Advanced Statistical Physics of Biological and Soft-Matter Systems

Summer Term 2020

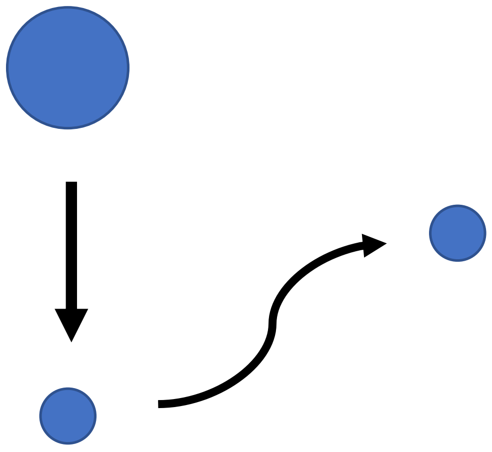
1. Physics of Evaporating and Diffusing Droplets, supervised by Prof. Roland Netz
2. Non-Ergodicity in 2D Diffusion Processes, supervised by Cihan Ayaz
3. Statistics of Gelation, supervised by Cihan Ayaz
4. Percolation Theory in Epidemics, supervised by Cihan Ayaz
5. The Statistical Mechanics of Self-Assembly, supervised by Cihan Ayaz
6. Oscillations in Chemical Systems, supervised by Maximilian Becker
7. Poisson-Boltzmann Modelling, supervised by Amanuel Wolde-Kidan
8. Evolutionary Game Theory, supervised by Shane Carlson
9. Barrier-Crossing Events, supervised by Florian Brünig
10. Random Networks, supervised Sina Zendehroud
11. Thermodynamics of small systems: Molecular Dynamics simulations of many-particle models, supervised by Philip Loche
12. Scale Invariance in Natural and Artificial Collective Systems, supervised by Laura Lavacchi
13. The Statistical Mechanics of Cell Migration, supervised by Bernhard Mitterwallner

Lifetime of virus-containing droplets diffusing and evaporating in air

Droplet radii produced by humans sneezing, coughing and speaking are between 1 and 500 μm . In fact, 95% of all droplets have radii below 50 μm, and most radii are around 5 μm.

A droplet with a radius of 5 μm released at an initial height of 2 meters stays suspended in air for 11 minutes before it falls to the ground, which is relevant for viral infection by aerosols.

Evaporation effects can be treated on the level of the diffusion equation in the stagnant approximation, i.e. neglecting the flow field around the droplet, and in the diffusion-limited evaporation regime. This approximation is accurate for droplet radii in the range 100 nm < R < 60 μm.



The time-dependent shrinking of the radius is given by

$$R(t) = R_0 \left(1 - t\frac{2D_w c_g v_w (1-RH)}{R_0^2}\right)^{1/2} = R_0(1 - \theta\, t(1-RH)/R_0^2)^{1/2} \quad .$$

Here R_0 is the initial droplet radius and the numerical prefactor is given by

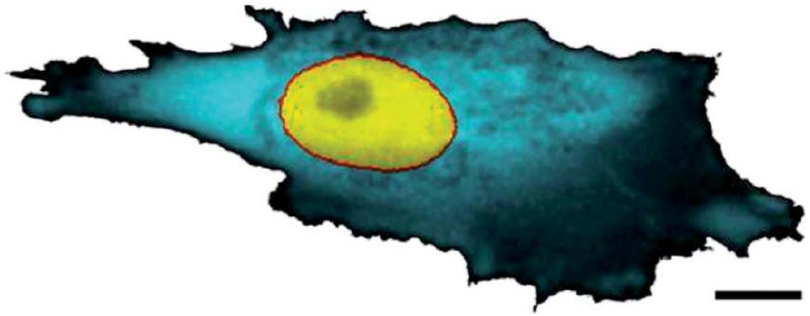
$$\theta = 2D_w c_g v_w = 1.1 \times 10^{-9} m^2/s \quad ,$$

where θ has units of a diffusion constant and the the water diffusion constant in air is D_w, the liquid water molecular volume is v_w and the saturated water vapor concentration is c_g

As a simple analysis shows, droplets smaller than R^{crit}= 67 μm will dry out before they hit the ground and shrink down to a radius that is predominantly determined by the solute content. Depending on the final size, they will be floating in air for an extended time. (R.R. Netz, preprint)

Non-Ergodicity in 2D Diffusion Processes

1. Ergodicity is an essential pillar in the application of Statistical Mechanics
2. Local diffusivity of proteins in bacterial cells shows non-ergodicity



