Statistical Mechanics E0415

Fall 2023, lecture 10 Out-of-equilibrium

… previous take home

“The article "Recovery of Equilibrium Free Energy from Nonequilibrium Thermodynamics with Mechanosensitive Ion Channels in E. coli" by Cetiner et al. published 2020 in physical review letters is about a method to get the free energy difference between closed and open states of mechanosensitive ion channles in a nonequilibrium work distribution.

Mechanosensitive ion channels serve as safety valves in a cell to regulate the osmotic pressure inside and outside of the cell. A common method to observe the change in free energy is by measuring the ion condictive as a function of the tension. If then the probability of finding a channel closed or opened is fitted onto a two-state “boltzmann distribution, then the changei n free energy can be determined. When triangular ramp protocool is applied, a clear hysteresis can be observed. In the publication, the thermodynamics of such ion channel gating is investigated with an alternative approach. The alternative approach is to observe the difference in free energy by a two equilibrium state systems A and B to the nonequilibrium duistribution of the work during the change in thermodynamic process relating A to B. Each channel can be seen as an independent event is therefore beneficial for the formalism which is normally problematic with the conventional approach.”

… examples…

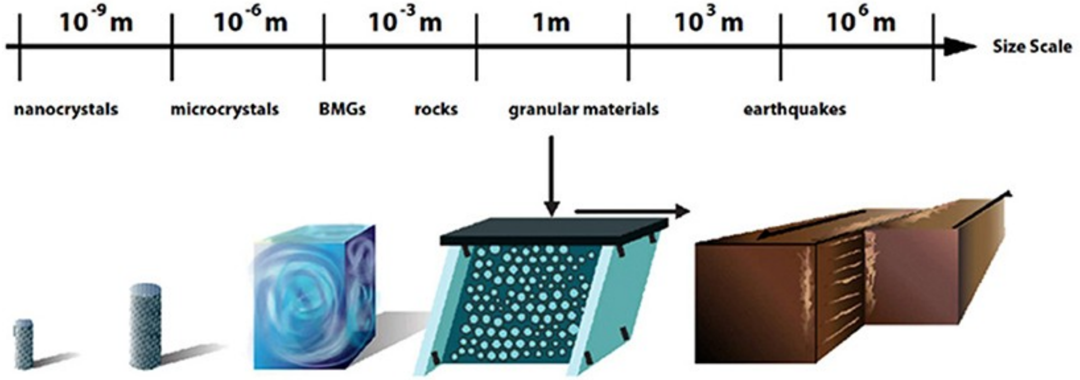
“The lecture notes begin with an example of when the microscopic and macroscopic worlds do not agree. If you stretch a rubber band very slowly, after you stop stretching it returns to the original state. However, if you stretch a microscopic rubber band like RNA molecule, you can unfold the twirls one at a time leading into multiple equilibrium states. So, the work done does not cancel out after the stretch. Now instead of just work, we need to concider the fluctuation in terms of the partition function, which leads into the Jarzynski equality. It holds in non-equilibrium thermodynamics, and is an important results to understand the dynamics on non-equilibrium thermodynamical systems. I learned that nonequilibrium steady states are such that the particle flow is constant or something alike this, where the thermodynamic quantites do not change anymore. The article of Jazynski derives a special relation for adiabatic processes.”

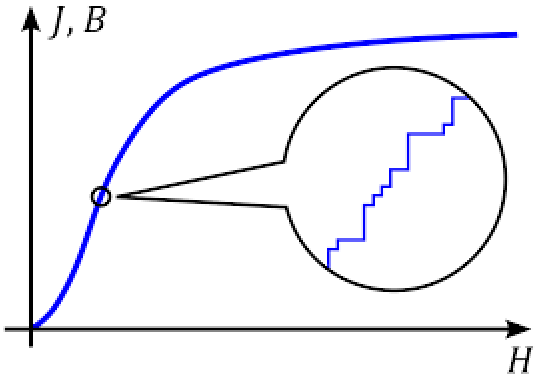
Lesson: JE says something about equilibrium by looking at things while not in equilibrium.

