DY 21 Statistical Physics in Biological Systems

Zeit: Samstag 08:30–11:15 Raum: TU H2032

DY 21.1 Sa 08:30 TU H2032

Maximum Prinzip für Sequenzraummodelle der Populationsgenetik — •Uwe Grimm[1], Tini Garske[1], Ellen Baake[2] und Michael Baake[3] — [1]Applied Mathematics Dept., The Open University, Milton Keynes MK7 6AA, UK — [2]Technische Fakultät, Univ. Bielefeld, Postfach 100131, 33501 Bielefeld, Germany — [3]Fakultät für Mathematik, Univ. Bielefeld, Postfach 100131, 33501 Bielefeld, Germany

Wir untersuchen Mutations-Selektionsmodelle für die Evolution zwei- oder vierbuchstabiger Sequenzen. Mutation wird dabei als Markovprozess modelliert, Selektion durch eine Fitnessfunktion, die jeder Sequenz eine reproduktive Fitness zuordnet. Wir betrachten Fitnessfunktionen, die permutationsinvariant sind, oder allgemeiner durch ein Hopfield-artiges Überlappmaß mit einer Anzahl vorgegebener Referenzsequenzen bestimmt sind. Für unendliche Sequenzlänge lassen sich Gleichgewichtseigenschaften der Sequenzraummodelle durch ein einfaches Maximumsprinzip beschreiben [1,2,3], welches zudem eine gute Näherung für den Fall endlicher Sequenzlängen liefert.

[1] T. Garske und U. Grimm, A maximum principle for the mutation-selection equilibrium of nucleotide sequences, *Bull. Math. Bio.* **66** (2004) 397–421.
[2] T. Garske und U. Grimm, Maximum principle and mutation thresholds for four-letter sequence evolution, *J. Stat. Mech.: Theor. Exp.* (2004) P07007.
[3] E. Baake, M. Baake, A. Bovier und M. Klein, An asymptotic maximum principle for essentially linear evolution models, *J. Math. Bio.* (im Druck); Preprint q-bio/0311020.

DY 21.2 Sa 08:45 TU H2032

Breather induced anomalous charge diffusion in a DNA model — •George Kalosakas[1], Kia Ngai[2], and Sergej Flach[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Str. 38, Dresden, 01187, Germany — [2]Naval Research Laboratory, Washington DC, 20375-5320, USA

We present results on the diffusive motion of a charge along a double stranded DNA, which interacts with the nonlinear opening dynamics of base pairs. Signatures of anomalous diffusive properties are found at relatively high temperatures. A sublinear diffusion and a plateau appears before the standard long-time diffusion during the evolution of the mean squared displacement and a significant degree of heterogeneity is exhibited among individual trajectories. Both properties are connected with the existence of vibrational hot-spots (breather or multibreather excitations). Transport parameters of the charge are strongly affected in this case, as can be exemplified by the significant suppression of the diffusion coefficient D. The variation of D with temperature follows a stretched exponential law. The results are contrasted with those of the linearized case, in the absence of breathers.

DY 21.3 Sa 09:00 TU H2032

Designability of RNA secondary structures — •Bernd Burghardt and Alexander K. Hartmann — Institut für Theoretische Physik, Universität Göttingen

Some RNA, e.g. ribozyme, provides by its secondary and tertiary structure enzymatic functionality. For a biologically relevant structure of an RNA sequence it is required that it is the most stable one, i.e. ground state, and that the ground state is unique, otherwise no definite functionality could be assigned to the sequence.

Given a RNA secondary structure the answer whether there is a RNA sequence which has this structure as its ground state structure or not, depends on the chosen energy model: for energy models with only pair contributions always such a sequence exits, while for energy models with stacking contributions there are structures that are not ground state of any RNA sequence. We numerically investigate whether this structures appear quite regularly in the space of all structures or are exceptional cases with an algorithm that exactly calculates the ground states in polynomial time. Because stacking contributions are always present in real RNA, this might have consequence for possible structures, and therefore functionality, of RNA structures.

