BP 33: Statistical Physics in Biological Systems IV (joint with DY)

Time: Friday 9:30–12:45 Location: H44

BP 33.1 Fri 9:30 H44

Range expansions in heterogeneous environments — •Wolfram Möbius[1], Andrew W. Murray[2], and David R. Nelson[1] — [1]Department of Physics and FAS Center for Systems Biology, Harvard University, Cambridge, MA, USA — [2]FAS Center for Systems Biology and Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA, USA

How species invade new territories and how these range expansions influence a population's genetic diversity are important questions in the field of population genetics. While the majority of work addressing these questions focuses on well-mixed environments, populations on a set of islands, or spatially uniform environments, much less is known about the consequences of an expanding population encountering obstacles such as lakes or mountain ranges.

We employ both experimental and theoretical methods to better understand range expansions in such types of environments. In particular, we established a system of bacteriophage T7 and *E. coli* as a bench-scale model system: The bacteriophage population spreads on a lawn of susceptible bacteria while a region of resistant bacteria poses an obstacle to the population wave and determines its shape. We use reaction-diffusion modeling and a phenomenological description to complement the experimental results. In addition, stochastic modeling allows us to study the fate of individual alleles in the course of the range expansion.

BP 33.2 Fri 9:45 H44

Chemical Warfare and Survival Strategies in Bacterial Range Expansions — Gabriele Poxleitner[1], •Markus Felix Weber[2], Elke Hebisch[1], Erwin Frey[2], and Madeleine Leisner[1] — [1]Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, D-80539 Munich, Germany. — [2]Arnold-Sommerfeld Center for Theoretical Physics and Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 Munich, Germany.

Bacterial communities represent complex and dynamic ecological systems. Different environmental conditions as well as bacterial interactions determine the establishment and sustainability of bacterial diversity. We study the competition of three Escherichia coli strains during range expansions on agar plates. In this bacterial model system, a colicin E2 producing strain C competes with a colicin resistant strain R and with a colicin sensitive strain S for new territory. Genetic engineering allows us to tune the growth rates of the strains and to study distinct ecological scenarios. These scenarios may lead to either single-strain dominance, pairwise coexistence, or to the coexistence of all three strains. In order to elucidate the survival mechanisms of the individual strains, we developed a stochastic agent-based model to capture the ecological scenarios in silico. In a combined theoretical and experimental approach we are able to show that the level of biodiversity depends crucially on the composition of the inoculum, on the relative growth rates of the three strains, and on the effective reach of colicin toxicity.

BP 33.3 Fri 10:00 H44

Efficacy of ribosome-targeting antibiotics determined by a non-linear molecular race — •Philip Greulich[1,2], Martin R. Evans[2], and Rosalind J. Allen[2] — [1]Cavendish Laboratory, University of Cambridge — [2]School of Physics and Astronomy, University of Edinburgh

Many antibiotics in current clinical use target bacterial ribosomes. We present a dynamical model for the response of a cell to a ribosome-targeting antibiotic. In this model, the efficacy of the antibiotic is determined by a non-linear "molecular race" between binding of the antibiotic to ribosomes and net production of new ribosomes. The model points to a non-trivial growth-rate dependence of the minimum inhibitory concentration (MIC) and predicts a discontinuous transition at the MIC when the antibiotic concentration is varied: the growth rate abruptly drops to zero at this point. Furthermore, the efficacy of an antibiotic treatment depends on both its intensity and duration, and we can determine the relation to critical pharmacokinetic/-dynamic parameters for cell killing.

BP 33.4 Fri 10:15 H44

Information-theoretic vs. thermodynamic entropy production in autonomous sensory networks — •Andre Cardoso Barato and Udo Seifert — Universität Stuttgart, II. Institut für Theoretische Physik, Pfaffenwaldring 57 / III, D-70550, Stuttgart, Deutschland

Acquiring and processing information about the instantaneous state of the environment is a prerequisite for survival for any living system. Sensory and signal transducting networks have evolved to achieve this task under a variety of external conditions as, e.g., the work on bacteria like Escherichia coli has demonstrated so beautifully [1,2].

We determine the rate with which sensory networks acquire information about the changing external conditions. Comparing this rate with the thermodynamic entropy production that quantifies the cost of maintaining the network, we show that there is no universal bound restricting the rate of obtaining information to be less than this thermodynamic cost. These results obtained within a general bipartite model consisting of a stochastically changing environment that affects the instantaneous transition rates within the system are illustrated with a simple four-states model motivated by cellular sensing. On the technical level, we require and justify a new conjecture on the mutual information rate involving a non-Markovian process.