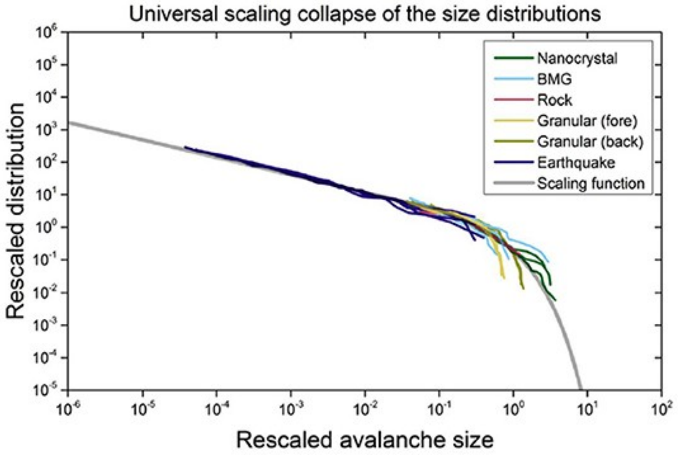
Non-equilibrium systems (“life”) stay so since they are kept out of equilibrium (e.g. flow of energy, matter)

Statistical mechanics for complex systems

Here are a few examples of "avalanching" systems: deformation up to earthquakes , Barkhausen noise (magnets), a real snow avalanche. How to understand such statistics?







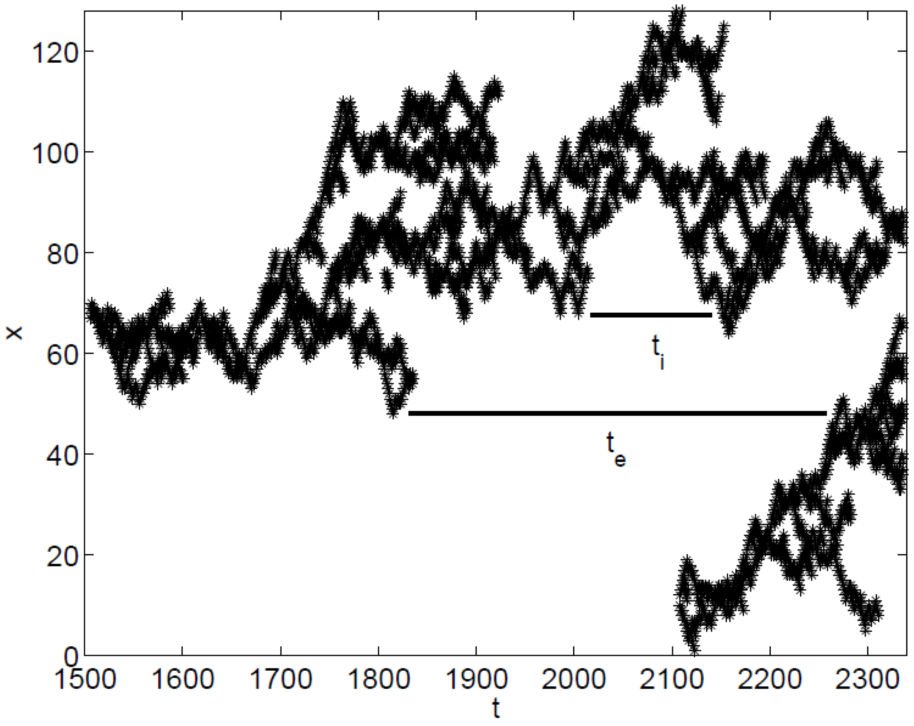
Activity map

A 1D model of activated random walkers.

Plot the locations where there is activity.

The pattern is (here) a self-affine fractal, since the system is in a (self-organized) critical state.

