BP 19: Posters - Computational Biophysics

Time: Tuesday 14:00–16:00 Location: P1A

BP 19.1 Tue 14:00 P1A

Morphological properties of the epithelial tissue — •Jakov Lovrić[1,2], Sara Kaliman[2], and Ana-Sunčana Smith[1,2] — [1]Institute Ruđer Bošković, Division of Physical Chemistry, Group for Computational Biosciencies, Zagreb, Croatia — [2]Institute for Theoretical Physics, PULS Group and Cluster of Excellence: EAM, FAU Erlangen-Nürnberg, Germany

Knowing the morphology of an epithelial tissue is important due to understanding proceses like growth and development of the tissue, wound healing and progression of the cancer.

We study the structure of the MDCK II epithelial cells in circular colonies. Cell nuclei can be approximated with ellipses and the Voronoi tesselation generated by those ellipses coincides well with the cell membranes. We compare the tissue cells to the Voronoi cells generated by randomly packed ellipses obtained from the cell nuclei. The comparison is done by studying the probability distributions of chosen morphological measures calculated from the cells. We find that randomly packed ellipses reproduce the morphology of the tissue well at the low cell density. At high cell density we observe more regular structure of the tissue an we see the deviations of the random model from the cell tissue.

BP 19.2 Tue 14:00 P1A

Structure formation of oligopeptides in the PRIME20 model — •Arne Böker and Wolfgang Paul — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Much effort has recently been put into understanding amyloid formation in polypeptides. The amyloid state is a structure in which polypeptides aggregate as a stack of β-sheets, which is usually not the native state, leading to loss of function. Amyloids can cause a variety of diseases (amyloidoses) such as Huntington's chorea, which is caused by an amyloidic state of expanded poly-Glutamine sequences.

The relation between conformations of a polypeptide is governed by local minima in the free energy function. Coarse-grained models tend to simplify the free energy in such a way that these local minima are ignored. To circumvent this problem, the level of coarse graining needs to be chosen appropriately. PRIME20[2] provides reasonable detail by mapping each amino acid to four beads, but keeps parameter space simple with the set of interactions reduced to 19 energy parameters.

We perform thermodynamic simulations of single PRIME20 chains using the "SAMC"[3] variation of Wang-Landau Monte Carlo sampling which provides insight in different statistical ensembles at the expense of dynamic information. The aforementioned poly-Glutamines are compared to poly-Alanines with a lower tendency to form β structure motifs.

[2]M. Cheon, , I. Chang, C. K. Hall, Proteins **78**(2010):2950

[3]B. Werlich, T. Shakirov, M. P. Taylor, W. Paul, Comp. Phys. Comm. **186**(2015):65

BP 19.3 Tue 14:00 P1A

Automated tracking of Adelie penguins — •Alexander Winterl[1], Daniel Zitterbart[1,2], Sebastian Richter[1], Richard Gerum[1], and Ben Fabry[1] — [1]Department of Physics, Biophysics Group, Friedrich-Alexander-University Erlangen-Nuremberg, 91052, Erlangen, Germany — [2]Alfred Wegener Institut, Helmholtz Zentrum für Polar und Meeresfoschung, 27568 Bremerhaven, Germany

Decision-making processes of colony-forming birds when they approach or leave their home colony e.g. during foraging are currently poorly understood and remain largely unexplored. To identify rules that govern such processes in Adelie penguins, we recorded high-resolution timelapse images of a colony near Dumont d'Urville, Antarctica, during January and February 2015. We then developed an automated tracking software to follow the movements of all birds outside the colony within the field of view. To correctly allocate crossing tracks when two penguins pass each other, we model the penguin movements by an auto-regressive random walk that assumes that penguins do not abruptly change their speed and direction. 12 ambiguous tracks were selected and analyzed by human observers who watched the full timelapse image sequence. Compared to this "ground truth", the assignment quality of the algorithm (25% error) was slightly inferior to human observers (17% error) when only the center of mass positions of the crossing tracks are provided. We conclude that reliable automated tracking of passing and crossing penguins requires the analysis of additional image information such as body posture and head orientation.

