# BP 18: Posters: Statistical Physics in Biological Systems

Time: Wednesday 17:30-19:30

BP 18.1 Wed 17:30 Poster A	BP 18.1	Wed 17:30	Poster A
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Adaptive walks and extreme value theory — •JOHANNES NEI-DHART and JOACHIM KRUG — Institut für Theoretische Physik, Universität zu Köln, Deutschland

We study biological evolution in a high-dimensional genotype space in the regime of rare mutations and strong selection. The population performs an uphill walk which terminates at local fitness maxima. Assigning fitness randomly to genotypes, we show that the mean walk length is logarithmic in the number of initially available beneficial mutations, with a prefactor determined by the tail of the fitness distribution. This result is derived analytically in a simplified setting where the mutational neighborhood is fixed during the adaptive process, and confirmed by numerical simulations.

#### BP 18.2 Wed 17:30 Poster A

**Emergence of stable epidemic oscillations due to a small** weather-based parametric excitation — •EUGENE POSTNIKOV and DMITRY TATARENKOV — Staatliche Universität Kursk, Kursk, Russland

The problem of mathematical description of seasonal epidemics of common diseases, e.g. flu, is one of hot topics joining mathematical epidemiology and theory of dynamical systems. The known results of stochastic simulations [Dushoff et al., 2004] demonstrate an evidence of 1:1 dynamical resonance between periods of parameter and solution variations. At the same time a deterministic model revealing this property is still an open problem.

We present the model based on SIRS (Susceptible-Infected-Recovered-Susceptible) approach:  $\dot{S} = -kIS + \theta^{-1}R, \dot{I}dt = kIS - \tau^{-1}I, \dot{R} = \tau^{-1}I - \theta^{-1}R (S + I + R = 1)$  with the variable parameter  $k = k_0 [1 + \delta \sin(\omega t)]$ . It has been shown that that this system can be transformed into the second-order non-autonomous ODE with free the term  $R_s \theta^{-1} \tau^{-1} \sin(\omega t)$ , where  $R_s$  is a fixed point for R in the case  $k = k_0 = \text{const.}$  In other words, the proposed coordinate transformation reveals the used parametrical excitation as a kind of outer one that allow us to clarify 1:1 character of the resonance.

To prove the obtained model, we analyze data on flu dynamics obtained from Google Flu Trends and corresponding weather conditions (mean temperature and humidity) from European Climate Assessment & Dataset. The processing of these curves confirms the proposed mathematical model.

# BP 18.3 Wed 17:30 Poster A

**Correlated mutations in protein sequences due to stability constraints** — •JONAS MINNING<sup>1</sup>, UGO BASTOLLA<sup>2</sup>, and MARKUS PORTO<sup>3</sup> — <sup>1</sup>Technische Universität, Darmstadt, Germany — <sup>2</sup>Centro di Biología Molecular, 'Severo Ochoa', CSIC-UAM, Madrid, Spain — <sup>3</sup>Universität zu Köln, Germany

Correlations between amino acids at different sites in protein sequences of the same protein family may yield important information on the protein three-dimensional structure and its evolution. We recently proposed an analytical approach which allows to quantitatively predict correlations that arise from selective constraints on unfolding and misfolding stabilities. Our approach is based on a cluster expansion of sequence entropy up to pairwise terms, with stability constraints represented through Lagrange multipliers. These Lagrange multipliers can be obtained either directly from data of correlated mutations or via the constraints on the cumulants of the partition function of the native and the misfolded ensemble, yielding very similar values. We show that in the latter case, the constraints can be written in good approximation as linear functions of the Lagrange multipliers, and that the coefficients quantify the strength of selective constraints on unfolding and misfolding stabilities on the correlation.

#### BP 18.4 Wed 17:30 Poster A

Emergence of robustness against noise: A structural phase transition in evolved models of gene regulatory networks — •TIAGO P. PEIXOTO — Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, D-28359 Bremen, Germany

We investigate the evolution of Boolean networks subject to a selective pressure which favors robustness against noise, as a model of evolved genetic regulatory systems. By mapping the evolutionary process into a statistical ensemble, and minimizing its associated free energy, we find the structural properties which emerge as the selective pressure is increased, and identify a phase transition from a random topology to a "segregated core" structure, where a smaller and more densely connected subset of the nodes is responsible for most of the regulation in the network. This segregated structure is identical to what is found in gene regulatory networks, where only a much smaller subset of genes — those responsible for transcription factors — is responsible for global regulation. We obtain the full phase diagram of the evolutionary process as a function of selective pressure and the average number of inputs per node. We compare the theoretical predictions with Monte-Carlo simulations of evolved networks, and with empirical data for Saccharomyces cerevisiae and Escherichia coli.

References:

[1] Tiago P. Peixoto, "Emergence of robustness against noise: A structural phase transition in evolved models of gene regulatory networks", arXiv:1108.4341

BP 18.5 Wed 17:30 Poster A Evolution of drug resistance in a spatially structured environment — •BARTLOMIEJ WACLAW, PHILIP GREULICH, and ROSALIND ALLEN — School of Physics, University of Edinburgh

Evolution of drug-resistant cells is an increasingly important problem in our quest to combat diseases such as bacterial infections or cancer. Many methods have been proposed to circumvent this problem, ranging from switching the drug periodically on and off, using a combination of drugs, or alternating drugs belonging to different classes. However, the majority of these studies (experimental and theoretical) have been carried out for well-mixed populations with spatially uniform distribution of the drug. Here we theoretically analyse the effect of a non-uniform distribution of a drug (e.g. an antibiotic) on the emergence of resistance to it, in a spatially structured population of malignant cells. Motivated by recent experiments on bacteria, we propose a simple stochastic model in which pathogenic microbes replicate, mutate, die and migrate in a box in which the antibiotic concentration changes in space from sub-lethal to overkill levels. We assume that resistance occurs by a sequence of consecutive mutations. Depending on the resistance levels of intermediate mutants (the "pathway to resistance"), we show that heterogeneous drug distribution can either dramatically speed up or slow down the evolution of resistance compared to the case of uniform distribution. We also discuss practical implications of our results for various modes of disease treatment.

