BP 22: Computational Biophysics II

Time: Wednesday 15:00–17:30 Location: H 1058

BP 22.1 Wed 15:00 H 1058

anionic and cationic gold nanoparticles in model lipid membranes: experiments and simulations — ESTER CANEPA[2], •SEBASTIAN SALASSI[1], FEDERICA SIMONELLI[1], RICCARDO FERRANDO[2], RANIERI ROLANDI[1], CHIARA LAMBRUSCHINI[2], ANNALISA RELINI[2], and GIULIA ROSSI[1] — [1]Physics department — [2]Chemistry department, University of Genoa, Genoa, Italy

Designing metal nanoparticles (NPs) with biomedical applications requires the molecular understanding of their interaction with cell membranes. We use fluorescence spectroscopy measurements and molecular dynamics (MD) simulations to study the interaction between charged monolayer-protected AuNPs and model POPC lipid bilayer[1-2]. We consider cationic (NP+) and anionic (NP-) NPs. The anionic ligands differ from the cationic ones for their terminal group, which is a carboxylate or a quaternary ammonium ion. We use fluorescence leakage assays to quantify the damage induced by NP- and NP+ to liposomes, and find that NP+ are more disruptive. MD simulations offer a molecular interpretation of this result. Assuming no changes of the charge of NP+ and NP- they interact with the bilayer with the same mechanism[3] and bilayer deformation. Our simulations, though, show that anionic ligands can be protonated when interacting with the lipid head. Once protonated, the NP- interact with the bilayer in a less disruptive way, without deforming or damaging it. This change of the pKa of the anionic ligands can explain the smaller leakage induced by NP-.

1.Tatur, S et all. Langmuir 2013. 2. Van Lehn,R. C. et all. Nano Lett. 2013. 3. Salassi, S. et all. JPCC 2017.

BP 22.2 Wed 15:15 H 1058

The effect of small molecules on lipid-domain formation studied by coarse-grained simulations — •ALESSIA CENTI, KURT KREMER, and TRISTAN BEREAU — Max Planck Institute for Polymer Research, Mainz, Germany

The lateral organisation of cell membranes is believed to play a key role in many biological processes, including protein trafficking, signal transduction as well as transport of viruses and pathogens. Small molecules, such as alcohols and anesthetics, can alter this lateral arrangement by preferentially partitioning between lipid domains, hence significantly affecting both membrane properties and functionalities. The process of domain stabilization/destabilization induced by small molecules has been widely investigated, both at experimental and computational level; however, its exact mechanism as well as the driving forces for it still remain elusive.

In this work, coarse-grained simulations based on the MARTINI force field have been used to try to shed light on the processes underlying domain reorganization mediated by small molecules. The approach used involves a combination of free energy calculations and replica exchange simulations; thereby, allowing to explore the effect of a multitude of parameters (e.g. type of lipids, solutes and relative concentrations) relevant for the process under evaluation at a reduced computational cost in comparison to atomistic simulations.

BP 22.3 Wed 15:30 H 1058

Performing cell-based tissue simulations to explore the impact of cell mechanics on anisotropic epithelial tissue growth — •ANNA STOPKA and DAGMAR IBER — D-BSSE, ETH Zürich, Schweiz

Understanding the anisotropic expansion of an embryonic tissue during organogenesis is a central challenge in developmental biology. Experimental studies increasingly provide quantitative data on cell behaviour during tissue growth. Computational models can help to interpret the acquired data and to infer underlying mechanisms. Our group has recently developed the 2D software framework LBIBCell to permit data-based simulations of tissue dynamics at cellular resolution [1]. LBIBCell represents cells as finely resolved polygons according to the Immersed Boundary (IB) method; membrane tension and cell-cell adhesion are represented via springs. The fluid behaviour inside and outside of the cells is described by the Lattice Boltzmann (LB) method. Cell growth is implemented via a fluid source inside the cells. Anisotropic outgrowth of epithelial tissues has been accounted to a range of mechanisms, including a bias in cell division orientation. We have used LBIBCell to investigate to what extent the mechanical properties of an epithelial tissue affect its capability to achieve anisotropic outgrowth via biased cell divisions. In our simulations we focused on the 2D apical plane where epithelial cells adhere tightly. We show that a bias in cell division orientation translates into a bias in outgrowth only for sufficiently stiff tissues. [1] S.Tanaka, D.Sichau, D.Iber, Bioinformatics (2015)

