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Fachverband Biologische Physik (BP)

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Overview of Invited Talks and Sessions

(Lecture halls H 0104, H 1012, H 1028, and H 2032; Poster B-F)

Invited Talks

BP 1.1	Mon	9:30–10:00	H 0112	**Co-evolution of RNA viruses and the human immune system** — •Richard Neher
BP 2.7	Mon	11:15–11:45	H 2032	**The fascinating membrane morphology of the endoplasmic reticulum** — •Reinhard Lipowsky
BP 5.6	Mon	16:30–17:00	H 0110	**Sculpting embryos through fluid-to-solid phase transitions** — •Otger Campas
BP 6.1	Mon	15:00–15:30	H 1028	**Proton:ion antiporters generate membrane potential, and thus proton motive force in E.coli** — •Teuta Pilizota
BP 10.7	Tue	11:15–11:45	H 0112	**RNA Contact Prediction by Data Efficient Deep Learning** — Oskar Taubert, Fabrice von der Lehr, Alina Bazarova, Christian Faber, Philipp Knechtges, Marie Weiel, Charlotte Debus, Daniel Coquelin, Achim Basermann, Achim Streit, Stefan Kesselheim, Markus Götz, •Alexander Schug
BP 11.1	Tue	9:30–10:00	H 2032	**Mechanochemical regulation of epithelial barrier formation and function** — •Carien Niessen
BP 17.5	Wed	10:30–11:00	H 2032	**Red photocontrollable fluorescent proteins in nanoscopy** — •Francesca Pennacchietti
BP 18.1	Wed	9:30–10:00	H 1028	**Production and applications of artificial spider silk fibers and hydrogels** — •Anna Rising
BP 23.1	Wed	15:00–15:30	H 2032	**Inhibitor-induced transitions in pattern formation and their role to morphogenesis robustness** — •Silvia Grigolon
BP 23.6	Wed	16:45–17:15	H 2032	**Bayesian inference of chromatin looping dynamics from live-cell measurements** — •Christoph Zechner, Michele Gabriele, Hugo B Brandão, Simon Grosse-Holz, Asmita Jha, Gina M Daily, Claudia Cattoglio, Tsung-Han Hsieh, Leonid Mirny, Anders S Hansen
BP 24.1	Wed	15:00–15:30	H 1028	**Steps towards the de-novo synthesis of life** — •Sijbren Otto
BP 27.7	Thu	11:15–11:45	H 0112	**Integrative dynamic structural biology with multi-modal fluorescence spectroscopy and nanoscopy: From single molecules to live cells** — •Claus Seidel
BP 28.4	Thu	10:30–11:00	H 2032	**Quantifying the actin cortex of cells in different states** — •Franziska Lautenschläger, Daniel Flormann, Christoph Anton, Rhoda Hawkins
BP 31.4	Thu	15:45–16:15	H 0112	**Polarizing nuclear spins at the interface between ESR and NMR spectroscopy** — •Marina Bennati
BP 33.1	Thu	15:00–15:30	H 1028	**Symmetry breaking in early embryonic organoids: bridging networks, mechanics and metabolism** — •Vikas Trivedi
BP 34.3	Fri	10:00–10:30	H 2032	**Bacterial transport in dilute and porous environments** — •Christina Kurzthaler
BP 35.7	Fri	11:15–11:45	H 1028	**Large scale collective dynamics of bacteria suspensions** — •Eric Clement, Benjamin Perez Estay, Anke Lindner, Carine Douarche, Jochen Arlt, Vincent Martinez, Wilson Poon, Alexander Morosov

BP 37.1	Fri	13:15–14:00	H 0104	**Virus traps and other molecular machines of the future** — •Hendrik Dietz

Invited Talks of the joint Symposium SKM Dissertation Prize 2024 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H 1012	**Nonequilibrium dynamics in constrained quantum many-body systems** — •Johannes Feldmeier
SYSD 1.2	Mon	10:00–10:30	H 1012	**Controlled Manipulation of Magnetic Skyrmions: Generation, Motion and Dynamics** — •Lisa-Marie Kern
SYSD 1.3	Mon	10:30–11:00	H 1012	**Interactions within and between cytoskeletal filaments** — •Charlotta Lorenz
SYSD 1.4	Mon	11:00–11:30	H 1012	**Field theories in nonequilibrium statistical mechanics: from molecules to galaxies** — •Michael te Vrugt
SYSD 1.5	Mon	11:30–12:00	H 1012	**Lightwave control of electrons in graphene** — •Tobias Weitz

Invited Talks of the joint Symposium New Trends in Nonequilibrium Physics: Conservation Laws and Nonreciprocal Interactions (SYNP)

See SYNP for the full program of the symposium.

SYNP 1.1	Thu	15:00–15:30	H 0105	**Universality classes of nonequilibrium phase transitions with conservation constraints** — •Walter Zimmermann
SYNP 1.2	Thu	15:30–16:00	H 0105	**The many faces of living chiral crystals** — •Nikta Fakhri
SYNP 1.3	Thu	16:00–16:30	H 0105	**Non-reciprocal pattern formation of conserved fields** — •Fridtjof Brauns, M Cristina Marchetti
SYNP 1.4	Thu	16:45–17:15	H 0105	**Phase transitions and fluctuations of nonreciprocal systems** — •Sarah A.M. Loos
SYNP 1.5	Thu	17:15–17:45	H 0105	**Chiral matters** — •William Irvine

Sessions

BP 1.1–1.10	Mon	9:30–12:45	H 0112	**Systems and Network Biophysics**
BP 2.1–2.12	Mon	9:30–13:00	H 2032	**Membranes and Vesicles I**
BP 3.1–3.12	Mon	9:30–12:45	H 1028	**Active Matter I (joint session BP/CPP/DY)**
BP 4.1–4.11	Mon	15:00–18:00	H 0112	**Computational Biophysics I**
BP 5.1–5.10	Mon	15:00–18:00	H 0110	**Tissue Mechanics I**
BP 6.1–6.10	Mon	15:00–18:00	H 1028	**Bacterial Biophysics I**
BP 7.1–7.12	Mon	15:00–18:30	BH-N 243	**Active Fluids and Microswimmers (joint session DY/BP/CPP)**
BP 8.1–8.44	Mon	18:00–20:30	Poster C	**Poster Session Ia**
BP 9.1–9.16	Mon	18:00–20:30	Poster D	**Poster Session Ib**
BP 10.1–10.11	Tue	9:30–12:45	H 0112	**Computational Biophysics II**
BP 11.1–11.10	Tue	9:30–12:45	H 2032	**Cell Mechanics I**
BP 12.1–12.13	Tue	9:30–13:00	H 1028	**Active Matter II (joint session BP/CPP/DY)**
BP 13.1–13.12	Tue	9:30–13:00	BH-N 334	**Statistical Physics of Biological Systems I (joint session DY/BP)**
BP 14.1–14.19	Tue	18:00–20:30	Poster E	**Poster IIa**
BP 15.1–15.28	Tue	18:00–20:30	Poster F	**Poster IIb**
BP 16.1–16.11	Wed	9:30–12:30	H 0112	**Membranes and Vesicles II**
BP 17.1–17.11	Wed	9:30–12:45	H 2032	**Bioimaging**
BP 18.1–18.12	Wed	9:30–13:00	H 1028	**Biomaterials and Biopolymers (joint session BP/CPP)**
BP 19.1–19.12	Wed	9:30–13:00	BH-N 334	**Active Matter III (joint session DY/BP/CPP)**
BP 20.1–20.37	Wed	11:00–14:30	Poster B	**Poster IIIa**
BP 21.1–21.34	Wed	11:00–14:30	Poster C	**Poster IIIb**
BP 22.1–22.8	Wed	15:00–17:15	H 0112	**Bacterial Biophysics II**
BP 23.1–23.8	Wed	15:00–17:45	H 2032	**Focus Session: Inference Methods and Biological Data (German-French Focus Session) (joint session BP/DY)**

BP 24.1–24.10	Wed	15:00–18:00	H 1028	**Synthetic life-like systems and Origins of Life**
BP 25	Wed	18:15–19:15	H 1028	**Members' Assembly**
BP 26.1–26.12	Thu	9:30–13:00	H 0111	**Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)**
BP 27.1–27.12	Thu	9:30–13:00	H 0112	**Single Molecule Biophysics**
BP 28.1–28.11	Thu	9:30–13:00	H 2032	**Cytoskeleton**
BP 29.1–29.9	Thu	9:30–12:00	H 1028	**Statistical Physics of Biological Systems II (joint session BP/DY)**
BP 30.1–30.11	Thu	9:30–13:00	BH-N 334	**Active Matter IV (joint session DY/BP/CPP)**
BP 31.1–31.10	Thu	15:00–18:00	H 0112	**Protein Structure and Dynamics**
BP 32.1–32.10	Thu	15:00–17:45	H 2032	**Tissue Mechanics II**
BP 33.1–33.8	Thu	15:00–17:30	H 1028	**Focus session: Physics of organoids**
BP 34.1–34.12	Fri	9:30–13:00	H 2032	**Statistical Physics of Biological Systems III (joint session BP/DY)**
BP 35.1–35.12	Fri	9:30–13:00	H 1028	**Active Matter V (joint session BP/DY)**
BP 36.1–36.11	Fri	10:00–13:00	H 0112	**Cell Mechanics II**
BP 37.1–37.1	Fri	13:15–14:00	H 0104	**Closing Talk (joint session BP/CPP/DY)**

Members' Assembly of the Biological Physics Division

Wednesday 18:15–19:15 H 1028

BP 1: Systems and Network Biophysics

Time: Monday 9:30–12:45 Location: H 0112

Invited Talk BP 1.1 Mon 9:30 H 0112

Co-evolution of RNA viruses and the human immune system — •Richard Neher — Biozentrum, University of Basel, Switzerland

Human influenza viruses and SARS-CoV-2 rapidly accumulate mutations to evade recognition by the human immune system, which allows these viruses to repeatedly infect individuals. Since circulation of a viral variant generates immunity against that variant, the resulting dynamics has features of rapid adaptive evolution as well as features of ecological interactions. With extensive surveillance of these human viruses, we can now track emerging variants in detail and quantify their competition. We also have more and more data on the diversity of human immune responses and molecular basis of viral immune escape. These data provide an opportunity to understand the co-evolutionary dynamics of humans and their viruses in quantitative terms. I will discuss the relative importance of adaptation and ecological dynamics for viral evolution and how it depends on the immunological diversity of the host population. Lastly, I will discuss implications of host diversity and ecological dynamics on predictability of the evolution of SARS-CoV-2 and influenza virus.

BP 1.2 Mon 10:00 H 0112

Non-determinism and Boltzmann ensembles in genotype-phenotype maps — •Nora S. Martin[1], Paula García-Galindo[2], and Sebastian E. Ahnert[2,3] — [1]CRG (Barcelona Collaboratorium for Modelling and Predictive Biology), Barcelona Institute of Science and Technology, Dr. Aiguader 88, Barcelona 08003, Spain — [2]Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, UK — [3]The Alan Turing Institute, 96 Euston Road, London NW1 2DB, UK

Over the last decades, analyses of genotype-phenotype (GP) maps have greatly contributed to our quantitative understanding of variation and its role in evolutionary processes. While the GP map of RNA secondary structure is maybe the best-studied example, many concepts have subsequently been applied to a range of further biological systems. However, most analyses neglect one key aspect of RNA folding that is also relevant in other systems: a genotype does not simply fold into a single structure (i.e. phenotype). Instead, its folding is more accurately described as a Boltzmann ensemble, i.e., a distribution of structures. This defines a different type of GP map, referred to as a "non-deterministic" map. In this contribution, I will describe definitions required for characterising these "non-deterministic" maps, and what patterns they reveal.

BP 1.3 Mon 10:15 H 0112

Unraveling the Influence of Geometry, Binding and Diffusion on Proteins in the Presynaptic Region — •Simon Dannenberg, Sarah Mohammadinejad, and Stefan Klumpp — Institut für Dynamik komplexer Systeme Georg-August-Universität Göttingen Friedrich-Hund-Platz 1 37077 Göttingen, Germany

The mobility of a protein is a key factor determining its availability for chemical reactions in a cell. It is influenced by many factors including the diffusion coefficient, binding to membranes and the geometry of the environment. In the presynaptic region of neurons, the latter varies widely between different synapses. Combined with the tremendous biological importance of this region it becomes a compelling quest to investigate mobility here. In our work we use simulations to disentangle the interplay of the aforementioned factors. We demonstrate that the binding to synaptic vesicles and the cytoplasmic diffusion of the protein give rise to a specific length scale that determines whether the recovery of protein material is dominated by protein redistribution inside the synapse or via fluxes from the axon. This length scale is comparable to the size of the presynaptic region, which makes the interpretation of common experimental techniques for mobility measurements such as FRAP challenging. However, our simulations enable suggestions to circumvent pitfalls in Experiments.

BP 1.4 Mon 10:30 H 0112

Elucidating the genetic determinants of antibiotic resistance evolution — •Gabriela Petrungaro, Theresa Fink, and Tobias Bollenbach — Institute for Biological Physics, University of Cologne, Germany

Biological evolution of bacterial populations under strong antibiotic selection can quickly lead to resistant populations that pose a threat to public health. To understand the evolutionary dynamics that lead to resistance, a thorough statistical characterization of this stochastic process is needed, which requires many repeats of the same experiments under tightly controlled conditions. Here, we report the results of 864 parallel automated evolution experiments with tight feedback control of population size and selection pressure. We investigate how the genetic background of an initially susceptible population constrains its ability to evolve resistance. To this end, we systematically compared 258 Escherichia coli strains that initially differ in single gene-deletions and evolve for two to three weeks under three clinically relevant antibiotics, one at a time. We find that evolution is highly parallel at the phenotypic and genotypic level, but the degree of parallelism varies among antibiotics. The evolutionary paths to resistance can be rationalized as biased random walks on a fitness landscape in genotype space. We find that certain gene deletions drastically alter these evolutionary paths, making new fitness peaks accessible and hampering others. Our results contribute to the understanding of repeatability in the evolution of antibiotic resistance and to the identification of possible targets for strategies to combat resistance.

15 min. break

BP 1.5 Mon 11:00 H 0112

Fluctuation-response relations for integrate-and-fire models with an absolute refractory period — •Benjamin Lindner[1,2] and Friedrich Puttkammer[1,2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Bernstein Center for Computational Neuroscience Berlin

For many systems in statistical physics it is known, that their spontaneous fluctuations and their response to a time-dependent perturbation are related via a fluctuation-dissipation theorem. For spike-generating nerve cells (neurons) such relations have been uncovered only recently (Lindner, PRL 2022) but these fluctuation-response relations (FRRs) were limited to a special class of stochastic neuron models, namely, integrate-and-fire (IF) neurons without a refractory period. Here we relax this restriction and derive FRRs for IF neurons with an absolute refractory period and a stereotypical spike shape for the action potential. The derived relations are exact for the case of an uncorrelated (white) intrinsic noise but only approximate if the intrinsic fluctuations are temporally correlated. All results are tested by comparison with stochastic simulations and reveal that even a small but nonvanishing refractory period leads to a significantly modified relation between fluctuation statistics and response statistics.

BP 1.6 Mon 11:15 H 0112

Nonrenewal spiking in Calcium signaling — •Lukas Ramlow[1,2,3], Martin Falcke[2,3], and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience, Berlin, Germany — [2]Department of Physics, Humboldt University, Berlin, Germany — [3]Max Delbrück Center for Molecular Medicine, Berlin, Germany

Inositol 1,4,5-trisphosphate-induced Ca^{2+} signaling is a second messenger system used by almost all eukaryotic cells. The agonist concentration that stimulates Ca^{2+} signaling is encoded in the sequence of Ca^{2+} concentration spikes. In response to the onset of stimulation, the times between spikes, the interspike intervals (ISIs), exhibit a distinct transient during which they gradually increase. In the steady state, this slow adaptation correlates the intervals and spiking is a nonrenewal process. We propose a stochastic model that can reproduce both stationary and transient statistics of experimentally observed ISI sequences. We derive approximate analytical expressions for the stationary ISI statistics and consider the response to the onset of a constant stimulus to estimate the length of the transient and the strength of the adaptation of the ISI. We show that the adaptation determines the coefficient of variation, in agreement with current ideas derived from experiments. Finally, we fit our model to reproduce the transient statistics of experimentally observed ISI sequences in stimulated HEK cells. The fitted model is able to qualitatively reproduce the relationship between stationary interval correlations and transient interval statistics.

BP 1.7 Mon 11:30 H 0112

Analysing biological systems via maximally informative representations — •Roberto Menichetti[1,2], Riccardo Aldrigo[1], and Raffaello Potestio[1,2] — [1]Physics Department, University of Trento, Trento, Italy — [2]INFN-TIFPA - Trento Institute for Fundamental Physics and Applications, Trento, Italy

The main challenge of an in silico investigation of biological systems is nowadays shifting from the generation of data to the problem of developing techniques enabling their rational interpretation. Often, the noise/signal discrimination passes through dimensionality reduction strategies; while such coarsening is necessary to interpret high-dimensional simulation datasets, it inevitably results in a loss of information on the system that critically depends on the choice of the low-dimensional projection [1]. We here discuss a recent workflow aimed at identifying simplified representations of a system that retain the largest amount of information on its statistical properties while reducing the observational level of detail [1,2]. The protocol is applied to proteins and memory-retrieving neural networks; in both cases, the resulting representations are shown to single out biologically relevant regions of the system, either in the form of functional chemical fragments in the analysed proteins or of strongly coupled neurons in the network. Our results suggest that this scheme can be employed to extract insight from large simulation datasets, further shedding light on the relation between dimensionality reduction and information loss. [1] Giulini M. et al., Front. Mol. Biosci. 8, 676976 (2021). [2] Giulini M. et al., J. Chem. Theory Comput. 16, 6795 (2020).

