DY 2: Statistical Physics of Biological Systems I (joint session of BP + DY)

Time: Monday 10:15–13:00 Location: H45

Invited Talk DY 2.1 Mon 10:15 H45

Noise during rest enables the exploration of the brain's dynamic repertoire — •Viktor Jirsa — Theoretical Neuroscience Group CNRS, ISM UMR6233, Marseille Luminy, France

At rest certain cortical regions of the human brain consistently show temporally coherent activity. In humans, these resting state networks have been shown to greatly overlap with functional architectures present during consciously directed activity, which motivates the interpretation of rest activity as day dreaming, free association, stream of consciousness, and inner rehearsal. Here, we show that comparable resting state networks emerge from a stability analysis of the network dynamics using biologically realistic primate brain connectivity, although anatomical information alone does not identify the network. We specifically demonstrate that noise and time delays via propagation along connecting fibres are essential for the emergence of the coherent fluctuations at rest. The combination of anatomical structure and time delays creates a space-time structure of the couplings in which the neural noise enables the brain to explore various functional configurations representing its dynamic repertoire.

DY 2.2 Mon 10:45 H45

Constrained Branching Random Walks as a minimal model for adaptive evolution — •Oskar Hallatschek — Biologische Physik und Evolutionäre Dynamik, MPI DS, Goettingen

Models of both sexual and asexual adaptation in well-mixed populations usually lead to solitary waves of adaptation. This means that the fitness distribution of the population assumes the form of a wave and moves to higher fitness at a certain speed of adaptation. This nonequilibrium steady state is easy to obtain in simulations but usually hard to analyze due to lack of detailed balance. Here, we introduce an analytically tractable minimal model that captures the essence of fitness waves of adaptation: i) a branching random walk of genotypes. ii) a global constraint that keeps the populations size finite. We show that for certain constraints an exact solution can be found. This exact solution, which can be summarized as a deterministic PDE with a peculiar cutoff, also turns out to approximate conventional models of adaptation in an unprecedented accuracy.

DY 2.3 Mon 11:00 H45

The number of adaptive paths in fitness landscapes with sign epistasis — •Jasper Franke[1], Alexander Kloezer[1], Joachim Krug[1], and J. Arjan G.M. de Visser[2] — [1]Institut für Theoretische Physik, Universität zu Köln — [2]Laboratory of Genetics, Wageningen University

A mutation of an organism's (genotypic or phenotypic) configuration has a higher probability of becoming fixed in the population if it increases the mutant's degree of adaptation to the environment (the organism's 'fitness'). A sequence of fitness-improving mutations forms an adaptive path along which the population can evolve. This concept of accessible paths plays an important role in determining the possible configurations that can be reached by evolutionary adaptation.

Since the mapping from configuration to fitness is biochemically only partially understood, several statistical models have been proposed trying to capture the essential features.

In this contribution, we consider the expected number of accessible paths and the probability of not having any accessible paths at all. We present analytic and numerical results for three statistical models for fitness landscapes and compare these results to data for the fitness landscape of the fungus *Aspergillus niger*.

DY 2.4 Mon 11:15 H45

Active Transport on Biological Networks — •Ines-Kristin Weber[1], Philip Greulich[1,2], and Ludger Santen[1] — [1]Department of Theoretical Physics, Saarland University, 66041 Saarbrücken — [2]Department of Theoretical Physics, Cologne University, 50937 Cologne

Active transport processes are vital for living cells. They are used, e.g. for structure formation, cell signaling and motion of cells. An large number of transport processes is carried out by molecular motors, i.e. specialized proteins that are able carry cargo along the cytoskeleton. The cytoskeleton is an inhomogeneous network of polar filaments which determines the cell shape and guides the motion of molecular motors.