3. In the article, the authors model viral transport via 2D model

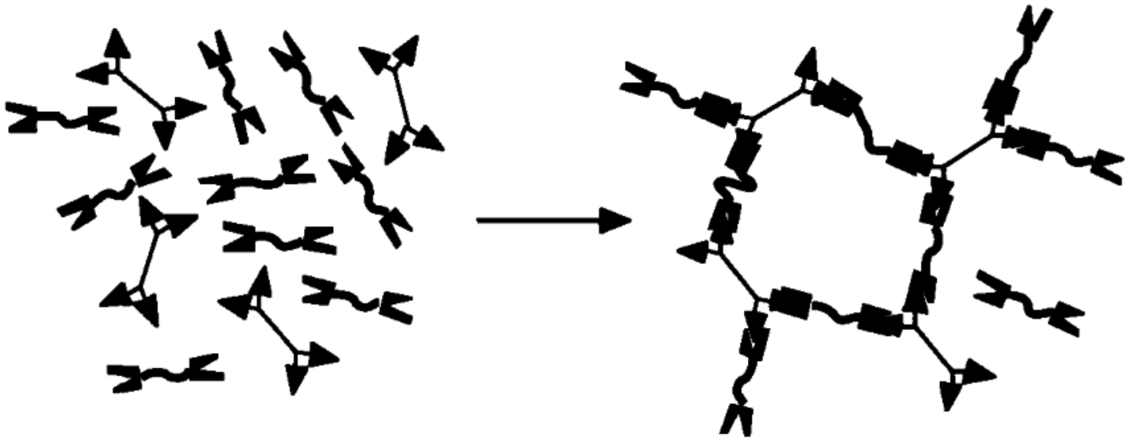
$$m\,\dot{\vec{v}}(t) = D(r)\overrightarrow{W}(t), \qquad \vec{v},\overrightarrow{W} \in \mathbb{R}^2$$

4. And they measure the EB (Ergodicity Breaking) parameter

Andrey G. Cherstvy, Aleksei V. Chechkin and Ralf Metzler, Soft Matter, 2014

The Statistical Mechanics of Gelation

1. A gel is a material composed of subunits that are able to bond with each other

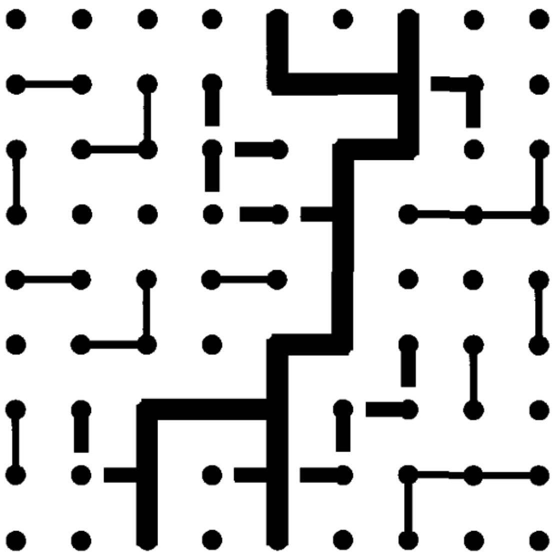


2. The statistical description of gel formation from a polymer system
3. Flory Stockmayer theory to estimate the gel point

Walter H Stockmayer, J. Chem. Phys., 1943

Percolation Theory in Epidemics

1. Model the percolation of a fluid through a random material

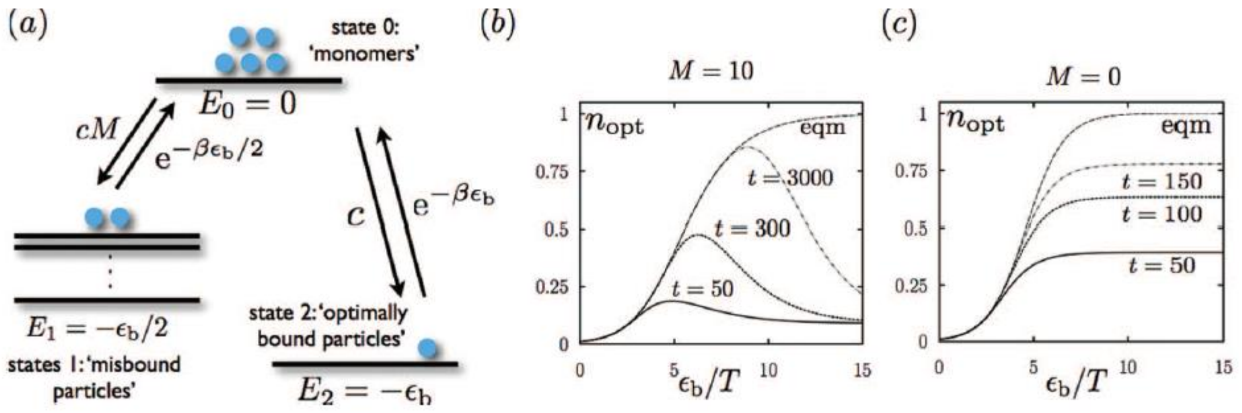


2. Estimate statistical quantities of the percolation process
3. Apply your result to the „percolation“ of a disease infecting a community

