DY 2: Statistical physics in biological systems I (joint session DY/BP)

Time: Monday 11:00–13:00 Location: ZEU 255

DY 2.1 Mon 11:00 ZEU 255

Segregation and long-range order in self-propelled particles with nematic interactions — •Markus Bär[1], Hugues Chate[2], Andreas Deutsch[3], Francesco Ginelli[2,4], and Fernando Peruani[4] — [1]Physikalisch-Technische Bundesanstalt, Berlin — [2]CEA Saclay, France — [3]ZIH, TU Dresden — [4]ICS Paris

Motivated by experiments on collective dynamics of gliding bacteria, we study collective phenomena in a two-dimensional stochastic system of self-propelled particles (SPP) interacting locally through an apolar, nematic alignment mechanism. Extensive simulations show that there are four qualitatively different regions of spatial organisation. At high noise intensity, disordered spatially homogeneous distributions are found, while at low noise intensity long-range nematic order is found. For intermediate noises and large enough system size, the system segregates into macroscopic areas with either high or very low particle density. The high density areas take the form of bands that can take on stable straight shapes or can be dynamically changing depending on the size of the system, band width and noise intensity.

DY 2.2 Mon 11:15 ZEU 255

Transport on inhomogeneous filament networks — •Philip Greulich and Ludger Santen — Fachrichtung Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

We present a model for intracellular vesicle transport on submembranal actin networks. These networks are created by stochastic growth dynamics of actin filaments leading to an inhomogeneous structure. The dynamics of vesicles are implemented by an interplay of active transport on filaments and diffusion in the cytosol, while steric interactions of vesicles are taken into account. One observes the formation of vesicle clusters in a wide range of parameter space. We investigate the distribution of cluster sizes and compare these results to a system without filaments but attractive interactions between vesicles.

DY 2.3 Mon 11:30 ZEU 255

Stochastic models for efficient intracellular transport — •Maximilian Ebbinghaus and Ludger Santen — Department of Theoretical Physics, Saarland University, 66041 Saarbruecken

Intracellular transport along microtubules is bidirectional although single motor proteins such as kinesin or dynein perform stochastic motion in a single direction. For several diseases, the breakdown of the bidirectional transport is known to be pathologic. It is thus of great importance to understand how cells organize their transport system in an efficient way and which influences might interfere. We approach this question by numerically examining one-dimensional lattice gas models with multiple filaments in parallel on which we assume hard core exclusion. Further particle-particle interactions are introduced in order to observe lane formation, i.e. filaments that are occupied by a single type of molecular motor. In this way, we find different transport regimes with highly different transport capacities. The surrounding cytoplasm is modeled by further tracks on which particles do not interact and perform undirected diffusion. This very simplified model of the cytoplasm is compared with the results of a model with similar dynamics on the filaments but in a three-dimensional cylinder.

DY 2.4 Mon 11:45 ZEU 255

Statistical mechanics description of the process of polypeptides and proteins folding — •Alexander Yakubovich, Ilia Solov'yov, Andrey Solov'yov, and Walter Greiner — Frankfurt Institute of Advanced Studies, Goethe—Universität Frankfurt, Ruth-Moufang Straße 1, D-60438 Frankfurt am Main, Germany

The conformational transitions in finite molecular systems, i.e. the transition from a stable 3D molecular structure to a random coil state or vice versa (also known as (un)folding process) occur or can be expected in many different complex molecular systems and in nano objects, such as polypeptides, proteins, polymers, DNA, fullerenes, nanotubes. Experimental studies of the recent years reveal new detailed mechanisms of such nanoscale transitions and challenge the development of new theoretical models for the description of these complex processes. We suggest a theoretical method based on the statistical mechanics for treating the helix↔random coil transition in polypeptides. We consider this process as a first-order phase transition in a finite system and develop a theory which is free of model parameters and is based solely on fundamental physical principles. It describes essential thermodynamical properties of the system such as heat capacity, the phase transition temperature and others from the analysis of the polypeptide potential energy surface calculated as a function of two dihedral angles, responsible for the polypeptide twisting. The developed formalism is extended for the description of helix↔coil transition in solvent. We also provide a recipe for the theoretical description of the folding↔unfolding processes in proteins.