[1] H. C. Berg and M. Purcell, Biophys. J. 20, 193 (1977).

[2] G. Lan, P. Sartori, S. Neumann, V. Sourjik, and Y. Tu, Nature Phys. 8, 422 (2012).

BP 33.5 Fri 10:30 H44

Optimality principles for bacterial quorum sensing — •Bastian Drees and Ilka Bischofs — BioQuant, Center for Quantitative Analysis of Molecular and Cellular Biosystems at Heidelberg University, Heidelberg

Bacterial signaling networks have to meet the challenge of gathering information from noisy biochemical signals. We introduce a theoretical framework to quantify the accuracy of a signaling process in the presence of noise by defining the resolving power R, the minimal difference between two inputs that is required to separate two outputs. We show that many natural quorum sensing systems - which regulate cell density dependent behavior in bacteria - tend to optimize R at their switching points. We furthermore study how differences in the physical network design affect R as a function of input strength. We find different network architectures to optimize R in different input regimes, which could explain the diversity of quorum sensing architectures that is observed in nature. Together our results suggest the existence of a physics-driven optimal design principle for quorum sensing networks, which could be exploited to facilitate rational design choices in synthetic biology applications.

BP 33.6 Fri 10:45 H44

In vivo facilitated diffusion model — •Maximilian Bauer[1,2] and Ralf Metzler[1,3] — [1]Institute for Physics and Astronomy, Potsdam University, Germany — [2]Physics Department, Technical University of Munich, Germany — [3]Physics Department, Tampere University of Technology, Finland

In vitro transcription factors (TFs) alternate between three-dimensional bulk diffusion and sliding along DNA in order to quickly find their target on DNA. Recent experiments showed that also in the crowded interior of living cells TFs employ this facilitated diffusion mechanism. For a theoretical description of the situation in vivo we use a simple model of the bacterial genome embedded in an experimentally identified subvolume of the cell. Explicitly taking into account the configuration of DNA, our findings agree with experimental results and suggest that cells operate near to conditions which are optimal for target localization.

References: M. Bauer and R. Metzler, Biophys. J. 102, 2321 (2012) and submitted (2012)

BP 33.7 Fri 11:00 H44

Random walks of bacteria: How the motility pattern affects diffusion and chemotaxis — •Johannes Taktikos[1,2], Holger Stark[2], and Vasily Zaburdaev[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institut für Theoretische Physik, Technische Universität Berlin

The motility patterns of many bacterial species can be described with

the help of random walk models. Swimming *E. coli* bacteria alternate almost straight runs with tumbling events, which randomize the direction of cell motion but keep a certain persistence. The majority of marine bacteria fully reverse their swimming direction after a tumbling event. However, the swimming strategy of the marine bacterium *V. alginolyticus* was recently discovered to consist of a strict sequence of reversal and completely randomizing flick events between the runs [Xie *et al.*, PNAS **108**, 2246 (2011)]. Remarkably, all these bacteria are capable to undergo chemotaxis – the ability to adjust their swimming direction to the concentration gradient of certain chemicals. We propose a generalized random walk model describing these motility patterns and use it to characterize the diffusion process of bacteria moving in chemically neutral environments. In the presence of a small gradient of a signaling chemical we calculate the chemotactic drift velocity along the gradient and analyze how it depends on the particular motility pattern. Our calculations show that the motility pattern alone cannot explain experimentally observed differences in the chemotactic behavior of *E. coli* and *V. alginolyticus* bacteria. This result suggests that the chemotactic internal response function of both bacteria differ.

15 min break

BP 33.8 Fri 11:30 H44

Impact of the cell division cycle on the dynamics of gene expression — •Veronika Bierbaum and Stefan Klumpp — Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Am Mühlenberg 1, 14476 Potsdam

Cell growth and division are elementary processes that influcence gene expression: While proteins are being synthesized, the change in cell volume due to cell growth leads to a dilution of protein concentration. To maintain a stable amount of protein, the protein content has to be doubled during the cell cycle. In this way, upon division, each daughter cell initiates the new cycle with the same amount of each protein. Protein synthesis and cell growth are typically not synchronous, such that the protein concentration varies over the cell division cycle. This variation may have an impact on the function of gene regulatory circuits.