S. R. Broadbent and J. M. Hammersley, Mathematical Proceedings of the Cambridge Philosophical Society, 1957
S. Davis, P. Trapman, H. Leirs, M. Begon and J. A. P. Heesterbeek, Nature, 2008

The Statistical Mechnics of Self-Assemply

1. Self-assembly describes the dynamical processes in which components of a system organize themselves, without external direction, into ordered patterns or structures.



2. Estimate statistical properties of a toy model analytically.
3. Compare results to a simple simulation of a 2D lattice gas.

James Grant, Robert L. Jack, and Stephen Whitelam, J. Chem. Phys., 2011

Nonlinear Dynamics

Oscillations in Chemical Systems. II. Thorough Analysis of Temporal Oscillation in the Bromate–Cerium–Malonic Acid System

Richard J. Field, Endre Körös, and Richard M. Noyes*

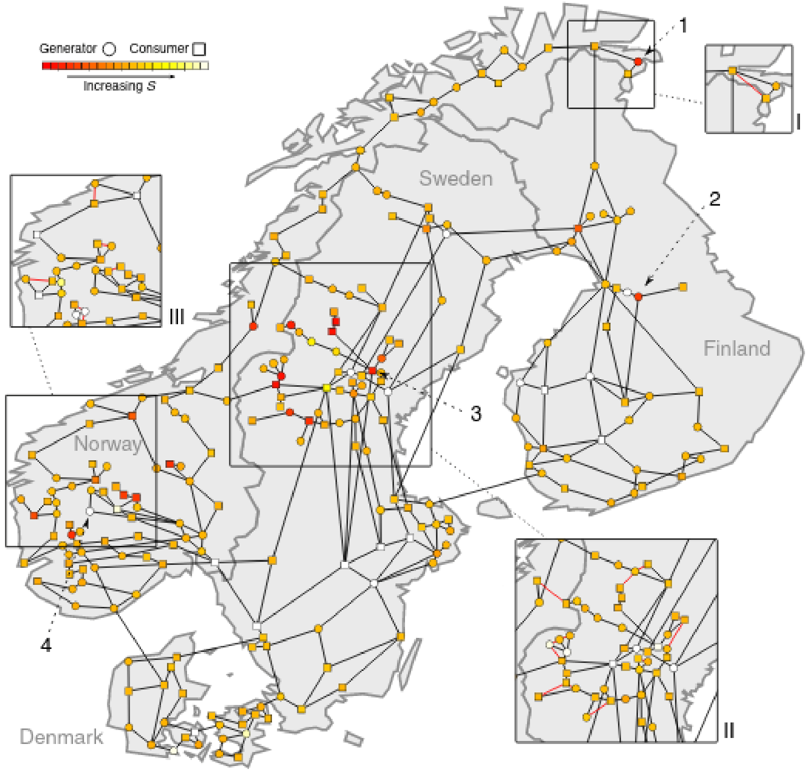
Contribution from the Department of Chemistry, University of Oregon, Eugene, Oregon 97403, the Institute of Inorganic and Analytical Chemistry, L. Eötvös University, Budapest, Hungary, and the Physical Chemistry Laborat Oxford University, Oxford, England. *Received April 3, 1972*

Received 2 Aug 2013 | Accepted 25 Apr 2014 | Published 9 Jun 2014

DOI: 10.1038/ncomms4969

How dead ends undermine power grid stability

Peter J. Menck[1,2], Jobst Heitzig[1], Jürgen Kurths[1,2,3] & Hans Joachim Schellnhuber[1,4]