15 min. break

BP 1.8 Mon 12:00 H 0112

The beginning of olfactory signal transduction: A theoretical model on the synergist-agonist threshold of G-protein-coupled receptors — •Won Kyu Kim — Korea Institute for Advanced Study, Seoul 02455, South Korea

We present a chemical reaction network theory for olfactory sensing processes of G-protein-coupled receptors (GPCRs) as olfactory receptors (ORs). The theory is applicable to mixtures of odorants and any number of ORs. It explicitly considers reactions of ORs with G-proteins, with and without odorants. The theory introduces an odor activity vector, representing strengths of odorant-induced signals from ORs relative to those from background G-protein activity. Each vector component follows a Michaelis-Menten form, accounting for cooperation or competition effects between different odorants. The theory's main features are illustrated for a two-odorant mixture, quantitatively describing known and potential mixture effects, such as suppression, shadowing, inhibition, and synergy. The effects of rate constants, basal activity, and G-protein concentration are also demonstrated.

BP 1.9 Mon 12:15 H 0112

A stochastic conductance-based model of the hawkmoth Manduca sexta olfactory receptor neuron — •Mauro Ariel Forlino, Aditi Vijayan, Katrin Schröder, Anna Schneider, Monika Stengl, and Martín García — Kassel University, Kassel, Germany

The long trichoid sensillum in male hawkmoths, Manduca sexta, is innervated by two olfactory receptor neurons (ORNs) that respond to the pheromone released by female moths to attract conspecific mates. In the absence of odor stimuli, pheromone-sensitive ORNs in hawkmoths exhibit non-randomly distributed spontaneous spikes. Analyzing spike distribution is crucial for identifying different mechanisms at play. The random opening and closing of ion channels introduce internal fluctuations in neurons, known as channel noise, which contributes to the variability in spike distribution and determines whether a single spike or a burst occurs. Furthermore, insect ORNs serve as endogenous peripheral circadian clock neurons, leading to the expression of daytime-dependent rhythmic spike distributions. In this study, we present a novel conductance-based model that incorporates the olfactory receptor coreceptor (ORCO) as a pacemaker ion channel with linear conductance dependent on cAMP concentration. Our model takes into account that cAMP express daytime-dependent rhythms with concentration being maximal during activity phase. By utilizing stochastic differential equations based on the microscopic Markovian states of ion channels, our model can reproduce the observed spike distribution with its circadian oscillations.

BP 1.10 Mon 12:30 H 0112

Inference of dynamical networks in biology with recurrent neural networks — •Pablo Rojas[1], Marie Kempkes[1], Claudia Arbeitman[1,2], and Martin Garcia[1] — [1]Theoretical Physics, University of Kassel, Kassel, Germany — [2]CONICET, Argentina

The inference of networks in dynamical systems is crucial to the mechanistic understanding of complex systems. Biological systems often rely on the emergent behaviour resulting from the interaction of multiple units. Inferring the existence of links between nodes of a network from measured time series is an inverse problem that becomes more complex under the presence of non-equilibrium, strong nonlinearity, noise, delays and large number of interacting nodes - frequent conditions in experimental time series. In this work, we present a method that uses recurrent neural networks to learn the underlying connections in a dynamical system from its multivariate time series. A key aspect of the method is that it does not assume a mathematical model, i.e. equations, defining the dynamics of the network. Thus, the method is model-free, which makes it applicable to a broader range of systems. We apply this method to a range of biological systems under far-from-ideal conditions to evaluate its performance. We sketch a comparison against other neural network architectures to showcase its advantages.

BP 2: Membranes and Vesicles I

Time: Monday 9:30–13:00 Location: H 2032

BP 2.1 Mon 9:30 H 2032

Membrane fusion as a pathway to fission — •Russell Spencer and Marcus Müller — Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

Remodeling of biological membranes, such as fusion and fission, is involved in a variety of basic, cellular processes. This work investigates the mechanisms and pathways for the fission of phospholipid membranes, in particular double-membrane fission as it occurs in mitochondrial division. We employ self-consistent field theory and utilize the string method to find the Minimum Free Energy Path (MFEP) in order to determine the most likely pathway for the transition. The complex landscape of possible rearrangements gives rise to multiple possible mechanisms for double membrane fission. The simplest pathway involves the local constriction, hemifusion and fission of the inner membrane, without contact with the outer membrane. Intriguingly, we also uncover a new mechanism whereby local fusion contact between the inner and outer membrane can catalyze the fission of the inner membrane. Not only does the new mechanism have a lower total free energy barrier, but also an intermediate metastable state, allowing the system to ratchet its way up the rate-limiting step.

BP 2.2 Mon 9:45 H 2032

Adhesion energy controls lipid binding-mediated endocytosis — R Groza[1], K Schmidt[1,2], P Müller[1], P Ronchi[3], C Schlack[1], U Neu[1], D Puchkov[4], R Dimova[2], C Matthaeus[5], J Taraska[5], T Weikl[2], and •H Ewers[1] — [1]Freie Universität Berlin — [2]MPI Colloids and Interfaces — [3]EMBL — [4]FMP — [5]National Institutes of Health

Many bacterial toxins and viruses deform membranes through multivalent binding to lipids for clathrin-independent endocytosis. How membrane deformation and endocytic internalization are mechanistically linked is unclear. Here we show that many lipid-binding virions induce membrane deformation for clathrin-independent endocytosis, suggesting a common mechanism based on multivalent lipid binding by globular particles. We create a synthetic cellular system consisting of a lipid-anchored receptor in form of GPI-anchored anti-GFP nanobodies and a multivalent globular binder with 180 regularly-spaced GFPs on its surface. We show that these 40 nm diameter particles bind to cells expressing the receptor, deform the plasma membrane upon adhesion and become endocytosed in a clathrin-independent manner. We explore the role of the membrane adhesion energy in endocytosis by using receptors with affinities varying over 7 orders of magnitude. Our

system shows that once a threshold in adhesion energy is overcome, membrane deformation and endocytosis occurs reliably. Membrane deformation by globular binders is thus sufficient for internalization to occur and is a common, purely biophysical mechanism for lipid-binding mediated endocytosis of particles.

BP 2.3 Mon 10:00 H 2032

Effect of the receptor nanoclustering on the activation of natural killer cells through biomechanical feedback — •Piotr Nowakowski[1], Ashish Pandey[2], Carlos Ureña Martin[2], Muhammad Abu Ahmad[3], Avishay Edri[3], Esti Toledo[2], Sivan Tzadka[2], Jonas Walther[4], Guillaume Le Saux[2], Angel Porgador[3], Mark Schvartzman[2], and Ana-Sunčana Smith[4,1] — [1]Division of Physical Chemistry, Institut Ruđer Bošković, Zagreb, Croatia — [2]Department of Materials Engineering, Ilse Katz Institute for Nanoscale Science and Technology, Ben-Gurion University of the Negev, Beer-Sheva, Israel — [3]Faculty of Health Sciences, Ben-Gurion University of the Negev, Beer-Sheva, Israel — [4]Institut für Theoretische Physik, IZNF, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Natural killer (NK) cells are part of the immune system responsible for rapid recognition and elimination of virus-infected or tumor cells. The exact mechanism of this recognition is not yet known but it is expected to be related to the observed formation of nanoclusters of receptors on the membrane of NK cell. We propose a phenomenological model of activity of NK cell based on biomechanical feedback between number of connected receptors, activity of NK cell, and fluctuations of the membrane. We test the model in experiment: using nanolithography we create patterns of ligands of various shapes and measure the activity of cells after binding to them. Our theoretical model qualitatively explanes the dependence of activity on the structure of nanoclusters and overall density of ligands that is observed in the experiment.

BP 2.4 Mon 10:15 H 2032

Polysaccharide functionalization reduces lipid vesicle stiffness — •Kevin Jahnke and David A. Weitz — Harvard University, Cambridge, USA

The biophysical properties of lipid vesicles are important for their stability and integrity, key parameters that control the performance when these vesicles are used for drug delivery. The vesicle properties are determined by the composition of lipids used to form the vesicle. However, for a given lipid composition, they can also be tailored by tethering polymers to the membrane. Typically, synthetic polymers like polyethyleneglycol are used to increase vesicle stability but the use of polysaccharides in this context is much less explored. Here, we report a general method for functionalizing lipid vesicles with polysaccharides by binding them to cholesterol. We incorporate the polysaccharides on the outer membrane leaflet of giant unilamellar vesicles (GUVs) and investigate their effect on membrane mechanics using micropipette aspiration. We find that the presence of the glycolipid functionalization produces an unexpected softening of GUVs with fluid-like membranes. By contrast, the functionalization of GUVs with polyethylene glycol does not reduce their stretching modulus. Furthermore, we explore the effect of polysaccharide functionalization of lipid vesicles for drug delivery. We find that it increases the uptake of small unilamellar vesicles (SUVs) by cells and leads to an improved transfection. This work provides the potential means to study membrane-bound meshworks of polysaccharides similar to the cellular glycocalyx; moreover, it can be used for tuning the mechanical properties of drug delivery vehicles.

BP 2.5 Mon 10:30 H 2032

Mechanical properties of pure protein membranes made from fungal hydrophobins — •Kirstin Kochems[1], Friederike Nolle[1], Hendrik Hähl[1], Michael Lienemann[2], and Karin Jacobs[1] — [1]Department of Experimental Physics & Center for Biophysics, Saarland University, Saarbrücken, Germany — [2]VTT Technical Research Centre of Finland Ltd., Espoo, Finland

As strongly amphiphilic proteins, fungal hydrophobins are known to self-assemble at water-interfaces into stable monolayer films. Contacting of two formed monolayers results in stable bilayers, that can be studied in a microfluidic surrounding or via atomic force microscopy (AFM)[1].

By transferring monolayer films from the water-air interface to perforated substrates, we can use force spectroscopy indentation measurements to examine the mechanical properties of pore-spanning hydrophobin mono- and bilayers. We find that the hydrophobin layers show a high stability and a higher Young's modulus in comparison with phospholipid membranes.

[1] Hähl, H. et al., Adv. Mater 29, 1602888 (2017).

BP 2.6 Mon 10:45 H 2032

Mechanical regulation of endocytosis by protein condensate capillary forces — •Max Ferrin[1,2,3], Tyler Harmon[2], David Drubin[3], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute Theory of Polymers, Leibniz Institute of Polymer Research, Dresden, Germany — [3]Department of Molecular and Cell Biology, University of California, Berkeley, CA, USA

Clathrin-mediated endocytosis (CME) is the primary pathway for internalization of extracellular and membrane cargo in eukaryotic cells. It is characterized by a patch of the plasma membrane invaginating and pinching off to generate a cytoplasmic vesicle. Recently, experimental evidence has begun to accumulate in support of proteins assembling into liquid-like condensates at nascent CME sites, but potential functional consequences are lacking in the literature. Given that condensate capillary forces influence membrane bending in other biological systems, we constructed a mathematical model to probe the mechanical influence of a protein droplet on endocytosis. Preliminary analysis of the model shows that a droplet can regulate the progression of endocytosis by stalling invagination until a threshold distance or droplet volume, and driving toward completion after passing the threshold. Further model analysis will characterize the critical parameters that set this regulatory behavior, as well as make predictions of CME dynamics that can be tested experimentally.

15 min. break

Invited Talk BP 2.7 Mon 11:15 H 2032

The fascinating membrane morphology of the endoplasmic reticulum — •Reinhard Lipowsky — Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

Our body contains an enormous number of biomembranes that enclose our cells and most intracellular organelles. A particularly intriguing example is provided by the membrane of the endoplasmic reticulum (ER), which extends throughout the whole cell as a bicontinuous network of membrane nanotubes connected by three-way junctions, thereby generating a surface with a very high topological genus. [1]

A long-standing puzzle of the ER morphology is the straight appearance of the nanotubes in the light microscope, which form contact angles close to 120 degrees. Another puzzling aspect are the nanoscopic shapes of the tubules and junctions. Furthermore, both the formation and the maintenance of the nanotubular networks require GTP and GTP-hydrolyzing membrane proteins. In fact, the nanotubes are destroyed when the supply of GTP is interrupted.

It has been recently argued [1] that all of these puzzling observations are intimately related to each other and to the dimerization of two membrane proteins anchored in the same membrane. The dimerization process can generate an effective membrane tension that stabilizes the ER geometry and prevents the tube destruction, thereby maintaining the integrity of the ER.

[1] R. Lipowsky, S. Pramanik, A. S. Benk, M. Tarnawski, J. P. Spatz, R. Dimova. Elucidating the Morphology of the Endoplasmic reticulum. ACS Nano 17:11957-11968 (2023) DOI: 10.1021/acsnano.3c01338

BP 2.8 Mon 11:45 H 2032

Biomolecular condensates on geometrically structured lipid membranes — •Katja Zieske — Biophysics, Max Planck Institute for the Science of Light, Erlangen, Germany

Biomolecular condensates are supramolecular assemblies of proteins and RNA molecules and have been studied extensively, due to their ability to spatially structure cells and to spatially confine biological reactions. However, little is known about the interactions of liquid-liquid condensates with geometrically structured lipid membranes and the consequences of these interactions on cellular length scales. Here, we used a cell-free bottom-up approach to reconstitute liquid-liquid condensates at geometrically structured lipid membranes. Our results demonstrate how lipid membranes and liquid-liquid condensates interact under various experimental conditions and point towards an important role of membrane geometry-controlled wetting-effects in intracellular organization.

BP 2.9 Mon 12:00 H 2032

Membranes interacting with biomolecular condensates: wet-

ting, remodeling, and damage stabilization — •Agustin Mangiarotti[1], Macarena Siri[1], Claudio Bussi[2], Nicky Tam[1], Leonel Malacrida[3,4], Maximiliano Gutierrez[2], Reinhard Lipowsky[1], and Rumiana Dimova[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]The Francis Crick Institute, London, UK — [3]Departamento de Fisiopatología, Hospital de Clínicas, Facultad de Medicina, Universidad de la República, Montevideo, Uruguay — [4]Advanced Bioimaging Unit, Institut Pasteur of Montevideo and Universidad de la República, Montevideo, Uruguay

Membrane wetting by biomolecular condensates recently emerged as an important phenomenon in cell biology, playing a key role in diverse processes across different organisms. By performing a systematic analysis of the interaction of protein and polymer condensates with giant unilamellar vesicles as model membranes, we have demonstrated that these interactions can lead to remodeling processes, which are governed by the interplay of adhesion, membrane elasticity, and interfacial tension. Moreover, we showed that condensate wetting can promote the stabilization of damaged membranes, uncovering a new mechanism for biomolecular condensates in cell physiology. Finally, we explored the interaction mechanism between condensates and membranes at a molecular scale, using nano-environmental sensors and state-of-the-art microscopy techniques combined with phasor analysis. With this approach, we found that biomolecular condensates can modulate membrane lipid packing and hydration by wetting.

BP 2.10 Mon 12:15 H 2032

Modeling the reshaping of membranes across the tree of life — •Felix Frey, Miguel Amaral, and Andela Saric — Institute of Science and Technology Austria, Klosterneuburg, Austria

All biological cells are defined by flexible lipid membranes that are constantly reshaped as cells divide or relay materials across them. Interestingly, various membrane designs have evolved across the tree of life. In archaea, one of the two prokaryotic domains that often live at extreme conditions, membranes are typically organized into monolayers. Therefore, archaeal membranes are supposed to react differently when subjected to curvature compared to bilayer membranes in eukaryotes. However, the physical behavior of archaeal monolayer membranes during bending deformations has never been characterized. Here, we develop the first particle-based model for archaeal monolayer membranes. Our computer simulations reveal how archaeal membrane monolayers self-assemble, how they withstand high temperatures and how they deform when they adsorb small particles. In addition, we explore how imposing external membrane curvature dictates the organization of membrane lipids and creates membrane plasticity. Our findings demonstrate that archaeal monolayer membranes behave significantly different from bilayer membranes, potentially explaining why various membrane designs have evolved across the tree of life.

BP 2.11 Mon 12:30 H 2032

Physicochemical properties of microplastic particles affect their cellular uptake and maturation — •Simon Wieland[1,2], Anja FRM Ramsperger[1,2], Wolfgang Gross[1], Matteo Kumar[1], Johanna Bodrogi[1], Christian Laforsch[2], and Holger Kress[1] — [1]Biological Physics, University of Bayreuth, Germany — [2]Animal Ecology I, University of Bayreuth, Germany

Microplastics are an abundant contaminant in the environment, raising concerns about harmful effects on organisms. Therefore, many studies investigating effects of microplastics on cells, tissues, and organisms were published. These studies often rely on commercial model microplastics, usually polystyrene microspheres. While nominally very similar, their physicochemical properties can differ, making it difficult to compare the results of different studies. We now show that nominally identical polystyrene microspheres from eight different manufacturers differ in their ζ-potential, which determines their cellular interactions and internalization by macrophages. We monitored the actin cytoskeleton during particle uptake and found that phagocytosis or macropinocytosis drive the internalization. The uptake time differed between particle types and was correlated with the particles ζ-potential. Furthermore, we examined the subsequent maturation and acidification of internalized microplastics. We found that the maturation kinetics strongly differed between particle types. Unraveling the kinetics and mechanisms of microplastic internalization and maturation in cells is essential to understand their potentially harmful effects.