In this work we investigate the relation between network structure and dynamics of molecular motors, whereat we consider computer generated filament networks as well as realistic structures of the cytoskeleton. The real cytoskeleton structures are obtained from light microscopy images which are preprocessed by automated image analysis procedures to localize fluorescent marked microtubules. Molecular motors are modeled as stochastic self-driven particles. By means of computer simulations and a phenomenological approach we investigate the formation of clusters on the different kinds of networks. We observe cluster formation at all size scales, even for small particle densities [1].

[1] P. Greulich, L. Santen, arXiv:0904.3890v1

DY 2.5 Mon 11:30 H45

Estimating molecule numbers based on fluctuations — •Andreas Ruttor and Manfred Opper — Technische Universität Berlin

Microarray experiments and other methods used to analyze biochemical systems are often not calibrated, so that results are given in arbitrary units. In this case the actual amount of molecules involved in the reactions remains unknown. However, fluctuations visible in the data set can be used to estimate it. For that purpose we use a diffusion model based on stochastic differential equations, which describe the dynamics of the reaction system. Here, two sources of fluctuations have to be taken into account: Observation noise, caused by the measurement process, is usually independent of the state of the system. But internal noise is the result of discrete reaction events occurring at random points in time. Therefore its size is directly related to the number of molecules per arbitrary unit, which is included in the model as a parameter. By solving the backward Fokker-Planck equation of the diffusion model in the weak noise limit, it is possible to calculate the likelihood of all observations. Maximizing this quantity with respect to the parameters leads to an estimate of the molecule numbers per arbitrary unit. Additionally, the uncertainty of this calibration can be obtained by calculating the Laplace approximation of the marginal posterior distribution.

DY 2.6 Mon 11:45 H45

Clustering in self-propelled particle systems — •Fernando Peruani[1] and Markus Baer[2] — [1]Service de Physique de l Etat Condense, CEA Saclay, 91191 Gif-sur-Yvette, France — [2]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

Self-propelled particle systems exhibit a rich irreversible clustering dynamics. Independently of the initial condition, these systems reach a steady state cluster size distribution which depends on particle density and noise intensity. We show that the aggregation process can be described by a set of Smoluchowski equations whose functional form is independent of the symmetry of the velocity alignment rule or interaction forces. For a given density (noise intensity) there is always a critical noise intensity (density) at which the cluster size distribution becomes critical, with a exponent 4/3. Below the critical point, the cluster size distribution is exponential and the system exhibits a characteristic cluster size. Above the critical point, the cluster size distribution can be well fitted by a power-law with a second peak at large cluster sizes. The exponent of the power-law is a function of the noise intensity, resp. of particle density.

DY 2.7 Mon 12:00 H45

A Colloidal Approach to Protein Adsorption — •Olaf Leidinger and Ludger Santen — Fachrichtung Theoretische Physik, Universität des Saarlandes

We investigate the unspecific adsorption of proteins, which are modeled as polydisperse colloidal particles. The particle-particle interactions are described in the framework of the DLVO theory, including steric repulsion, electrostatic and van der Waals interactions. Furthermore we introduce internal degrees of freedom representing different conformations of the model proteins at the surface.

By means of extensive Monte Carlo simulations we reproduce the experimentally observed characteristics of the biofilm-formation[1,2]. The adsorption kinetics can be divided into three intervals: Initially the adsorption is limited by the flux of particles to the surface. At low concentrations the proteins spread at the surface in order to opti-

mize the binding to the surface. At higher concentrations the adsorbed proteins are compacted due to particle-particle interactions and finally the surface coverage saturates. These dynamical regimes can be identified in experimental and theoretical investigations of the adsorbed amount. The comparison between experimentally and theoretically generated biofilms is completed by a detailed analysis of the point patterns connected to the adsorbed particles, which is carried out by means of integral measures.

