

DY 32: Statistical Physics in Biological Systems III (joint with BP)

Time: Thursday 15:00–17:30

Location: H46

DY 32.1 Thu 15:00 H46

On the Fourier spectra of fitness Landscapes — ●JOHANNES NEIDHART, IVAN SZENDRO, and JOACHIM KRUG — Institut für Theoretische Physik, Universität zu Köln, Deutschland

Fitness Landscapes are a well established tool in the analysis of evolutionary processes. In order to extract important information, graph theoretical Fourier decomposition has proven to be very useful. In order to compare experimental data with stochastic models, we analyse several models, amongst others Kauffmann's *LK* model and present exact results for the Fourier spectra as well as a comparison to experimental data.

DY 32.2 Thu 15:15 H46

On the existence of accessible paths in trees — ●STEFAN NOWAK and JOACHIM KRUG — Institute for Theoretical Physics, University of Cologne

The study of accessible paths is a new type of percolation problem which is inspired by evolutionary biology. To each node of the underlying graph a random number is assigned and a path through the graph is called accessible if all random numbers along the path are in ascending order. We will give an exact expression for the second moment of the number of accessible paths from the root to the leaves in n -trees and an asymptotic expression for the probability that there is at least one accessible path. Furthermore, we will show that there is a percolation threshold if the random variables are Gumbel distributed and a linear drift is added.

DY 32.3 Thu 15:30 H46

A new evolutionary food web model — ●KORINNA T. ALLHOFF¹, DANIEL RITTERSKAMP², CHRISTIAN GUILL³, and BJÖRN C. RALL³ — ¹Institute of Condensed Matter Physics, TU Darmstadt — ²Institute for Chemistry and Biology of the Marine Environment, Carl von Ossietzky University of Oldenburg — ³J. F. Blumenbach Institute for Zoology and Anthropology, Georg-August-University Göttingen

Understanding the conditions that are required for complex ecosystems to persist despite changes in species composition and anthropogenic perturbations, is of utmost importance in order to conserve these systems. Evolutionary food web models provide a mechanistic tool to understand how complex ecosystems emerge and how they react to changes in their composition. We present such an evolutionary food web model, where each species is characterized by three key traits: its own body mass, its preferred prey body mass, and the width of its potential prey body mass spectrum. The model contains allometric effects on feeding and competition interactions and determines dynamically whether a species is viable or goes extinct. The evolutionary processes that enable new species to enter the system as mutants of already existent ones, also follow allometric rules. The food web structure emerges as a highly nontrivial result from the combined effect of population dynamics and evolution. We present computer simulations of different model modifications and show how they influence network structure and stability.

DY 32.4 Thu 15:45 H46

The influence of chaos on the stability of small food webs — ●FANNY GROLL and ALEXANDER ALTLAND — Institut für Theoretische Physik, Universität zu Köln, Germany

Ecological networks can show different types of dynamics. Experiments have demonstrated that they can actually be governed by deterministic chaos. In that case the population numbers evolve along a chaotic attractor; they show large fluctuations but do not go extinct.

We examine a mathematical model of a simple food web consisting of two prey and one predator population. In this model a control parameter triggers the onset of chaos via bifurcation. Such dynamics have already been observed in an aquatic system of few competing species.

In studying this system we aim to find a catalogue of techniques to approach such a system and to analyze its features. Starting from a general master equation approach we have explored routes to chaos in few-species ecological systems. Emphasis has been put on the mechanisms leading to chaotic attractors. Under ambient conditions ecological systems are subject to demographic and environmental fluctuations. We explore the stability and persistence of populations in

chaotic regimes compared to more regular types of dynamics.

DY 32.5 Thu 16:00 H46

The effect of migration between patches on the stability of foodwebs — ●SEBASTIAN PLITZKO and BARBARA DROSSEL — Institut für Festkörperphysik, TU Darmstadt, Germany

During recent years, several factors that stabilize food webs have been identified. Among these are allometric scaling of metabolism with body size and adaptive foraging. So far, food web models rarely take space into account. However, it is known that being distributed over several spatial patches can have positive as well as negative effects on the stability of metacommunities.

Using computer simulations for the population dynamics of systems with many species, we investigate the stability of food webs that are distributed over several patches that are connected by migration. We evaluate species persistence in dependence of food-web complexity, patch arrangement, and migration rule. In particular, we study conditions under which migration alone, without the above-mentioned additional stabilizing factors, can increase food-web stability. We also determine whether food webs that already have a high stability can gain further by being distributed over several patches.

DY 32.6 Thu 16:15 H46

The effect of predator limitation on the dynamics of simple food chains — ●CHRISTOPH SCHMITT¹, STEFAN SCHULZ¹, JONAS BRAUN¹, CHRISTIAN GUILL², and BARBARA DROSSEL¹ — ¹Physics Department, TU Darmstadt — ²Institute for Zoology and Anthropology, University of Göttingen

We investigate the influence of competition between predators on the dynamics of predator-prey systems and of tritrophic food chains. Competition between predators is implemented either as interference competition, or as a density-dependent mortality rate.

With interference competition, the paradox of enrichment is reduced or completely suppressed, but otherwise the dynamical behavior of the system is not fundamentally different from that of the Rosenzweig-MacArthur model, which contains no predator competition.