BP 18.6 Wed 17:30 Poster A Fluctuations in meta-population transport models — •TOBIAS GALLA — Complex Systems and Statistical Physics Group, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom

We introduce meta-population models of transport processes. Particles move along a chain of cells, each of which can hold a number of particles up to a maximum carrying capacity. Particles can only advance along the chain if the patch ahead is not fully occupied. Viewing each patch as a separate population of particles this effectively generates a 'population of interacting populations', hence the term meta-population. Based on a master equation approach and a subsequent system-size expansion we compute the spectral properties of fluctuations in such models about their naive deterministic limit. This naive limit corresponds to models with an infinite patch size. The other extreme, a carrying capacity of one, on the other hand reproduces commonly used single-occupancy models. Our approach allows one to interpolate between the two limits. Specific applications we will discuss include asymmetric exclusion processes with single or multiple types of particles, frequently used as stylized models of biological transport.

BP 18.7 Wed 17:30 Poster A Thin Films of chiral Fluids — •SEBASTIAN FÜRTHAUER<sup>1,2</sup>, MARIA STREMPEL<sup>1,2</sup>, STEPHAN W. GRILL<sup>1,2</sup>, and FRANK JÜLICHER<sup>1</sup> — <sup>1</sup>Max Planck Institut für die Physik komplexer Systeme, Dresden — <sup>2</sup>Max Planck Institut für Molekulare Zellbiologie und Genetik, Dresden

Hydrodynamic flows in biological systems are often generated by active chiral processes near or on surfaces. Important examples are beating cilia, force generation in actomyosin networks, and motile bacteria in-

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teracting with surfaces. We develop a coarse grained description of active chiral films that captures generic features of flow and rotation patterns driven by chiral motors. We discuss force and torque balances within the film and on the surface and highlight the role of the intrinsic rotation field. We arrive at a two dimensional effective theory and discuss our results in the context of ciliary carpets and thin films of bacterial suspensions.

# BP 18.8 Wed 17:30 Poster A

Nucleation of ligand-receptor-domains in membrane adhesion — ●TIMO BIHR<sup>1</sup>, UDO SEIFERT<sup>1</sup>, and ANA-SUNČANA SMITH<sup>2</sup> — <sup>1</sup>II. Institut für Theoretische Physik, Universität Stuttgart — <sup>2</sup>Institut für Theoretische Physik and Excellence Cluster: Engineering of Advanced Materials, Universität Erlangen-Nürnberg

We investigate the nucleation of adhesion domains consisting of ligandreceptor bonds forming between membranes that also interact by a nonspecific potential. We first determine the critical size of the nucleus within the capillary approximation. The time evolution of the nucleation process is considered to take place in a number of ratedependent coupled stochastic events, each denoting the association or dissociation of a bond. The effective rates for each of these events are calculated by taking into account the membrane deformation and fluctuations. Based on these rates, we construct a discrete master equation from which the characteristic nucleation time is obtained numerically or as an analytic estimate. We validate our model by performing extensive Langevin simulations of an adherent fluctuating membrane, including the ligand-receptor unbinding. We find excellent agreement between the different approaches, particularly in the regime of strong intra-bond correlations.

We show that for experimentally relevant parameters a stable nuclei consists typically of only a few bonds. Furthermore, we find a strong dependence of the characteristic nucleation time on the distance between the receptors which could explain some of the recurrent threshold length-scales in cell adhesion assays.

#### BP 18.9 Wed 17:30 Poster A

The effect of metabolic theory on life histories — •YIXIAN SONG<sup>1</sup>, STEFAN SCHEU<sup>3</sup>, and BARBARA DROSSEL<sup>2</sup> — <sup>1</sup>Max Planck Institute for Evolutionary Biology, Plön, Germany — <sup>2</sup>Institute for Condensed Matter Physics at Darmstadt University of Technology, Darmstadt, Germany — <sup>3</sup>J.F. Blumenbach Institute of Zoology and Anthropology at Georg-August University of Göttingen, Göttingen, Germany

We explore the consequences of metabolic theory on life histories and life history evolution. We use a mathematical model for an iteroparous species and its resources, taking into account the allometric scaling of consumption, metabolism and mortality with consumer body mass. Mortality is assumed to be density-dependent, and the dynamics of resources are explicitly modeled. We find that populations that have more or faster growing resources have a shorter life span and a higher mortality, and that populations with a larger adult biomass have a larger number of offspring per female and a larger biomass density. When we allow the adult body mass to evolve, it increases with time without limits. When we allow the offspring body mass to evolve, it becomes smaller. Both trends result from the allometric scaling of mortality and are kept in limits by trade-offs other than those included in our model.

# $BP 18.10 \quad Wed 17:30 \quad Poster A$

Nonequilibrium clustering of self-propelled particles — •FERNANDO PERUANI<sup>1</sup> and MARKUS BÄR<sup>2</sup> — <sup>1</sup>Universite de Nice -Sophia Antipolis, France — <sup>2</sup>Physikalisch-Technische Bundesanstalt, Braunschweig und Berlin, Germany

It is known from simulations and experiments that many systems of interacting self-propelled particles (SPP) exhibit two phases: i) a monodisperse phase where the cluster size distribution (CSD) is dominated by an exponential tail, and ii) an aggregated phase characterized by the presence of non-monotonic cluster size distributions with a peak at large cluster sizes. At the transition between these two phases, the CSD has a power-law shape with a critical exponent. This qualitative change in the functional form of the CSD can be used as a criterion to define the onset of collective motion in SPP systems as this change in the cluster-size distribution is connected with a strong increase of average cluster sizes. This criterion is particularly useful for application in experimental SPP system where other quantities indicating collective motion like a global orientational order parameter are often not observed. We show that a simple kinetic theory is sufficient to reproduce this transition and allows prediction of the exponent of the power-law of the CSD.