Invited Talk BP 22.4 Wed 15:45 H 1058

Complex shapes and dynamics of red blood cells in shear flow under physiological conditions — JOHANNES MAUER[1], SIMON MENDEZ[2], LUCA LANOTTE[3], MANOUK ABKARIAN[3], GERHARD GOMPPER[1], and •DMITRY A. FEDOSOV[1] — [1]Institute of Complex Systems, Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Institut Montpellierain Alexander Grothendieck, CNRS, University of Montpellier, 34095 Montpellier, France — [3]Centre de Biochimie Structurale, CNRS, University of Montpellier, 34090 Montpellier, France

Red blood cells (RBCs) constitute the major cellular part of blood and are mainly responsible for the transport of oxygen. They have a biconcave shape with a membrane consisting of a lipid bilayer with an attached cytoskeleton formed by a network of the spectrin proteins. The RBC membrane encloses a viscous cytosol (hemoglobin solution), so that RBCs possess no bulk cytoskeleton and organelles. Experiments on RBCs under shear flow reveal that the viscosity contrast between cytosol and blood plasma is an essential factor which determines their shape and dynamics. Under physiological conditions with a viscosity contrast of about five, RBCs first tumble, then roll, transit to a rolling and tumbling stomatocyte, and finally attain polylobed shapes at high shear rates. Our study based on microfluidic experiments and two different simulation techniques results in a complete diagram of RBC shapes and dynamics in shear flow as a function of shear rate and viscosity contrast. We will discuss potential mechanisms, which may lead to the variety of novel shapes, and compare the diagram for RBCs to that for vesicles.

BP 22.5 Wed 16:15 H 1058

On how the CSF flows in the ventral third ventricle of brain — •YONG WANG[1], CHRISTIAN WESTENDORF[1], REGINA FAUBEL[2], GREGOR EICHELE[3], and EBERHARD BODENSCHATZ[1] — [1]MPI for Dynamics and Self-Organization, 37077 Göttingen, Germany — [2]Department of Developmental Biology, U Pittsburgh, Pittsburgh PA 15201, USA — [3]MPI for Biophysical Chemistry, 37077 Göttingen, Germany

A complex transport network driven by coordinated motile cilia inside the ventral third ventricle (v3V) of mammalian brain was reported recently. This network generates cerebrospinal fluid (CSF) flow patterns such as a separatrix and a whirl that establish intraventricular boundaries. The CSF flow in the whole three-dimensional v3V cavity was studied numerically. Specifically, experimental trajectory data obtained by tracking fluorescent beads were converted to 2D velocity fields. The velocity maps were then refined by considering divergence-free and projected onto a curved virtual surface as boundary conditions. Three-dimensional flow features with likely physiological consequences were uncovered numerically. We thank the Max Planck Society for financial support. This work is conducted within the Physics and Medicine Initiative at Goettingen Campus between Max Planck Society and University Medicine Center.

BP 22.6 Wed 16:30 H 1058

Memoryless navigation with limited sensing capacity — LUIS GÓMEZ NAVA, •ROBERT GROSSMANN, and FERNANDO PERUANI — Université Côte d'Azur, Nice, France

How should an active walker detect a target in a complex landscape, e.g. the maximal chemical concentration, given that (i) only local values of this external signal are instantaneously accessible, but no gradients, and (ii) there is no memory? This question is of broad relevance, from bacterial chemotaxis to the design of self-controlled microrobots that are supposed to perform complex tasks autonomously. The latter area of application is particularly important with regard to today's medicine aiming at fabricating micrometer-sized robots for target-specific drug-delivery, for example. Motion on the micronscale is, however, subject to a series of constraints: viscous forces dominate over inertial ones and thermal fluctuations are relevant. Navigation under these physical conditions is hence a nontrivial task. In this talk, we provide basic theoretical guidelines how to design active particles

with internal states which are able to execute complex tasks such as adaptive gradient-following. We analytically link their internal dynamics of these particles to their motility properties such as drift and diffusivity enabling us to discuss how to tune the internal dynamics given a specific task. These findings are important in the design of simple navigation algorithms for robotic engineering and, moreover, may be present in various microbiological systems.