Correlation functions…. Avalanche distributions.

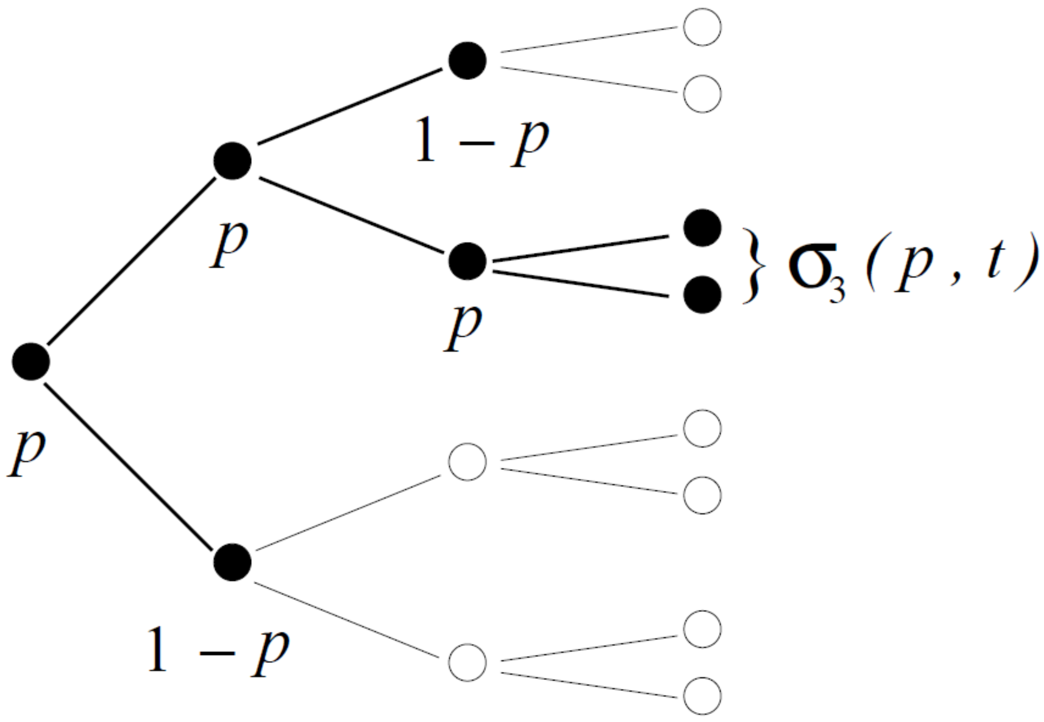


Branching process on a tree

Size of the avalanche? ”7”

Number of generations? 4 (0…3 counting also the seed).

Limit of infinite dimensions: the avalanche never re-visits the same location.