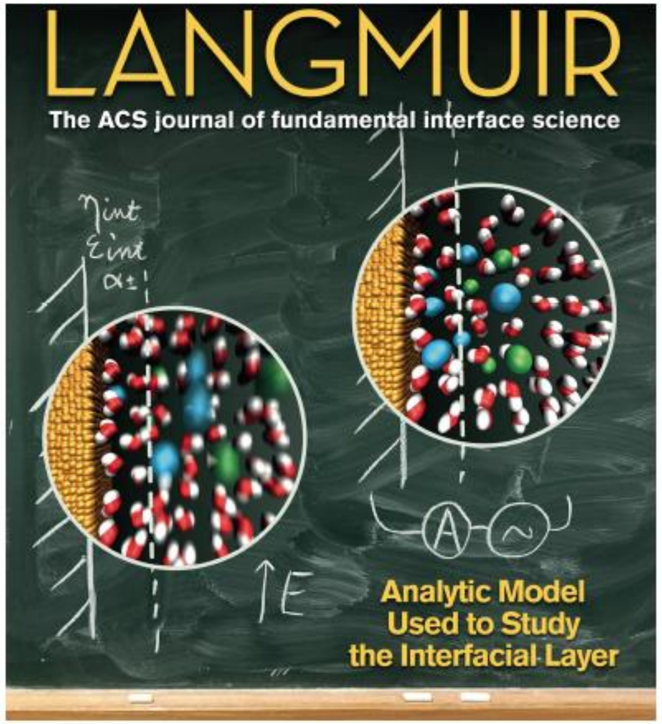
https://doi.org/10.1021/acs.langmuir.7b04171

Poisson-Boltzmann Modelling

Theory

Electrostatics: Poisson's Equation + Thermodynamics: Boltzmann Distribution

$$\Delta\varphi = -\frac{\rho}{\varepsilon\varepsilon_0} \qquad n = N_0 e^{-\beta E}$$

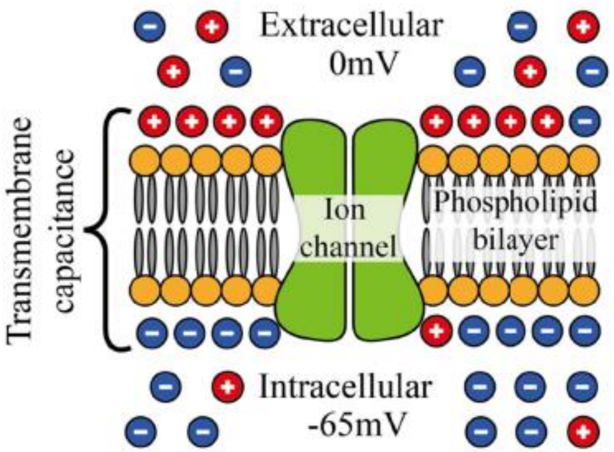


Applications

Capacitances

- ➢ Industrial Capacitors
- ➢ Carbon Nanotubes

Cellular Membranes



- ➢ Nerve Signaling
- ➢ Ion-Lipid Interactions

Evolutionary Game Theory

Game theory: models consist of agents interacting with different strategies. Gives insight into e.g.

- economies consisting of people and corporations
- ecosystems consisting of animals
- interactions among nations/governments

Classic example: Prisoner's dilemna

Evolutionary game theory: looks at adapting/learning of agents in repeated games. Keyword: evolutionarily stable strategy (ESS)

1. G. Szabo, C. Toke, "Evolutionary prisoner's dilemma game on a square lattice" *Physical Review E* **58** 1 (1998) 69
2. G. Szabo, G. Fath, "Evolutionary games on Graphs" *Physics Reports* **446** 4-6 (2007) 97
3. C.P. Roca, J. A. Cuest, A. Sanchez, "Evolutionary game theory: Temporal and spatial effects beyond replicator dynamics" *Physics of Life Reviews* **6** (2009) 208

"In its evolutionary form and especially when the interacting agents are linked in a specific social network the underlying solution concepts and methods [of game theory] are very similar to those applied in non-equilibrium statistical physics. [2]"