BP 18.11 Wed 17:30 Poster A Directed Transport of Confined Brownian Particles with Torque – •PAUL RADTKE and LUTZ SCHIMANSKY-GEIER — Institute of Physics, Humboldt University at Berlin, Newtonstr. 15, D-12489 Berlin, Germany

We consider the motion of Brownian particles who are confined in tunnel with differently shaped walls. The particles are driven by random fluctuations modeled by the Ornstein-Uhlenbeck process with given correlation time  $\tau_c$ . It is implemented as both a thermal and nonthermal process. Furthermore, the particles' trajectories possess a nonzero mean curvature.

We investigate numerically whether the particles diffuse symmetrically in both directions, or a net transport into one direction emerges. In this case our setup realizes a ratchet mechanism; random fluctuations in the thermodynamic nonequilibrium are rectified. For the nonthermal noise we find the emergence of transport. It is investigated with respect to the correlation time, the mean curvature and the tunnel's geometry. Eventually, the mechanism of the symmetry breaking is elucidated.

BP 18.12 Wed 17:30 Poster A Single-molecule FRET experiments analyzed by likelihoodbased methods — •BETTINA G. KELLER and FRANK NOÉ — Freie Universität Berlin, Arnimallee 6, 14195 Berlin

The conformational equilibrium of single molecules can be probed by a variety of experimental techniques, such as fluorescence resonance energy transfer (FRET) spectroscopy, fluorescence quenching or atomic force experiments. However, constructing a consistent kinetic model from the measured data is difficult because (i) the conformational states of the molecule are typically related to overlapping value ranges of the observable, (ii) single-molecule experiments suffer from a lowsignal to noise ratio, and (iii) the influence of measurement errors, as for example spectral cross-talk, on the signal is sizable. Likelihoodbased analysis methods, such as hidden Markov models, are much more apt in dealing with overlapping states than conventional histogram analyses. However, due to problems ii and iii, their application to experimental data has remained challenging. Using a novel likelihood function, which explicitly accounts for the background noise in the experimental signal, we have constructed hidden Markov models of single-molecule FRET data of two experimental systems: the presumed two-state folder rRNA three-helix junction and the ribozyme Diels-Alderase, known to show a complex folding behavior. The analyses reveal multi-state kinetic networks including transition rates, state life times, and associated FRET efficiencies. The networks are hierarchically organized, such that at low state resolution the results of conventional histogram analyses are largely recovered.

BP 18.13 Wed 17:30 Poster A Heterogeneous short-term plasticity enables spectral separation of information in the neural spike train — •FELIX DROSTE, TILO SCHWALGER, and BENJAMIN LINDNER — Bernstein Center for Computational Neuroscience, Haus 2, Philippstrasse 13, 10115 Berlin, Germany

In order to understand how information is processed in the brain, i.e. how signals are encoded, transmitted, and gated, it is vital to investigate how a single neuron responds to inputs that encode multiple signals. Here, we study a scenario in which a neuron receives two stimuli through populations of facilitating and depressing synapses, respectively. We show that this leads to a spectral separation of information into high and low frequency bands. This spectral separation is based on the respective other signal acting as a kind of noise in the disfavored frequency band. We also show that the total information transfer about one signal can still benefit from the presence of the other signal through a form of stochastic resonance.

BP 18.14 Wed 17:30 Poster A Dynamics of resting brain fluctuations — •VESNA VUKSANOVIC<sup>1,2</sup> and PHILIPP HÖVEL<sup>1,2</sup> — <sup>1</sup>Technische Universität Berlin, Germany — <sup>2</sup>Bernstein Center for Computational Neuroscience Berlin, Germany

Despite important progress over the last few years, brain functional connectivity at rest "i.e." under no stimulation and in the absence of any overt-directed behaviour, is still not well understood. In studies on goal-directed mental activity, spontaneous brain activity at rest has been considered as random enough to be averaged out across many trials. However, well organized spatio-temporal low-frequency fluctuations (<0.1 Hz) have been observed in blood-oxygen-level-dependent (BOLD) fMRI signal of human subjects during rest. These well organized patterns of activity, suggest the existence of underlying dynamics that governs intrinsic brain processes. Here, we address resting brain fluctuations in fMRI data proposing some possible routes of studying the underlying dynamics.

## BP 18.15 Wed 17:30 Poster A

**Understanding electrical currents in DNA translocation experiments** — •STEFAN KESSELHEIM and CHRISTIAN HOLM — Institut für Computerphysik, Universtät Stuttgart

DNA translocation through synthetic nanopores is considered a technologically promising candidate for rapid DNA sequencing and is physically interesting because the experiments allow to probe single DNA molecules. The most important observable, the electrolyte-based conduction is only partly understood. We analyze this situation from different perspectives and show many different effects are important: We discuss an complex interplay of attraction of counterions, steric exclusion of ions, hydrodynamic interactions, ion correlations and electrofriction. Our analysis tool is molecular dynamics simulation including hydrodynamic interaction by means of the Lattice-Boltzmann method.

#### BP 18.16 Wed 17:30 Poster A

Influence of dielectric background on biophysical simulations — •FLORIAN FAHRENBERGER and CHRISTIAN HOLM — Institut für Computerphysik, Universität Stuttgart, Deutschland

In today's computer simulations, especially in but not limited to biophysics, electrostatic interactions play a crucial role in the behaviour of experimentally relevant systems. They also take up a major amount of the computation time and are very complicated to parallelize.

We present an electrostatics algorithm that is intrinsically local and therefore straight forward to parallelize. One of the main advantages of the algorithm's locality is that one can apply spatially varying dielectric properties to the simulation background. For many coarse-grained simulations of biophysical systems this is of high interest, since the dielectric permittivity is directly dependent on the salt concentration in water, which can vary significantly in inhomogeneously distributed systems.

We present the theory behind this algorithm and show the influence of variations in salt concentration in some typical simulation setups.