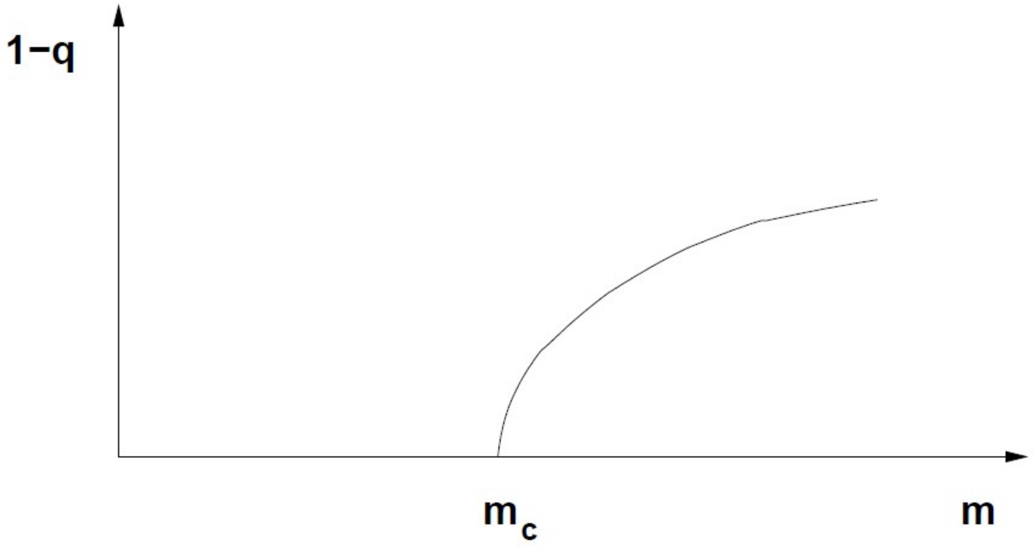


Critical properties

$$\text{Prob(survival)} = \begin{cases} 0, & m \leq m_c \\ (m - m_c)^\beta, & m > m_c. \end{cases}$$

Order parameter: survival probability.

Critical point value, order parameter exponent β.



Properties of critical branching processes

The statistics can be solved with the aid of the generating functions of the stochastic process as a function of generation n, and looking at the scale-free, Fixed-Point solution.

$$f(x,p) = \frac{1-\sqrt{1-4x^2p(1-p)}}{2xp}.$$

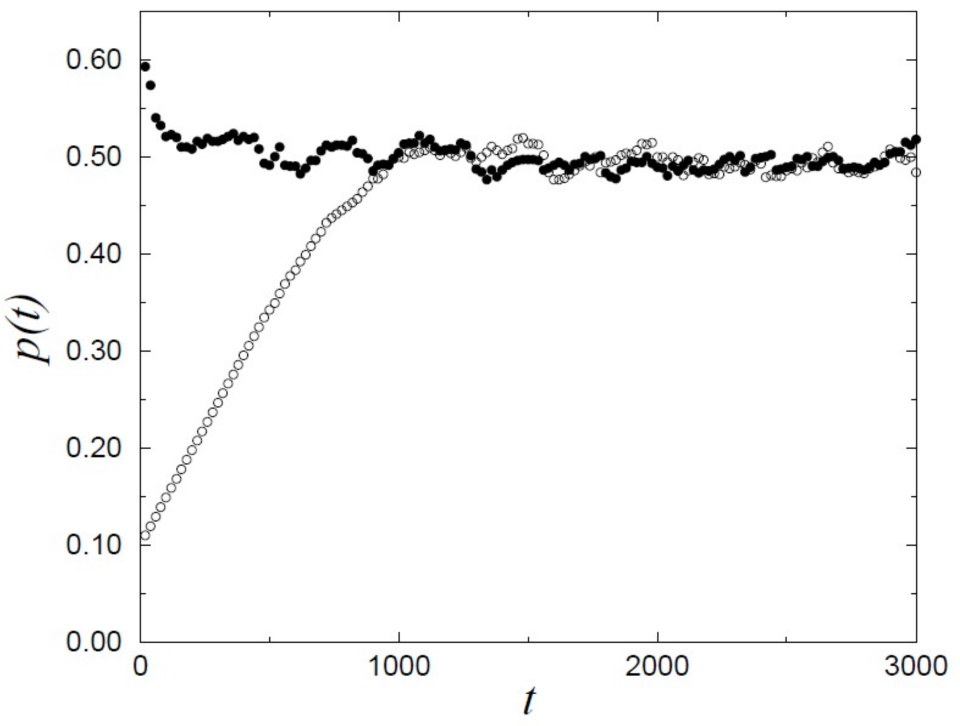
$$P_n(s,p) = \frac{\sqrt{2(1-p)/\pi p}}{s^{3/2}} \exp\left(-s/s_c(p)\right).$$

This shows that indeed, the avalanches are scale-free apart from a cut-off function.

Self-organized Branching Process

At a fixed n, we study the effect of the initial condition on the time-dependent branching probability p(t) (above and below the critical value).

