CPP 4: Statistical Physics in Biological Systems (joint session DY, BP, CPP)

Time: Monday 9:30–12:15 Location: BH-N 243

Invited Talk CPP 4.1 Mon 9:30 BH-N 243

Chemical warfare and survival strategies in bacterial range expansions — Markus F Weber, Gabriele Poxleitner, Elke Hebisch, Erwin Frey, and •Madeleine Opitz — Center for NanoScience, Faculty of Physics, Ludwig-Maximilians-Universität München, Munich, Germany

Spreading of species into uncolonized territory is a fundamental ecological process in the evolution and maintenance of biological diversity. Although interactions between species have experimentally been identified as major determinants of species coexistence in spatially extended populations, their role in spatially expanding populations is largely unknown. Here, we address the roles of resource and interference competition by genetically tuning a bacterial model system of three Escherichia coli strains: a toxin (colicin) producing strain, a sensitive strain, and a resistant strain. We show that maintenance of biodiversity is determined by three strongly interdependent ecological factors: the relative ratio of the competing strains, their growth rates and the strength of toxicity. Our mathematical analysis suggests, that despite general expectations, a non-hierarchical interaction network is not a necessary prerequisite for biological diversity. Moreover, we find that robust three-strain coexistence requires a balance between growth rates and a small enough toxicity range or, alternatively, a reduced initial ratio of the colicin-producing strain. We expect that the approach presented in this study will be useful to identify further mechanisms for the maintenance of biodiversity in microbial communities.

CPP 4.2 Mon 10:00 BH-N 243

A New Dimension: The Influence of Two Dimensional Niche Space on Evolutionary Food Web Models — •Daniel Ritterskamp and Bernd Blasius — ICBM, University Oldenburg, Germany

Food webs encode feeding interactions of ecological communities, originating from an intricate interplay of evolutionary and ecological processes. This dynamic can be described by evolutionary food web models, in which feeding interactions between species are related to the relative distance of their adaptive traits (e.g., body size) on a niche axis. However, not much is known about evolutionary food web dynamics in space.

Here, we go beyond traditional approaches and develop an evolutionary food web model in a two dimensional niche space, where the additional niche axis might describe a spatial coordinate or an environmental variable. Using numerical simulations, we investigate population dynamics, evolutionary behaviour and the emerging community structure in space. The model is able to produce both static and dynamic food webs, depending on the width of the interaction kernel; whereas food web complexity is determined mainly by the interaction strength.

We observe rich dynamics including: spatio-temporal patterns, arms races, red queen dynamics, as well as sub-food webs moving in space. By sampling the spatial axis, local food webs are recovered, which can be related to empirical data. We conclude that the additional niche-dimension is essential to capture realistic patterns of spatially structured food webs.

CPP 4.3 Mon 10:15 BH-N 243

Biodiversity and ecosystem functioning in evolving food webs — •Korinna T. Allhoff and Barbara Drossel — TU Darmstadt, Germany

We analyze an evolutionary food web model where each species is characterized by three traits, namely its own body mass, its preferred prey body mass, and the width of its potential prey body mass spectrum. Population dynamics includes feeding and competition interactions and determines which species are viable and which ones go extinct. On a timescale much slower than population dynamics, new species emerge as modifications of existing species. The network structure emerges according to the interplay between population dynamics and evolutionary rules and shows an ongoing species turnover. The model thus gives insights into how the functional diversity changes during the initial network buildup as well as due to extinction avalanches. We investigate the relation between the functional diversity and five community level measures of ecosystem functioning. These are the metabolic loss of the predator community, the total biomasses of the basal and the predator community and the consumption rates on the basal community and within the predator community.

CPP 4.4 Mon 10:30 BH-N 243

Efficiency of cellular information processing — •David Hartich, Andre C. Barato, and Udo Seifert — II. Institut für Theoretische Physik, Stuttgart, Germany

We study theoretical models inspired by the *E. coli* sensory network, using the framework of stochastic thermodynamics for bipartite systems [1]. More precisely, we model the sensory system by an internal process measuring an external process, which is a ligand concentration jumping at random between two values. We show that the rate of conditional Shannon entropy reduction, characterizing the learning of the internal process about the external process, is bound by the thermodynamic entropy production [2]. This approach allows for the definition of an informational efficiency that can be used to study cellular information processing. We start with a simple model for which ATP must be consumed so that a protein inside the cell can learn about the external environment. A further discussion illustrates, *inter alia*, that a non-zero learning rate without dissipation inside the cell can only be obtained if the external process compensates for it.

[1] DH, ACB and US, J. Stat. Mech., P02016 (2014)
[2] ACB, DH and US, New J. Phys. **16**, 103024 (2014)

CPP 4.5 Mon 10:45 BH-N 243

Tackling your free energy estimates with pyfeat — •Antonia Mey, Christoph Wehmeyer, Fabian Paul, Hao Wu, and Frank Noé — Institut für Mathematik, FU Berlin

Understanding the equilibrium properties of physical systems is of general interest in many different areas of physics. In complex systems, equilibrium properties can often only be evaluated by means of numerical simulations, which are frequently plagued by rare event dynamics. One approach to circumvent rare event dynamics is to use enhanced sampling methods (e.g. replica exchange methods or umbrella sampling).