### BP 18.17 Wed 17:30 Poster A

A facilitated diffusion model with two conformational states — ●MAXIMILIAN BAUER<sup>1</sup> and RALF METZLER<sup>2,3</sup> — <sup>1</sup>Physics Department, Technical University of Munich, Germany — <sup>2</sup>Institute for Physics and Astronomy, Potsdam University, Germany — <sup>3</sup>Physics Department, Tampere University of Technology, Finland

Transcription factors (TFs) such as the lac repressor find their target sequence on DNA at remarkably high rates. In the established facilitated diffusion model for this search process the TF alternates between three-dimensional diffusion in the bulk solution and one-dimensional sliding along the DNA chain. In similar models the TF was considered as being present in two conformations (search state and recognition state) between which it switches stochastically. Combining both approaches we obtain a generalised model, that comprises the previous models as special cases. We treat the bulk excursions explicitly for rod-like chains arranged in parallel and consider a simplified model for coiled DNA.

## BP 18.18 Wed 17:30 Poster A

Reduction of Scattered Light by Müller Cells in the Human Retina — •OLIVER BENDIX, RAGNAR FLEISCHMANN, and THEO GEISEL — Max Planck Institute for Dynamics und Self-Organization, Göttingen, Germany

It is a long standing question why in the mammalian eye photoreceptors are positioned at the back of the retina, forcing photons to travel through various neuronal layers of the retina before the light-sensitive rods and cones can detect them. Recent studies suggest that certain retinal glial cells – called Müller cells (MCs) – play an important role in answering that question. Recent experiments have suggested that MCs extracted from the retina can act as optical fibers [1].

To understand the light guiding properties of the MC in the natural

fluctuating optical environment, we developed a model to analyze the light reflection and transmission of MCs embedded in a random medium neuronal tissue. With these quantities and a simplified geometrical eye model we study how light is scattered in the eye. We found that MCs can lead to a substantial increase of the signal-tonoise ratio (SNR), the ratio of the intensity of direct incident light at a photoreceptor to the intensity of back-scattered light from other areas of the retina. The SNR is most pronounced in the vicinity of the fovea and can be more than an order of magnitude.

#### References

[1] Franze et. al., Müller cells are living optical fibers in the vertebrate retina. Proc. Natl. Acad. Sci. U.S.A. **104**, 2007.

BP 18.19 Wed 17:30 Poster A Short Range Interaction Dynamics of Colloidal Particles in a Single Optical Potential — •BENJAMIN TRÄNKLE and ALEXAN-DER ROHRBACH — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

In many biological systems, binding and unbinding events are of vital importance. Here, the accomplishment of initial contacts not only depend on a time independent association probability, but also on time dependent conformational changes of the interaction partners and therefore on a interaction duration  $\tau_{on}$ . Furthermore, interaction dynamics are affected by long and short ranging forces, such as hydrodynamic, entropic and steric forces. Colloidal particles can serve as a model system for the investigation of such interaction events. We measure the 3D trajectories of two particles in a single potential, which is generated by an oscillating optical line trap. In this geometry, the reaction rate is increased due to the confined space, while rotational and translational degrees are preserved. With our setup, we can trap multiple beads and analyse particle motions at a spatial precision in the nanometer range and scanning frequencies up to 10 kHz. We show how various controls, i.e. the reaction volume or inter-particle potentials affect the interaction duration  $\tau_{on}$ .

BP 18.20 Wed 17:30 Poster A Neural dynamics during sleep: state switching and oscillations — •JENS CHRISTIAN CLAUSSEN — Institut für Neuro- und Bioinformatik, Universität zu Lübeck

The mammalian brain during sleep exhibits various interesting dynamical phenomena including switching processes from the neural microscale [1] to collective phase transitions, which, including regulatory mechanisms, give rise to the sleep-wake cycle. In addition, sleep state switching shows stochasticity [2,3]. On the time scale, the processes are separated from spikes (1ms) to spindle and burst lengths (1s) [4,5] via sleep states (100-10000s) to the ultradian (1.5h) and circadian rhythm. Sleep-associated oscillations are also separated in the frequency domain, and show rich complexity [3] including entrainment of spindles (12-15 Hz) by slow oscillations (0.8 Hz) [6]. In some cases, these oscillations can be influenced by electrical stimulation, observing a significant phase-dependence [4].

J. Mayer et al, PRE 73, 0131908 (2006), [2] Lo et al. EPL 57, 625 (2002), [3] E. Olbrich, J.C. Claussen, P. Achermann, Phil. Trans. Roy. Soc. A 369, 3884 (2011), [4] A. Weigenand, T. Martinetz and J.C. Claussen (subm.), [5] H.-V. Ngo et al, EPL 89, 68002 (2010), [6] J. Mayer et al, PRL 99, 068102 (2007)

BP 18.21 Wed 17:30 Poster A Effects of interactions between ion channels on neuronal dynamics — •Ekaterina Zhuchkova, Dmitry Zarubin, and Susanne Schreiber — Institute for Theoretical Biology, Humboldt-Universität zu Berlin and BCCN Berlin, Germany

Electrical signaling in our brain and heart relies on the opening or closing of individual stochastic units, so-called ion channels. Since Hodgkin and Huxley's model of action potential (AP) initiation, the prevailing assumption is that ion channels act independently; they change their open probability in response to a common signal such as the membrane voltage, but do not directly influence each other. However, evidence for additional interactions between channels accumulates.

Consequences of such enhancing or hindering interactions between ion channels for neuronal spiking dynamics can be expected. Nevertheless, they have so far received relatively little attention in the analysis of excitable membranes. Here, we use bifurcation analysis and stochastic simulations of an extended Morris-Lecar model to understand how cooperative and anticooperative gating between ion channels changes basic sub- and suprathreshold voltage dynamics. The effects of channel interactions include the modification of the range of sustained firing and cell-intrinsic noise, the prolongation of AP duration, the occurrence of multistability and type-3-like firing. We hypothesize that channel interactions could be an efficient mechanism to regulate neuronal activity.

Acknowledgments.—Funded by BMBF (01GQ0901, 01GQ1001A, 01GQ0972).