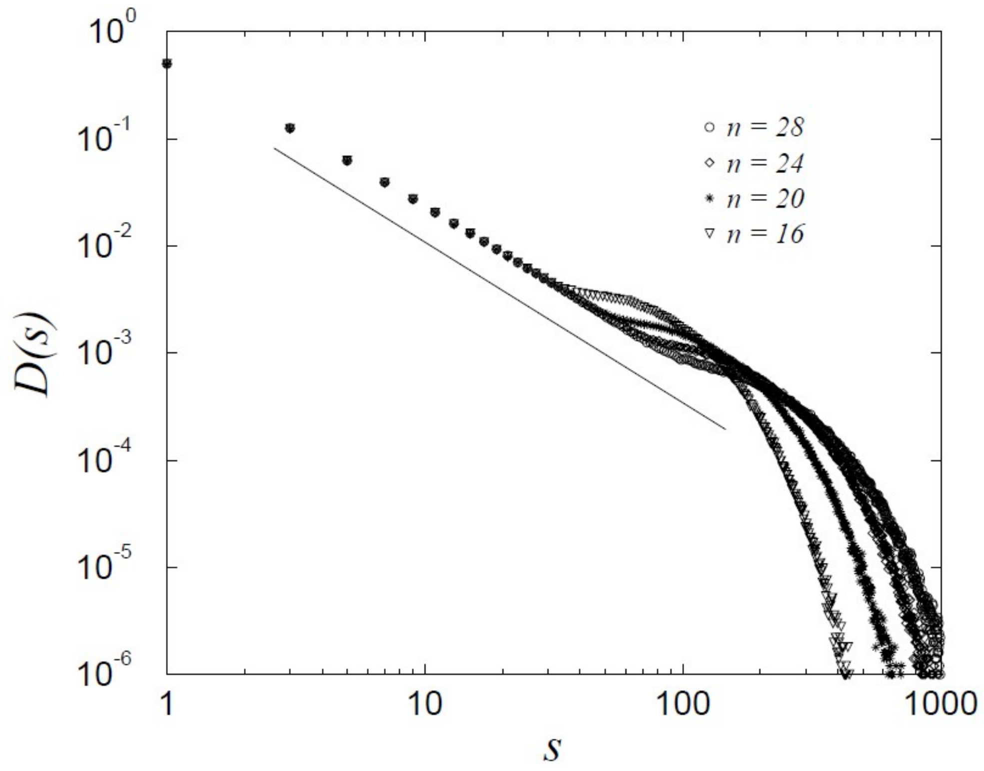
After transient periods, a fluctuating steady-state is reached.



SOBP: avalanches

At finite n, the avalanches follow the theoretical prediction (exponent -3/2, exponential cut-off).