[1] A. Quinn et al 2008 EPL 81 56003 (6pp)
[2] M Bellion et al 2008 J. Phys.: Condens. Matter 20 404226 (11pp)

DY 2.8 Mon 12:15 H45

All-or-none protein-like folding transition of a flexible homopolymer chain — •Wolfgang Paul[1], Mark Talor[2], and Kurt Binder[3] — [1]Institut für Physik, Martin-Luther-Universität, 06099 Halle — [2]Department of Physics, Hiram College, Hiram, Ohio 44234, USA — [3]Institut für Physik, Johannes-Gutenberg-Universität, 55099 Mainz

We report a first-order all-or-none transition from an expanded coil to a compact crystallite for a flexible polymer chain. Wang-Landau sampling is used to construct the complete density of states for square-well chains up to length 256. Analysis within both the microcanonical and canonical ensembles shows a direct freezing transition for finite length chains with sufficiently short-range interactions. This type of transition is a distinctive feature of "one-step" protein folding and our findings demonstrate that a simple homopolymer model can exhibit protein-folding thermodynamics. We also discuss how this finding depends on the range of the attractive interaction. Chains assume an expanded coil conformation at high temperatures and a crystallite structure at low temperatures. For large well diameters, with decreasing temperature a chain undergoes a continuous coil-globule (collapse) transition followed by a discontinuous globule-crystal (freezing) transition. For small well diameters the collapse transition is preempted by the freezing transition and thus there is a direct first-order coil-crystal phase transition.

DY 2.9 Mon 12:30 H45

Genome Folding at the 30 nm Scale — •Philipp M. Diesinger[1] and Dieter W. Heermann[2] — [1]Institute of Theoretical Physics, Heidelberg, Germany / MIT, Cambridge, USA — [2]Institute of Theoretical Physics, Heidelberg

We present a Monte Carlo model for genome folding at the 30-nm scale with focus on linker-histone and nucleosome depletion effects. Depletion of linker histones and nucleosomes affects, massively, the flexibility and the extension of chromatin fibers. Increasing the amount of nucleosome skips can lead either to a collapse or to a swelling of chromatin fibers. We show that depletion effects may even contribute to chromatin compaction. Furthermore, we find that predictions from experimental data for the average nucleosome skip rate lie exactly in the regime of maximum chromatin compaction.

We determine the nucleosome pair distribution function of chromatin. We show that chromatin nanostructure might in principle be accessible by 2D high-resolution light microscopy: Our simulations show that even in the case of fibers with depletion effects and after a projection, the main dominant peaks can still be identified.

Furthremore, we compare our simulations with 5C data of a gene desert as well as FISH data and find that only fibers with random depletion of linker histones or nucleosomes can explain the probability of random chromatin contacts on small length scales that play an important role in gene regulation. Missing linker histones and nucleosomes might not just be randomly occuring simple unavoidable defects but instead they might even play a regulatory role in gene expression.

DY 2.10 Mon 12:45 H45

Statistical aspects of trypanosome's motility — •Vasily Zaburdaev[1,2], Sravanti Uppaluri[3], Thomas Pfohl[3,4], Markus Engstler[5], Holger Stark[2], and Rudolf Friedrich[6] — [1]Harvard University, Cambridge, USA — [2]Technical University of Berlin, Berlin, Germany — [3]MPI for Dynamics and Self-Organization, Göttingen, Germany — [4]University of Basel, Basel, Switzerland — [5]University of Würzburg, Würzburg, Germany — [6]University of Münster, Münster, Germany

Trypanosome is a parasite causing the sleeping sickness. The way it moves in the blood stream and penetrates various obstacles is the area of active research. Our goal was to investigate a free trypanosomes' motion in the planar geometry. Our analysis of trypanosomes' trajectories reveals that there are two correlation times - one is associated with a fast motion of its body and the second one with a slower rotational diffusion of the trypanosome. We propose a system of Langevin equations to model such motion. One of its peculiarities is the presence of multiplicative noise predicting higher level of noise for higher velocity of the trypanosome. Theoretical and numerical results give a comprehensive description of the experimental data such as the mean squared displacement, velocity distribution and auto-correlation function.