BP 19.4 Tue 14:00 P1A

Physical Analysis of One-Component Signaling in Bacteria — •Linda Martini and Ulrich Gerland — Physics of Complex Biosystems, Department of Physics, Technical University of Munich

Adaptation to changing environments is of vital importance to bacterial cells and is enabled by sophisticated signal transduction systems. While classical two-component signaling is well studied, the mechanisms of one-component systems, where a single protein implements both sensing and response regulation, are mostly uncharacterized.

One such one-component system is the membrane-integrated protein CadC, which is part of the pH-stress response system in E. Coli. As it directly binds to the genomic DNA to regulate transcription, it faces a target search problem the dynamics of which are still to be understood.

Using kinetic Monte Carlo simulations of a lattice model, we focus on a characterization of the coupled stochastic dynamics of the DNA and the proteins, and its dependence on the system parameters. Understanding the kinetics of membrane-localized proteins specifically binding to a dynamic DNA will be important to interpret corresponding *in vitro* experiments and more generally to understand the biophysics of one-component signal transduction.

BP 19.5 Tue 14:00 P1A

Huddle-behavior simulation of emperor penguins — •Florian Morawetz[1], Klaus Morawetz[2,3,4], and Daniel Zitterbart[5,6] — [1]University of Rostock, Wismarsche Straße 8,18057 Rostock, Germany — [2]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [3]International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [4]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [5]Department of Physics,University of Erlangen-Nuremberg,Henkestrasse 91,91052 Erlangen, Germany — [6]Alfred Wegener Institut für Polar- und Meeresforschung, AmHandelshafen 12, 27570 Bremerhaven, Germany

Despite the deadly environmental conditions in the Antarctic, emperor penguins have developed a surviving strategy which allows them to breed the eggs during 4 months of winter time. This is realized by a huddle of huge numbers of tightly grouped penguins. Though no individual has the overview to realize an optimized strategy of the whole huddle, it behaves according to certain rules which are vital for the survive. These rules are found employing a cellular automates model. First, each individual feels attracted by the most nearest *and* next-but-next-nearest neighbors which creates the attraction of the huddle. If a stress situation occurs like created by external enemy, the individuals cease to see the next-but-next-nearest neighbor but see only the next neighbors which leads to an expel of the crowed. Second, there is a pushing of an individual in front if too many sides of the individual are uncovered.

BP 19.6 Tue 14:00 P1A

Adaptive Resolution Simulations of Biomolecular Systems — •Raffaele Fiorentini, Aoife Fogarty, Raffaello Potestio, and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Mainz, Germany

A fully atomistic modelling of many biophysical and biochemical processes at biologically relevant length- and time-scales is beyond our reach with current computational resources. One approach to overcome this difficulty is the use of multiscale simulation techniques in which different system components are simultaneously modelled at different levels of resolution, these being smoothly coupled together. In the case of biomolecules, functionally relevant parts of the system are modelled at as high a level of detail as necessary, while the remainder of the system is represented using less expensive models. Such a multiscale simulation can employ an adaptive resolution scheme, in which system components change their resolution on the fly during the simulation. Recently, the existing adaptive resolution (AdResS) methodology has been extended to biomolecular systems. We now demonstrate how the AdResS approach applies to the calculation of thermodynamical properties of such biomolecular systems.

BP 19.7 Tue 14:00 P1A

Classificatory Analysis of Biological Autofluorescence Spectra — •Ignas Ciplys[1,2], Vilmantas Gegzna[1,2], Darius Varanius[1,2], Aurelija Vaitkuviene[1], Gunoras Terbetas[3], Ruta Kurtinaitiene[4], Jurgita Usinskiene[5], and Juozas Vilmantis Vaitkus[1] — [1]Institute of Applied Research, Vilnius University, Vilnius, Lithuania — [2]Life Sciences Center, Institute of Biosciences, Vilnius University, Vilnius, Lithuania — [3]Clinics of Neurology and Neurosurgery, Vilnius University, Vilnius, Lithuania — [4]Hospital Santariskiu Klinikos, Vilnius University, Vilnius, Lithuania — [5]National Cancer Institute, Vilnius University, Vilnius, Lithuania

This research deals with auto-fluorescence of biological specimens and its relations to medical diagnostics. The purpose of this study is to collect auto-fluorescence spectra from gynecological and intervertebral disc related specimens in various medical conditions and extract diagnostically relevant information through computational methods. The methods used include non-linear, univariate as well as multivariate statistical techniques focused on performance of classification and identification of the most informative spectral ranges. The main result: the fluorescence spectroscopy analysis might be recommended for medical practice, as well as at a point of care, and the efficiency of diagnostics expressed via balanced accuracy is up to 0,75-0,90. Further results and interpretation of analysis will be demonstrated during conference. The collected data base has to be increased to achieve more precise results.