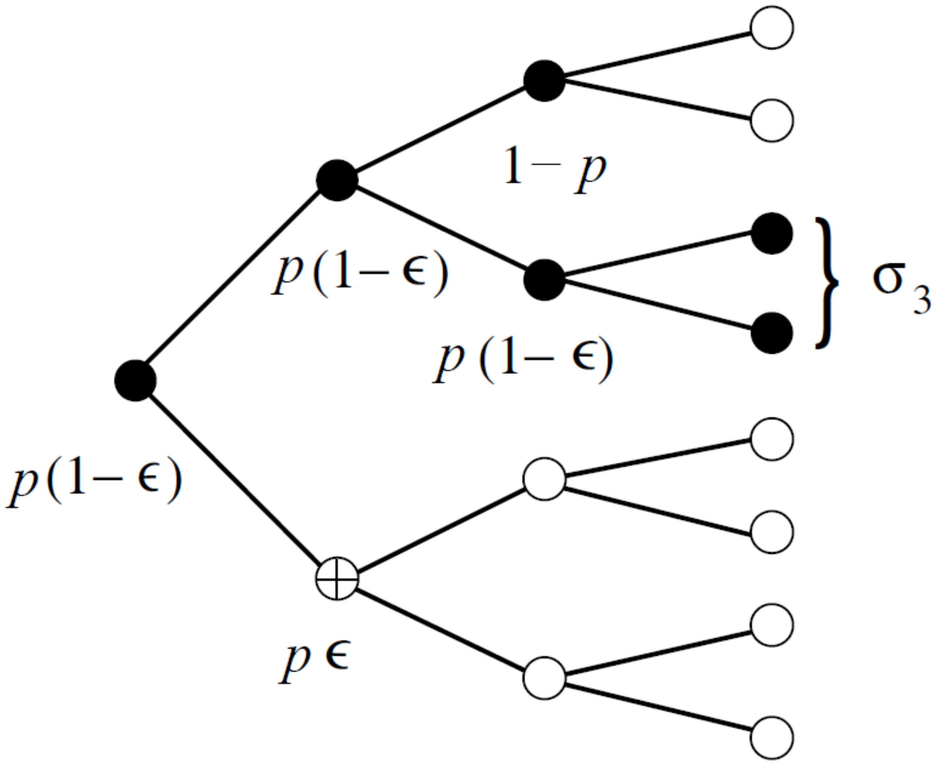
Similar results for durations T.



SOBP with dissipation

How does dissipation (of particles, energy…) influence the critical properties.

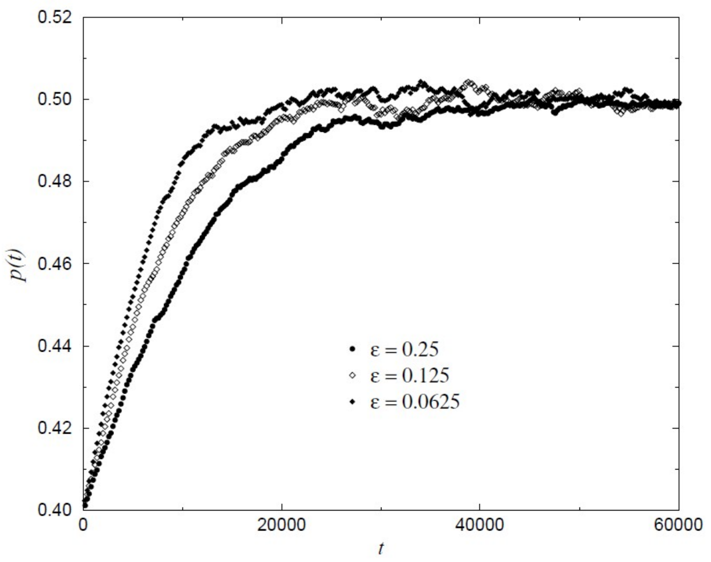
In the tree/mean-field picture this, “ε”, is easy to add to the process dynamics.