# BP 18.22 Wed 17:30 Poster A

Modeling the swimming African Trypanosome using mulitparticle collision dynamics — •SUJIN BABU and HOLGER STARK — Institute for Theoretical Physics, Technische University Berlin, D-10623 Berlin, Germany

The African Trypanosome is a unicellular organism which attacks the central nervous system of humans, causing the deadly disease called the sleeping sickness. The spindle-shaped flexible cell body of the African Trypanosome possesses some bending rigidity due to its cytoskeleton. A single flagellum runs from the posterior end to the anterior end of the cell body and is firmly attached to it. By propagating a wave along the flagellum from the anterior to the posterior end, the Trypanosome propels itself. However, the details of how the flagellum is attached to the cell body and its propulsion mechanism is still under debate. Our goal is to study a model Trypanosome in its viscous environment. We model the cell body and the flagellum (attached either straight or helical to the cell body) as a mesh of vertices connected by springs with some resistance to bending. A bending wave passing through the flagellum propels the organism in the direction opposite to the propagating wave. We simulate the flow field around the model Trypanosome using the method of multi-particle collision dynamics, which is an effective solver for the Navier-Stokes equations. We will demonstrate that our model is able to reproduce the experimental results both qualitatively and quantitatively. We will also show that the so called sperm number used in resistive force theory reveals a characteristic scaling in the dynamics of such a self-propelled elastic body.

#### BP 18.23 Wed 17:30 Poster A

Identification of Metastable States through dynamical clustering of Free Energy Landscape of Biomolecules — • ABHINAV JAIN and GERHARD STOCK — Biomolecular Dynamics, Institute of Physics, Albert Ludwigs University, 79104 Freiburg.

Recent simulation of peptides, proteins and RNA have shown that in many cases the free energy landscape can be well characterized in terms of metastable conformational states. They can be employed to construct transition networks of the system, reveal relevant pathways, and influence the average folding times by means of kinetic traps. We introduce a new approach that consists of (i) initial preprocessing to reduce the dimensionality of the data via principal components analysis, followed by k-means clustering to generate microstates [1], (ii) the most probable path algorithm to identify the metastable states of the system, and (iii) boundary corrections of these states to obtain the correct dynamics. The potential of the method is demonstrated with application to the villin headpiece subdomain.

[1] Jain; Hegger; Stock. J. Phys. Chem. Lett. 2010, 1, 2769 - 2773

BP 18.24 Wed 17:30 Poster A

Poisson ratio and local stress in the phospholipid membrane — •TAYEBEH JADIDI<sup>1</sup>, ALIREZA MASHAGHI<sup>2,3</sup>, HAMID SEYYED-ALLAEI<sup>4</sup>, PHILIPP MAASS<sup>1</sup>, and MOHAMMAD REZA RAHIMI TABAR<sup>1,4</sup> — <sup>1</sup>university of osnabrueck, osnabrueck, Germany — <sup>2</sup>FOM Institute AMOLF, Science Park 104, 1098XG Amsterdam, The Netherlands — <sup>3</sup>ETH Zürich, Department of Materials, Wolfgang-Pauli-Strasse 10, CH-8093 Zürich, Switzerland — <sup>4</sup>Department of Physics, Sharif University of Technology, 11365-9161, Tehran, Iran

We calculate the poisson's ratio and local stress tensor of the lipid bilayer membrane at gel-, fluid-, interdigitated- and ripple phases. We propose a general algorithm for calculating Poisson's ratio for membranes with periodic boundary conditions; we show that gel-phase lipid membranes has a positive Poisson's ratio and therefore do not behave like crystalline (polymerized) membranes. The distribution of locally stored energy is calculated from the stress tensor for membrane at different phases and the stability of the ripple phase is studied by determining the ripple-gel transition energy barrier. Finally we report on the thermal expansivity of the lipid membrane.

BP 18.25 Wed 17:30 Poster A Stochastic bifurcations in biological systems — •Anna Zakharova<sup>1</sup>, Aneta Koseska<sup>1</sup>, Juergen Kurths<sup>2,3</sup>, and Tatyana  $\label{eq:Vadivasova} \begin{array}{l} {\rm Vadivasova}^4 ~ - ~^1{\rm Center} ~ {\rm for} ~ {\rm Dynamics} ~ {\rm of} ~ {\rm Complex} ~ {\rm Systems}, ~ {\rm University} ~ {\rm of} ~ {\rm Potsdam}, ~ {\rm Potsdam}, ~ {\rm Germany} ~ - ~^2{\rm Potsdam} ~ {\rm Institute} ~ {\rm for} ~ {\rm Climate} ~ {\rm Impact} ~ {\rm Research}, ~ {\rm Potsdam}, ~ {\rm Germany} ~ - ~^3{\rm Institute} ~ {\rm of} ~ {\rm Physiscs}, ~ {\rm Humboldt} ~ {\rm University} ~ {\rm Berlin}, ~ {\rm Berlin}, ~ {\rm Germany} ~ - ~^4{\rm Saratov} ~ {\rm State} ~ {\rm University}, ~ {\rm Saratov}, ~ {\rm Russia} ~ {\rm Saratov}, ~ {\rm Saratov}$ 

The influence of noise on nonlinear dynamical systems is one of the most relevant and intensively developing research directions of nonlinear dynamics. The investigation of stochasticity is very important for understanding the dynamical features of real systems, since they are inevitably affected by noise. In the present work we define a concept of stochastic bifurcations as an approach to the analysis of noisy systems. First, we apply this method to a Duffing-Van der Pol oscillator and further extend it to biological systems. On the example of gene relaxation oscillator we demonstrate that a concept of stochastic bifurcations is suitable to investigate the dynamical structure of cellular networks. Furthermore, we show that under stochastic influence the expression of given proteins is defined via the probability distribution of the phase variable, representing one of the genes consisting the system. Moreover, for the isochronous case we found out the presence of coherence resonance-like (CR-like) effect. We also show that under changing stochastic conditions the probabilities of expressing certain concentration values are different, leading to different functionality of the cells, and thus to differentiation of the cells in the various types.