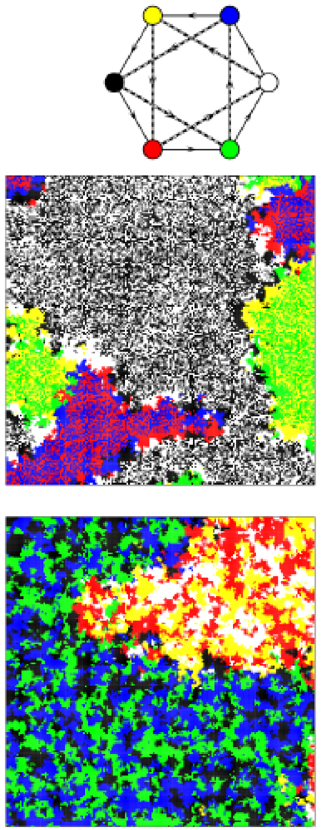
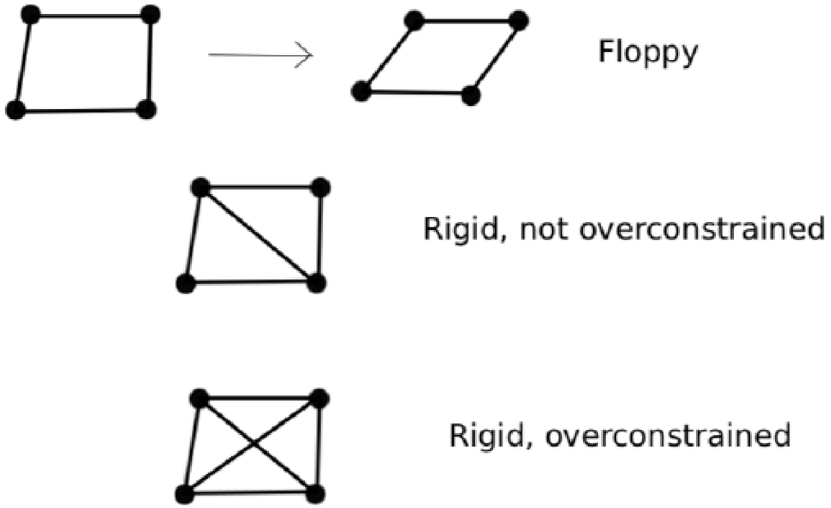
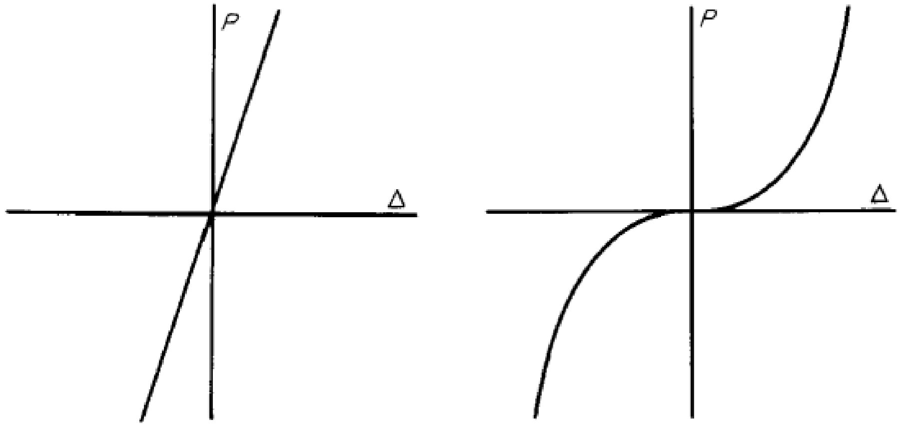


Figure: Snapshots of two different lattice simulations of a six-species predator-prey model defined by the food web above. [2]

Rigidity of Random Networks

- Structure consisting of *nodes* randomly connected by *edges*
- When is such a structure rigid?



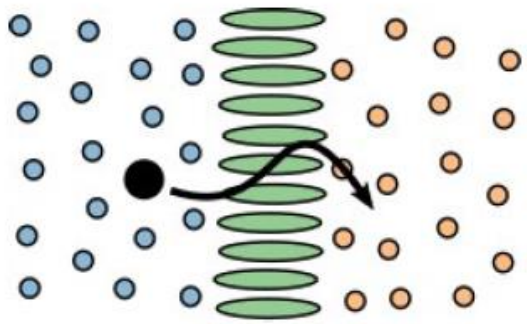


- *Rigid* and *floppy* modes
- Applications:
  - Structural engineering
  - Glasses
  - Soft matter (biomembranes, proteins, …)

Modelling of rare events / barrier-crossing rates

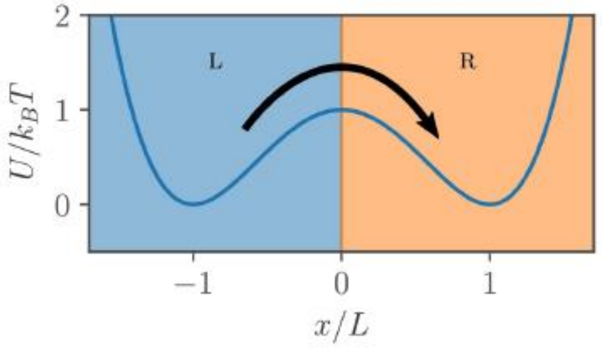
A fundamental question in biophysical applications (reactions, protein folding, diffusion processes):

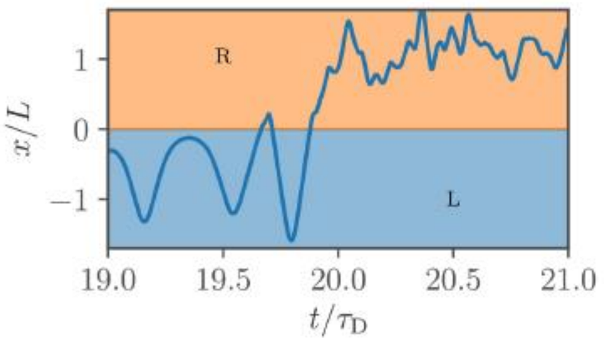
What is the mean barrier-crossing time?