BP 19.8 Tue 14:00 P1A

Optical-tweezer controlled translocation of DNA-bound proteins in MoS2 nanopores — •Andreas J Meyer and Peter Reimann — Universität Bielefeld, Germany

Atomic monolayer MoS2 membranes promise great sensitivity improvements in nanopore experiments compared to commonly used, much thicker silicon-nitride membranes.

We study the translocation dynamics of DNA and DNA-bound proteins in ultra-thin MoS2 nanopores. Employing a worm-like chain model and Brownian dynamics we examine effects like two-state hopping and force hystereses, as were previously reported in SiN nanopores [1].

[1] A. Spiering, S. Getfert, A. Sischka, P. Reimann, and D. Anselmetti, Nano Lett., 11, 2978 (2011)

BP 19.9 Tue 14:00 P1A

Lateral trapping of DNA inside voltage gated nanopores — •Thomas Töws and Peter Reimann — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

We consider a rigid cylinder, modelling a section of DNA, inside a solid state nanopore which is electrically gated by an all-around electrode integrated into the membrane. We study the interaction of DNA with the pore wall by means of potential energy landscapes. For this purpose we solve the fully 3D Poisson-Nernst-Planck and Stokes equations numerically and complement it by a 2D model and a 1D analytical calculation. We find that the DNA can be efficiently trapped parallel to the wall and off the symmetry axis of the pore by a proper choice of the gate voltage. Due to the hence induced confinement of accessible space lateral fluctuations of the DNA will be reduced. Furthermore we elucidate the dislike charge repulsion behaviour close to the wall which is necessary for such local minima of the potential energy.

BP 19.10 Tue 14:00 P1A

Cycle-based non-equilibrium Markov state modeling for periodic driving — •Fabian Knoch and Thomas Speck — Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany

A major current challenge in statistical mechanics poses the systematic construction of coarse-grained Markov State Models [1] that are dynamically consistent, and, moreover, might be used for systems driven out of thermal equilibrium. We previously introduced a novel prescription that extends the Markov state modeling approach to systems with dynamicas breaking detailed-balance [2,3]. Here, we show that our approach also holds for systems driven by a time-dependent periodic protocol. In partiucular, we apply the methodology to alanine dipeptide exposed to an oscillating electric field. Markov state modeling allows us to examine how the frequency of the external field influences the long term dynamics without conducting new simulations.

[1] Prinz, J.-H., Wu, H., Sarich, M., Keller, B., Senne, M., Held, M., Chodera, J. D., Schütte, C. and Noé, F. Markov models of molecular kinetics: Generation and validation. JCP 134(17), 2011

[2] Knoch, F. and Speck, T. Cycle representatives for the coarse-graining of systems driven into a non-equilibrium steady state. New Journal of Physics 17(11), 2015

[3] Knoch, F. and Speck, T. Non-Equilibrium Markov State Modeling of the Globule-Stretch Transition. arXiv:1611.02990, 2016

BP 19.11 Tue 14:00 P1A

Large Deviation Properties of RNA Neutral Set Size — •Charlotte J. Beelen and Alexander K. Hartmann — Institute of Physics, University of Oldenburg

The functionality of noncoding RNA molecules is mainly determined by their structure. Sequences with the same structure form the *neutral set*. The neutral set may be partitioned into several components, called neutral networks, traversable by structure-preserving point mutations. The neutral network size is biologically relevant: large neutral networks appear to be favourable in terms of mutational robustness and evolvability. We investigate the neutral set and neutral network size using computer simulations.

