BP 26: Posters: Statistical Physics of Biological Systems

Time: Tuesday 14:00–16:00 Location: Poster A

BP 26.1 Tue 14:00 Poster A

Broken detailed balance in active fluctuations of semiflexible filaments — •Jannes Gladrow[1], Nikta Fakhri[2], Chase P. Broedersz[3], Fred C. MacKintosh[4], and Christoph F. Schmidt[1] — [1]Georg-August Universität Göttingen, Germany — [2]Massachusetts Institute of Technology, USA — [3]Princeton University, USA — [4]Vrije Universiteit, Netherlands

Non-equilibrium microscopic force generation in cells often results in stochastic steady-state fluctuations. In the cell cytoskeleton, for example, cytoplasmic myosins can drive vigorous conformational fluctuations of actin filaments and microtubules. We here present an analytical and numerical analysis of randomly driven shape fluctuations of semiflexible filaments in a viscoelastic environment. To detect and quantify non-equilibrium dynamics, we focus on the breaking of detailed balance in a conformational phase space subtended by eigenmodes of the beam equation. Molecular dynamics simulations reveal a non-zero circulatory flux in phase space induced by motor activity. Furthermore, we derived an analytical expression of nonequilibrium mode correlations that allows us to predict temporal effects of active molecular motors.

BP 26.2 Tue 14:00 Poster A

Thermodynamic uncertainty relation for biomolecular processes — •Andre C. Barato and Udo Seifert — II. Institut für Theoretische Physik, Stuttgart, Germany

Biomolecular systems like molecular motors or pumps, transcription and translation machinery, and other enzymatic reactions can be described as Markov processes on a suitable network. We show quite generally that in a steady state the dispersion of observables like the number of consumed/produced molecules or the number of steps of a motor is constrained by the thermodynamic cost of generating it. An uncertainty ϵ requires at least a cost of $2k_BT/\epsilon^2$ independent of the time required to generate the output.

BP 26.3 Tue 14:00 Poster A

Statistical classification of small microbial food webs — •Fanny Groll and Alexander Altland — Institut für Theoretische Physik, Universität zu Köln, Germany

We identify classes of food webs with regard to their stability and species diversity. Food webs are characterised by the topology of their inter-species relations, e.g. feeding on products of metabolism of another species or competition on nutrients or via a common predator. To gain insight into these structures we pursue a statistical approach: the starting point is the numerical implementation of food webs of with given inter-species network dependence. We consider different aquatic microbial communities. Each species is defined by parameters determining its attributes. A whole distribution of parameter combinations is then randomly generated and tested according to its temporal evolution. Individual systems evolve for some time in simulations and the outcome is monitored. Specifically, we deduce probabilities for the survival of a given number of species over distributions of network parameters at fixed network topology.

BP 26.4 Tue 14:00 Poster A

How molecular knots can pass through each other — •Jonathan Siebert[1], Benjamin Trefz[1,2], and Peter Virnau[1] — [1]Department of Physics, Johannes Gutenberg University of Mainz, D-55128 Mainz, Germany — [2]Graduate School Materials Science in Mainz, D-55128 Mainz, Germany

In our work a method is proposed that allows two molecular knots on a DNA strand to pass through each other. This results in interchanging their positions along the strand. By expanding its size, one of the knots allows the other to diffuse along its contour.

As explained in *PNAS*, 111(22), 7948-7951 the free energy barrier for this particular mechanism only amounts to a few k_BT. Therefore, it is not only of aesthetic interest, but may also play a role in technological applications, e.g. nanopore sequencing.

BP 26.5 Tue 14:00 Poster A

Rigorous combination of molecular dynamics and biased or multi-temperature simulations with pytram — •Christoph Wehmeyer, Antonia Mey, Fabian Paul, Hao Wu, and Frank Noé — Institut für Mathematik, Freie Universität Berlin

The reliable estimation of equilibrium and kinetic properties of complex dynamical systems is of general interest in the physical and life sciences. Despite well established theoretical frameworks, the underlying complexity in general renders analytical predictions impossible and requires a numerical treatment instead; which can still be costly due to rare events dynamics.

Enhanced sampling and multi-ensemble methods (e.g. parallel tempering, Hamiltonian replica exchange, or umbrella sampling) allow to sample such rare events feasibly in many cases and, in this way, to calculate equilibrium properties. In general, however, the simultaneous analysis of molecular dynamics and biased simulations lacks a rigorous and broadly applicable protocol.

To this aim, we present TRAM, a fully rigorous approach to combine molecular dynamics and multi-ensemble simulations to estimate equilibrium and kinetic properties of systems with rare event dynamics using the Markov state model framework.

The TRAM method is implemented in the pytram package, available at https://github.com/markovmodel/pytram.