Widely used model: Kramers' rate [1,2]

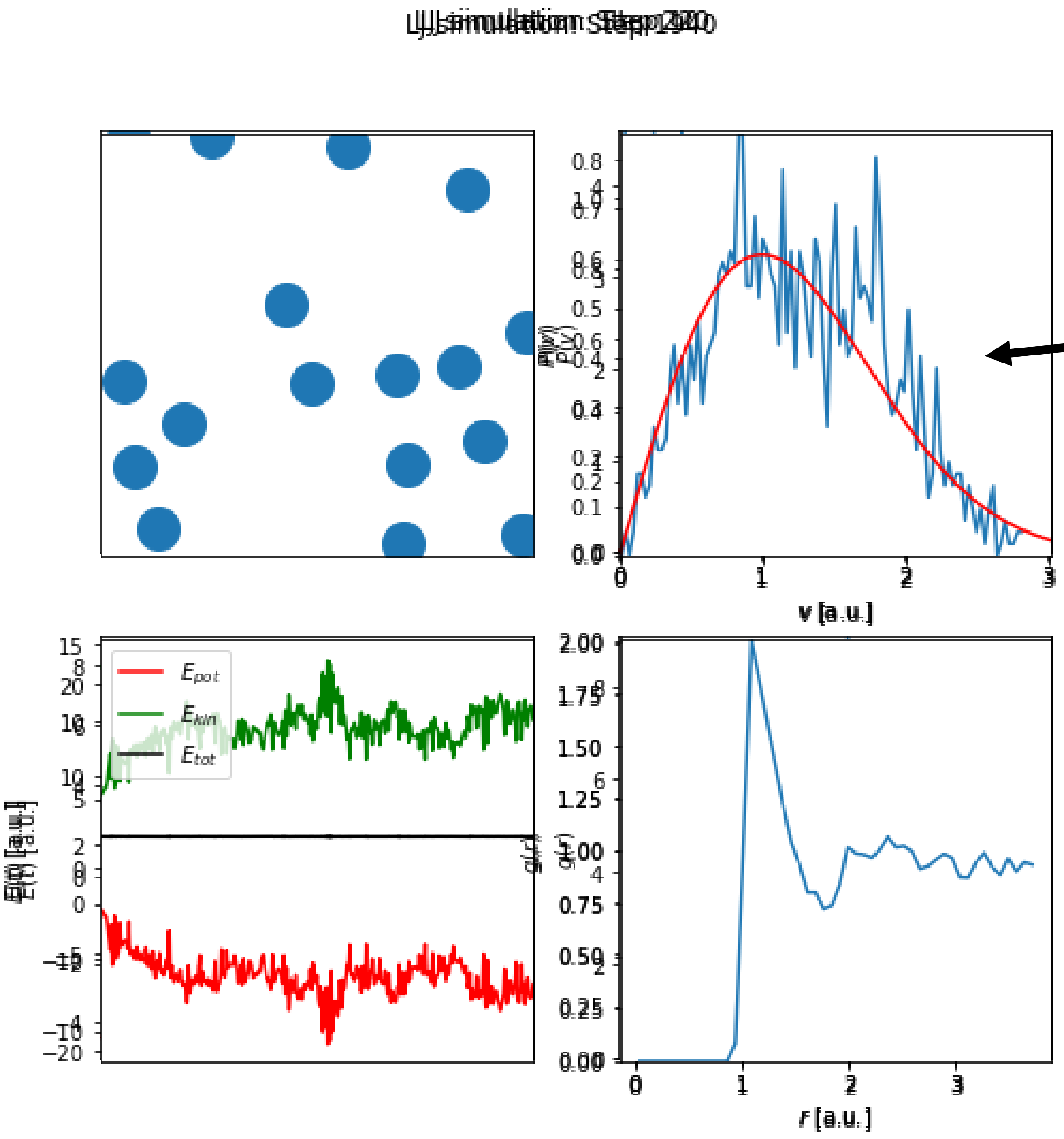
$$\tau_{\mathrm{Kr}} = \frac{2\pi\gamma}{\sqrt{U''_{\mathrm{max}} U''_{\mathrm{min}}}} e^{U_0/(k_B T)}$$