BP 2.12 Mon 12:45 H 2032

Understanding the Interface of Plastic Nanoparticles and Biomimetic Cell Membranes — •Una Janke, Emma Weilbeer, Wanda Levin, Norman Geist, and Mihaela Delcea — Institut für Biochemie, Felix-Hausdorff-Str. 4, 17489 Greifswald

Plastics and the release of polymeric particles into the environment is a burning issue, not least because plastic nanoparticles (NPs) are potentially harmful to both the surrounding and human health. As soon as they enter the body, NPs have contact to various biological fluids (e.g. blood) and with cell membranes containing different types of lipids and numerous membrane proteins. To understand the complex interaction of NPs with the cellular interface, we have chosen a representative model system comprising of the commonly used plastic polystyrene and an artificial biomimetic membrane containing the platelet receptor integrin αIIbβ3 which undergoes conformational dynamics, e.g. in the presence of manganese ions. The combination of biophysical methods, such as dynamic-light-scattering, enabled the characterisation of the protein corona around the polystyrene nanoparticles (PS-NPs) with different surface charges and its stability over time. Moreover, the interaction of the PS-NPs with the engineered biomimetic membranes was analysed by quartz-crystal-microbalance and the results were confirmed by cell interaction analyses and molecular dynamic simulations studies. Our results reveal that protein corona formation prevents unspecific binding of PS-NPs to membranes, whereas the absence of corona induces surface charge-dependent aggregation of PS-NPs, as well as strong binding to model cell membranes.

BP 3: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: H 1028

BP 3.1 Mon 9:30 H 1028

Active Colloids as Tunable Swarmalators — •Veit-Lorenz Heuthe[1,2] and Clemens Bechinger[1,2] — [1]Fachbereich Physik, Universität Konstanz — [2]Centre for the Advanced Study of Collective Behaviour, Universität Konstanz

The complexity and functional advantages in various systems from groups of organisms to robotic swarms and digital networks hinge on spatiotemporal patterns arising from the interactions of their constituents. One approach to gain understanding of how these patterns emerge are so-called swarmalators. In this conceptual framework, individual entities exhibit both oscillatory behavior and translational motion, coupled based on their relative phase and position, yielding a diverse array of complex patterns. Here, we introduce a system of active colloids that both oscillate and translate and are coupled to each other in both speed and phase through hydrodynamic interactions. Despite the physical nature of the interactions, the system retains tunability, enabling us to systematically study the behavior of swarmalators in a real system.

BP 3.2 Mon 9:45 H 1028

Electric field driven active colloids moving in polymeric environments — •venkata manikantha sai ganesh tanuku, peter vogel, and thomas palberg — Institute of Physics, Johannes Gutenberg University

A dilute suspension of Janus particles (JPs) in a dense viscoelastic fluid, forms a natural setting to study their dynamics in surrounding doped with macromolecules such as polymers is crucial, as most of the target application media are complex in nature. In this study, we investigate the motion of AC electric field driven SiO2-Au JPs in the presence of concentrated amounts of poly (ethylene glycol) (PEG). The transport of active particles is strongly influenced by the viscous medium and shows a dynamical jamming transition as a function of activity and medium density. For low activity, the active particle gets self-trapped in a cavity of its own making. Conversely, higher activity causes JP to push through the fluid, leaving behind a porous trail. At the given concentration of the PEG studied within these experiments two intriguing outcomes emerge: firstly, a JP can be immobilized and secondly, when two JPs move in the same direction, an unusual at-

traction occurs, causing the trailing JP to eventually catch up with the leading one in finite time.

BP 3.3 Mon 10:00 H 1028

Lorentz reciprocal theorem in fluids with odd viscosity — •Yuto Hosaka[1], Ramin Golestanian[1,2,3], and Andrej Vilfan[1,4] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom — [3]Institute for the Dynamics of Complex Systems, University of Göttingen, 37077 Göttingen, Germany — [4]Jozef Stefan Institute, 1000 Ljubljana, Slovenia

The Lorentz reciprocal theorem – that is used to study various transport phenomena in hydrodynamics – is violated in chiral active fluids that feature odd viscosity with broken time-reversal and parity symmetries. Here we show that the theorem can be generalized to fluids with odd viscosity by choosing an auxiliary problem with the opposite sign of the odd viscosity [1]. We demonstrate the application of the theorem to two categories of microswimmers. Swimmers with prescribed surface velocity are not affected by odd viscosity, while those with prescribed active forces are. In particular, a torque-dipole can lead to directed motion.

[1] Y. Hosaka, R. Golestanian, and A. Vilfan, Phys. Rev. Lett. 131, 178303 (2023).

BP 3.4 Mon 10:15 H 1028

A Stochastic Bubble Model in MIPS Active systems — •Mingqi Yan[1,2,3,4], Erwin Frey[1,4], Marcus Müller[2,4], and Stefan Klumpp[3,4] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, D-80333 München, Germany — [2]Institut für Theoretische Physik, Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [3]Institut für Dynamik komplexer Systeme, Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [4]Max Planck School Matter to Life, Hofgartenstraße 8, D-80539 München, Germany

Motility-Induced Phase Separation (MIPS) is a notable phenomenon in which self-propelled particles undergo phase separation solely due to their intrinsic motility. This behavior starkly contrasts with passive systems, where active systems constantly form bubbles in liquids. Here, we introduce a stochastic bubble model to elucidate the changes in bubble area within Active Brownian Particle systems. We demonstrate that the bubble-area evolution can be described by a Langevin equation. Notably, this equation characterizes a unique category of stochastic systems: while it possesses an absorbing state, it concurrently maintains a stable nonequilibrium steady state distribution of areas.

BP 3.5 Mon 10:30 H 1028

Dynamics and phase separation of active Brownian particles on curved surfaces and in porous media — •Priyanka Iyer, Roland Winkler, Dmitry Fedosov, and Gerhard Gompper — Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich

In biophysical systems, active particles are often exposed to curved geometries and confinement. This prompts a crucial question: How does curvature influence the emergent collective behavior of active particles? We study this question by considering the effect of curvature on an ensemble of repulsive active Brownian particles (ABPs) moving on a spherical surface. Surface curvature affects the dynamics of ABPs, as it introduces a new time scale $\tau = R/v_0$, with curvature radius R and propulsion velocity v_0, in addition to the rotational diffusion time τ_r. The time scale τ is related to a stop-and-go motion caused by the recurrent alignment of the propulsion direction with the surface normal. This implies that motility-induced phase separation (MIPS) disappears for large curvature. Moreover, the phase-separation boundary at low area fraction ϕ attains a turning point for small R, allowing for the possibility of a re-entrant behavior. The findings also have implications for understanding how curvature influences ABP dynamics in porous media, as demonstrated through a paradigmatic example involving two connected pores. Surprisingly, it is found that the different curvatures of the two pores can facilitate particle flux towards regions of high particle density and induce transient MIPS states.

[1] Iyer et al. Phys. Rev. Res. **5**, 033054 (2023).

BP 3.6 Mon 10:45 H 1028

Giant Activity-Induced Stress Plateau in Entangled Polymer Solutions — Davide Breoni[1], Christina Kurzthaler[2], Benno Liebchen[3], Hartmut Löwen[2], and •Suvendu Mandal[3] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöhnitzer Straße 38, 01187 Dresden, Germany — [3]Technische Universität Darmstadt, Karolinenplatz 5, 64289 Darmstadt, Germany

Highly entangled active polymer solutions play vital roles in various biological processes, spanning from the intricate mechanisms of cell mitosis to the regulation of genetic transcription. We study the viscoelastic properties of highly entangled, flexible, self-propelled polymers using Brownian dynamics simulations. Our results show that the active motion of the polymer increases the height of the stress plateau by orders of magnitude due to the emergence of grip forces at entanglement points. Identifying the activity-induced energy of a single polymer and the ratio of polymer length to self-propulsion velocity as relevant energy and time scales, we find the stress autocorrelation functions collapse across Peclet numbers [1]. We predict that the long-time viscosity scales with polymer length squared, in contrast to equilibrium counterparts that scale with the cube of the polymer length [1]. These insights offer prospects for designing new materials with activity-responsive mechanical properties.

[1] D. Breoni, C. Kurzthaler, B. Liebchen, H. Löwen, and S. Mandal, https://doi.org/10.48550/arXiv.2310.02929

15 min. break

BP 3.7 Mon 11:15 H 1028

Gravitactic bioconvection drives emergent transport and mixing in harmful algal blooms — •Soumitree Mishra[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg

Bioconvection, the active self-sustaining transport phenomenon triggered by the accumulation of motile microbes, has been long studied. Yet, if and how this collective behavior, driven by competing physico-chemical cues, impacts ecological processes including Harmful Algal Blooms (HABs) remains unexplored. Here, using a bloom-forming model phytoplankton, we present a comprehensive mechanistic study on the biophysical factors governing the emergent collective patterns and capture the eco-physiological implications of bioconvective flows. Leveraging our Ocean-On-Chip platform, together with particle tracking velocimetry (PTV) and particle image velocimetry (PIV), we uncover flow fields around isolated self-organized microbial plumes, using which we extract the spatial range of active transport. Using data-backed fluid dynamic simulations, we extract the Lyapunov exponents, revealing the mixing capacity of such plumes in confined environments. Our findings significantly advance our understanding of bioconvection's functional role in ecological contexts[1], providing a novel playground where ecology meets active matter. [Reference 1] Bioconvection mediates transport and mixing dynamics within harmful algal blooms: S. Mishra & A. Sengupta (manuscript in preparation).

BP 3.8 Mon 11:30 H 1028

Energetic cost of microswimmer navigation: the role of body shape — •Lorenzo Piro[1,2], Andrej Vilfan[1,3], Ramin Golestanian[1,4], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany — [2]Department of Physics and INFN, University of Rome Tor Vergata, Via della Ricerca Scientifica 1, 00133 Rome, Italy — [3]Jozef Stefan Institute, 1000 Ljubljana, Slovenia — [4]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We study the energetic efficiency of navigating microswimmers by explicitly taking into account the geometry of their body. We show that, whereas arguments based solely on propulsion efficiency lead to the conclusion that needle-like swimmers are most energetically efficient, disk-like swimmers rotated by flow gradients naturally follow time-optimal trajectories. The coupling between body geometry and hydrodynamics thus leads to a generic trade-off between the energetic costs associated with propulsion and navigation, which is accompanied by the selection of a finite optimal aspect ratio. We derive from optimal control theory the steering policy ensuring overall minimum energy dissipation and characterize how navigation performances vary

with the swimmer shape. Our results highlight the important role of the swimmer geometry in realistic navigation scenarios.

BP 3.9 Mon 11:45 H 1028

Optimal motility strategies for self-propelled agents to explore porous media — •Christoph Lohrmann and Christian Holm — Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany

Micro-robots for, e.g., biomedical applications, need to be equipped with motility strategies that enable them to navigate through complex environments. Inspired by biological microorganisms we recreate motility patterns such as run-and-reverse, run-and-tumble or run-reverse-flick applied to active rod-like particles in silico. We investigate their capability to efficiently explore disordered porous environments with various porosities and mean pore sizes ranging down to the scale of the active particle. By calculating the effective diffusivity for the different patterns, we can predict the optimal one for each porous sample geometry. We find that providing the agent with the ability to sense position for a certain time and to make a decision based on its observation yields a motility pattern outperforming the biologically inspired patterns for all investigated porous samples[1].

[1] Lohrmann, Holm: Optimal motility strategies for self-propelled agents to explore porous media, arXiv:2302.06709, 2023

BP 3.10 Mon 12:00 H 1028

Chemotaxis of an active particle attached to a semiflexible cargo — •Shashank Ravichandur[1], Abhinav Sharma[2,1], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Universität Augsburg, Augsburg, Germany

The chemotaxis of synthetic active particles in activity gradients, achieved by connecting them to other active/passive particles to form simple dimers, has been demonstrated in recent studies. These studies have been extended to synthetic active particles connected to each other to form polymer chains, which also exhibit chemotaxis. However, the study of these polymer chains in activity gradients has been limited to the Rouse model, wherein the particles are connected to each other via springs, and the excluded volume interactions are ignored. To obtain a more realistic description, we consider an active synthetic particle connected to a passive tail that is semiflexible. In such a system, the configuration of the passive tail affects the motion of the active particle. Using Langevin dynamics simulations, we show that these polymers also exhibit chemotaxis in activity gradients despite the coupling between the active particle and the passive tail. We also study the effects of the chain length and bending rigidity on the chemotactic behavior.

BP 3.11 Mon 12:15 H 1028

How cell shape guides gliding motility — •Leon Lettermann[1], Falko Ziebert[1], Mirko Singer[1], Friedrich Frischknecht[2], and Ulrich S. Schwarz[2] — [1]IPT & Bioquant, Heidelberg University — [2]CIID, Heidelberg University

Cell motility comes in many different types, including swimming, crawling and gliding. The latter term denotes movement on surfaces or through tissues without appreciable changes in cell shape and is usually based on some kind of surface flow. Gliding motility is often used by cells that need to accomplish high speeds, including myxo- or flavobacteria as well as eukaryotic parasites from the phylum apicomplexa, in particular the causative agents of malaria and toxoplasmosis. We have developed an active particle theory which connects the self-organized surface dynamics to the global motility patterns of the glider. Our theory demonstrates that the resulting trajectories depend strongly on glider shape. Our analytical solutions and numerical simulations show that straight motion to get from A to B is unstable and predict the rotational and helical trajectories which are observed experimentally for gliding bacteria and apicomplexan parasites.

BP 3.12 Mon 12:30 H 1028

Impact of non-reciprocity on the self-aggregation of an anisotropic colloidal system — •Salman Fariz Navas and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Non-reciprocal interactions have been demonstrated to introduce interesting collective behaviour in many-body systems[1]. Recent studies involving non-reciprocal colloidal particle systems have shown to induce propulsion mechanisms[2] and cause enhanced diffusion of tracer particles[3]. Such effects can have an impact on aggregation mechanisms as well[2]. Here, we introduce non-reciprocal interactions to a self-aggregating colloidal system with direction dependent, field-induced interactions[4]. In stark contrast to the passive (reciprocal) case, non-reciprocity induces a propulsion mechanism when a pair of particles belonging to different species come in contact. We show that at low degrees of non-reciprocity the aggregation is accelerated. At higher degrees of non-reciprocity, the system even tends to phase separate leading to the coexistence of dilute, freely moving particles and dense clusters.

[1] M. Fruchart, R. Hanai, P. B. Littlewood, and V. Vitelli, Nature 592, 363 (2021).
[2] S. Fehlinger and B. Liebchen, Phys. Rev. Research 5, L032038 (2023).
[3] A. Benois, M. Jardat, V. Dahirel, V. Démery, J. Agudo-Canalejo, R. Golestanian, and P. Illien, Phys. Rev. E 108, 054606 (2023).
[4] F. Kogler, O. D. Velev, C. K. Hall, and S. H. L. Klapp, Soft Matter 11, 7356 (2015).

BP 4: Computational Biophysics I

Time: Monday 15:00–18:00 Location: H 0112

BP 4.1 Mon 15:00 H 0112

Efficient radial-shell model for 3D tumor spheroid dynamics with radiotherapy — •Florian Franke[1], Soňa Michlíková[2,3], Sebastian Aland[1,4,5], Leoni A. Kunz-Schughart[2,6], Anja Voss-Böhme[1], and Steffen Lange[1,2] — [1]HTW Dresden - University of Applied Sciences — [2]OncoRay, Natl. Center for Radiation Research in Oncology, TU Dresden — [3]Helmholtz-Zentrum Dresden - Rossendorf, Germany — [4]TU Bergakademie Freiberg — [5]Center for Systems Biology, Dresden — [6]Natl. Center for Tumor Diseases, Dresden, Germany

Approximately 50% of patients diagnosed with cancer receive radiotherapy at least once during their disease. Experiments with sophisticated in-cellulo assays to improve radiotherapeutic outcomes are still challenging, and some critical details of tumor cell dynamics still need to be explored. To enhance the informative value of such approaches and support future therapeutic study designs, we developed an efficient mathematical model for three-dimensional multicellular tumor spheroids, which reflect microregions within a large tumor or avascular micrometastases and which are an auspicious experimental framework to pre-assess the curative effect of radio(chemo)therapy. We validate our mathematical model using experimental tumor spheroid growth data of several cell lines with and without radiotherapy and observe equal or better performance than previous models. Moreover, our model allows for efficient parameter calibration within previously reported and/or physiologically reasonable ranges. Based on this data-driven approach, we can explain the mechanism of the characteristic dynamics at small tumor volumes.

BP 4.2 Mon 15:15 H 0112

Leveraging Point Cloud Transformers and Simulation-based Inference for Enhanced Parameter Inference in Tumor Growth Modeling — •Julian Herold[1], Eric Behle[2], and Alexander Schug[2] — [1]Kalrsruhe Institut für Technologie (KIT), Karlsruhe, Germany — [2]Jülich Supercomputing Centre (JSC), Jülich, Germany

Computational modeling serves as a cornerstone in unraveling the intricate dynamics of living tissues. However, the challenge of deriving quantitatively meaningful parameters from experimental data persists. Conventional methods, such as ABC, rely on summary statistics, introducing inherent limitations in the selection of relevant metrics. To address these challenges, we advocate for the adoption of Simulation-based Inference (SBI), harnessing the capabilities of deep learning techniques to navigate the complexities associated with parameter inference. In this study, we present utilizing point cloud transformers directly on positional data extracted from in-vitro spheroids, circumventing the reliance on summary statistics and thus overcoming the limitations of traditional methods. Our methodology integrates the training

of neural networks into the parameter inference pipeline of CellsInSilico (CiS), a high-performance framework designed for large-scale tissue simulations. Not only does this yield superior results in terms of inference accuracy, but it also enhances computational efficiency compared to conventional methodologies, empowering researchers to explore critical biological questions. Demonstrated utility includes investigating the interplay between the extracellular matrix and tumor invasion.