We apply a dynamic programming approach [1] to obtain the secondary structures of RNA sequences. The neutral set size can be estimated using a *Nested Set Monte Carlo* Simulation [2]. We implemented a combination of the algorithm with the *Ballistic Search* approach to estimate the neutral network size. The distribution of neutral set and network sizes is determined for randomly generated RNA and compared to biological RNA molecules. To improve the accuracy in the tails of the distribution, large-deviation simulations are used [3]. Furthermore, the correlation of the neutral set size to other observables like the number of base-pairs is investigated.

[1] M. Zuker and P. Stiegler, Nucl. Acids Res. **9**(1), 133-148 (1981)
[2] T. Jörg, O.C. Martin and A. Wagner, BMC Bioinf., **9**:464 (2008)
[3] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

BP 19.12 Tue 14:00 P1A

Computational prediction of alternative σ factor control — •Hao Wu, Angelika Diehl, and Georg Fritz — LOEWE Center for Synthetic Microbiology, Philipps University Marburg, Germany

Evolutionary co-variation of residues has been extensively exploited to predict conserved interaction of proteins. Here we used this method to study bacterial alternative σ factors. These subunits of RNA polymerases determine its specificity of promoter recognition and are involved in many gene regulation processes crucial for bacterial survival. One important player in the regulation of σ factor activity are anti-σ factors, which sequester their cognate σ factors in the absence of a stimulus, but to date the determinants of binding specificity are poorly understood. Our computational analysis revealed the interacting pairs of residues featuring crucial domains in σ factors. The amino acid pairs are either positively and negatively charged, or hydrophobic, depending on the phylogenetic group of the σ factor. Furthermore, a few alternative σ factor groups contain no anti-σ factor and instead feature a protein domain fused C-terminally to the σ factor as well as a highly conserved gene in its genomic context. Our analysis suggests a cluster of interactions interfacing between the σ domain and the C-terminal domain of the σ-factor. The second protein is also predicted to contact a number of residues at the same interface, suggesting a function as a co-factor. This study helps us to deepen our understanding of the specificity of interactions between σ factor and anti-σ factor, and provides novel insights into the regulatory mechanism employed by different alternative σ factor groups.

BP 19.13 Tue 14:00 P1A

Interactions of polyatomic anions with proteins depend strongly on sodium — Sadra Kashefolgheta and •Ana Vila Verde — MPIKG, Theory and Bio-Systems Dept., Am Mühlenberg 1 OT Golm, 14476 Potsdam, Germany

Polyatomic ions such as sulfates, phosphates or sulfonates are key players in biological processes but the molecular mechanisms by which these ions act are currently incompletely understood. We use molecular simulations and classical, atomistic models with fixed-charge and explicit solvent representation to clarify the molecular mechanisms of interaction between cationic amino acids and sulfates, phosphates and sulfonates, in their methylated and non-methylated forms and in the presence of excess counterions. This works goes beyond prior reports on the topic in that it uses a newly developed, internally consistent force field for all ions, which correctly captures the energy magnitude and length scale of anion-cation interactions. Our results suggest a possible molecular origin of previously unexplained experimental observations: anions that, according to experiment, differ strongly in the

magnitude of their interaction with cationic amino acids have in fact very similar interactions with those amino acids, but different interactions with sodium; the presence of excess sodium in the experiments thus determines the experimental outcome due to competition with the cationic sites on the protein.

BP 19.14 Tue 14:00 P1A

In Silico Model for Vesicle Blebbing — •Sebastian Hillringhaus, Dmitry A. Fedosov, and Gerhard Gompper — Institute of Complex Systems, Forschungszentrum Juelich, Juelich, Germany

Experiments with vesicles that incorporate an action network show complex behavior and the formation of blebs when they are actively contracted through motor proteins [Loiseau et. al., *Science Advances*, 2016]. To understand the mechanics that lead to this observations, we employ a coarse-grained cell model which incorporates the membrane properties similar to the RBC-model [Turlier et. al., *Nature Physics*, 2016] and an elastic inner mesh to include the actin network. The model is formulated in the framework of the dissipative particle dynamics simulation method. To connect both the membrane and the actin network, we use the Two-Pathway Model [Pereverzev et. al., *Biophysical Journal*, 2005] which can model different behavior under tension. We perform various tests to evaluate the best parameters for this model to match the observed experimental data. We observe that the model of Catch-Slip bonds lead to the best fit with the experimental data.