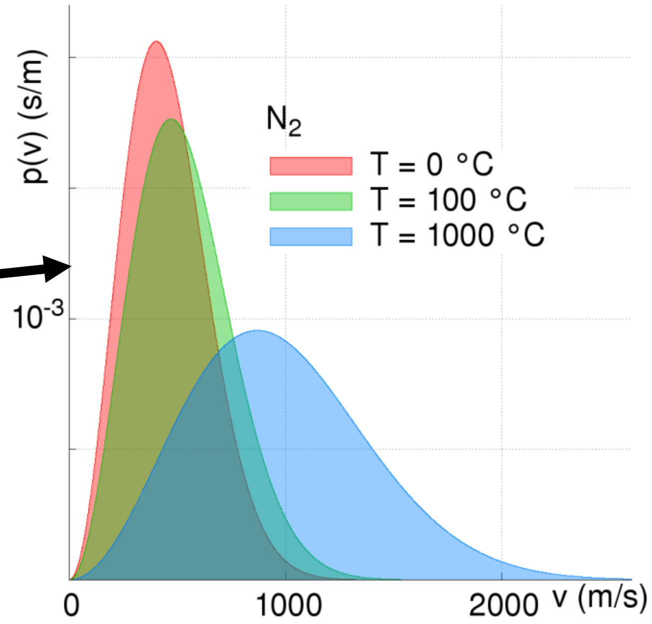


[1] Kramers, H. A. (1940). Physica, 7(4), 284–304.
[2] Zambelli, S. (2010). Archive for History of Exact Sciences, 64(4), 395–428.

Thermodynamics of small systems:
Molecular Dynamics simulations of many-particle models



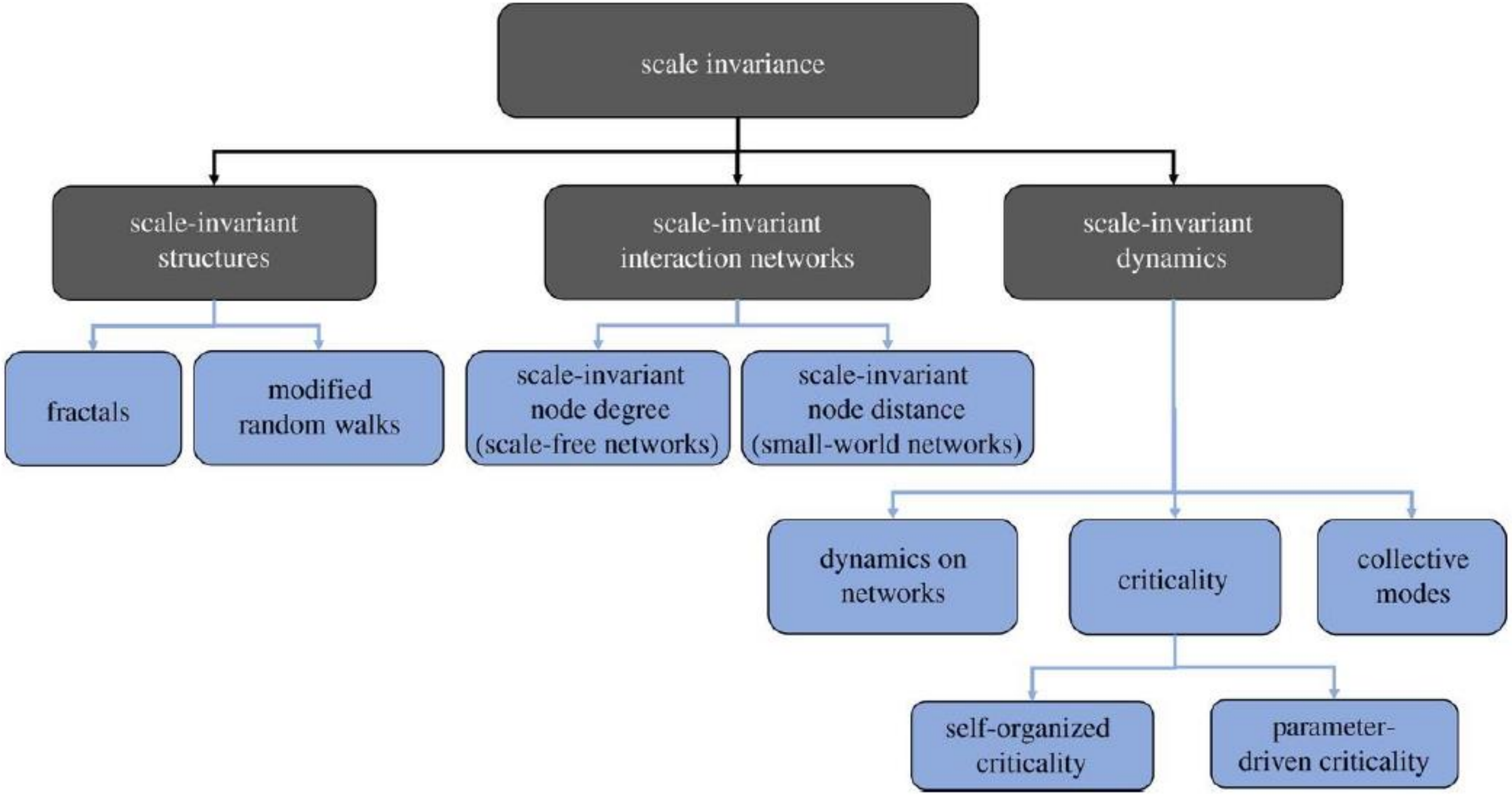
Speed distrbution of particles is according to the Maxwell-Boltzman (MB).