The range of established analysis methods to optimally estimate equilibrium properties from multi-ensemble simulations often requires an expert user for their implementation or even usage. Here, we introduce a new software package, the python free energy analysis toolkit – pyfeat, that facilitates the analysis of multi-ensemble simulation. Pyfeat provides an easy-to-use interface to well established methods such as WHAM or MBAR, as well as the recently introduced transition-based reweighting analysis methods (TRAM), which borrow ideas from Markov state models. The software's straight forward usability makes comparing different estimation method applied to the same input data trivial.

Generally, any multi-ensemble simulation can be used for the analysis ranging from all-atom protein molecular dynamics simulations to simulations of condensed matter systems. Pyfeat is available for download at: https://github.com/markovmodel/pyfeat.

15 min. break

CPP 4.6 Mon 11:15 BH-N 243

Lateral domain formation in membranes coupled to curvature — •Sina Sadeghi, Marcus Müller, and Richard Vink — Institute of Theoretical Physics, Georg-August-Universität Göttingen, Göttingen, Germany

The lateral heterogeneity in the plasma membrane of eukaryotic cells is an important factor for regulating biological functions. As opposed to plasma membranes, model membranes (either artificially prepared membranes, or membranes extracted from living cells) typically phase separate. To address this paradox, we present computer simulations of a coarse-grained membrane model that undergoes macroscopic phase separation at low temperature. Considering a coupling between local composition and local curvature of the membrane, we show that the system exhibits composition fluctuations with a nontrivial length scale, resembling microemulsion. The latter is identified as a region where lipid rafts can form. We furthermore probe the nature of phase transition between the phase-separating regime and the mixed state. This transition is continuous and belongs to the two-dimensional Ising universality class for weak coupling to curvature, but becomes first-order for strong curvature-composition coupling.

CPP 4.7 Mon 11:30 BH-N 243

DNA denaturation transition: environmental effects on scaling — •Christian von Ferber[1] and Yurij Holovatch[2] — [1]Coventry University, UK — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, UA

The Poland and Scheraga model for the DNA denaturation transition is reconsidered taking into account environmental effects. We apply field theoretical methods to discuss environmental effects on the nature of the transition. In particular we discuss variants of the transition that may occur due to particular properties of the environment. These are the presence of uncorrelated and power-law long-range correlated disorder which influences the transition as function of the power law exponent, the quality of the solution which may affect the self- and mutual interaction of both single and double strands and combination of these. All these have significant effects on the transition.

CPP 4.8 Mon 11:45 BH-N 243

Variational approach to molecular dynamics — •Bettina Keller — Freie Universität Berlin, Institut für Chemie und Biochemie, Takustraße 3, 14195 Berlin

The eigenvalues and eigenfunctions of the classical molecular dynamics propagator contain the essential information about the molecular thermodynamics and kinetics. A matrix representation of the propagator can be constructed by partitioning the conformational space into discrete states and estimating the state-to-state transition probabilities from molecular dynamics simulations, yielding a so-called Markov state model (MSM). The precision of an MSM depends sensitively on on how well the discretization reproduces the shape of the dominant eigenfunctions. The difficulty to find a suitable discretization has limited the routine use of MSMs. Moreover, most discretizations are data-driven, impairing the comparison between MSMs and the interpretation of the eigenvectors in terms of structural transitions.

Using a recently published variational approach, it is possible to construct a matrix representation of the propagator using an arbitrary basis set, allowing to use basis functions with gentle slopes. This reduces the discretization error. More importantly, the user can define basis sets which have a chemical meaning and can be used for entire classes of molecules, thereby allowing for direct comparison of the kinetic models. I will give an overview of the variational principle for the classical molecular dynamics propagator and propose a basis set for peptide dynamics which is based on the dominant eigenfunctions of individual amino acids

CPP 4.9 Mon 12:00 BH-N 243

Simple association-dissociation-aging process: recursive solution — •Thomas Niedermayer and Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

The simple association-dissociation-aging process (SADAP) is characterized by the coupling of stochastic growth and shrinkage of one-dimensional structures to the random aging of the constituting subunits. Most prominently, SADAPs capture the essential features of the polymerization of actin filaments and microtubules. Previously employed mean field methods fail to describe the dynamics of SADAPs. We found an ansatz for the full master equation which allows us to study SADAPs analytically and derive a recursion relation for the steady state solution which enables the calculation of all emergent quantities with increasing accuracy. In particular, our method allows, for the first time, the precise calculation of the boundary between the growth and shrinkage regime, in excellent agreement with results from stochastic simulations.