BP 4.3 Mon 15:30 H 0112

Modeling and simulation of red blood cells aggregation in cardiovascular networks — •Fouzia Imharken[1,2], Chaouqi Misbah[1], and Hamid Ez-zahraouy[2] — [1]Interdisciplinary Laboratory of Physics (LIPhy)-UGA-Grenoble- French — [2]Laboratory of Condensed Matter and Interdisciplinary Sciences-Mohamed 5 University-Morocco

Cardiovascular dysfunctions due to undesirable adhesion among blood elements (like red blood cells-RBCs) are the main causes of mortality in the world. In our study, we intend to develop simple models to better understand the perfusion of blood in microcirculation by considering a complex geometry under several conditions (shear, confinement, pressure, etc.) in the presence of adhesion among RBCs using an immersed boundary-lattice Boltzmann method. Our primary results show that the aggregation of RBCs and their mechanical properties has a strong impact on their distribution in the network. For stiff RBCs (due to a disease) a weak adhesion leads to super diffusion instead of ballistic transport, as compared to the case without adhesion.

BP 4.4 Mon 15:45 H 0112

Validating the Protein Hydration Shell against Small-angle Scattering Data - Effects of Water Models, Force Fields, and Surface Composition — •Johanna-Barbara Linse and Jochen S. Hub — Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, 66123, Germany

The proteins hydration shell plays key roles in protein stability and function. So far, it remained unclear whether hydration shells predicted by explicit-solvent molecular dynamics (MD) simulations match experimental conditions, as precise experimental data on hydration shell structures were limited. Small-angle scattering (SAS) experiments provide insight into hydration shell properties, because the detected radius of gyration (R_g) and zero-angle scattering (I_0) depend on the contrast between the hydration shell and the solvent. Using explicit-solvent MD simulations and SAS calculations, we calculated R_g values for five proteins, evaluating 18 combinations of protein force fields and water models. Validation of the results against consensus data from a round-robin benchmark project revealed remarkable agreement between MD simulations and experiments, depending on the choice of force field and water model. Furthermore, we investigated the influence of amino acid surface composition of proteins on the hydration shell contrast, providing contrast scores for 20 amino acids. Our studies show that explicit-solvent SAS calculations and consensus SAS data provide a novel routes for scrutinizing the proteins hydration shell and for predicting the amino acid effects on the hydration shell structure.

BP 4.5 Mon 16:00 H 0112

Chromatic medium under active perturbation — •Rakesh Das — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany — Mechanobiology Institute, National University of Singapore, Singapore 117411

Chromatin organization inside a cell nucleus and its coordination with subnuclear compartments (SNCs) play crucial roles in genome regulation. However, numerous enzymes act inside the nucleus that actively perturb the medium. We investigated the effect of such active perturbations (AP) on the compartmentalization of chromatin into eu- and hetero-chromatin phases and the SNC-dynamics embedded therein. We use a polymer physics framework, where the chromatin is perturbed through a non-localized active mechanism mimicking the action of TopoisomeraseII enzyme. Computer simulations show the emergence of characteristic phase separation morphologies, viz., wall-like organization of euchromatin with negative nematic ordering of the euchromatic segments due to such active perturbations. A simplified equilibrium model can catch the essence of the phase separation but fails to explain such emergent features. This highlights the critical role of AP in chromatin organization. Using a similar computational setting, we show that the SNC-dynamics in such a complex medium can be described as a combination of three modes linked with different physical aspects of the embedding medium. Under AP, mainly a slow mode associated with remodeling of chromatic meshes enhances SNC-dynamics. This may provide an insight into the role of global AP on regulating the target-searching processes in the chromatic medium.

BP 4.6 Mon 16:15 H 0112

Kinetics of radiation-induced DNA double-strand breaks through coarse-grained simulations — •Manuel Micheloni[1,2], Lorenzo Petrolli[1,2], Gianluca Lattanzi[1,2], and Raffaello Potestio[1,2] — [1]Physics Department, University of Trento, via Sommarive, 14 I-38123 Trento, Italy — [2]INFN-TIFPA, Trento Institute for Fundamental Physics and Applications, I-38123 Trento, Italy

Double-strand breaks (DSBs), the covalent cut of the DNA backbone over both strands, are a detrimental outcome of cell irradiation. The earliest stages of the irradiation of DNA feature fast and localized processes, hardly characterizable by conventional experimental techniques, but viable for *in silico* assessments; mean-field descriptions have been extremely insightful at correlating irradiation regimes and macroscopic observables (i.e. cell survival), albeit neglecting structural, mechanical and kinetic implications associated with lesioned DNA molecules. In fact, in spite of their biological significance, the dynamical evolution of DSBs is still largely uncertain. *Via* coarse-grained molecular dynamics simulations, we have addressed the mechanical rupture of a DNA molecule by diverse DSB motifs, i.e., within a range of distances between strand breaks (DSB distance). We have shown the cooperative nature of the process, characterized by an abrupt transition driven by the disruption of the residual interactions between DNA moieties, governed by Poisson statistics. Moreover, we have accessed the timescales of the rupturing process, inferring an exponential dependence of the characteristic rupture times on the DSB distances, typically associated with an Arrhenius-like law of thermally-activated processes.

15 min. break

BP 4.7 Mon 16:45 H 0112

Computational design of graphene nanopores for amino-acid detection — •Longlong Li and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Germany

Nanometer-sized pores, the nanopores, opened in two-dimensional (2D) materials have been shown to enhance biosensing due to their atomic-layer resolution. Using density-functional theory and the non-equilibrium Green's functions approach, we perform systematic simulations to investigate the electronic and transport properties of graphene nanopores in which single amino acids are placed. The simulations aim to gain an in-depth understanding of the interaction between these biomolecules and graphene nanopores and reveal amino-acid specific characteristics. The results indicate the significant role of these biomolecules, their structure and properties in modulating the electronic structure and transport of the pristine nanopores. Our research provides valuable insights into designing graphene nanopore-based biosensing devices, with precise control over their electronic and transport properties.

BP 4.8 Mon 17:00 H 0112

Tensile strength of water with organic impurities — •Marin Šako and Matej Kanduč — Jožef Stefan Institute, Ljubljana, Slovenia

The stability of water is a long-standing problem in physics, studied since the 17th century and continuing to be a subject of investigation today. There is a notable discrepancy between experimental findings and theoretical predictions, as well as inconsistency in measurements across different experiments. While theory predicts that water should be remarkably stable against cavitation, experiments show quite the opposite. In this talk, I will present our work on the conditions that lead to catastrophic cavitation events in decane and water. Additionally, I will discuss how the tensile strength of water is influenced by hydrocarbon impurities, such as oil droplets. We use a framework that combines classical nucleation theory with molecular dynamics simulations. We find that while pure bulk water is exceptionally stable against cavitation, the presence of even tiniest amounts of decane is enough to destabilize water and reduce its tensile strength to experimentally measured lower values. Using our numerical analysis, we find that a decane droplet of a radius of around 1 nm in a macroscopic volume of water is enough to destabilize the system. This is the reason why even in ultra-pure water, the measured tensile strength is significantly lower compared to theoretical predictions. We also find that the curvature correction of surface tension is important to take into

account when studying cavitation, nanodroplets, or nanobubbles.

BP 4.9 Mon 17:15 H 0112

Introducing the Automated Ligand Searcher — Luise Jacobsen[1], Jonathan Hungerland[2], •Vladimir Bačić[2], Luca Gerhards[2], Fabian Schuhmann[3], and Ilia A. Solov'yov[2] — [1]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, 5230 Odense M, Denmark — [2]Institute of Physics, Carl von Ossietzky Universität, 26129 Oldenburg, Germany — [3]Niels Bohr International Academy, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark

The Automated Ligand Searcher (ALISE) is designed as an automated computational drug discovery tool. To approximate the binding free energy of ligands to a receptor, ALISE includes a three-stage workflow, with each stage involving an increasingly sophisticated computational method: molecular docking, molecular dynamics, and free energy perturbation, respectively. To narrow the number of potential ligands, poorly performing ligands are gradually segregated out. The performance and usability of ALISE are benchmarked for a case study containing known active ligands and decoys for the HIV protease. The example illustrates that ALISE filters the decoys successfully and demonstrates that the automation, comprehensiveness, and user-friendliness of the software make it a valuable tool for improved and faster drug development workflows.

BP 4.10 Mon 17:30 H 0112

Radial dependence of X-ray induced ionization clusters around a gold nanoparticle — •Leo Thomas[1,2], Hans Rabus[1], and Miriam Schwarze[1] — [1]National Metrology Insititute, Berlin Germany — [2]Dept. II, Technical University of Berlin, Germany

One strategy to improve the efficacy of radiotherapy for cancer is increasing the tumor*s sensitivity to irradiation, e.g., by introducing gold nanoparticles (GNPs) into cancer cells [1].

This work explores the enhancement of ionization clusters around a GNP, which are considered to be indicative of the induction of DNA lesions [2], a potential trigger for cell-death-inducing damage [3].

Monte Carlo track structure simulations were performed in a two-step-approach. The produced ionizations were scored using Associated Volume Clustering [4] to obtain the radial profile of ionization clusters frequency.

The influence of the GNP on the electron fluence spectrum is relatively small and occurs mainly at energies below 10 keV. Accordingly, increased ionization clustering is limited to a range up to about 200 nm. Here, smaller GNPs (radii up to 10 nm) cause noticeable peaks in the frequency ionization clusters upon occurrence of a photon interaction at distances around 50 nm from the GNP surface.

[1] J. Hainfeld et al.,Nanomedicine (Lond), 8 (2013) 1601-9 [2] A. Rucinski et al., Phys Med Biol, 66 (2021) 24TR01 [3] M. Lomax et al., Clin Oncol, 25 (2013) 578-85. [4] K. R. Kase et al., The dosimetry of ionizing radiation Vol 1 (1985) Chap. 2

BP 4.11 Mon 17:45 H 0112

Cationic and anionic lipid mixing favors the lamellar-to-hexagonal phase transition in coarse-grained molecular dynamics simulations — •David Noel Zimmer[1,2], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Physics Department Johannes Gutenberg University Mainz — [2]Faculty of Physics and Astronomy Ruhr University Bochum

Lipid-based nanoparticles (LNPs) are used as delivery vehicles for RNA-therapeutics, a potentially broad class of drugs including COVID-19 vaccines as well as drugs against genetically inherited diseases and cancer. LNPs are produced by rapid mixing the cargo RNA at low pH with a lipid formulation containing ionizable cationic lipids, helper and PEGylated lipids. The lipid formulation helps to compact the RNA, to screen it from degradation and to deliver it to the target cell. LNPs' mechanisms of action is not yet well understood. Here, we use coarse-grained molecular dynamics simulation to investigate the effect of the fusion process between the LNP and the endosomal membrane following cellular uptake of the LNP. The simulations show that the mixing of the anionic lipids of the endosome with the cationic lipids of the LNP leads to a stabilization of the hexagonal phase versus the lamellar phase. Analysis of the hexagonal phase shows that cationic lipids tend to accumulate in the space between three adjacent tubules, while anionic lipids distribute more uniformly around the tubules, indicating a lack of correlation in the position of the two oppositely charged lipids.

BP 5: Tissue Mechanics I

Time: Monday 15:00–18:00 Location: H 0110

BP 5.1 Mon 15:00 H 0110

Polydispersity-Mediated Crystallization in the Developing Fruit Fly Wing — •Kartik Chhajed[1], Marko Popović[1], and Frank Jülicher[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden — [2]Center for Systems Biology Dresden, Pfotenhauerstraße 108, 01307 Dresden

During development of the fruit fly wing the cellular packing in the wing epithelium transitions from a disordered packing to an ordered, crystalline packing. We investigate biophysical mechanisms controlling this crystallization process. While previous studies highlight the role of tissue shear flow in establishing the ordered cell packing, we find that in fly wings where tissue flows have been inhibited the cells still transition from disordered to an ordered packing. Instead, we propose that the transition is controlled by the cell size heterogeneity, which is quantified by the cell size polydispersity. We use vertex model of epithelial tissues to show that there is a critical value of cell size polydispersity above which cellular packings are disordered and below which they form a crystalline packing. Furthermore, by analyzing experimental data we find that cell size polydispersity indeed decreases during the fly wing development in the wild-type wings, while in perturbed wings where cells remain heterogenous in size cellular packing remains disordered. Finally, we find that although tissue flows do not control the transition they do significantly enhance the tissue scale order as they help align locally ordered crystallites on the tissue scales.

BP 5.2 Mon 15:15 H 0110

The fluid mechanics of the first folding event of the zebrafish forebrain — Angus Inman[1], Judith E. Lutton[2], Elisabeth Spiritosanto[1], Masazumi Tada[3], Till Bretschneider[2], •Pierre A. Haas[4,5,6], and Michael Smutny[1] — [1]Centre for Mechanochemical Cell Biology and Division of Biomedical Sciences, Warwick Medical School, University of Warwick — [2]Department of Computer Science, University of Warwick — [3]Department of Cell and Developmental Biology, University College London — [4]Max Planck Institute for the Physics of Complex Systems — [5]Max Planck Institute of Molecular Cell Biology and Genetics — [6]Center for Systems Biology Dresden

The formation of complex tissues during development relies on robust spatiotemporal coordination of mechanical forces between different tissues or in complex geometries.

Here, I will show how such inter-tissue forces underpin the first folding event in the developing zebrafish forebrain [bioRxiv:2023.06.21.545965v1]. I will develop a fluid mechanical model of tissue flows during zebrafish gastrulation to identify the minimal set of spatiotemporally varying regularised force singularities required to reproduce the topological features of the observed tissue flows qualitatively. I will then discuss how we have tested these predictions in vitro and in silico: I will show in particular that this minimal set of singularities is also sufficient to reproduce the observed tissue flows quantitatively and I will explain how our combined experimental and theoretical results show that the coordination of different mechanical processes in different tissues is required for correct folding of the zebrafish forebrain.

BP 5.3 Mon 15:30 H 0110

Minimal vertex model explains how the amnioserosa tissue remains solid during Drosophila dorsal closure — •Daniel Haertter[1,2], Indrajit Tah[3], Janice M. Crawford[4], Daniel P. Kiehart[4], Christoph F. Schmidt[2], and Andrea J. Liu[3] — [1]Institute of Pharmacology and Toxicology, University Medical Center Göttingen, Germany — [2]Department of Physics, Duke University, NC, USA — [3]Department of Physics and Astronomy, University of Pennsylvania, PA, USA — [4]Department of Biology, Duke University, NC, USA

Dorsal closure is a process in *Drosophila melanogaster* embryogenesis during which the amnioserosa (AS), a one-cell-thick epithelial tissue that fills the dorsal opening, shrinks as the lateral epidermis sheets converge and eventually fuse. This process results in a significant increase in the aspect ratio of the AS cells. Contrary to predictions of the standard vertex model, which suggests tissue fluidization by cell rearrangement, the AS retains its elastic solid properties without such changes. We introduce a two-dimensional cellular vertex model that accounts for the ability of the AS to sustain this behavior. The model demonstrates that the continuous decrease in preferred cell perimeter and variability in cell perimeter size are key factors in maintaining the solid state of the AS. Our model effectively replicates observed changes in cell shape and orientation and indicates a non-uniform pattern of junctional tension, which we verify through laser ablation experiments.

BP 5.4 Mon 15:45 H 0110

Quantification of Glioblastoma Mechanics in Brain Organoids Using Ferrofluid Droplets — •Michael Frischmann[1,2], Elijah R. Shelton[1], Achim T. Brinkop[1], Sofia Kalpazidou[3], Jovica Ninkovic[3], and Friedhelm Serwane[1,4] — [1]Faculty of Physics and Center for NanoScience, LMU Munich, Germany — [2]Faculty of Medicine, LMU Munich, Germany — [3]Biomedical Center, LMU Munich, Germany — [4]SyNergy and GSN, LMU Munich, Germany

Glioblastoma, a highly malignant brain tumor, has a median patient survival of a few months untreated, due to its rapid, infiltrative and destructive growth. Although its molecular biology is well described, knowledge about the mechanical properties and forces that enable its invasive spread is limited. We used cerebral organoids derived from induced pluripotent stem cells (iPSCs) and implanted with patient-derived glioblastoma cells as an *in vitro* model. To measure its viscoelastic properties, ferrofluid droplets were utilized. The mechanical properties were determined from the droplets' dynamic strain curves via a custom modular analysis pipeline developed in Python. This approach allowed quantifying viscous behavior of the tumor tissue on time scales from seconds to minutes. At short time scales, we determined an elastic modulus of $E = (0.96 \pm 0.27)$ kPa, which is consistent with previous elasticity measurements performed in patient tissue. Moreover, we find a long-term viscosity of $\eta = (17.6 \pm 3.9)$ kPa s in the core tumor. A viscoelastic model of glioblastoma enhances our understanding of how brain tumors mechanically affect their environment, which is crucial for targeting the infiltration mechanism.