DY 2.5 Mon 12:00 ZEU 255

Protein folding dynamics in a simplified model — •Katrin Wolff[1], Michele Vendruscolo[2], and Markus Porto[1] — [1]Institut für Festkörperphysik, TU Darmstadt, Germany — [2]Department of Chemistry, University of Cambridge, Cambridge, UK

The study of all-atom protein folding dynamics is usually restricted to conformations close to the native state as it requires significant computational efforts and its force fields may not be accurate for unfolded structures. Coarse-grained models are therefore of great interest to capture essential features of the free energy landscape. We employ the tube model [1], describing a protein as a chain of uniform thickness with bending rigidity, and a bias towards the native structure to investigate protein folding dynamics from completely unfolded to folded native structure. The structural bias is based on a one-dimensional representation of the structure (structure profile) which is conceptually very different from the use of the contact map as in Gō-models. Unlike Gō-models, which favour the formation of contacts between specific residues, our approach mediates 'connectivity' of residues, that, much like hydrophobicity, describes a residue's propensity to have many contacts. We show that the 'effective connectivity' profile [2] constitutes a suitable bias towards the native structure and explore the free energy landscape and folding dynamics of this model [3].

[1] T.X. Hoang *et al.*, Proc. Natl. Acad. Sci. USA **101**, 7960 (2004).
[2] U. Bastolla *et al.*, Proteins **73**, 872 (2008).
[3] K. Wolff, M. Vendruscolo, and M. Porto, PMC Biophysics **1**, 5 (2008)

DY 2.6 Mon 12:15 ZEU 255

Funnels in energy landscapes — •Konstantin Klemm[1], Christoph Flamm[2], and Peter Florian Stadler[1,2] — [1]Bioinformatics Group, Leipzig University, Germany — [2]Theoretical Chemistry Group, University of Vienna, Austria

Local minima and the saddle points separating them in the energy landscape are known to dominate the dynamics of biopolymer folding. Here we introduce a notion of a folding funnel that is concisely defined in terms of energy minima and saddle points, while at the same time conforming to a notion of a folding funnel as it is discussed in the protein folding literature.

DY 2.7 Mon 12:30 ZEU 255

Selectively accessible paths in fitness landscapes — •Jasper Franke and Joachim Krug — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

A mutation of an organism's genome changing one nucleotide in the DNA has a higher probability of becoming fixed in the population if it increases the mutant's degree of adaptation to the environment (it's 'fitness'). A sequence of mutations that each increase the fitness of the respective mutant therefore forms a selectively accessible trajectory in the (generally very high-dimensional) space of sequences. This concept of accessible paths plays an important role in determining the possible configurations that can be reached starting from a given position in the sequence space.

Since the mapping from genotype to fitness is rather intricate and only partially understood, the fitness landscape can be modelled as a random landscape with a certain amount of correlation between the fitness values of different genotypes. The NK- Modell introduced by Kauffman was used to generate this family of fitness landscapes with tunable degree of correlation and thus tunable ruggedness.

In this talk, we present numerical results on the statistics of the selectively accessible paths in these fitness landscapes depending on the ruggedness.

DY 2.8 Mon 12:45 ZEU 255

A simple model for stress reactions in cellular regulation — •Andreas Ruttor[1], Guido Sanguinetti[2], Cedric Archambeau[3], and Manfred Opper[1] — [1]Technische Universität Berlin, Germany — [2]University of Sheffield, UK — [3]University College London, UK

Microarray experiments show that some cells can quickly respond to external stimuli, e.g. sudden environmental changes, by switching between different regulatory regimes. This stress reaction is achieved by activating a transcription factor, which changes the transcription rates of certain proteins. We present a simple model for such a bistable regulatory system. Production and degradation of mRNA and proteins are described by differential equations, as their concentrations change continuous in time. But we assume that there are only two possible states for the transcription factor, either active or inactive. Therefore its activity, which is difficult to observe in microarray experiments, is modelled as a random telegraph process. We find that this stochastic process can be reconstructed using only noisy measurements of the mRNA concentrations at discrete points in time. Our solution to this problem is based on calculating effective jump rates for the hidden activity of the transcription factor. This can be done by using the backward Chapman-Kolmogorov equation directly or an efficient approximate algorithm. Afterwards it is possible to estimate the time evolution of the posterior process and parameters of the regulatory system. Simulation results indicate that our approach works well.