BP 18.26 Wed 17:30 Poster A Non-Equilibrium Phase Transition in a Biofilm Growth Model — •FLORENTINE MAYER and ERWIN FREY — Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), Department of Physics, Ludwig-Maximilians-Universität München, Germany

Biofilms show remarkable resistance to environmental stress as, for example, introduced by antibiotics. This is because biofilms promote growth by diversifying cells: faster growing, more sensitive phenotypes are protected by resistant phenotypes. As environmental conditions change, the fitness of phenotypes may change, which increases the benefit of heterogeneous populations. While models for well-mixed systems reproduce the advantage of heterogeneity in changing environments, the situation for spatial settings has received less attention so far. To analyze biofilm growth we set up a two-species automaton model in which growth and death rates depend on the environmental conditions. These fluctuate, resulting in periodically interchanged growth and death rates of the two phenotypes. Depending on the rates we find either fast extinction or thriving biofilms with intriguing spatio-temporal patterns. Close to the region of extinction patterns become self-affine, which is the hallmark of a phase transition to an absorbing state (i.e. an empty lattice). Employing extensive stochastic simulations we measure critical exponents of our non-equilibrium phase transition and find universal scaling behavior, which characterises the universality class of our model.

BP 18.27 Wed 17:30 Poster A Physical description of centrosome assembly using a phase separation process — •DAVID ZWICKER<sup>1</sup>, MARKUS DECKER<sup>2</sup>, STEFFEN JAENSCH<sup>2</sup>, ANTHONY HYMAN<sup>2</sup>, and FRANK JÜLICHER<sup>1</sup> — <sup>1</sup>Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — <sup>2</sup>Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

The size of many cell organelles is strongly correlated with cell size. Achieving this requires a robust mechanism for organizing and scaling subcellular structures. Here, we propose a theoretical description of the growth phase of the centrosome, an organelle involved in mitosis. We identify a possible mechanism based on phase separation by which the centrosome volume may be controlled. Specifically, a chemical reaction driving the phase separation process accounts for the temporal and spatial evolution observed in experiments. We also take surface tension effects into account.

Our theory explains the growth dynamics of centrosomes for all cell sizes down to the sixteen cell stage of the C. elegans embryo, and it also accounts for data acquired in experiments with aberrant numbers of centrosomes and altered cell volumes. Furthermore, the model can describe the dissolution phase occurring during cell division and unequal centrosome sizes observed in cells with disturbed centrioles.

BP 18.28 Wed 17:30 Poster A **Cell-Cell-Desynchronization in Yeast Cell Populations** — •ANDRÉ WEBER<sup>1,2</sup>, WERNER ZUSCHRATTER<sup>2</sup> und MARCUS HAUSER<sup>1</sup> — <sup>1</sup>Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany —  $^2 {\rm Leibniz-Institut}$ für Neurobiologie Magdeburg, Germany

Colonies of the yeasts Saccharomyces carlsbergensis and Saccharomyces cerevisiae have been used as stable model organisms to investigate glycolytic oscillations over years. The dynamics of the cell population depend on the cell density: At high cell densities all cells of the population show synchronous and coherent oscillations, which can be detected as global oscillations. The collective behaviour ceases at a critical, low cell density, but the nature of the dynamics at single cell level remained an open question. Recent reports predicted a 'quorum sensing' mechanism, where all cells stop oscillating synchronously below the quorum. Using single photon counting fluorescence microscopy, we study the dynamics of individual yeast cells at low cell densities for both yeast strains. Our focus lies in elucidating the mechanism of the transition between individual and collective dynamics. At very low cell densities, the individual cells still perform metabolic oscillations, the frequencies of which show a very broad distribution. Thus the cells oscillate in a desynchronous fashion. As the cell density increases, we observe that the frequency distribution narrows and synchronized collective behaviour sets in. We can preclude a dynamical quorum sensing phenomenon for glycolytic oscillations in yeast strains S. carlsbergensis and S. cerevisiae.

## BP 18.29 Wed 17:30 Poster A

**Dynamics of a spherical microswimmer in Poiseuille flow** — •ANDREAS ZÖTTL and HOLGER STARK — Institut für Theoretische Physik, TU Berlin

Microorganisms in the human body have to respond to confining boundaries and fluid flow, like sperm cells in the Fallopian tube or pathogens in blood vessels. Also, artificial microswimmers would have to swim in narrow channels like arteries if one day they may be used as drug deliverers in the human body. Due to vorticities in the flow field and hydrodynamic interactions with bounding surfaces, microswimmers change their swimming speeds and orientations.

To capture both effects of fluid flow and confinement, we analyze the dynamics of a spherical microswimmer in Poiseuille flow, moving in a cylindrical microchannel. Neglecting the finite extent of the swimmer and its hydrodynamic interaction with the bounding wall, the dynamic equation for a swimmer in 2D is given by a simple pendulum equation. Swimmers swing around the centerline of the channel while oriented upstream, or tumble when the flow is strong enough. In 3D the swimmer can perform helical and helical-like trajectories while its angular momentum is conserved. Accounting also for hydrodynamic interactions between the swimmer and the wall, we show that *pushers* such as sperm cells or bacteria and *pullers* like the algae *Chlamydomonas* show different behavior. We find that upstream motion in the center of the channel is stabilized for pullers but becomes unstable for pushers which move on a stable limit cycle.

## BP 18.30 Wed 17:30 Poster A

Langevin Modeling of Biomolecular Dynamics — •NORBERT SCHAUDINNUS<sup>1</sup>, RAINER HEGGER<sup>2</sup>, and GERHARD STOCK<sup>1</sup> — <sup>1</sup>Biomolecular Dynamics, Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — <sup>2</sup>J.W. Goethe University, Institute for Physical and Theoretical Chemistry, Maxvon-Laue-Str. 7, 60438 Frankfurt/Main

Principal component analysis is widely used to obtain coordinates that monitor essential dynamics of high-dimensional biomolecular systems. Applying this technique to MD simulations of various peptides allows a separation of slow large-amplitude motions and high-frequency fluctuations [1]. A Langevin simulation on the first few principal components using local estimates of drift and diffusion fields is shown to reproduce the conformational dynamics of those peptides [2]. Particularly, a set of short trajectories can be used instead of one continuous trajectory as input. We demonstrate thermodynamical characteristics of the studied peptide systems revealed by this method. Furthermore, we present first attempts to construct an analytical model to characterize the free energy landscape.