Program/Set up a simulation of a 2D Lennard-Jones particle system (Good model for a nobel gas).

- How many particles and simulation steps are necessary to obtain the MB distribution?
- How does the radial distribution function (RDF) compares to the RDF of real nobel gases?
- How does the RDF change with temperature (phase transition)?

Critical phenomena, scale invariance, scaling relations

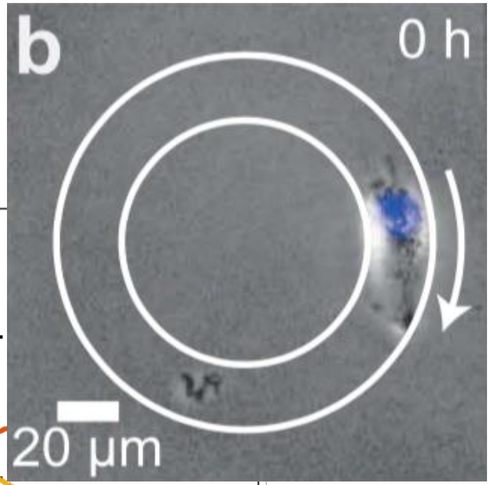


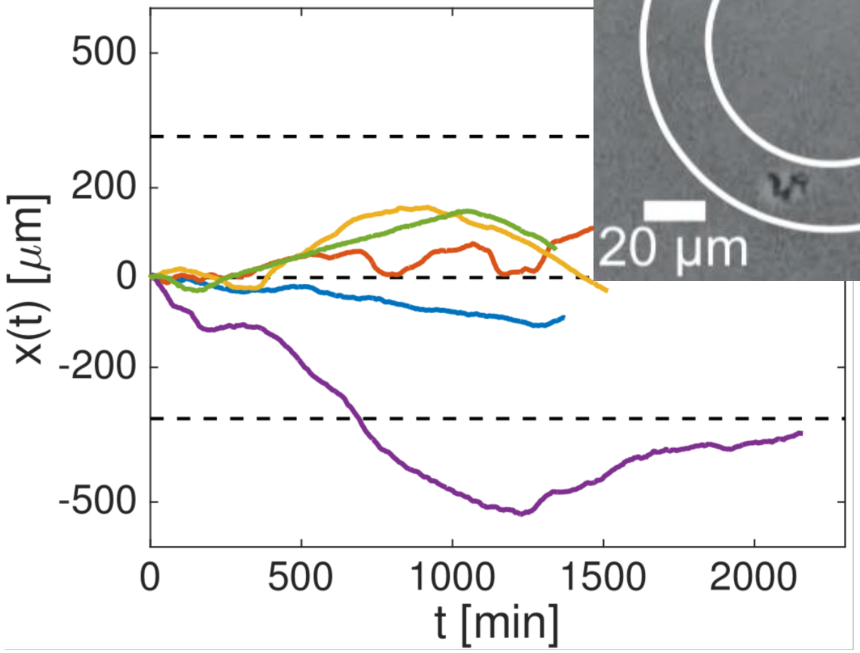
Scale invariance in natural and artificial collective systems:
Yara Khaluf, Eliseo Ferrante, Pieter Simoens and Cristián Huepe
Published:01 November 2017

Stat. Mech. Of Cell Migration

Schreiber et. al , Sci. Rep., 6, 26858 (2016)

$$x(t) = r_0 \varphi(t)$$





- Equation of Motion for migrating cells?
- Difference between Brownian motion of "passive" particles vs. "active" motion of living cells
- Inferring theories from experimental data

$$\ddot{x}(t) = -\frac{1}{\tau_p}\dot{x}(t) + F_R(t), \quad \langle F_R(t) F_R(0) \rangle = \frac{2B}{\tau_p}\delta(t)$$

Die Brownsche Bewegung bei Berücksichtigung einer Persistenz der Bewegungsrichtung. Mit Anwendungen auf die Bewegung lebender Infusorien.

Von **Reinhold Fürth.**

Mit zwei Abbildungen.

Aus dem physikalischen Institut der deutschen Universität in Prag.

(Eingegangen am 26. Juni 1920.)