We have developed a theoretical description of genetic regulatory systems that explicitly considers the cell division cycle to investigate its impact onto both simple and regulated systems of gene expression. We calculate the cell-to-cell variations in protein content of cells at different stages in the division cycle, and discuss to which extent these variations contribute to the extrinsic noise observed in single-cell experiments. While positive autoregulation can amplify the variation in protein concentration over the division cycle, negative autoregulation buffers against such variation. In addition, we investigate how the variability in the concentration influences the stability phases of bistable autoregulated systems.

BP 33.9 Fri 11:45 H44

Deducing underlying mechanisms from protein recruitment data — •Laurin Lengert and Barbara Drossel — TU Darmstadt, Hessen

The technique of fluorescently labelling proteins made it possible to visualize cellular proteins and to measure their distribution and dynamics within the cell. We focus on protein recruitment to a region in the cell following a triggering event, such as irradiation. Often mechanistic models are used to fit the recruitment data. In such models, differential equations describe the changes in the concentrations of activated or bound proteins in the region of interest. The aim of such mechanistic models consists in evaluating rate constants, in identifying the proteins and reactions that are essential for the investigated process, and in obtaining evidence for processes that are not directly visible. By analyzing in a systematic way the recruitment curves generated by different simple models, we explain how the features of the recruitment curves reflect the properties of the underlying processes. This analysis also shows that a distinction between different models is not always possible from a given set of data. However, in many cases it is possible to suggest additional experiments with different protein concentrations that allow to distinguish between different models.

BP 33.10 Fri 12:00 H44

Scaling behaviour of knotted polymer rings in semidilute solutions — •Benjamin Trefz and Peter Virnau — Johannes Gutenberg Universität Mainz

Recently, the study of ring polymers and in particular their scaling behaviour in semidilute solutions [1, 2] has attracted considerable attention as a potential model system for the organization of DNA in chromosome territories. Building upon these studies, we investigate the influence of topology in melts of rings, which contain a certain knot type. These molecular dynamics simulations typically require around half a million particles as well as long run times and have been performed on graphic cards. Just like their unknotted counterparts, knotted rings form crumpled globules in the large N-limit. Knots tend to take up a large fraction of the chain for small rings, but become localized in the thermodynamic limit.

[1] J. Halverson, W. Lee, G. Grest, A. Grosberg, and K. Kremer, "Molecular dynamics simulation study of nonconcatenated ring polymers in a melt. I. Statics," The Journal of chemical physics, vol. 134, p. 204904, 2011.

[2] D. Reith, L. Mirny, and P. Virnau, "GPU Based Molecular Dynamics Simulations of Polymer Rings in Concentrated solution: Structure and Scaling," Progress of Theoretical Physics Supplement, vol. 191, pp. 135-145, 2011.

BP 33.11 Fri 12:15 H44

Molecular knots can pass through each other — •Peter Virnau and Benjamin Trefz — Uni Mainz

We propose a novel mechanism in which two molecular knots can pass through each other and effectively swap positions along a polymer strand. Associated free energy barriers in our molecular dynamics simulations only amount to a few k_BT, which may enable the interchange of knots on single DNA strands.

BP 33.12 Fri 12:30 H44

Sequence depending membrane-activity of amphiphilic polymers — •Marco Werner[1,2] and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Technische Universität Dresden, Germany

Using the bond fluctuation model with explicit solvent we investigate self-assembled bilayer membranes interacting with random copolymers of hydrophilic/-phobic monomers under variation of the fraction of hydrophobic monomers, H. Our simulation data indicates that polymers localize at the membrane-solvent interface for values of $H \gtrsim 1/2$, where the polymer forms excess blobs in the solvent- and lipid tail phases to increase the number of preferred contacts to both environments. Excess blobs with hydrophobic majority are inhibited to freely expand in the lipid tail phase due to the self-organized packing of lipids. Therefore, the number of preferred polymer-environment contacts is balanced on both sides for values of H slightly larger than $H = 1/2$. Here, the polymer shows the largest membrane-activity as indicated by a maximum of polymer-induced permeability for solvent. Testing a larger population of random polymer sequences we demonstrate that heterogeneity of the amphiphilic components of the polymer on a scale smaller than the lipid tail length is a key feature for polymer-induced bilayer perturbations. This seems to be confirmed by testing polymers with alternating sequences with hydrophobic blocks of size smaller than the lipid tail length, for which the polymer-induced membrane permeability for solvent is larger than on average for the population of random copolymers.