[1] A. Altis, M. Otten, P.H. Nguyen, R. Hegger and G. Stock, J. Chem. Phys. 128, 245102 (2008)

[2] R. Hegger and G. Stock, J. Chem. Phys. 130, 034106 (2009)

BP 18.31 Wed 17:30 Poster A The dynamics of stochastic slowdown in evolutionary processes — •PHILIPP M. ALTROCK<sup>1</sup>, TOBIAS GALLA<sup>2</sup>, and ARNE TRAULSEN<sup>1</sup> — <sup>1</sup>Max-Planck-Institute Evolutionary Biology, Plön — <sup>2</sup>School of Physics & Astronomy, University of Manchester We study the stochastic dynamics of evolutionary games, and focus on the so-called 'stochastic slowdown' effect, previously observed in (Altrock et al. 2010, PRE 82, 011925) for simple evolutionary dynamics. Slowdown here refers to the observation that a neutral mutation may fixate quicker than a beneficial one under certain forms of frequency dependent selection. More precisely the fixation time, conditioned on paths in which the mutant takes over, has a maximum value at intermediate selection strength. This phenomenon is present in the prisoners dilemma game. Additional analysis of a co-existence game reveals even more intricate behavior of the fixation times. In small populations, the conditional average fixation time shows multiple extrema as a function of the selection strength. We establish the microscopic origins of these phenomena and calculate the mean conditional sojourn times, identifying those transient states which contribute most to the slowdown effect.

BP 18.32 Wed 17:30 Poster A Predictability of evolution depends nonmonotonically on population size —  $\bullet$ Ivan G. Szendro<sup>1</sup>, Jasper Franke<sup>1</sup>, J. Ar-JAN G.M. DE VISSER<sup>2</sup>, and JOACHIM KRUG KRUG<sup>1</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Cologne, Germany — <sup>2</sup>Laboratory of Genetics, Wageningen University, The Netherlands

We study Wright-Fisher dynamics on an empirical 8-locus fitness landscape (FL) obtained experimentally for the filamentous fungus Aspergillus Niger. In order to measure predictability, we define entropy measures on the observed paths. We find a non monotonic dependance of the entropy on population sizes, N, for fixed mutation rates,  $\mu$ . The initial decrease of entropy and the subsequent increase, for ever larger N, are governed by the scales  $N\mu$  and  $N\mu^2$ , respectively, and the amplitude of this pattern is determined by the magnitude of  $\mu$ . We also study the departure from the strong selection weak mutation regime, when increasing N, for the probability of the largest subpopulation to end up on the wild type genotype. To show that our observations are generic, we compare our findings for the experimental FL with data obtained on a simple model landscape.

For optical neurostimulation, holograms have proven to be particularly efficient. Fast and flexible stimulation is crucial for e.g. controlled synaptic learning experiments. Since a spatial light modulator used for hologram generation can only shift phases, hologram computation is a complex process. Up to now, no direct method to determine a corresponding phase mask exists. Current algorithms consist of a series of iterative fourier transforms and projections, with sometimes very slow convergence speeds. Fortunately, the matrix formulation of existing algorithms is data-parallel and thus can directly be implemented on a GPU. We present a CUDA-based implementation for computing phase-only holograms which are used for a selective excitation of individual light-sensitive neurons. We focussed on a modular structure to be flexible for changing experimental hardware or for incorporating advancements in parallel computing or new algorithms. We compare the performance of the well-known GS algorithm [1] with the recently introduced Relaxed Averaged Alternating Reflections [2].

[1] R. W. Gerchberg and W. O. Saxton, Optik 35, 237 (1972)

[2] D. R. Luke, Inverse Problems **21**,37 (2005)

BP 18.34 Wed 17:30 Poster A **Describing non-linear attentional modulation patterns through ring-architecture neural circuits** — •MARKUS HELMER<sup>1,4</sup>, VLADISLAV KOZYREV<sup>2,3</sup>, STEFAN TREUE<sup>2,4</sup>, THEO GEISEL<sup>1,4</sup>, and DEMIAN BATTAGLIA<sup>1,4</sup> — <sup>1</sup>Max Planck Institute for Dynamics and Self-Organization, Göttingen — <sup>2</sup>Deutsches Primatenzentrum, Göttingen — <sup>3</sup>Institute of Neuroinformatics, Ruhr-University Bochum — <sup>4</sup>BCCN, Göttingen

We analyzed recordings in area MT from macaque monkeys performing a transparent motion task. They were presented random-dotpatterns (RDP) at two distinct locations within the receptive field of the recorded cell. Attention was directed to a fixation spot or to only one of the two RDPs. The angle between the two RDPs was kept fixed at 120 degrees so that covarying the motion directions provided tuning curves with two peaks. We found that the positions of the response peaks were different from what the single-motion orientationpreferences of the cell predicted. Furthermore they depended on the attentional condition, showing strong signatures of non-linear interactions during the integration of the two stimuli by MT neurons, including peak repulsion or attraction. By using a mean-field ring model, we could reproduce all the observed response non-linearities independently in broad regions of the parameter space. However, to find the specific combination of non-linearities observed across attentional conditions a fine tuning of the parameters was required. We explored therefore multi-areal network models with multiple coupled rings to achieve a more robust description of non-linear attentional modulation patterns.

## BP 18.35 Wed 17:30 Poster A

Modeling of the theta rhythm patterns in septo-hippocampal area — •SEBASTIAN MILSTER, ANASTASIA LAVROVA, and LUTZ SCHIMANSKY-GEIER — HU Berlin, Institut für Physik

Theta (3 - 12 Hz) and gamma (30 - 70 Hz) oscillations in rodent's hippocampal and septal areas have been throuroughly studied in vivo as well as in vitro. They occur during distinct cognitive states. It has been shown that theta and gamma oscillations in hippocampus are modulated by inhibitory inputs from the septum.