BP 5.5 Mon 16:00 H 0110

Poking a very soft elastic shell — •Shiheng Zhao[1,2,3] and Pierre Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Biological tissues are very soft materials: Their linear elastic constants tend to be several orders of magnitude smaller than those of conventional soft materials. At the same time, biological tissues undergo large deformations during development, suggesting that their nonlinear elastic behaviour is much more important than that of conventional soft materials.

Here, we therefore consider the simplest model of an elastic material with zero linear shear modulus, i.e. of a purely nonlinearly elastic material. We extend the paradigmatic "Pogorelov dimple" problem of classical elasticity [1] to this "supersoft" material: An elastic spherical shell is poked by a concentrated, point force. Strikingly, our numerical calculations reveal novel scaling behaviour of the force-displacement relation, with an exponent 3/2 for this "supersoft" material, different from the classical exponent 1/2. We develop an elastic shell theory and a scaling argument to explain this exponent, and we characterise numerically the transition between the two scaling regimes as a small, nonzero linear shear modulus is added. Excitingly, the results suggest that the nonlinear contributions to tissue elasticity can be measured from the scaling behaviour in poking experiments.

[1] A. V. Pogorelov, Bendings of surfaces and stability of shells (American Mathematical Society, Providence, RI, 1988).

15 min. break

Invited Talk BP 5.6 Mon 16:30 H 0110

Sculpting embryos through fluid-to-solid phase transitions — •Otger Campas — Physics of Life Excellence Cluster, TU Dresden, Germany

During embryonic development, cells self-organize to build functional structures, like tissues and organs, and progressively shape the organism. While many key molecular players that orchestrate embryonic development are known, the physical mechanisms underlying embryonic morphogenesis remain unclear. Performing direct measurements of the tissue physical state in situ and in vivo using microdroplet techniques, I will show that embryonic tissues undergo fluid-to-solid (rigidity) transitions that are controlled in space and time to guide morphogenesis. First, I will discuss body axis elongation in vertebrates and show that posterior tissues are fluid-like at their elongating end and become solid-like as they mature anteriorly through a jamming transition of the cell collective. Beyond axis elongation, I will discuss a new nuclear jamming transition that controls tissue architecture during vertebrate eye and brain organogenesis.

BP 5.7 Mon 17:00 H 0110

Mechanically-driven stem cell separation in tissues caused by progeny outflux — •Johannes C. Krämer[1], Edouard Hannezo[2], Gerhard Gompper[1], and Jens Elgeti[1] — [1]Theoretical Physics of Living Matter (IBI-5/IAS-2), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Science and Technology Austria, 3400 Klosterneuburg, Austria

The homeostasis of epithelial tissue relies on a balance between the self-renewal of stem cell populations, cellular differentiation, and loss. We expand the two particle growth model [1,2] to incorporate the text book picture of tissue renewal by stem cells and the corresponding differentiation cascade [3], and find that the model generates unexpected dynamic features: stem cells repel each other in the bulk tissue and are thus found rather isolated, as in a number of in vivo contexts. We demonstrate that this repulsion can be quantitatively described by mapping it to an ensemble of passive Brownian particles with effective repulsive interactions. The effective interaction potential between a pair of stem cells decays exponentially with a characteristic length that spans several cell sizes, corresponding to the outflux volume of differentiated cells generated per stem cell division. By introducing stochastic cell fate decisions we find that tissue pressure controls the stem cell number. Our findings may help understanding the dynamics and evolution of normal and cancerous epithelial tissues.

[1] M. Basan et al 2011 Phys. Biol. 8 026014;
[2] N. Podewitz et al 2015 EPL 109 58005
[3] J. C. Krämer et al 2023 arXiv:2310.04272 [physics.bio-ph]

BP 5.8 Mon 17:15 H 0110

Wrinkling instability in unsupported epithelial sheets — •Urska Andrensek[1,2], Primoz Ziherl[1,2], and Matej Krajnc[1] — [1]Jozef Stefan Institute, Ljubljana, Slovenia — [2]Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

We investigate the elasticity of an unsupported epithelial monolayer and we discover that unlike a thin solid plate, which wrinkles if geometrically incompatible with the underlying substrate, the epithelium may do so even in absence of the substrate. From a cell-based model, we derive an exact elasticity theory and discover wrinkling driven by the differential apico-basal surface tension. Our theory is mapped onto that for supported plates by introducing a phantom substrate whose stiffness is finite beyond a critical differential tension. This suggests a new mechanism for an autonomous control of tissues over the length scale of their surface patterns.

BP 5.9 Mon 17:30 H 0110

A model of epithelial folding through local degradation of an elastic basement membrane plate — •Karla Yanin Guerra Santillan[1,2], Caroline Jantzen[1], Christian Dahmann[1,2], and Elisabeth Fischer-Friedrich[1,2,3] — [1]Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden, Germany. — [2]School of Science, Technische Universität Dresden, Dresden, Germany. — [3]Biotechnology Center, Technische Universität Dresden, Dresden, Germany.

Epithelia are polarized flat layers of cells that line the surfaces of organs. On the basal side, the epithelial cell layer is supported by a basement membrane - a thin polymeric layer of self-assembled extracellular matrix (ECM) that plays a crucial role in shaping healthy organs during organism morphogenesis. Previous research on the larval wing disc of Drosophila melanogaster notes a connection between localized basement membrane degradation and epithelial folding.

In this study, we introduce a unique approach to understanding epithelial folding by integrating a plate theory model of the basement membrane with experiments. Our theoretical model considers force balance within the basement membrane and interactions with the cell

layer, explaining epithelial folding during local plate degradation with a preexisting balance of active and passive mechanical prestress.

To validate our theoretical framework, we conducted experiments exploring the influence of cell-internal hydrostatic pressure and basolateral contractility on fold depth, confirming their pivotal roles in fold shape.

BP 5.10 Mon 17:45 H 0110

The Geometric Basis of Epithelial Convergent Extension — Fridtjof Brauns[1], Nikolas H. Claussen[2], and •Boris I. Shraiman[1,2] — [1]Kavli Institute for Theoretical Physics, University of California Santa Barbara, Santa Barbara, California 93106, USA — [2]Department of Physics, University of California Santa Barbara, Santa Barbara, California 93106, USA

Animal development requires large numbers of cells to choreograph their force generation in order to sculpt tissues and organs. Leveraging the fact that cellular forces equilibrate rapidly compared to the speed of development, we formulate a geometrical model for the network of balanced active tensions in an epithelial sheet. Within this framework, we can investigate how cells remodel the tension network to change tissue shape. A simple "winner-takes-all" mechanical feedback loop can self-organize complex cell movement, matching experimental data on the cell and tissue scale. We find that the ability to self-organize depends on initial order in the cellular packing. Our model explains how genetic patterning, embryo geometry, and cellular packing geometry combine to determine tissue shape change.

BP 6: Bacterial Biophysics I

Time: Monday 15:00–18:00 Location: H 1028

Invited Talk BP 6.1 Mon 15:00 H 1028

Proton:ion antiporters generate membrane potential, and thus proton motive force in E.coli — •Teuta Pilizota — Centre for Engineering Biology, University of Edinburgh, Edinburgh, UK

To stay outside of thermodynamic equilibrium, all living cells need energy. Arguably the main energy source of life is the electrochemical potential of a given ion, so-called ion motive force, with the ATP molecule being the other. Because bacteria are unicellular the energy production is tightly linked with all the other processes in the cell. For example, the electrochemical potential of a given ion is composed of two parts. The electrical potential across the membrane, which is generated by the charge accumulated at the membrane, and 'drives' all ions. But also the specific chemical concentration differences of a given ion, where the exact concentration of ions in the cell matters, particularly that of protons. Lastly, bacteria maintain significant osmotic pressures, which depend on the difference between the extracellular and intracellular concentrations of all solutes, including ions. The result is a non-trivially intertwined set of physiological variables, yet, the bacterial cell does it; it achieves the necessary homeostasis of them all. How?

To begin answering the question here I'll focus on the bacterium Escherichia coli and show how it achieves a sufficient electrical potential, and in turn the electrochemical gradient of protons. The results champion a shift of perspective in the fundamental principle driving pH regulation.

BP 6.2 Mon 15:30 H 1028

Understanding the mechanisms of novel and existing antibiotics at the single-cell level — •Lars Renner[1], Felix Wong[2], James Collins[2], Jens Friedrichs[1], and Ralf Helbig[1] — [1]Leibniz-Institute of Polymer Research, Max Bergmann Center of Biomaterials, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, MA, USA

Many existing antibiotics are becoming increasingly ineffective causing antibiotic resistance in bacteria. Antibiotics have different molecular targets, however, even after decades of medical use, many effects of antibiotics on bacteria are still unknown. We investigate the mechanistic mode of action of antibiotics, particularly at the single cell level. Using various techniques, we are corroborating the cellular physiology and biochemical regulation as well as the different molecular mechanism downstream caused by the application of antibiotics, specifically for aminoglycoside, beta-lactams and quinolones. We have observed that cell death is preceded by cytoplasmic condensation for aminoglycosides and quinolones. When beta-lactams are used, cell wall synthesis is significantly disrupted, resulting in cellular lysis, which we are studying both in bulk and at the single cell level. By elucidating the molecular effects, we hope to address the problem of antibiotic misuse and the associated potential antibiotic resistance. In addition, we are using machine-learning approaches to determine structure-function relationships which in turn are used to identify and discover novel, underutilized or untouched structural classes of antibiotics with explainable deep learning to fight the antibiotic resistance crisis.

BP 6.3 Mon 15:45 H 1028

Genealogical organization in growing bacterial colonies — Garima Rani[1] and •Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg

Spatio-temporal organization of individuals within growing bacterial colonies is a key determinant of intraspecific interactions and colony-scale heterogeneities. The evolving cellular distribution, in relation to the genealogical lineage, is thus central to our understanding of bacterial fate across scales. Yet, how bacteria self-organize genealogically as a colony expands has remained unknown. In this work we report recent results obtained using a custom-built label-free algorithm to track bacterial genealogy in growing colonies. Our results reveal emergence of distinct self-similar genealogical enclaves, whose dynamics are governed by biological activity. The enclaves boundaries are populated by topological defects, which tune finger-like morphologies of the active interfaces. Estimation of the Shannon entropy of cell arrangements show a reduction over time; with faster dividing cells possessing higher spatial affinity to genealogical relatives, at the cost of a well-mixed, entropically favorable state. We complement the experimental results with a coarse-grained lattice model, demonstrating that the genealogical enclaves emerge due to an interplay of division-mediated dispersal, stochasticity of division events, and cell-cell interactions. Our study reports so-far hidden emergent self-organizing features which modulate genealogical distances within growing bacterial colonies.

BP 6.4 Mon 16:00 H 1028

Exploiting Spatial Dynamics to Optimize Evolution-Based Therapy Strategies in Dense Cellular Populations — Nico Appold[1,2], Serhii Aif[1,2], and •Kayser Jona[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max Planck Zentrum für Physik und Medizin, Erlangen, Germany

The ubiquitous emergence of resistant mutants in pathogenic cellular populations is one of the primary challenges for modern antibiotic or anti-cancer therapies. Despite advances in evolution-based adaptive therapies and mathematical or computational models, a gap remains in translating these findings to clinical application. Empirical investigations are particularly challenging for densely packed cellular communities, such as microbial biofilms or solid tumors, as a result of their inherently complex spatio-temporal dynamics. Addressing this, we introduce a yeast-based model system tailored for the systematic study of resistant mutant emergence and therapy failure dynamics in dense populations. This model combines the precise tracking of de novo mutant clones with an accurate control over temporally varying fitness landscapes. Applying concepts from active granular matter physics and collective growth dynamics, our research uncovers a previously unidentified mode of competitive release. We then integrate our results with a tailored reinforcement learning approach to optimize the balance between immediate efficacy and long-term control of population size. Our findings underscores the importance of integrating physical principles of population dynamics into the design of evolution-based treatment strategies.

BP 6.5 Mon 16:15 H 1028

Beta-lactamase induced social dynamics of E. Coli — •Rotem Gross[1], Muhittin Mungan[1], Suman G. Das[2], Tobias Bollenbach[1], Joachim Krug[1], and J. Arjan G. M. de Visser[3] — [1]Institute for Biological Physics, University of Cologne, Köln, Ger-

many — [2]Institute of Ecology and Evolution, University of Bern, Bern, Switzerland — [3]Labaratory of Genetics, Wageningen University & Research, Wageningen, The Netherlands

Treating Escherichia coli with the antibiotic cefotaxime at sub-lethal concentration leads to a complex response: cells are filamenting, a known mechanism related to delayed lysis and enhanced antibiotic tolerance. Moreover, near lethal concentrations, the population displays complex dynamics, with a crossover from filamented to normal-sized cells after about 14 hours of exposure. Our experiments show that the filamentation causes an active break-down of the antibiotic by a chromosomally encoded enzyme. In fact, freshly introduced bacteria grow in this spent medium and survive at antibiotic concentrations higher than twice the lethal dose. Combining experimental results with theoretical modeling, we explore the biological and chemical pathway through which the bacterial colony inactivates the antibiotic. We argue that this pathway is ancient and common across a wide range of bacteria and constitutes a first line of defense which is triggered even when it is not necessarily effective against the cause of stress.

BP 6.6 Mon 16:30 H 1028

Evaluation of nanoparticle influence on living microorganisms — •Stefanie Schuba, Rico Illing, Xinne Zhao, Jürgen Fassbender, Larysa Baraban, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf

The discovery of antibiotics against bacterial infections has led to a higher life expectancy and quality of life for people worldwide. However, a major issue with using antibiotics is they also cause an increase resistance in bacterial pathogen resistance. The search for alternatives to classical active substances is pushing nanoparticles (NP) into the focus of scientific research. Particular attention is being paid to Nano-Silver (Ag-NP) due to its biocide and antibacterial effect, which is used in many medical products and consumer goods. But how reliable is Ag-Np? Conventional methods are used to analyze NPs, but these are limited in terms of labor, material costs, and statistical power. To tackle these limitations, we have developed a droplet-based millifluidic analysis platform as a tool to elucidate the effects of NPs on microorganisms (MO) with high statistical evaluation and detection power, enabling the separation of MO into individual droplets as bioreactors. In this work, we focus on the screening of the metabolism of gram-negative bacteria in the presence of NP under different stress factors. With the influence of Ag-NP, an inhibited bacterial activity was observed, which indicates the antibacterial effect of NP could be confirmed in our analysis platform. Further experiments are needed to clarify the stability of this effect.

15 min. break

BP 6.7 Mon 17:00 H 1028

Ultrasensitive dependence of fitness costs on membrane protein overexpression — •Janina Müller, Andreas Angermayr, Gerrit Ansmann, and Tobias Bollenbach — Institute for Biological Physics, University of Cologne

Perturbing expression levels of genes is a key technique for studying their function. In E. coli, strong overexpression of gratuitous proteins leads to fitness costs that are partially predictable from bacterial growth laws and sector models of proteome allocation. Here, we systematically quantified the precise dependence of fitness costs on the level of overexpression using a genome-wide library. Our results confirm that the fitness cost for membrane proteins is extremely high compared to cytosolic proteins, and reveal that this cost is ultrasensitive to the expression level. To elucidate the mechanisms underlying this ultrasensitive response to membrane protein overexpression, we characterized the role of membrane translocation by examining the fitness costs of mutants of a model membrane protein with different translocation requirements, resulting in a reduction in translocation success. Single-cell experiments to detect membrane localization using protein-GFP fusions further demonstrated that overexpression of membrane proteins leads to displacement of other membrane proteins. This displacement closely coincides with the abrupt collapse of the growth rate. A minimal physical model can explain these observations and suggests that the abrupt growth collapse is caused by zero-order ultrasensitivity in the translocation pathway.

BP 6.8 Mon 17:15 H 1028

Using simulations to investigate the mechanical properties of peptidoglycan — •Marco Mauri[1], Abimbola F. Adedeji Olulana[2], Jamie K Hobbs[2], Sheila Hoshyaripour[1], and Rosalind J Allen[1] — [1]FSU Jena - Balance of the Microverse — [2]University of Sheffield

In bacteria, the peptidoglycan (PG) cell wall consists of a mesh of glycan strands crosslinked by short peptides. PG counteracts the internal turgor pressure and its integrity is necessary to prevent cell lysis; indeed, many antibiotics target PG synthesis. The mechanical properties of the PG mesh are important for understanding the biophysics of cell growth, cell shape and antibiotic action: yet these properties are hard to measure experimentally.

Here, we present a coarse-grained molecular simulation model for the PG mesh in Gram negative bacteria such as *E. coli*. Inspired by previous works, we model PG as a network of beads and springs governed by a system of overdamped Langevin equations. However, our model incorporates real PG configurations, informed by AFM and biochemical measurements.

We use dynamical simulations to study how a patch of PG responds to biochemical perturbations. We predict the mechanical effects of antibiotic action via uncontrolled hydrolase enzymes, and explore the role of biophysical properties of the mesh, such as connectivity, on mechanical stability. Our work provides a connection between the molecular-scale PG configuration and the macro-scale mechanical properties of the cell wall.