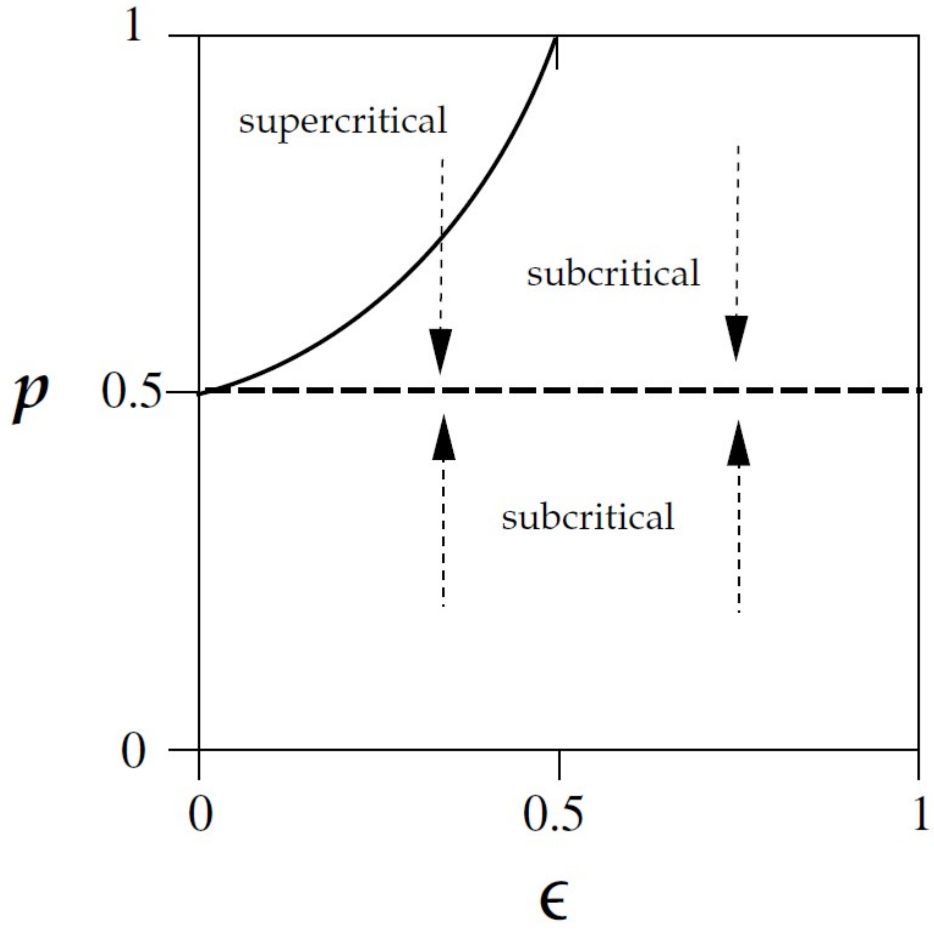


Phase diagram in the presence of dissipation

Dynamical equation for p(t): steady-state.

Resulting phase diagram.