DY 21.4 Sa 09:15 TU H2032

Comparison of RNA secondary structures with and without pseudoknots — •Alejandro Morales Gallardo, Bernd Burghardt, and Alexander K. Hartmann — Institut für Theoretische Physik, Universität Göttingen

RNA plays an important role in the biochemistry of all living systems. It does not only transmit pure genetic information, but, e.g. works as a catalyst. While for the former the primary structure, i.e. the sequence of the bases, is relevant, for the later the kind of higher order structures, i.e. secondary and tertiary structures, are relevant. While most studies concentrate on plain secondary structures without pseudo knots, we allow some special kinds of pseudo knots, which makes the computational problem more demanding, e.g. the effort for finding the ground state energy increases from $\mathcal{O}(L^3)$ without pseudo knots to $\mathcal{O}(L^6)$ the sequence length L. We have done numerical studies on statistical quantities, where we used algorithms that are able to calculate the ground-state energy exactly in polynomial time. We concentrate on the difference between models with and without pseudo knots.

DY 21.5 Sa 09:30 TU H2032

The dynamical lattice model of proteins — •Frank Dressel and Sigismund Kobe — Institut für Theoretische Physik, TU Dresden, D-01062 Dresden, Germany

Lattice models are used to investigate the energy landscape, folding properties and thermodynamics of proteins. The main disadvantage of such up to now considered rigid models is the disability to characterize the real structure. We propose a model, which is more appropriate to deal with biological conformations. The real positions of the amino acids are dynamically simulated using fixed bond lengths between the atoms and an angle distribution taken from Ramachandran plots. Data of the pairwise interactions between the amino acids are based on results of biological investigations [1]. The exact ground state (energy and conformation) is calculated using methods of optimization algorithms with respect to the global energy. Results for different proteins up to a chain length of 40 amino acids are obtained. The comparison with experimentally found biological structures [2] are in good accordance with respect to the secondary structure elements. As an example we discuss the Alzheimer's disease amyloid A4 peptide (residues 1-40).

[1] R. I. Dima, G. Settanni, C. Micheletti, J. R. Banavar, A. Maritan, J. Chem. Phys. 112 (2000) 9151.
[2] H.M. Berman, J. Westbrook, Z. Feng, G. Gilliland, T.N. Bhat, H. Weissig, I.N. Shindyalov, P.E. Bourne: The Protein Data Bank. Nucleic Acids Research 28 (2000) 235.

DY 21.6 Sa 09:45 TU H2032

Transition from local to global events in a stochastic medium — •Martin Falcke and Rüdiger Thul — Hahn Meitner Institut, Glienicker Str.100, 14109 Berlin

In the last 2-3 years, it could be shown by a sequence of simulations and analytic calculations that intracellular calcium dynamics is a stochastic nonlinear system. Spatial and temporal structures arise due to fluctuations only. The biological function of intracellular calcium dynamics is to generate transients of high calcium concentration or oscillations. Repetitive wave nucleation is one possibility to achieve this goal. A global event starts from a local fluctuation and travels through the whole system. We investigate the prerequisites for wave nucleation with master and Fokker Planck equations for calcium channel clusters and calculate average frequencies for the occurence of local events.

DY 21.7 Sa 10:00 TU H2032

Tumor induced angiogenesis: A theoretical model for neo-vascularization and tumor growth — •Heiko Rieger[1], Deok-Sun Lee[1], Raja Paul[1], and Katalin Bartha[2] — [1]Theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany — [2]Department of Medical Biochemistry, Semmelweis University, Budapest, Hungary

Tumor-induced angiogenesis is the formation of new blood vessels from pre-existing capillaries around a growing tumor in a hypoxic (oxygen-depleted) microenvironment. Hypoxia induces growth factor (GF) synthesis and release from tumor cells (TC), that act on endothelial cells (EC) of nearby blood vessels. Angiogenic sprouting, new vessel formation

and vessel dilatation is the result of this interaction leading to favorable tumor growth conditions. We introduce a stochastic hybrid cellular automaton model to describe quantitatively how vascularization develops in a melanoma type tumor. We present results for the spatio-dynamic evolution of the microvascular and tumor density, which reflect a compartmentalization of the tumor into rapidly vascularizing periphery and necrotic regions. Biological implications and possible physical universality classes are discussed.