The focus of this work is to study the influence of the connection between the septum and the hippocampus CA3 area. We use the Hodgkin-Huxley equations to construct a minimal septo-hippocampal circuit. By changing the coupling strengths between the cells we define the parameter range at which different oscillatory regimes emerge. We analyze how the main characteristics of self-sustained oscillations as phase shift and frequency change at the switching between different rhythms. The model is to examine the mechanism of disinhibition and its contribution to the modulation of these rhythms.

## BP 18.36 Wed 17:30 Poster A

**Biocompatibility of Parylene-coated GaAs Substrates and Microtubes** — •CORNELIUS BAUSCH, ERIC STAVA, and ROBERT BLICK — Institute for Applied Physics, University of Hamburg

The strain caused by the mismatch of the lattice constants of two epitaxially grown semiconductor layers can be exploited to roll up microtubes. Recently, arrays of such semiconductor tubes have been fabricated as a method to create three-dimensional spatial confinement for in vitro neurite outgrowth. Thereby, the tube walls resemble the myelin sheath, which accelerates signal propagation through the axon.

Our rolled-up microtubes are fabricated from gallium arsenide, which is known to be toxic. Parylene C, a biocompatible, chemical vapor deposited poly(p-xylylene) polymer, can be used as a coating to prevent the poisonous effects of As. We test the biocompatibility of GaAs substrates coated with parylene by means of cell culture. Additionally, we test the layer quality of the parylene coating on the outside and inside of GaAs-semiconductor tubes.

[1] Yu, M. R. et al., Semiconductor Nanomembrane Tubes: Three-Dimensional Confinement for Controlled Neurite Outgrowth. Acs Nano 5, 2447-2457 (2011)

### BP 18.37 Wed 17:30 Poster A

Virtual Networks of In Vitro Neurons by Patterned Photostimulation — •KAI BRÖKING<sup>1,3,6</sup>, AHMED ELHADY<sup>1,2,5,6</sup>, RAGNAR FLEISCHMANN<sup>1</sup>, THEO GEISEL<sup>1,3,5,6</sup>, WALTER STÜHMER<sup>2,5,6</sup>, FRED WOLF<sup>1,3,5,6</sup>, and GERT RAPP<sup>4</sup> — <sup>1</sup>MPI für Dynamik und Selbstorganisation, Göttingen — <sup>2</sup>MPI für experimentelle Medizin, Göttingen — <sup>3</sup>Fakultät für Physik, Georg-August-Univ. Göttingen — <sup>4</sup>Rapp Opto-Electronic GmbH, Hamburg/Wedel — <sup>5</sup>Bernstein Center for Computational Neuroscience, Göttingen —  $^6\mathrm{Bernstein}$  Focus for Neurotechnology. Göttingen

Transfecting neurons with light-gated ion channels and -pumps, e.g. Channelrhodopsin2 [1], makes it possible to precisely control their activity noninvasively, by means of photostimulation.

Here, we present an experimental setup for the patterned photostimulation with continuous signals which can be modulated on the millisecond-scale. It allows to artificially link biological neurons into virtual networks of arbitrary topology. The setup consists of an LEDbased multi-spot illumination device, a data aquisition and processing unit, and a software system for input-driven stimulus generation. Local neural activity measured from neurons living on a grid of electrodes in a Multi-Electrode Array (MEA) is used to induce activity elsewhere in the culture by means of generating dynamic photostimulation signals as live feedback. We characterize the performance and limitations of our closed-loop feedback system with respect to latency, long-term stability, and photoelectric articfacts. [1] Boyden, E., et.al., Nat Neurosci 8, 1236-1268(2005), doi:10.1038/nn1525

BP 18.38 Wed 17:30 Poster A Modeling of rhythmic patterns in hippocampus — •ANASTASIA LAVROVA<sup>1</sup>, MICHAEL ZAKS<sup>2</sup>, and LUTZ SCHIMANSKY-GEIER<sup>1</sup> — <sup>1</sup>Institut für Physik, HU — <sup>2</sup>Institut für Mathematik

The hippocampal circuit can exhibit network oscillations in different frequency ranges (\*gamma\* - 30-80 Hz; \*theta\* - 4-12 Hz; as well as \*theta/gamma\* or a bursting regime) both in vivo and in vitro and switch between them. . The hippocampal neuronal network consists of various types of connected cells, which allows them to provide oscillations with different periods, amplitudes, and phase shifts.

We propose the minimalistic model for the description of generation of such polyrhythmic signals in the hippocampal area CA3. The network includes two fast- and two slowly-spiking cells which are described by the FitzHugh-Nagumo equations and coupled by means of synaptic connections. We analyze the influence of synaptic strengths on the synchronization in the network. Mechanisms of switching between different rhythms are discussed.

Signal processing in the brain builds up on biophysical principles that are the bases for essential features like protein targeting, voltage sensing and signal propagation amongst many others. Many open questions remain that are difficult to attack as the cellular environment is inherently complex.

In this study, an ex-vivo, bottom-up approach was pursued by reconstituting the purified voltage sensitive potassium channel of Aeropyrum pernix (KvAP) into cell-sized artificial lipid vesicles (giant unilamellar vesicles - GUVs). The next step is to gain electrical control over the system to investigate the function of voltage-gated ion channels (here KvAP), but also pumps and porins in the controlled ex-vivo environment. The prospect is then to create a model system for action potential propagation in a biomimetic axon that can be formed by pulling a lipid nano-tube from the giant vesicle thus providing a biomimetic neuronal geometry in which membrane curvature, lipid composition and protein concentration can be controlled in contrary to an in-vivo Neuron.

This work will contribute to our understanding of the effect of membrane morphology on ion channels distribution and provide experimental data for the theory of signal propagation with respect to axon diameter, morphology and stochastic noise.