DY 46: Statistical Physics of Biological Systems II (joint session DY/BP)

Time: Friday 11:30–13:00 Location: H43

Invited Talk DY 46.1 Fri 11:30 H43

Equilibrium and non-equilibrium dynamics of biological systems with memory — •Roland Netz — Freie Universität Berlin, Fachbereich Physik, Berlin

Biological systems are many-body systems. Thus, their dynamics, when described in terms of a low-dimensional reaction coordinate, is governed by the generalized Langevin equation (GLE), an integro-differential equation of motion which contains friction memory [1]. Two examples will be discussed:

Protein-folding kinetics is standardly described as Markovian (i.e., memoryless) diffusion in a one-dimensional free-energy landscape. By analysis of molecular-dynamics simulation trajectories of fast-folding proteins the friction is demonstrated to exhibit significant memory with a decay time of the same order as the folding and unfolding times [2,3,4]. Memory friction leads to anomalous and drastically modified protein kinetics: the folding and unfolding times are not dominated by free-energy barriers but rather by non-Markovian friction.

Active motion of organisms obviously is far from equilibrium. The parameters of an appropriate non-equilibrium GLE are extracted from trajectories. It is demonstrated that the motion of single-cellular algae is characterized by pronounced memory friction, which allows to classify and sort individual cells.

[1] Memory and Friction: From the Nanoscale to the Macroscale, BA Dalton, A Klimek, H Kiefer, F N Brünig, H Colinet, L Tepper, A Abbasi, RR Netz, https://arxiv.org/pdf/2410.22588

DY 46.2 Fri 12:00 H43

Mean transient drift of synaptic weights in feed-forward spiking neural networks with spike-timing-dependent plasticity — •Jakob Stubenrauch and Benjamin Lindner — BCCN Berlin and Physics Department HU Berlin, Germany

Spike-timing dependent plasticity (STDP) [1] is a phenomenological model for the dynamics of single synaptic weights. This concise microscopic (single-synapse) description allows for the derivation of macroscopic network theories, capturing for instance learning, forgetting, and representational drift.

For the development of such theories it is important to characterize the stochastic process of synaptic weights. Early attempts capture this process for Poissonian presynaptic spikes and conditionally Poissonian postsynaptic spikes [2]. However, since STDP depends on fine spike-timing differences below 20 ms [1], it is important to characterize the synaptic dynamics for neuron models that describe the fast response mechanistically.

Leveraging a recent theory [3] as well as established results for the leaky integrate-and-fire neuron [4,5], we analytically compute the drift and diffusion of feed-forward synapses in a setup where a layer of presynaptic Poisson processes feeds into a recurrent network of leaky integrate-and-fire neurons.

[1] Bi and Poo, J. Neurisci. (1998) [2] Kempter et al., Phys. Rev. E (1999) [3] Stubenrauch and Lindner, Phys. Rev. X (2024) [4] Brunel et al., Phys. Rev. Lett. (2001) [5] Lindner and Schimansky-Geier, Phys. Rev. Lett. (2001)

DY 46.3 Fri 12:15 H43

A Biophysical Model for Temperature-Sensitivity of Neurons — •Julian Voits[1], Wojciech Ambroziak[2,3], Jan Siemens[2,4], and Ulrich S. Schwarz[1,5] — [1]Institute for Theoretical Physics, University of Heidelberg, Germany — [2]Department of Pharmacology, University of Heidelberg, Germany — [3]Department of Translational Disease Understanding, Grünenthal GmbH, Aachen, Germany — [4]Molecular Medicine Partnership Unit (MMPU), European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [5]BioQuant-Center for Quantitative Biology, University of Heidelberg, Germany

Control of body temperature is essential for our well-being and especially important during periods of fever or heat acclimation, e.g. due to traveling or climate change. An essential element of body temperature control are temperature-sensitive neurons, particularly warm-sensitive ones in the preoptic area of the hypothalamus. Since the discovery of temperature-sensitive ion channels, it has become clear that the underlying molecular mechanisms are rather diverse. In this work, we introduce a mathematical model based on a reduced version of the Hodgkin-Huxley model that can predict the frequently observed linear dependence of spiking rates on temperature in warm-sensitive neurons. Additionally, we present data showing how neurons adapt to varying temperatures over time, along with evidence of hysteresis in many temperature-sensitive neurons.

DY 46.4 Fri 12:30 H43

Position-Dependent Non-Markovian Effects Improve Protein Folding Simulations — •Lucas Tepper, Cihan Ayaz, Benjamin Dalton, and Roland Nezt — Freie Universität Berlin

It's common to project a protein's full atomic resolution onto a one-dimensional reaction coordinate to capture key aspects of its folding process. As a direct consequence of this dimensionality reduction, non-Markovian memory effects emerge. Accounting for memory effects in the framework of the generalized Langevin equation (GLE) with linear friction has proven efficient, accurate and insightful. However, recent advances in deriving GLEs with non-linear, position-dependent friction kernels raise questions about their applicability to protein folding simulations. We derive a novel method to extract position-dependent friction kernels from time series data via conditional Volterra equations. When applied to two protein test systems, the position- and time-dependent friction is strongest for long memory times in the folded states, where atoms are tightly packed. Additionally, we propose a novel and numerically efficient GLE simulation setup, confirming the accuracy of the extracted kernels. Compared to linear friction GLE simulations, our results show that position-dependent non-Markovian effects are critical for accurately reproducing protein folding kinetics when using low-dimensional reaction coordinates.

DY 46.5 Fri 12:45 H43

Multicomponent mixtures exhibit a vast nucleation-and-growth regime — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Phase coexistence is crucial for understanding how cells regulate biomolecular condensates. Despite of the multicomponent and multiphase nature of such condensates, the direct study of coexisting phases is limited to only few components since the parameter space is high-dimensional. So far, no theory provides a direct and concrete estimation of the phase coexistence behavior of multicomponent mixtures. As a first-level description of multicomponent phase behavior, we derive scaling relations for the number of coexisting phases in typical multicomponent mixtures in equilibrium. The scaling relations reveal that the interactions required to have many coexisting phases only scales very weakly with the number of components, whereas the stability analysis of the homogeneous state suggests a much stronger scaling. This discrepancy implies that large parts of the phase diagram of multicomponent mixture are in the nucleation-and-growth regime, where the homogeneous state is locally stable while multiple coexisting phases are preferred energetically. This suggests that multicomponent mixtures can achieve versatility and controllability in phase behavior with moderate interactions, which might be utilized by cells to create or destroy biomolecular condensates.