SYFP 1: Physics of Fluctuating Paths

Time: Tuesday 9:30–12:15 Location: HSZ 01

Invited Talk SYFP 1.1 Tue 9:30 HSZ 01

Time at which a stochastic process achieves its maximum — •Satya Majumdar — Lptms, Universite paris-saclay, Bat 530, Rue Andre Riviere, Orsay 91405, france

For any stochastic time-series of duration T, the time $t_{\max}$ at which the process achieves its maximum is an important observable. For example, for a stock price over a trading period T, one would like to sell the stock at the time when the price is maximal. I'll discuss the statistics of $t_{\max}$ for a variety of stochastic processes. In particular, for several stationary processes, both in and out of equilibrium systems, we show that the distribution of $t_{\max}$ over $[0, T]$ exhibits a universal and interesting edge behavior (near 0 and T).

Invited Talk SYFP 1.2 Tue 10:00 HSZ 01

Fluctuations and molecule-spanning dynamics of single Hsp90 proteins on timescales from nanoseconds to days — •Thorsten Hugel — Institute of Physical Chemistry, University of Freiburg, Germany — Signalling research centers BIOSS and CIBSS, University of Freiburg, Germany — Cluster of Excellence livMatS @ FIT, University of Freiburg, Germany

Protein dynamics have been investigated on a wide range of timescales. Nano- and picosecond dynamics have been assigned to local fluctuations, while slower dynamics have been attributed to larger conformational changes. However, it is largely unknown how local fluctuations can lead to global changes and on which timescales the proteins dynamics are ergodic and if they show ageing. These questions become even more challenging if ATP hydrolysis is involved.

Here we set out to understand the fluctuations and conformational dynamics in the molecular machine and heat shock protein Hsp90. Therefore, we measure the dynamics of single Hsp90s on timescales from nanoseconds to days with a combination of single-molecule fluorescence, Neutron scattering and Plasmon resonance supported by MD simulations.

I will show that molecule-spanning dynamics on the 100 ns timescale likely precede hierarchical allosteric processes on slower timescales. Then the very good statistic on the even slower conformational dynamics allows us to discuss directionality, ergodicity and ageing in this fascinating ATP fueled molecular machine.

Invited Talk SYFP 1.3 Tue 10:30 HSZ 01

Path reweighting for Langevin dynamics — •Bettina Keller — Freie Universität Berlin, Berlin, Germany

Transition processes in molecular dynamics are investigated by simulating the molecular dynamics as underdamped Langevin dynamics on a high-dimensional energy surface. The accuracy of the rate estimates depends critically on the number of transitions observed in the simulated trajectories. However, the relevant molecular timescales are often beyond the reach of molecular simulations - even when the simulation is conducted on a supercomputer. Slow molecular processes include formation of molecular complexes, transitions through membranes, or phase transitions in crystalline materials. By biasing the potential energy one can sample transitions of rare events, but the rate estimates are distorted. Path reweighting techniques [1, 2] unbias the rate estimates by explicitly calculating the path probability density in the original and biased potential, and thus enable us to characterize slow molecular processes. While the path probability density for overdamped Langevin dynamics is well-documented, little information is available on the path probability densities for underdamped Langevin dynamics [3]. This hampers the use of path reweighting in molecular simulations. I will focus on Langevin integrators constructed via the operator splitting technique, and derive their path probability density. An important intermediate result is the single-step transition probability which maps a point in state space to another point in state space. The image of this function determines whether the integrator can be used (efficiently) for path reweighting. I will demonstrate the results on model potentials and molecular examples.

[1] Luca Donati and Bettina G Keller. Girsanov reweighting for metadynamics simulations. The Journal of Chemical Physics, 149(7):072335, 2018.

[2] Luca Donati, Marcus Weber, and Bettina G Keller. A review of Girsanov reweighting and of square root approximation for building molecular Markov state models. Journal of Mathematical Physics, 63(12):123306, 2022.

[3] Stefanie Kieninger and Bettina G Keller. Path probability ratios for Langevin dynamics exact and approximate. The Journal of Chemical Physics, 154(9):094102, 2021.

15 min. break

Invited Talk SYFP 1.4 Tue 11:15 HSZ 01

Out-of-equilibrium dynamics of trapped Brownian particles — •Raul A. Rica — Universidad de Granada, Granada (Spain)

Micro and nanoparticles can be individually manipulated by different trapping mechanisms, among which optical tweezers and Paul traps are the most extended approaches. Trapped particles are subject to Brownian motion due to collisions with the molecules of the dispersing medium. Once trapped, the particles can be driven out of equilibrium under the action of external fields, giving rise to very rich dynamics. In this talk, we will discuss some of our work with trapped nanoparticles dispersed in different media, including water, air, and vacuum. We will present recent experimental results demonstrating the occurrence of anomalous relaxation processes, time asymmetries, and bistability with trapped particles.

Invited Talk SYFP 1.5 Tue 11:45 HSZ 01

Thermodynamics of Clocks — •Patrick Pietzonka — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The thermodynamic uncertainty relation (TUR) establishes a seemingly universal trade-off between cost and precision for classical nonequilibrium systems in a steady state. Applied to clocks subject to thermal noise, it states that the product of the energy used for the driving and the squared relative uncertainty of the displayed time is always greater than $2k_{\mathrm{B}}T$. The TUR has been proven for models based on Markov jump dynamics or overdamped Brownian motion. It had also been conjectured to hold for underdamped Brownian dynamics, i.e., systems where inertia plays a role. This conjecture can now be disproven. I will present a counterexample that is inspired by a pendulum clock, consisting of an underdamped oscillator and a discrete counter, with thermal noise accounted for in both degrees of freedom. As it turns out analytically, this classic design principle of a clock allows one to overcome the bounds on precision set by the TUR . Beyond the minimal model, I also show numerically that the TUR can be broken in a fully continuous model with two underdamped degrees of freedom. Finally, I present a new bound valid for time-symmetric observables, which shows that for overdamped systems there is a minimal cost for producing a precise sequence of "ticks".