BP 22.7 Wed 16:45 H 1058

How does reducible defense alter predator-prey dynamics? — •Tatjana Thiel, Andreas Brechtel, Adrian Brückner, Michael Heethoff, and Barbara Drossel — Technische Universität Darmstadt, Germany

In nature, numerous animal species use defense mechanisms like hardening or chemical secretions to defend against attacks of predators. However, there is yet no theoretical study of defensive mechanisms where protection is permanent, but diminished with attacks, which has been termed "reducible defense". This kind of defense mechanism is common among arthropods and is likely to change the dynamics and stability of the system.

We propose a predator-prey model where prey use a reducible defense mechanism (i.e. reservoir-based chemical defense). The prey excretes a certain amount of secretion upon attack and is therefore not consumable while it is armed. The predator has to attack often enough to disarm and consume prey, before the secretion is biosynthetically restored. We will discuss the behavior of our model under parameter changes and compare it to a conventional predator-prey system. We show that predator and prey can become considerably more abundant by taking reducible defense into account. Furthermore, we consider payoffs between fast replenishment of secretion and larger storage volume, and between investment in offspring vs investment in defense. For the latter, we find that prey should invest more in defense when resources are scarce, but completely in offspring when plenty of resources are available.

BP 22.8 Wed 17:00 H 1058

Trade-off shapes diversity in eco-evolutionary dynamics — •Farnoush Farahpour[1], Mohammadkarim Saeedghalati[1], and Daniel Hoffmann[1,2,3] — [1]Bioinformatics and Computational Biophysics, Uni. Duisburg-Essen, DE — [2]CCSS, Uni. Duisburg-Essen, DE — [3]ZMB, Uni. Duisburg-Essen, DE

Over the last decades one of the main drivers of research in biodiversity has been to explain the naturally observed diversity and coexistence of competing species specially in well-mixed systems. In this project we propose a simple solutions for paradoxical question of diversity in competitive communities in a bare-bone and generic model. We introduce an Interaction and Trade-off based Eco-Evolutionary Model (ITEEM), in which species are competing for resources in a well-mixed system, and their evolution in interaction trait space is subject to a life-history trade-off between replication rate and competitive ability. We demonstrate that the strength of the trade-off has a fundamental impact on eco-evolutionary dynamics, as it imposes four phases of diversity, including a sharp phase transition. Despite its minimalism, ITEEM produces without further ad hoc features a remarkable range of observed patterns of eco-evolutionary dynamics. Most notably we find self-organization towards structured communities with high and sustainable diversity, in which competing species form interaction cycles similar to rock-paper-scissors games. Our approach to study the role of trade-offs in diversity provides a general framework to study assembly process of competitive communities and investigate the mechanisms responsible for resistance and resilience of their networks.

BP 22.9 Wed 17:15 H 1058

Interplay between Spatial Dynamics and Lifetime Distributions in an Evolutionary Food Web Model — •Tobias Rogge[1], Korinna T. Allhoff[2], David Jones[1], and Barbara Drossel[1] — [1]Institut für Festkörperphysik, Technische Universität Darmstadt, Germany — [2]Institute of Evolution and Ecology (EvE), University of Tübingen, Germany

We study the meta-network dynamics emerging in an evolutionary food web model on a system of coupled patches in space. Species are characterized by their body mass and the body-mass interval that specifies their prey. Each patch hosts a food web that contains several trophic layers, and the species composition in the patches changes due to ongoing processes of species addition ("mutation"), migration, and interaction-dependent extinction.

The model is able to sustain a complex food web structure on each patch, while undergoing continued species replacement dynamics. In particular, we evaluate species-lifetime distributions (how long is the time span that a species can survive in the system?) and species-area relationships SAR (how many species can we find in a given area?). All these relationships resemble power laws over appropriately chosen parameter ranges and thus agree qualitatively with empirical findings. We observe strong finite-size effects, and a dependence of the relationships on the trophic layer of the species. More precisely, we find that species with larger body masses on higher trophic position generate steeper SAR.