuous Time Random Walk model

on a graph:

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

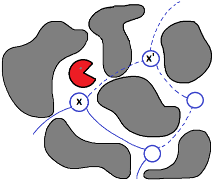
The generalized transition matrix

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




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

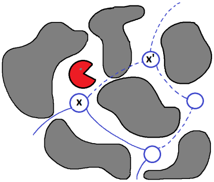
# Analytical results for HCTRW model




**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** $\tilde{P}_{x_0 x}(s)$:

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

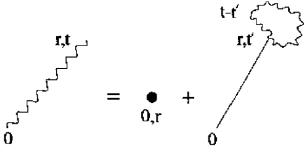
where $\tilde{Q}_{xx'}(s) = Q_{xx'} \tilde{\psi}_{xx'}(s)$.

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

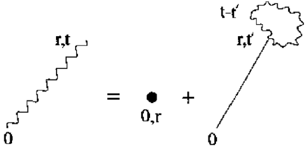
$$\boxed{\tilde{P}_{x_0 x}(s) \simeq \underbrace{p_{st}(x)}_{stat.dist.} + t(x) \sum_{k>0} \frac{u_{0k}^{\dagger}(x)\, v_{0k}(x_0)}{\lambda_{0k} + s\lambda_{1k}}} \qquad (2)$$

$\lambda_{0k}$ 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

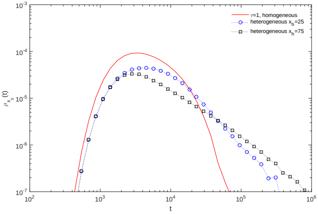


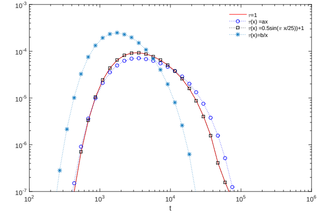
# First passage time




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

**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)

# 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]

# Some references

1. L. Tupikina, K. Rehfeld, N. Molkenthin, V. Stolbova, N. Marwan, and J. Kurths, ''Characterizing the evolution of climate networks'', Nonlin. Processes Geophys., 21, 705-711 (2014)
2. H. Bunina, L. Tupikina, ''Authomorphisms of the semigroup of nonnegative invertible matrices of order 2 over rings'', Journal of Mathematical Sciences, 183, 305-313 (2012)
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)
4. J.F. Donges, J. Heitzig, B. Beronov, M. Wiedermann, J. Runge, Q.-Y. Feng, L. Tupikina, V. Stolbova, R.V. Donner, N. Marwan, H.A. Dijkstra, and J. Kurths, ''Unified functional network and nonlinear time series analysis for complex systems science: The pyunicorn package'', Chaos 25, 113101-1-25 (2015)
5. L.Tupikina, N. Molkenthin, C.Lopez, E.Hernandez-Garca, N.Marwan and J.Kurths, ''Correlation networks from flows. The case of forced and time-dependent advection-diffusion dynamics'', Plos One, 0153703 (2016)
6. H.Kutza, N. Molkenthin, L. Tupikina, N.Marwan, J.Donges, U.Feudel, J. Kurths, R.Donner, ''A geometric perspective on spatially embedded networks. Quantification of edge anisotropy and application to flow networks'', Chaos 27, 035802 (2017)
7. **L.Tupikina**, ''Dynamics on networks: case of Heterogeneous opinion state model (on graphs)", arxiv 1708.01647
8. P.Holme, L.Tupikina "Explicit solutions for SIS model" arxiv.org 1802.08849
9. R.Donner, M.Lindner, N.Molkenthin, **L.Tupikina** "From nonlinear dynamics to complex systems: A Mathematical modeling approach" Springer book chapter, Cham, pp. 197-226 (2019)
10. D.Grebenkov, **L.Tupikina**, "Heterogeneous continuous time random walk" Phys. Rev. E 97, 012148 (2018)
11. **L.Tupikina**, D.Grebenkov "Continuous limits of Heterogeneous continuous time random walk", (in prep.)
12. M. Kang, **L. Tupikina**, G. Berthelot, C. Nicolaides, D. Grebenkov, B. Sapoval "Universality of resistor scale-free networks" (in prep.)
13. M.Stella, M.Porter, L.Tupikina, C. Cramer, "Multilayer network between science and education", Proceedings of NetSci (2018)

# Main Collaborators

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