BP 6.9 Mon 17:30 H 1028

Heterogeneity in Bacterial Contact Formation — •Johannes Mischo[1], Samer Alokaidi[1], Cao Nguyen Duong[2], Markus Bischoff[3], and Karin Jacobs[1] — [1]Experimental Physics, Center for Biophysics, Saarland University, 66123 Saarbrücken, Germany — [2]INM Leibniz Institute for New Materials, Campus D2 2, 66123 Saarbrücken, Germany — [3]Institute of Medical Microbiology and Hygiene, Saarland University, 66421 Homburg (Saar), Germany

Bacteria adhere to virtually every surface and promote the formation of sometimes desirable but often unwanted biofilms. As the adhesion of a single bacterial cell is the critical initial step in biofilm formation, we analyse the adhesion properties using single cell force spectroscopy. The contact formation is mainly attributed to bacterial cell wall macromolecules: Their nature and their distribution on the cell wall are a highly individual property of the bacterial cells and define the contact formation properties of the respective cell. We showed that Staphylococcus aureus cells have several distinct spots of high adhesion capability causing heterogeneous distributions of adhesive strength on the cell wall [1]. During cell division, bacteria synthesise about 33 - 50 % fresh cell wall structures, leading to further heterogeneity within individual cells [2]. We combine Atomic Force Microscopy of single S. aureus cells with high resolution fluorescence microscopy to investigate the influence of cell wall age on the adhesion capability of individual cells. [1] Spengler, C. et.al., DOI: 10.1039/d3sm01045g [2] Monteiro, J. M. et.al NatCom. 2015., DOI: 10.1038/ncomms9055.

BP 6.10 Mon 17:45 H 1028

Bacteria in shear flow — •Pierre Martin[1], Tapan Chandra Adhyapak[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Indian Institute of Science Education and Research (IISER), Tirupati, India

This study aims to investigate the behavior of flagellated bacteria under shear flow conditions, focusing on the specific case of E. coli bacteria. E. coli employs a rotating bundle of helical flagella for self-propulsion, and its ability to alter direction is facilitated by the reversal of flagellar rotation, a process known as tumbling.

In the presence of shear flow, helical objects, experience a chirality-induced drift force propelling them in the direction of vorticity. Additionally, objects in shear flow exhibit the well-known Jeffery orbit causing them to rotate. However, due to the helical bundle driving a non-chiral head, E. coli experiences a rheotactic torque and aligns along the vorticity axis. A phenomena known as rheotaxis.

To gain insights into these phenomena, we conducted a detailed analysis using a realistic model of E. coli coupled with fluid flow at low Reynolds numbers. The fluid flow was simulated using the method of multi-particle collision dynamics and Lees-Edwards boundary conditions were implemented to reproduce a planar shear flow in bulk.

Our research contributes to a deeper understanding of the complex interplay between flagellated bacteria and shear flow, shedding light on the responses of E. coli in such environments.

BP 7: Active Fluids and Microswimmers (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: BH-N 243

Invited Talk BP 7.1 Mon 15:00 BH-N 243

Control of active turbulence — •Holger Stark — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Active turbulence is one of the prominent features of active matter and occurs in diverse systems such as bacterial suspensions, biopolymeric assemblies, and tissues. One of the current challenges is to control these turbulent flow patterns for powering processes at small scales.

In the first part of the talk we rely on a continuum description of active paranematics, the Doi-Edwards theory supplemented by an active stress tensor [1]. We characterize the occuring turbulent flow for extensile active stresses. Then, motivated by the possibility to control the activity of bacteria by light, we consider a square lattice of spots, where activity drops to zero. Depending on the lattice constant and the size of the spots, we identify a trapped-vortex and, most interestingly, a multi-lane flow state. The latter consists of lanes with opposite flow directions separated by a street of vortices. It displays multistability and can also appear transiently.

Second, we perform hydrodynamic simulations of a collection of active or squirmer rods moving in their fluid environment [2]. We classify their dynamic states for the pusher/puller type as a function of density and aspect ratio of the rods and observe clustering and swarming. In particular, pusher rods show active turbulence as a compromise of disordering hydrodynamic and aligning steric interactions.

[1] A. Partovifard and H. Stark, submitted.

[2] A.W. Zantop and H. Stark, Soft Matter **18**, 6179 (2022).

BP 7.2 Mon 15:30 BH-N 243

Entropy production in active turbulence — •Byjesh N. Radhakrishnan, Thomas L. Schmidt, and Etienne Fodor — Department of Physics and Material science, University of Luxembourg

Active particles like bacteria and sperm cells sustain a continuous intake and dissipation of energy. Consequently, they are intrinsically out of equilibrium which leads to a non-vanishing entropy production rate (EPR) even in steady states. Quantifying how the EPR varies in different collective phases is crucial in developing a thermodynamic framework for active matter. In this work, we look at the EPR in active turbulence. We use Active Model H, a continuum model for active particles in a momentum-conserving fluid, to study turbulence in contractile scalar active systems. We measure the local EPR in numerical simulations, which unveils the relation between the magnitude of entropy production and $+1/2$ topological defects in the system. Also, we study how EPR and the properties of defects such as mean square displacement and defect lifetime vary with the activity parameter.

BP 7.3 Mon 15:45 BH-N 243

Active turbulent mixing — •Till Welker[1], Malcolm Hillebrand[2], Ricard Alert[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, TU Berlin, Germany — [2]MPI for the Physics of Complex Systems, Dresden, Germany

Mixing on the mesoscale is crucial for both microfluidic devices and living cells. Experiments backed by simulations show a significant increase in mixing efficiency caused by active turbulence.

Our goal is to enhance the theoretical understanding of active turbulent mixing by transferring theories and concepts originally developed for inertial turbulent mixing. We therefore study a defect-free active nematic model known to show universal scaling of the energy spectrum with a passive chemical diffusing and advecting in the flow.

The efficiency of mixing χ rises with both activity of the nematic A and diffusion coefficient of the chemical D. Intriguingly, as D approaches zero, mixing efficiency converges to a non-zero value $\chi_0(A)$ because smaller D are compensated by larger concentration gradients. This presents an attractive mechanism to mix poorly diffusive substances, and is also observed in inertial turbulent mixing.

The scaling of the concentration spectrum $E_c(q)$ is of great interest and has been extensively studied in the context of inertial turbulence. We demonstrate that Batchelor-Howells-Townsend theory and Batchelor theory for strongly and poorly diffusive substances can be transferred to active turbulence. As a consequence of the universal energy scaling of our active nematic, we predict universal scaling regimes for $E_c(q)$ which we validate in simulations.

BP 7.4 Mon 16:00 BH-N 243

Simultaneous emergence of active turbulence and odd viscosity in a colloidal chiral active system — •Joscha Mecke[1,2], Yongxiang Gao[1], Gerhard Gompper[2], and Marisol Ripoll[2] — [1]Institute for Advanced Study, Shenzhen University, China — [2]Institute of Biological Information Processing and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

Active fluids display collective phenomena such as active turbulence or odd viscosity, which refer to spontaneous complex and transverse flow. We report the simultaneous emergence of these seemingly separate phenomena in experiment for a chiral active fluid composed of a carpet of standing and spinning colloidal rods, and in simulations for synchronously rotating hard discs in a hydrodynamic explicit solvent (see also Commun. Phys. 6, 324 (2023), https://doi.org/10.1038/s42005-023-01442-3). Stresses among the colloids encompass rotational and odd shear contributions absent in usual fluids. Rotational viscosity couples the colloids' rotation to translation, causing active turbulence. Odd viscosity involves a perpendicular coupling of shear stresses, leading to an effective pressure pointing into or out of the emergent vortices. We quantify the two phenomena in experiments and simulation using the same setup. Both rotational and odd viscosity originate from the same source and the system behaviour hinges on the propagation of odd stresses via long-ranged hydrodynamics. Our findings are relevant for the understanding of biological systems and for the design of microrobots with collective self-organised behaviour.

BP 7.5 Mon 16:15 BH-N 243

Hydrodynamic synchronization of elastic cilia: How flow confinement and boundary conditions determine the characteristics of metachronal waves — Albert von Kenne, •Markus Bär, and Thomas Niedermayer — Physikalisch-Technische Bundesanstalt, Berlin, Germany

We model hydrodynamically interacting cilia by a coupled phase oscillator description by reducing the dynamics of hydrodynamically interacting elastic cilia to the slow time scale of synchronization [1]. In this framework, we determine analytical metachronal wave solutions as well as their stability and perform simulations in a periodic chain setting. The flow confinement at the wall stabilizes metachronal waves with long wavelengths propagating in the direction of the power stroke and, moreover, metachronal waves with short wave lengths propagating perpendicularly to the power stroke. In open chains of phase oscillators, the dynamics of metachronal waves is fundamentally different. Here, the elasticity of the model cilia controls the wave direction and selects a particular wave number: At large elasticity, waves traveling in the direction of the power stroke are stable, whereas at smaller elasticity waves in the opposite direction are stable. In addition, coexistence of waves traveling in opposite directions and irregular, chaotic dynamics are observed. [1] A. von Kenne, M. Bär and T. Niedermayer. Preprint, https://www.biorxiv.org/content/10.1101/2023.10.20.563276v1.full.pdf.

BP 7.6 Mon 16:30 BH-N 243

Pattern formation in non-Newtonian active suspensions — •Henning Reinken and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Controlling spatiotemporal patterns in active matter is of essential importance in view of prospective applications. In contrast to previous studies utilizing external control such as geometrical constraints [1], we here explore the possibility of controlling suspensions of microswimmers via the internal rheological properties of the suspension. Recent work has focused on the impact of viscoelastic and non-Newtonian behavior on the dynamics of single swimmers [3], but only a limited number of studies explores the consequences for collective motion and emergent patterns. Here, employing a recent continuum model for mesoscale turbulence in microswimmer suspensions [4], we investigate the impact of non-Newtonian behavior on the pattern formation. In particular, we focus on the stabilization of regular vortex structures in otherwise turbulent suspensions without the need for external intervention.

[1] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. **3**, 76 (2020)

[3] G. Li, E. Lauga, and A. M. Ardekani, J. Non-Newton. Fluid Mech.

297, 104655 (2021)
[4] J. Słomka and J. Dunkel, Eur. Phys. J. ST **224**, 1349 (2015), Phys. Rev. Fluids **2**, 043102 (2017), Proc. Natl. Acad. Sci. U.S.A. **114**, 2119 (2017)

15 min. break

BP 7.7 Mon 17:00 BH-N 243

Bacterial swimming strategies in a shear flow — •Valeriia Muraveva, Agniva Datta, and Carsten Beta — Potsdam University, Potsdam, Germany

By changing the configuration of their flagella, bacterial swimmers can control their direction and speed of locomotion. The soil bacterium Pseudomonas putida pushes itself forward by counterclockwise (CCW) rotation of its flagellar bundle, while clockwise (CW) rotation pulls the cell body in the opposite direction. Additionally, P. putida can wrap its bundle of flagella around the cell body to move in a screw thread fashion. However, the benefits of having different modes of swimming still remain unclear. Here, we used microfluidics in combination with fluorescence microscopy to show how the swimming behavior changes under laminar shear flow conditions. Compared to a fluid at rest, we found that in flow, swimmers prefer the pull configuration over the wrapped one (both emerging under CW flagellar rotation). Moreover, we investigated flow-induced alignment effects and compared the distributions of swimming modes and velocities in the bulk fluid and close to the fluid-substrate interface. Our results provide first insights into how bacteria adapt their swimming strategy under different flow conditions at the single-cell level.

BP 7.8 Mon 17:15 BH-N 243

Artificial Microswimmers in locally-tuneable hydrodynamic flow fields — •Lisa Rohde and Frank Cichos — Molecular Nanophotonics Group, Peter-Debye-Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Biological components on the microscale, which constantly consume energy can organize themselves into functional structures through interaction with their environment. Interaction potentials, temperature or composition gradients as well as flow fields play an important role in this structure formation. We would like to transfer such self-organization principles to synthetic active particles, which are a model system to mimic the function of motors in biology, but yet have only limited functionality. Here, we expose thermo-phoretic Janus particles to an environment with tuneable hydrodynamic flow fields generated by local temperature gradients. A heated paramagnetic silica particle acts as a heat source and generates a thermo-osmotic flow field due to a temperature gradient on the substrate. By controlling the temperature of the heat source, we are able to locally change the generated hydrodynamic flow field. We study the orientational dynamics and the distance of the Janus particles relative to the heat source in dependence of temperature and laser intensities. The interplay of the local flow fields with the activity of the Janus particles results in a potential that traps the Janus particles in a configuration around the heat source. We find a polarisation of the Janus particles that align with the flow field having a stable orientation relative to the heat source.

BP 7.9 Mon 17:30 BH-N 243

Run-and-tumble motion of ellipsoidal swimmers — •Gordei Anchutkin[1], Viktor Holubec[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Department of Macromolecular Physics, Faculty of Mathematics and Physics, Charles University, CZ-180 00 Praha, Czech Republic

The characteristic motion of bacteria, the so-called "run-and-tumble" motion, is a hallmark of living active particles. It consists of a sequence of linear directional movements and random rotations that constantly alternate based on a biochemical feedback process. In contrast to bacteria, synthetic active particles do not exhibit run-and-tumble motion, except they are forced to do so by sophisticated optical control feedback loops.

In this study, we show that self-thermophoretic Janus ellipsoids can carry out run-and-tumble-like dynamics under strong confinement. Our Janus ellipsoids are propelled along the short axis and exhibit long periods of directed motion before reversing the propulsion direction. We show that a bimodal out-of-plane angular distribution arises at high propulsion velocities, which is mainly the result of hydrodynamic wall interactions. We evaluate hydrodynamic interactions, and gravitational and optical forces to give a quantitative model of the observed dynamics. These interactions together with the slow rotational diffusional dynamics around the short ellipsoid axis provide the basis of the run-and-tumble dynamics.

BP 7.10 Mon 17:45 BH-N 243

Microswimming under a wedge-shaped confinement — •Alexander R. Sprenger and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

Microswimmers, both living and artificial, frequently navigate through diverse and often confined environments. Their out-of-equilibrium nature of self-propulsion and associated fluid flows lead to complex hydrodynamic interactions with their surroundings. Understanding the impact of various confinements on the behavior of self-propelled particles is crucial for gaining insights into biological phenomena and motivating advancements in microtechnologies.

In this contribution, we study the low-Reynolds-number dynamics of microswimmers confined within a wedge-shaped free-slip boundary [1]. Such scenarios naturally occur in experiments on inhomogeneously evaporating fluid flows, which form a free-standing confinement between two converging interfaces. Additionally, wedge-shaped environments possess distinctive geometric trapping and guiding properties relevant to various microfluidic applications.

Here, we present an exact solution for the resulting flow fields for various opening angles of the wedge employing the method of images. In this manner, we investigate the hydrodynamic interactions between each swimmer and the confining interfaces. We find either attraction or repulsion towards the tip of the wedge, depending on the propulsion mechanism (pusher or puller) and the opening angle of the wedge.

[1] A. R. Sprenger, A. M. Menzel (submitted).

BP 7.11 Mon 18:00 BH-N 243

AcoDyn: Efficient computer simulations of acoustically propelled microparticles — •Adrian Paskert and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany

For future applications in science and engineering, active microparticles have great potential. Acoustically propelled microparticles are particularly advantageous for medical applications because they operate well within medically safe intensity ranges and are generally considered biocompatible. However, due to the complexity of the flow fields generated around these particles and the high computational cost of direct computer simulations even for simple 2D particle geometries, the theoretical understanding of the particles' propulsion and dynamics is still very limited. In this talk, we will give an overview of how these particles can be simulated efficiently to enable the numerical study of complex 3D particles. Moreover, our novel software solution `AcoDyn` will be presented, along with key results we have obtained through its application.

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BP 7.12 Mon 18:15 BH-N 243

Opto-fluidic dynamic patterning of microparticles — •Elena Erben[1], Weida Liao[2], Antonio Minopoli[3], Nicola Maghelli[4], Eric Lauga[2], and Moritz Kreysing[1] — [1]IBCS-BIP, KIT, Karlsruhe, Germany — [2]DAMTP, University of Cambridge, UK — [3]University of Pisa, Pisa, Itlay — [4]Fondazione Human Technopole, Milano, Italy

Techniques for the precise manipulation of microscopic objects bear great potential for application in a wide range of fields, from basic biological research to microfabrication. Our method uses rapid scanning of an infrared laser beam to optically generate thermoviscous flows [1] within a sample. Combined with closed-loop control this enables the automatic positioning of a single microparticle, with a precision of up to 24 nm [2]. Our approach can be multiplexed to manipulate up to 15 particles in a parallel and dynamic fashion. Furthermore, we have found that the positioning of multiple particles can be greatly accelerated by exploiting the complex flow patterns that result from the time-sharing of different laser scan paths. We plan to combine our approach with a full analytical model of the flows [3], which we expect will further increase the precision and speed of this manipulation method, facilitating its translation to applications in the life sciences and beyond.

[1] Weinert et al. Phys. Rev. Lett. 2008; [2] Erben et al. Opt. Express 2021; [3] Liao et al. Phys. Rev. Fluids 2023.

BP 8: Poster Session Ia

Cytoskeleton, Membranes and Vesicles, Cell Mechanics. Additional posters on Cell Mechanics in Poster Session Ib.