In contrast, with density-dependent predator mortality the predator-prey system shows a surprisingly rich dynamical behavior. In particular, decreasing the density regulation of the predator can induce catastrophic shifts from a stable fixed point to a large oscillation. Furthermore, the model shows several other types of nonlocal bifurcations, the coexistence of several attractors, and different types of regime shifts. In tritrophic food chains chaos can occur in both models.

DY 32.7 Thu 16:30 H46

Score statistics of multiple sequence alignments — ●PASCAL FIETH and ALEXANDER K. HARTMANN — Institute of Physics, University of Oldenburg

Optimally aligned sequences of amino acids [1] can be studied numerically [2] in the biologically relevant high scoring region by means of parallel tempering simulations [3]. Preceding studies have shown that the scores of gapped pairwise sequence alignments of finite-length sequences follow a Gumbel extreme value distribution, modified by a Gaussian correction [4] rather than a simple Gumbel extreme value distribution as previously predicted for ungapped pairwise alignments. In this study these methods are applied to the case of multiple sequence alignment (MSA). Here the distributions of the sum-of-pair scores of the MSA of more than two sequences are studied. In particular the distribution of protein MSA-scores using different common substitution matrices (BLOSUM and PAM) are analysed for protein background frequencies of real sequences.

[1] R. Durbin et al., *Biological sequence analysis*, (Cambridge University Press, 1998)

[2] A.K. Hartmann, *Practical Guide to Computer Simulations*, (World Scientific, 2009)

[3] A.K. Hartmann and Heiko Rieger, *Optimization Algorithms in Physics*, (Wiley-VCH, 2001)

[4] S. Wolfshheimer et al., *Local Sequence Alignments Statistics: Deviations from the Gumbel Statistics in the Rare-Event Tail*, (Algorithms for Molecular Biology, 2007)

DY 32.8 Thu 16:45 H46

Understanding evolutionary conserved contacts by structure based models. — ●ABHINAV VERMA¹, BENJAMIN LUTZ¹, MARTIN WEIGT², and ALEXANDER SCHUG¹ — ¹Karlsruhe Institute of Technology, Karlsruhe, Germany — ²Université Pierre et Marie Curie, Paris, France

The evolution of a protein family leaves a fingerprint in databases of protein sequences. In a recent study, Direct Coupling Analysis (DCA) has been shown to accurately identify co-evolving residue pairs preserved as spatial contacts in their three dimensional fold [1]. Such DCA-derived contacts can be combined with molecular dynamics simulations to predict experimentally inaccessible transiently occupied active states [2]. Only a fraction of a contact map, however, is identified by DCA. Here we attempt to understand the evolutionary constraints leading to the conservation of these specific contacts by native structure based models [3]. We compare simulations with DCA derived contact maps to randomly chosen subsets of contacts.[unpublished data]

[1] Marcos et. al. , PNAS, 2011, 108, E1293

[2] Dago et. al. , PNAS, 2012, 109, E1733

[3] Whitford et al. Proteins, 2009 75, 430

DY 32.9 Thu 17:00 H46

Symmetry Breaking of Sequence Information in Catalytic Polymer Soups — ●SHOICHI TOYABE and DIETER BRAUN — Systems Biophysics, Ludwig-Maximilians-University Munich, Munich

One of the most distinguished properties of living systems is that they sustain genetic information and reproduce it. However, its origin remains elusive; how can information emerge in the chaotic molecular soup in the prebiotic earth? We discuss models and preliminary experiments to show the emergence of order in a catalytic polymer solution. We argue that template-directed copolymerization of diverse polymers is a promising route. Autocatalytic copolymerization extends polymers stochastically. Interestingly, a numerical simulation shows that the polymers self-organize into an ordered state where a stochastically

chosen small set of sequence motifs become dominant. This spontaneous symmetry breaking occurs because autocatalytic chain reactions in the reaction network interact competitively and amplify strands beyond exponential growth. This amplifies spontaneous fluctuations and sustains it by Darwinian selection against other sequences. The transition to the ordered state is accompanied by a population inversion, i.e. the length distribution of polymers was biased to the longer side at the ordered state. In order to demonstrate the symmetry breaking by experiments, we performed ligase chain reactions of DNA strands with semi-random sequences. Under nonequilibrium driving of material flux and temperature cycles, we observed a population inversion, which implies the breaking of the symmetry. Furthermore, we analyzed the sequences to confirm the symmetry breaking by on the basis of PCR.

DY 32.10 Thu 17:15 H46

Characteristics of the formation of oligomers in a primordial broth — ●SABRINA SCHERER — Biologische Experimentalphysik, Universität des Saarlandes

We analyse the energetically driven emergence of spontaneous and dynamic states of order in prebiotic, complex systems. We perform Miller-Urey-type experiments: simple anorganic molecules driven by electric discharges and form complex, organic reaction mixtures. The process is analysed by real-time mass spectroscopy. The spectra reveal the formation of a time-dependent order of molecules in the reaction mixture. The peak intensities of several oligomeric molecules oscillate over time. Some oligomers vanish after their first occurrence to reform again later. The increase and decrease of these intensities follow exponential and sigmoid courses. This points towards autocatalytic processes. In contrast to the original Miller-Urey-experiment which consists of the constituents methane, ammonia, hydrogen and water, we add other biologically relevant elements like phosphor and sulfur to observe their influence on the stability of the oligomer oscillations.