DY 21.8 Sa 10:15 TU H2032

Positioning the division plane in *Escherichia coli* — •Giovanni Meacci[1], Markus Bär[1,2], and Karsten Kruse[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin

During division of the bacterium *Escherichia coli*, the correct position of the division plane is determined in part by the Min proteins. For this purpose, pole-to-pole oscillations of these proteins are important. Here, a phenomenological description for these oscillations is presented, where lateral interactions between proteins on the cell membrane play a key role. The phenomenological parameters used can be linked to microscopic physical quantities and thus allow for a quantitative comparison with experimental results. To study the effects of fluctuations due to low protein numbers, we consider a Langevin equation for the fluctuating protein concentrations. It is derived through coarse graining of the microscopic master equation.

DY 21.9 Sa 10:30 TU H2032

Stable and unstable attractors in critical Boolean networks — •Konstantin Klemm[1] and Stefan Bornholdt[2] — [1]Bioinformatik, Universität Leipzig, Kreuzstr. 7b, 04103 Leipzig — [2]Theoretische Physik, Universität Bremen, Otto-Hahn-Allee, 28334 Bremen

Studying the dynamics of Boolean networks, we check the stability of the attractors against small perturbations. We perturb the synchrony in the model by slightly accelerating or decelerating the update of a subset of units. This set of perturbations is motivated by the noisy delay time with which a biological switch (neuron, expressed gene) responds to a changing input. An attractor is called stable if after any such perturbation synchrony is regained. In random Boolean networks at the critical point (connectivity K=2) the number of stable attractors grows sublinearly with increasing system size [1], while the growth of the total number of attractors is superpolynomial. Thus in large systems almost all attractors considered earlier are artefacts arising from the synchronous clocking mode.

[1] K. Klemm and S. Bornholdt, preprint cond-mat/0411102

DY 21.10 Sa 10:45 TU H2032

Theorie der AFM-Kraftspektroskopie an Rezeptor-Liganden-Systemen — •Martin Raible und Peter Reimann — Fakultät für Physik, Universität Bielefeld, PSF 100131, 33501 Bielefeld

Einzelmolekülprozesse in Rezeptor-Liganden-Systemen können mit dynamischer AFM-Kraftspektroskopie experimentell untersucht werden. In den meisten Fällen benutzt man dabei ein Rasterkraftmikroskop (AFM), wobei die einwirkende Kraft (approximativ) linear mit der Zeit zunimmt: $F(t) = \mu \cdot t$. Die allgemein akzeptierte Grundannahme [1] in allen diesbezüglichen Untersuchungen ist ein Ratengesetz mit einer nur von der momentan wirksamen Kraft $F(t)$ abhängigen Zerfallsrate $\nu(F(t))$. Bei der Anwendung einer neuen Methode [2] zur Auswertung der Kraftprokolle auf gemessene Daten [3] zeigte sich eine Inkompatibilität mit dieser Grundannahme [4]. Ein erfolgversprechender Ansatz zur Erklärung dieser Inkompatibilität wird diskutiert.

[1] E. Evans and K. Ritchie, Biophys. J. **72**, 1541 (1997).
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[3] F.W. Bartels, B. Baumgarth, D. Anselmetti, R. Ros, and A. Becker, J. Struct. Biol. **143**, 145 (2003).
[4] M. Raible et al., J. Biotechnology **112**, 13 (2004).

DY 21.11 Sa 11:00 TU H2032

Assessment of Parameters of Neural Ensembles for the Calibration of Modification Techniques — •Oliver Holzner[1], Alexander Kleinsorge[1], Eckehard Schöll[1], and Peter Tass[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Institut für Medizin, Forschungszentrum Jülich, D-52425 Jülich, Germany

Differential equations modeling neural ensemble behavior generally contain a multitude of parameters governing the ensemble's behavior. Their corresponding neurophysiological parameter values vary substantially between individuals, and even within one individual over time. The problem of calibrating these parameters without dissecting the system ("in-vivo") is solved by using nonlinear response theory in conjunction with calculating non-autonomous attractor landscapes for the dynamical system considered. Functioning of calibration by means of elementary versus feedback-looped input signals is demonstrated in the presence of various types of noise.