Time: Monday 18:00–20:30 Location: Poster C

BP 8.1 Mon 18:00 Poster C

Microtubule dynamics in the presence of an actin network — •Saheli Dey, Tiago Mimoso, and Sarah Köster — Georg-August-Universität Göttingen

The eukaryotic cytoskeleton is a composite network of biopolymers of variable flexibilities. It drives many important biological processes such as cell division and motility. In response to external and internal stimuli, the cytoskeleton rapidly rearranges itself. This property is achieved with the aid of microtubules and actin filaments, which are the dynamic components of the cytoskeleton. Since these biopolymers co-exist in a cell, our focus lies on understanding microtubule dynamics in a composite network system. Using a bottom-up approach, we investigate whether actin filaments influence microtubule dynamics. Total internal reflection fluorescence (TIRF) microscopy serves as an essential tool to capture the dynamics of the microtubules in our experiments. Based on our analysis from kymographs, we quantify the polymerization and depolymerization rates of microtubules. Furthermore, rescue and catastrophe frequencies indicate the influence of actin filaments on the stability of microtubules. Till now studies have shown interaction between these two cytoskeletal filaments in the presence of motor proteins or cross-linkers. Complementary to those results, our study provides insight into direct filament-filament interactions and will answer the question of whether actin filament networks stabilize dynamic microtubules against depolymerization.

BP 8.2 Mon 18:00 Poster C

Imaging F-Actin arrangement via homo-FRET using 2D polarization fluorescence microscopy — Lukas Spantzel[1,2], Chen Sun[3], Lena Jesse[1,2], Yunhao Mei[1,4], Yutong Wang[1,4], Shangjun Cheng[1,2,4], Mohammad Soltaninezhad[1,4], Michael Börsch[1,2], Rainer Heintzmann[1,4], Ivan G. Scheblykin[3], Adrian T. Press[1,2], and •Daniela Täuber[1,4] — [1]Friedrich Schiller University, Jena — [2]University Hospital Jena — [3]Lund University, Sweden — [4]Leibniz Institute of Photonic Technology, Jena, Germany

Polymicrobial infection affects the organization of F-Actin in the cytoskeleton and the cortex causing cell death. We use 2-dimensional polarization fluorescence imaging (2DPOLIM) to visualize the aggregation of phalloidin-dye labeled F-Actin via Förster Resonance Energy Transfer (homo-FRET). The homo-FRET efficiency observed from fibrillar structures in mouse embryonal fibroblasts agrees well with that of single fibrillar F-Actin synthesized from non-muscle Actin. Higher values are observed from other structures inside the cells, representing a more dense aggregation of the F-Actin in those regions.

BP 8.3 Mon 18:00 Poster C

Influence of the cytoskeletal surrounding on microtubules in cells — •Anna Blob[1], Roman David Ventzke[1,2], Thomas Giacomo Nies[2], Axel Munk[2], Laura Schaedel[3], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]Institute for Mathematical Stochastics, University of Göttingen — [3]Center for Biophysics, Saarland University

The cytoskeleton in eucaryotic cells determines essential cellular functions and properties. It is an intricate network of three different filamentous proteins, microtubules, actin filaments and intermediate filaments, each of which has unique features. Microtubules are important for intracellular transport and withstand compressive forces while exhibiting characteristic bending and buckling in cells. Interactions between cytoskeletal filaments have been found, such as the templating of microtubules by vimentin intermediate filaments in cells. Yet, the scope and consequences of such cytoskeletal interdepence are not fully understood. Here, we investigate how the orientation and bending of microtubules in cells is influenced by actin and vimentin intermediate filaments. We compare microtubule networks in vimentin-knockout and wildtype mouse fibroblasts on micropatterns and disturb the actin network chemically. We find that microtubules are radially oriented regardless of the presence of vimentin or actin. The local curvature of microtubules is not influenced either, even if the cells are under mechanical compression. Our study suggests that the organization and mechanical behavior of microtubules in cells may be more independent of the surrounding cytoskeleton than expected.

BP 8.4 Mon 18:00 Poster C

Keratin and actin networks in epithelial cells under uniaxial strain — •Ruben Haag[1], Ruth Meyer[1], Peter Luley[1], Nicole Schwarz[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]Institute of Molecular and Cellular Anatomy, RWTH Aachen University

The cytoskeleton is mainly made up of microtubules, actin and intermediate filaments (IFs). The composition of the IF-network is cell-type specific and influences the viscoelastic properties of cells. In some epithelial cell types, the keratin IFs forms a rim close to the F-actin cortex. It is hypothesized that this so-called "IF-cortex" is linked to radial keratin spokes, forming a "rim-and-spokes"-structure. This hypothesis leads to the question of how the IF and actin cortices complement each other. Furthermore, it was previously observed that keratin IF, unlike actin filaments, survive being stretched to high strains. We now ask the question of whether this unique force-extension behavior of keratin is also relevant in whole cells, and of how both the IF and the actin cortices interact. In order to investigate the extension behavior of whole cells, we design a uniaxial cell-stretcher compatible with fluorescence and atomic force microscopy, enabling us to stretch cells up to high strains of 80%. Subsequently, we analyze the cells both in 2D and in 3D at different strains. To achieve this goal, we first deconvolve the images, then segment the individual cells and finally analyze the cell shape and the keratin-actin colocalization.

BP 8.5 Mon 18:00 Poster C

Active microrheology on in vitro cytoskeletal networks — •Shanay Zafari, Pratima Sawant, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

The cytoskeleton plays a crucial role in maintaining cell shape and overall structural integrity. It consists of three types of filaments including actin filaments (AFs) and intermediate filaments (IFs). Notably, IFs stand out for their exceptional extensibility and remarkable resistance against rupture at high strains, while AFs break at low strains. Composite networks of these two different kinds of filaments may lead to emergent mechanical properties. Here, we examine the mechanical properties of actin and vimentin networks separately by performing active microrheology with optical tweezers. We quantify the viscoelastic properties of the networks by fitting the force-strain curves with a power-law decay function. Our results indicate different viscoelastic behavior for pure actin and pure vimentin networks. This sets the stage for a comprehensive study of combined networks in order to understand the role of intermediate filaments in composite cytoskeletal networks at high strain.

BP 8.6 Mon 18:00 Poster C

Response of confined vimentin intermediate filament networks to applied strain — •Pratima Sawant, Shanay Zafari, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

Eukaryotic cells undergo high strains during division, motility, wound healing and numerous other cellular processes. The mechanical integrity of cells under these conditions is maintained by the cytoskeleton, mainly comprising actin filaments, intermediate filaments (IFs), and microtubules. Among these three filament types, IFs are the most extensible ones. However, the role of IFs in modulating the mechanical response of cells under strain still remains unclear. In vitro studies on single vimentin IFs show that they exhibit tensile memory and can dissipate more than 70% of the input energy. Since these filaments form networks in cells, it is crucial to extend this analysis to study network behaviour. Here, we present a microfluidic device that is compatible with fluorescence microscopy. We image reconstituted networks of vimentin encapsulated in microfluidic droplets. Flowing these droplets through constricted channels ensures the application of a global strain. Furthermore, the networks are suspended within the droplets and not attached to a substrate in this set-up. Thus, this approach enables us to probe the mechanical properties of vimentin IF networks in a

confined environment with the ability to manipulate the degree and nature of strain and buffer conditions.

BP 8.7 Mon 18:00 Poster C

Unveiling microtubule fracture dynamics: A comprehensive examination of the influence of lattice defects on the breakage process of microtubules — •Amir Zablotsky and Karin John — Université Grenoble Alpes / CNRS, LIPhy, Grenoble, France

Microtubules (MTs), crucial to many cellular functions, are tube-like structures formed by a quasi-crystalline arrangement of $\alpha\beta-$tubulin heterodimers.

Two parameters that are major determinants for MT stability and dynamics are the lattice binding energy and anisotropy (defined as the ratio between the longitudinal and lateral binding energies).

Despite considerable effort on comprehending the dynamics of the MT tip, in particular the so called dynamic instability, the dynamics within the "bulk" MT lattice have received little attention.

Recent experimental findings revealed that MTs often present dimer and monomer sized vacancies along their shaft, resulting in structural defects that compromise their shaft integrity and may interfere with the dynamic instability at the tip.

Here we employ kinetic Monte Carlo simulations, as well as analytical approaches, to study the defects dynamics in the MT shaft and their effects on MT breakage in the absence of free tubulin dimers.

Our findings highlight the significant role of initial defects in the fracture propagation dynamics. Furthermore, comparison with experiments allows us to identify lattice binding energies and anisotropies that accurately reproduce experimental observations of fracture times and lengths.

BP 8.8 Mon 18:00 Poster C

The structure and mechanics of the actin cortex in different adhesion states — •Christoph Anton[1], Lucina Kainka[1], Sandra Iden[2,3], and Franziska Lautenschläger[1,3] — [1]Department of Physics, Saarland University, Saarbrücken, Germany — [2]Center of Human and Molecular Biology (ZHMB), Saarland University, Homburg, Germany — [3]Center for Biophysics, Saarland University, Saarbrücken, Germany

Transitions between different cellular adhesion states are essential for many biological processes e.g. metastasis. These transitions involve drastic changes of the actin cortex, a submembraneous network of actin filaments. Our aim is to characterize the properties of the actin cortex in single adherent cells and cells within a monolayer. We use scanning electron microscopy and atomic force microscopy to quantify the structure and mechanics of the actin cortex. We investigate how the structural and mechanical properties are related to each other and how they are influenced by the amount of filamentous actin and the amount of actin bundles within the cortex. Furthermore, we investigate the role of specific proteins (e.g. the cell-cell adhesion protein E-cadherin) by using different inhibitors and chemical compounds. Generally, it is our aim to control state transitions by controlling the actin cortex via compounds that affect the amount of filamentous actin and the actin bundles.

BP 8.9 Mon 18:00 Poster C

Membrane Stiffness and Formation of Microtentacles — •Yannic Veit[1], Lucina Kainka[1], Christoph Anton[1], and Franziska Lautenschläger[1,2] — [1]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Center for Biophysics, Saarbrücken, Germany

Microtentacles (McTNs) are microtubule-based membrane protrusions. They are found in circulating tumour cells (CTCs) and are assumed to promote reattachment of the CTCs to the vessel walls and facilitate the extravasation from the blood stream.

We previously found that McTNs grow from actin-rich sites (actin patches). There is a force balance between the microtubules and the cell barrier, which consists of the actin cortex and the cell membrane. During the formation of microtentacles, that barrier exerts a counterforce depending on its stiffness on the microtubules. This led us to a question: Does decreased actin patch area decrease membrane stiffness and influence McTN formation?

To disentagle the influence of the two components of the barrier, we tackled actin directly by depolymerisation using latrunculin A, and the membrane stiffness itself by depleting it of cholesterol with methyl-beta-cyclodextrin. The membrane stiffness was quantified via tether rupturing using atomic force microscopy.

We found that decreasing the actin patch area decreases the membrane stiffness while depleting the membranes of cholesterol increases the stiffness. We found that an increase in membrane stiffness inhibits microtentacle formation.

BP 8.10 Mon 18:00 Poster C

Quantitative description of cellular adhesion forces and corresponding focal adhesions — •Kathi Michèle Kaiser[1], Carsten Baltes[1], Ben Wieland[2], Gubesh Gunaratnam[2], and Franziska Lautenschläger[1,3] — [1]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Institute for Medical Microbiology and Hygiene, Saarland University, Homburg, Germany — [3]Center of Biophysics, Saarland University, Saarbrücken, Germany

The adhesion force of a cell has a huge impact on various processes linked to adhesion, for example in metastasis. Controlling the adhesion force means controlling the balance between adhesive and non-adhesive forces which could help to prevent the formation of metastasis.

The adhesion of cells to the extracellular matrix is mediated by integrin receptors, which link the cytoskeleton of the cell to the extracellular environment. On the cytoplasmic side these receptors are connected to actin filament bundles via an assembly of proteins forming the focal adhesions (FA).

My aim is to find a correlation between the number and size of the FAs and the adhesion force of a cell. Different compounds, which alter the dynamics of actin, were used to change the properties of the FAs. With a TIRF microscope the FAs could be imaged. To measure the adhesion force of single cells a fluid force microscope was used. These measurements enabled us to quantitatively describe and correlate the adhesion forces corresponding to the properties of the FAs. Once we understand this correlation, we will be able to understand an altered adhesion in a pathogenic context or to actively influence adhesion.

BP 8.11 Mon 18:00 Poster C

Mechanical properties of microtubule in actin network — •Komal Bhattacharyya, Sarah Köster, and Stefan Klumpp — University of Göttingen, Göttingen, Germany

The cytoskeleton provides structural support and facilitates dynamic cellular processes such as growth and migration. Actin and microtubules are key components of the cytoskeleton. Actin, characterized by its semi-flexible nature, contrasts with the stiff, rod-like structure of microtubules. The synergy between these two elements plays a pivotal role in numerous biological phenomena. For instance, microtubules exhibit enhanced resistance to compressive forces when integrated into an actin network. In our research, we use Cytosim[1] to simulate the networks formed by actin and microtubules. Specifically, we analyze the buckling behavior of microtubules under varying compressive forces. The objective is to unravel the specific interactions between actin and microtubules that contribute to the observed mechanical responses within composite networks.

[1] Francois Nedelec and Dietrich Foethke 2007 New J. Phys. 9 427

BP 8.12 Mon 18:00 Poster C

Interactions between synaptic vesicles and cytoskeletal filaments — •Tiago Mimoso[1], Rajdeep Chowdhury[2], Saheli Dey[1], Christian Hoffmann[3], Dragomir Milovanovic[3], Silvio Rizzoli[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Institute for Neuro- and Sensory Physiology, University Medical Center Göttingen, Germany — [3]Laboratory of Molecular Neuroscience, DZNE, Germany

Signal transmission of neurons occurs both electrically and chemically. The chemical signal is transported by synaptic vesicles (SVs) via the synaptic cleft to an adjacent neuron. Thus, these SVs are found in the synapse, within the so-called synaptic bouton. Here, the SVs are surrounded by cytoskeletal filaments, including dynamic microtubules (MTs) that undergo rapid assembly and disassembly. Some studies suggest interactions between SVs and the cytoskeletal filaments. Therefore, we now ask the question of what influence the presence of SVs has on microtubules. We employ a reconstituted in vitro system, by attaching the SVs to the surface and imaging the dynamic microtubules by total internal reflection fluorescence microscopy to obtain the growth rate, disassembly rate, catastrophe frequency and rescue frequency. We present an approach for attaching SVs to a surface using protein G and a primary antibody targeting a membrane protein in SVs. The MT are attached using biotin-neutravidin complex. This method grants control over the SVs and MT positioning, enabling a comprehensive study of their dynamic interactions.

BP 8.13 Mon 18:00 Poster C

Influence of perfluorocarbon on the structural changes of lipid monolayers and on protein adsorption — •Jaqueline Savelkouls, Christian Albers, Gordon Scholz, Eric Schneider, and Michael Paulus — Maria-Goeppert-Mayer-Straße 2, 44227 Dortmund

Perfluorocarbons (FCs) have high medical potential, serving as therapies in ophthalmology and respiratory diseases by replacing liquid FC ventilation and unsafe lung surfactant (LS) substitutes in the future [1]. We analysed the influence of the FC F-Decalin on the structural changes of model membranes of LS like anionic DPPA and zwitterionic DPPC monolayers at different initial surface pressures as well as on the adsorption of the surface-active proteins human serum albumin and lysozyme at beamline ID10 with a photon energy of 22 keV at the European Synchrotron Radiation Source (Grenoble, France). All samples were measured in situ at ambient temperature and pressure using a combined grazing incidence X-ray diffraction and X-ray reflectivity study. In summary, surface-active proteins adsorb to the lipid membrane either with and without a FC atmosphere. F-Decalin itself adsorbs to the interface between the head and tail groups of the lipid monolayer as well as to the hydrophobic regions of the lipid and protein. This leads to a compression of the lipid and protein layer. F-Decalin reduces the size of the crystalline domains, the surface tension of the monolayers and induces a fluidisation of the lipid monolayer. This effect is observed for monolayers with initially high surface tensions. [1] M. P. Krafft, DOI: 10.1002/pola.21937

BP 8.14 Mon 18:00 Poster C

Investigating the Fusion Efficiency of Respiratory Virus-Like Particles with Model Cell Membranes — •Mahsa Mohammadian[1], Chetan S Poojari[2], Ralf Seemann[1], Jochen Hub[2], and Jean-Baptiste Fleury[1] — [1]Department of Experimental Physics and Center for Biophysics, Saarland University, Germany — [2]Theoretical Physics and Center for Biophysics, Saarland University, Germany

Viral infections are initiated when a virus attaches to a host cell membrane, and then penetrates the cell through a process called membrane fusion. The fusion process depends on specific fusion proteins located on the viral particle surface, which contain a short, relatively hydrophobic segment called "fusion peptide" that binds to the host membrane. To investigate the fusion efficiency of various fusion peptides, we create non-infectious virus-like particles (VLPs) decorated with different fusion peptides and fuse them with an artificial cell membrane. For this purpose, 3D microfluidic devices are used to create either supported or free-standing lipid bilayers and the fusion process is then studied using fluorescence microscopy. Furthermore, molecular dynamics (MD) simulations are employed to provide structural and energetic insights into the effect of fusion peptides on stalk-formation. Our study provides structural insights into the interactions between virus particles and cell membranes, which can facilitate the development of new therapeutic strategies and more effective viral vectors for therapeutic applications.

BP 8.15 Mon 18:00 Poster C

Structure and Electrostatics in Monolayers of Raft-Forming Lipid Mixtures Containing GM1 — •Miriam Grava[1], Valeria Rondelli[2], and Emanuel Schneck[1] — [1]Technische Universität Darmstadt, Germany — [2]Università degli Studi di Milano, Italy

Lipid rafts are membrane domains with specific lipid composition and high sterol content, that can host certain membrane protein. Important examples are lipid domains enriched in glycosphingolipids such as ganglioside GM1 with negatively chargeable sialic acids, whose protonation state can depend on lipid packing and on the type and concentration of counterions.