BP 26.6 Tue 14:00 Poster A

Specialization and bet hedging in heterogeneous populations — •Steffen Rulands[1,2], Benjamin D. Simons[1], and Erwin Frey[1] — [1]Cavendish Laboratory, Department of Physics, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, UK — [2]Department of Physics, Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstrasse 37, D-80333 München, Germany

How can cells specialize to a niche and at the same time be able to survive in a variety of different environments? In recent years it has become increasingly clear that bacterial, stem cell and even tumor cell populations exhibit a surprisingly high degree of heterogeneity. Genetic diversity and phenotypic heterogeneity are commonly used as a strategy to rapidly adapt to changing conditions. For example, some bacteria switch between phenotypic states in order to survive antibiotic attacks and embryonic stem cell populations exhibit heterogeneous capacities for pluripotency.

We investigate how and under which conditions genetic diversity and phenotypic heterogeneity develop and sustain. Studying paradigmatic ecological scenarios we show that the degree of genetic diversity and the persistence of phenotypic heterogeneity qualitatively change with type of competition between cells and the degree of diffusive motion in the population. While direct competition generally promotes persistence of phenotypic heterogeneity, specialization dominates in models with indirect competition irrespective of the degree of mobility.

BP 26.7 Tue 14:00 Poster A

Knotted protein folding as an ordered sequence of events — •Saeed Najafi and Raffaello Potestio — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

A small but relevant number of proteins whose native structure is known features nontrivial topology, i.e. they are knotted. Understanding the process of folding from a swollen conformation to the biologically-relevant conformation is, for these proteins, particularly difficult, due to the complex pathways leading to entangled state.To shed some light into this problem we introduced a native structure-based coarse-grained model of the protein, in which the information about the folded conformation is encoded in local, short-ranged interactions. Making use of a stochastic search scheme in the parameter space we can identify a set of interactions that maximize the folding probability to the native state.

BP 26.8 Tue 14:00 Poster A

Influence of genetic interactions schemes on adaptive walks — •Stefan Nowak and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln

The NK landscape is a model for a genotype to fitness mapping where epistatic interactions between loci can be explicitly defined. We study adaptive walks on this landscape to analyse the effects of different interaction schemes. For simple versions of the model, the length of the walk and the attained fitness can be computed exactly. For general NK landscapes, we show by Monte Carlo simulations that these quantities

are strongly correlated to the so-called rank of the interaction scheme.

BP 26.9 Tue 14:00 Poster A

Phase transition in random adaptive walks on correlated fitness landscapes — Su-Chan Park[1], Ivan Szendro[2], •Johannes Neidhart[2], and Joachim Krug[2] — [1]The Catholic University of Korea, Bucheon, Korea — [2]Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study biological evolution on a random fitness landscape with linear fitness gradient. When selection is strong and mutations rare the dynamics is an uphill walk that terminates at a local fitness maximum. The mean walk length is a function of the genome size L. We show that if and only if the random contribution to the fitness is exponentially distributed, the mean walk length displays a phase transition as a function of the strength of the fitness gradient. For all other distributions only a single phase exists. The considered process is equivalent to a zero temperature Metropolis dynamics for the random energy model in an external magnetic field which leads to a connection to the aging dynamics of spin glasses. See also arXiv:1408.4856.

BP 26.10 Tue 14:00 Poster A

Statistical properties of Fisher's geometric model — •Sungmin Hwang, Ivan Szendro, and Joachim Krug — Insitute for Theoretical Physics, University of Cologne, Germany

Fisher's geometric model has played an important role for providing a connection between the phenotypic space and the fitness landscape while it remains simple enough to be analytically tractable. As complete or partial structures of fitness landscapes in many microbial organisms have been experimentally explored, the extensive effort has been made to understand the epistasis of the fitness landscape, i.e., the genetic interaction among mutations. In this work, we calculated the properties of epistasis distribution under various conditions in the frameworks of Fisher's geometric model. Especially, we focus on the case where the two single mutants have the same selection coefficient in order to analyze how epistasis varies in terms of the selection coefficient of the single mutants. Finally, we compare this result with experimental data to check the validity of our result.

BP 26.11 Tue 14:00 Poster A

Theory of rapid force spectroscopy — •Jakob Tómas Bullerjahn, Sebastian Sturm, and Klaus Kroy — Universität Leipzig, Faculty of Physics & Earth Sciences, Institute for Theoretical Physics, Brüderstr. 16, 04103 Leipzig, Germany

Dynamic force spectroscopy allows the experimentalist to gauge the underlying free energy landscape of single molecular bonds by enforcing their rupture with external loading. At low loading rates, the experimentally measured distributions of rupture forces can be analysed using Kramers' theory of spontaneous unbinding, whereas the extreme forces observed in full-scale molecular simulations can be treated with deterministic methods. Starting from a rigorous probabilistic model of bond dynamics, we develop a unified systematic theory [1] that provides exact closed-form expressions for the rupture force distributions and mean unbinding forces, valid for all loading rates save for a narrow region close to a critical loading rate. Our results, in combination with Bayesian methods of data analysis, yield an accurate tool for analysing and comparing force spectroscopy data from a wide range of experiments and simulations.

[1] J. T. Bullerjahn, S. Sturm & K. Kroy, Nat. Comm. 5, 4463 (2014).