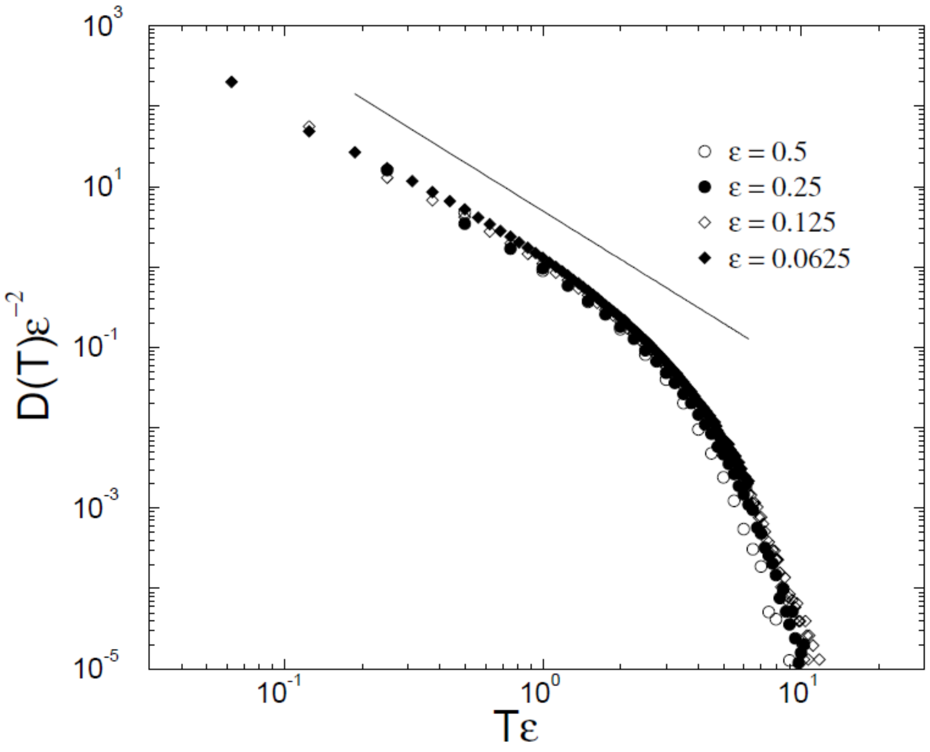


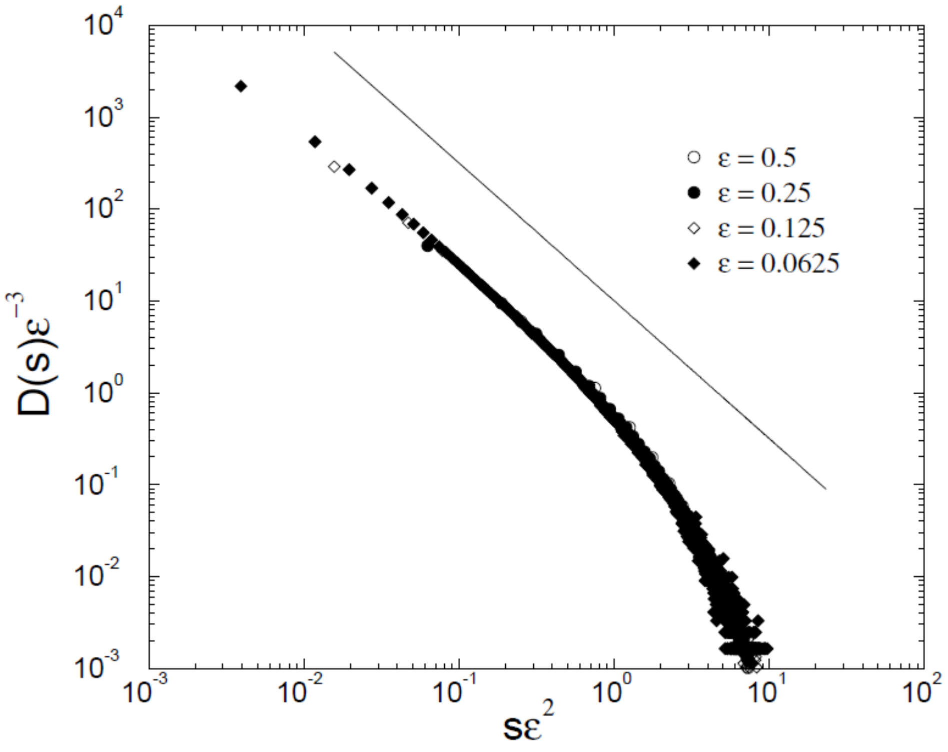


Avalanche distributions with dissipation

Distributions of durations, sizes with varying dissipation.

Rescaling/collapse of statistics (cf. x/y-axis).





Last take home

This time we study out-of-equilibrium systems that exhibit what is called crackling noise or bursts of activity. Such phenomena arise in many contexts (materials, astrophysics, geophysics - earthquakes, neuroscience, biology).... and so forth. The material for this lecture is a set of lecture notes.

The key points are: understand some mechanisms (there are more) by which systems in nature produce such behavior. If you are really interested and want more depth you may have a look at the very recent review article in https://www.frontiersin.org/articles/10.3389/fphy.2020.00333/full

To finish off the take homes, we have again then a pick of THREE recent papers for you. These illustrate (all from 2020) the applications of such ideas to various fields.

We start from neuroscience

https://arxiv.org/abs/2011.03263

... move over to the deformation of materials....

https://advances.sciencemag.org/content/6/41/eabc7350

... and finish with earthquake (prediction) in a laboratory.

https://arxiv.org/abs/2011.06669

And your task is like the previous time "2+8" sentences on the selection and main points.

… end of the course…

On the 8th of December presentations of the computational projects.

We will that week let you know of your projected total score for the course.

Enjoy!