BP 26.12 Tue 14:00 Poster A

Increasing complexity of linear, prevailing, autocatalytical molecules — •Philipp Zimmer[1], Emanuel Gregor Worst[2], Eva Wollrab[2], Albrecht Ott[2], and Karsten Kruse[1] — [1]Universität des Saarlandes, Theoretische Physik, Postfach 151150, 66041 Saarbrücken — [2]Universität des Saarlandes, Biologische Experimentalphysik, Postfach 151150, 66041 Saarbrücken

Two common concepts of Darwinian evolution are mutation and selection. In natural evolution, these processes have permanently generated increasingly complex species. Nevertheless evolution has maintained to avoid dead ends such that a further development is proceeding. This process is not well understood. Performing stochastic simulations as well as experiments with DNA, we find that our system evolves reproducibly towards consecutive states of increasing complexity, if the autocatalytic activity exceeds a critical value.

BP 26.13 Tue 14:00 Poster A

Modeling chromosomes during meiosis in fission yeast — •Wenwen Huang[1], Yen Ting Lin[1], Daniela Frömberg[1], Petrina Delivani[2], Mariola Chacón[2], Iva Tolic[2], Frank Jülicher[1], and Vasily Zaburdaev[1] — [1]Max Planck Institute for the Physics of Complex Systems, 01187, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, 01307, Dresden, Germany

During the prophase of meiosis in fission yeast, both ends of chromosomes are bound to the spindle pole body (SPB) and form a ring-like structure. Furthermore, the whole nucleus oscillates, moving from one pole of the zygote to the other. The dramatic movements of the nucleus are believed to promote the chromatin alignment and are required for proper recombination. Our goal is to understand the physical picture of chromosome alignment during nuclear oscillations. We perform extensive Brownian dynamics simulations of three pairs of homologous chromosomes during the oscillations. An individual chromosome is represented by a bead-rod ring, where the SPB is a special common bead shared by all the rings. A periodic force is applied to the SPB, which pulls the chromosomes through the viscous nucleoplasm and under the confinement of the cell walls. By setting parameters based on estimation of the available experimental data, we analyze the distance between the homologous loci as the function of time and amplitude of oscillations and compare it to the experimental data. Our results provide a quantitative characterization of of chromosome movements and help to understand the role of nuclear oscillations on the alignment of chromosomes during meiosis.

BP 26.14 Tue 14:00 Poster A

Evolutionary accessibility in the NK Model for fitness landscapes — •Benjamin Schmiegelt — Institute for Theoretical Physics, Cologne, Germany

Fitness landscapes are biological evolution's equivalent to energy landscapes, on which populations move as genotype distribution clouds [1]. In the limit of weak mutation and strong selection, the population's dynamic can be described by an uphill climb. Accessibility refers here to the probability that the landscape's global maximum is reachable from the antipodal genotype [2]. The NK model for such a landscape with L binary loci resembles a spin glass where each spin/locus interacts with k other spins/loci. A key determinant of evolutionary accessibility is the degree of sign epistasis, the fraction of loci having both positive and negative fitness effects depending on the state of other loci. Using that the NK model at fixed k for $L \to \infty$ almost surely exhibits global reciprocal epistasis, i.e. reciprocal sign epistasis between two loci on all generic background, it is shown that the accessibility tends to zero, and does so faster than in the House-of-Cards model (random energy model), generalizing results obtained previously for a special case of the NK-model where the groups of interacting loci are disjoint [3].

[1] J.A.G.M. de Visser and J. Krug, Nature Reviews Genetics 15, 480-490 (2014)

[2] J. Franke, A. Klözer, J.A.G.M. de Visser and J. Krug, PLoS Computational Biology 7, e1002134 (2011).

[3] B. Schmiegelt and J. Krug, Journal of Statistical Physics 154, 334-355 (2014).

BP 26.15 Tue 14:00 Poster A

Stochastic Terminal Dynamics in Epithelial Cell Intercalation — •Matthias Häring[1], Stephan Eule[1], Jakob Metzger[1], Lars Reichl[1], Deqing Kong[2], Yujun Zhang[2], Jörg Grosshans[2], and Fred Wolf[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg, 37077 Göttingen, Germany — [2]Institute for Developmental Biochemistry, Medical School, University of*Göttingen, Justus-von-Liebig Weg 11, 37077 Göttingen, Germany

We found that the constriction of epithelial cell contacts during intercalation in germ band extension in Drosophila embryos follows intriguingly simple quantitative laws. The mean contact length $\langle L \rangle$ follows $\langle L \rangle(t) \sim (T-t)^{\alpha}$, where T is the finite collapse time; the time dependent variance of contact length is proportional to the square of the mean; finally the time dependent probability density of the contact lengths remains close to Gaussian during the entire process. These observations suggest that the dynamics of contact collapse can be captured by a single stochastic differential equation in a small noise regime. Here, we present such a model, providing an effective description of the non-equilibrium statistical mechanics of contact collapse. All model parameters are fixed by measurements of time dependent mean and variance of contact lengths. Our model predicts the existence of a quasi-stationary distribution of contact lengths. We investigate this quasi-stationary distribution numerically and present an analytical solution for model parameters that are close to the measured values.