Here, we use mixed lipid monolayers to mimic GM1-containing rafts in the mammalian nervous system and investigate them with synchrotron-based x-ray scattering and x-ray fluorescence, to elucidate their structural and electrostatic characteristics under various biologically relevant conditions.

The experiments reveal electron density profiles, in-plane lipid ordering, and the surface charge density. The absence of a pronounced charge inversion in the presence of divalen cations indicates that a considerable fraction of ions bridges two negatively charged GM1 molecules.

BP 8.16 Mon 18:00 Poster C

Cavitation in lipid systems: Insights from molecular dynamics — •Marin Šako and Matej Kanduč — Jožef Stefan Institute, Ljubljana, Slovenia

Liquids under tension are found in many systems in nature as well as in technology. Examples include lithotripsy and sonoporation of cell membranes, octopus suckers, catapulting mechanisms of fern spores, and the hydraulic system in plants. Such systems under these metastable conditions are vulnerable to cavitation. Lipid membranes, as part of cell membranes, are found in almost every biological system. The study of cavity formation in lipid membranes under tension plays an important role in the research of biological systems. In this context, lipid-lipid adhesion energy, as well as adhesion energy between lipids and other surfaces, is a crucial physical property as it tells us a lot about the strength of interaction between lipids and other matter.

In this poster I present our work on adhesion of lipid systems obtained from molecular dynamics simulations. More specifically, I will examine the lipid-lipid adhesion energy as well as lipid-surface adhesion energy and how it depends on the surface properties. Additionally, I will discuss how the adhesion energy and surface properties affect cavitation in lipid bilayers and lipid-substrate systems.

BP 8.17 Mon 18:00 Poster C

The Mechanics of Pancake-like Adhered Vesicles — •Gianna C. Wolfisberg[1], Hendrik T. Spanke[1], Jaime Agudo-Canalejo[2], Eric R. Dufresne[1,3], Robert W. Style[1], and Aleksander A. Rebane[1,4] — [1]Department of Materials, ETH Zürich, Switzerland — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Germany — [3]Department of Physics, Cornell University, USA — [4]Programs in Chemistry and in Physics, New York University Abu Dhabi, United Arab Emirates

Eukaryotic cells contain various lipid membrane-bounded organelles that possess unique biochemical identities. However, it remains often unclear how the organelle shapes are generated and what role the shapes play in function. An important example is the Golgi Apparatus, which has a highly conserved architecture comprising a stack of pancake-like sub-compartments (cisternae) that are adhered to each other and whose function is to process, sort, and transport freshly synthesized proteins via mechanisms that remain mysterious. Here, we develop an in vitro approach to study the mechanics of cisternae by creating flattened vesicle shapes of high surface-to-volume ratio achieved through adhesion and osmotic deflation. We compare our experimental shapes with the spontaneous curvature model. We find simple relations of aspect ratio and size that govern the mechanical properties of adhered pancake-like vesicles. We apply these simple relations to Golgi cisternae and find that the estimated adhesion strength between cisternae in cells is insufficient to create these flat shapes, suggesting that the shape is maintained by the cell using other mechanisms.

BP 8.18 Mon 18:00 Poster C

Flow Dynamics in the Capillary Network of Different Blood Cell Types — •khadija larhrissi[1], Christian Wagner[1], Felix Milan Maurer[1], Selina Wrublewsky[2], Yazdan Rashidi[1], Alexis Darras[1], and Matthias Laschke[2] — [1]Department of Experimental Physics, University Campus, Saarland University, 66123 Saarbrucken, Germany — [2]Institute for Clinical and Experimental Surgery, Saarland University, 66421 Homburg, Germany

Red blood cells (RBCs) constitute the majority of cells in the blood and play a key role in transporting oxygen to tissues and organs. On the other hand, leukocytes, also known as white blood cells, make up approximately 1% of the total blood volume in most mammals. The flow of these cells ensures the body's defence against various viral and bacterial infections. The White blood cells (WBCs) exhibit two modes of motion: a fast flow mode where they move with the surrounding fluid, and a slower rolling mode where they partly adhere to the wall, whereas Red Blood Cells (RBCs) simply flow with the surrounding fluid.

In this study, our objective is to examine the influence of geometry and distribution on the flow of white blood cells (WBCs) and to explore how the rigidity of red blood cells (RBCs) alters flow dynamics. To achieve this, we used Golden Syrian Hamsters as a model system to quantify the flow of cells by fluorescence microscopy and compare their behavior in different networks of vessels. Additionally, since some WBCs are larger in size than the capillaries they pass through, we will examine the impact of this size difference on their flow.

BP 8.19 Mon 18:00 Poster C

Exploring Cell Shapes and Dynamics Through Discrete Differential Geometry — •Mauricio Rojas-Vega, Andela Šarić, and Christopher Wojtan — Institute of Science and Technology,

Klosterneuburg, Austria

Our study utilizes the Canham-Helfrich bending energy model to validate anticipated cellular phenomena within membrane structures, identifying three primary equilibrium shapes. Introducing an external cargo attracted to the membrane confirms established interactions, resulting in observed budding and wrapping. These findings solidify our model's robustness in encapsulating known cellular behaviors.

Additionally, our research explores controlled membrane manipulations, enhancing the model's representation of fluid-like behavior. Future work aims to incorporate non-reciprocal interactions for exploring non-equilibrium cell shapes and validating the inside-out model.

This research consolidates understanding of established cellular interactions, offering avenues to explore non-equilibrium cellular phenomena, thereby advancing our comprehension of cellular dynamics.

BP 8.20 Mon 18:00 Poster C

The Role of Perilipin 5 for the Contact Sites between Lipid Droplets and Bilayer: Protein Tether, or Lipid Bridge? — •Shima Asfia, Mahsa Mohammadian, Ralf Seemann, and Jean-Baptiste Fleury — Department of Experimental Physics and Center for Biophysics, Saarland University, Germany

Lipid droplets (LDs) play a pivotal role in cellular energy storage and supplying components for the structure of organelle membranes. As the biology of lipid droplets relies on close coordination and communication with other cellular organelles, it is important to take a look at this interaction. In particular, the role of the protein Perilipin 5 (PLIN5), which is known as a mediator in regulating LDs dynamics and metabolism in cells is of interest. To investigate the impact of PLIN5 on the formation of contact sites between LDs and a bilayer, LDs (triolein oil droplets) surrounded by a phospholipid monolayer with and without PLIN5 are brought in contact with single unilamellar vesicles (SUV)s with a composition close to the ER membrane. To detect different contact interactions of SUVs with the monolayer coating the LDs, the SUVs were double fluorescent labeled with a phospholipid Rhodamine dye in the bilayer and Cy5 dye in the core. Protein tethers can be assumed when the SUVs stay in contact with LDs via protein attachment; in this case, spots with both fluorescent dyes are observed on the surface of the LDs. Lipid bridges can be assumed when SUVs fuse to the LD monolayer, and a colored *Rhodamine ring* appears on the surface of LDs revealing that only the phospholipid dye of the SUVs merged with LDs monolayer.

BP 8.21 Mon 18:00 Poster C

Modulating self-organizing protein patterns by controlling the number of membrane linkers and the membrane charge — •Katharina Esch[1,2], Mergime Hasani[1,2], and Katja Zieske[1,2] — [1]Biophysics and Optogenetics, Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander Universität Erlangen Nürnberg, Erlangen, Germany

In nature, patterns occur on many different scales and are an expression of nature's ability to self-organize. Understanding the mechanisms regulating such patterns is an intriguing challenge in biophysics. The Min protein system is one of the best-studied examples of protein self-organization, and Min proteins self-organize into spiral waves on a model lipid membrane. In this study, we investigate the effects of biophysical membrane parameters on Min protein waves using purified proteins and a model lipid membrane. First, we demonstrate that an increase in protein-membrane interaction induces patterns of different geometry. Specifically, we observe not only wave-like patterns but also snowflake-like and flower-like patterns in dependence on the number of membrane linkers. Second, we demonstrate that these snowflake-like patterns not only occur on E. coli membranes but also on a minimal membrane composition of DOPC and PG. Finally, membrane charge modulates the complexity of protein patterns. Our results demonstrate that the regulation of membrane charge and linkers is an intriguing mechanism to regulate cellular pattern formation on the mesoscale.

BP 8.22 Mon 18:00 Poster C

Formation of supported artificial Membranes of Lipid Raft Models by Physical Vapor Deposition — •Nancy Gomez-Vierling[1], Daniel Saavedra[1], Marco Soto-Arriaza[2], Marcelo A. Cisternas[3], Nicolás Moraga[1], Tomás P. Corrales[4], and Ulrich G. Volkmann[1] — [1]Instituto de Física and CIEN-UC, Pontificia Universidad Católica de Chile (UC), Santiago, Chile — [2]Facultad de Medicina y Ciencia, Universidad San Sebastián, Santiago, Chile — [3]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Santiago, Chile — [4]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile

The study focuses on advancing the development of rapid and cost-effective biosensors through the exploration of artificial membranes. The researchers, particularly from SurfLab UC, aim to create a Supported Lipid Bilayer (SLB) mimicking the Lipid Rafts model in cellular membranes. They employ the vapor-phase deposition method to determine optimal temperatures for evaporation rates of cholesterol, DOPC, and sphingomyelin molecules within a high vacuum chamber. The research delves into understanding the phases formed by these molecules at different temperatures. The obtained critical information guides the deposition of these molecules onto a silicon substrate, alongside DPPC molecules, to form self-assembling artificial bilayers resembling lipid rafts. The significance of this research lies in providing solvent-free alternatives for designing, fabricating, and storing phospholipid bilayer-based devices, including sensors and biomimetic devices. Acknowledgements: ANID Ph.D. Fellowships (NGV, DS, NM).

BP 8.23 Mon 18:00 Poster C

Superstructure in lipopolymer monolayers at the air/water interface — •Issam Assi, Heiko Ahrens, and Christiane A. Helm — Institute of Physics, University of Greifswald, 17489 Greifswald, Germany

Lipopolymers with covalently bound poly(ethylene oxide) (EO_N)head groups have been introduced to stabilize bilayer membranes. Langmuir monolayers of the lipopolymer DSPE-EO_N at the air/water interface show in the isotherm a transition from the liquid expanded to the liquid condensed phase, which is confirmed by in-situ Grazing Incidence X-ray Diffraction (GID). A laterally inhomogeneous film of condensed ordered alkyl chains embedded in a matrix of solvated polymers is formed. Small Angle GID shows that these lipid domains are ordered with a lattice constant of about 12 nm. Hexagonally ordered lipid domains were observed in situ with GID, which changed on further compression to a lamellar phase (nanostripes). The films stayed homogeneous on the micrometer scale as observed with Brewster Angle Microscopy. On transferred monolayers, these supramolecular phases were observed with AFM. The enthalpy of the phase transition was determined from isotherms at different temperatures for several EO degrees of polymerization (N between 6 and 112). The lattice constants of the hexagonally ordered lipid domains and the nanodomains changed very little.

BP 8.24 Mon 18:00 Poster C

Nobody is perfect: inspecting the defects of lipid membrane stacks by STED microscopy and X-ray diffraction — •Sarah Becker, Jette Alfken, and Tim Salditt — Institute for X-Ray Physics, University of Göttingen, Göttingen, Germany

Solid-supported lipid membranes are an important model system for biological membranes. A commonly used method to study the structure of lipid bilayers is x-ray reflectometry which yields averaged information such as the number of membranes deposited, the bilayer thickness, and the density profile. However, information regarding single defects in membranes is not accessible by this ensemble averaging technique based on diffraction. Now, we have applied different fluorescence microscopy techniques such as epifluorescence, confocal and STED microscopy, in order to examine local defects in oligo lipid membrane stacks. The high resolution STED images extend the multiscale structural characterization of membrane stacks by brightfield microscopy and x-ray reflectometry, which we also have applied. The study shows that the idealized assumption of perfect stacks without defects is not warranted and that (partial) dewetting effects can easily be encountered when preparing bilayers by spin coating.

BP 8.25 Mon 18:00 Poster C

Studying extracellular vesicle-mediated cell communication in flow networks for drug delivery system development — •Jan Jedryszek, Fatemeh Mirzapour, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Extracellular vesicles (EVs) are membrane-bound particles produced by cells and released into the bloodstream, functioning as vital information carriers within the body. They transfer molecules like proteins and RNA, significantly influencing intercellular communication and physiological processes. Functioning similarly to data packets in a network, EVs are key in cell-to-cell signaling. EVs from immune cells, such as dendritic cells and B cells, are pivotal in transferring molecules for adaptive immune responses against pathogens and tumors.

Our research focuses on elucidating this mechanism of long-range

cellular communication and leveraging these insights to enhance drug delivery methods. We are investigating both natural EV*s and synthetic vesicles, the latter of which are loaded with surface proteins and CRISPR-Cas12 gene editing tools, infused into a vasculature-on-a-chip system developed in our lab. By analyzing binding and fusion rates in a flow network, we intend to deepen our understanding of the natural role of extracellular vesicles in intercellular communication within the body and advance drug delivery techniques.

BP 8.26 Mon 18:00 Poster C

Properties of Long-Chain Lipid Enriched Regions in Biological Membranes: Insights from MD Simulations — •Annemarie Quas, Clara Rickhoff, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Corrensstraße 28/30, 48149 Münster

In the yeast plasma membrane, domains rich in long-chain sphingolipids are observed[1]. Our study employs molecular dynamics (MD) simulations to explore the influence of these lipids on membrane properties. We utilize both coarse-grained and all-atom models, employing a simplified lipid composition with varying concentrations of long-chain lipids in the outer leaflet. Initially, the sphingolipids are represented by long-chain phosphatidylinositols. The equilibration steps are performed with the coarse-grained model. Subsequently, back-mapping techniques are utilized to obtain the corresponding all-atom system. This enables extended simulation times and a comparison between all-atom and coarse-grained results. We assess the impact on diverse parameters such as order parameter, membrane thickness, and interdigitation to unravel the relationship between long-chain lipid concentrations and membrane properties. Our findings aim to enhance result interpretation and to provide approaches for new experiments.

[1] Aresta-Branco *et al.*, *J. Biol. Chem.* **2011**, 7, 5043-5054

BP 8.27 Mon 18:00 Poster C

Fungal hydrophobins as building blocks for rigid, water-impermeable pure protein bilayers and vesicles — Friederike Nolle, Kirstin Kochems, Karin Jacobs, and •Hendrik Hähl — Experimental Physics & Center for Biophysics, Saarland University, Saarbrücken, Germany

Hydrophobins are a class of small, strongly amphiphilic and extremely stable proteins formed mainly by filamentous fungi. Similar to surfactant molecules like phospholipids they self-assemble in monolayer films at water interfaces. Contacting two films, stable membranes resembling lipid bilayers are obtained, and subsequently also vesicles can be formed. These hydrophobin bilayers exhibit a similar thickness to lipid bilayers allowing for an incorporation of simple ion channels [1].

Due to their natural biocompatibility, higher stability in comparison to lipid bilayers and versatility gained through bioengineering, the application potential for hydrophobin bilayers and vesicles is vast. Many properties of this new type of membrane are, however, still to be characterized. We report here on mechanical testing via atomic force microscopy on pore-spanning films and determination of the water permeability in a droplet interface bilayer setup. We find that the layers exhibit a finite elasticity and high stability, withstand by far larger osmotic pressures than lipid bilayers, and are nearly impermeable to water [2]. Yet, by disturbing the molecular packing in the bilayer, the permeability can be tuned.

[1] H. Hähl et al., Adv Mater **29**, 1602888 (2017).
[2] F. Nolle et al., Langmuir **39**, 13790 (2023).

BP 8.28 Mon 18:00 Poster C

Molecular Dynamics Simulations as a tool to investigate the impact of imidazole-based cholesterol in lipid bilayers — •Clara Rickhoff, Azadeh Alavizargar, and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Münster, Germany

Cholesterol is an important component of plasma membranes in mammalian cells having a significant impact on their fluidity and structure. Experiments aiming at a deeper understanding of the effect of cholesterol are facing the difficulty of tracking this non-fluorescent component of lipid bilayers. In order to overcome this problem, different imidazole-based cholesterols were developed. These modifications allow to add different functionalities to the cholesterol analog without changing the backbone of cholesterol which is embedded in the membrane. [Matos et al, Commun Biol, 2021, 4, 720] In this work Molecular Dynamics simulations of the non-charged imidazole-based cholesterol analog were conducted. This molecule was previously synthesized in the Glorius group (University of Münster). Our simulations aim to investigate the impact of this cholesterol analog on the structure of lipid bilayers and on the stability of lipid rafts. The results of this study allow a more precise assessment of how accurate this analog mimics cholesterol in terms of order parameter, tilt angle and position within the bilayer also in comparison with the positively charged imidazolium-based cholesterol analog.

BP 8.29 Mon 18:00 Poster C

Elevating Understanding of Membranes: How Spectroscopic Techniques can draw from Super-Resolution Microscopy Principles — •Simone Ezendam[1], Jonatan Alvelid[1], Andrea Volpato[2], and Ilaria Testa[1] — [1]Department of Applied Physics and Science for Life Laboratory, KTH Royal Institute of Technology, Stockholm, Sweden — [2]Department of Women's and Children's Health and Science for Life Laboratory, Karolinska Institut, Stockholm, Sweden

Membranes and vesicles play pivotal roles in cellular processes, operating across various scales and intricately interacting with proteins. Super-resolution microscopy has transformed our understanding of membrane dynamics by providing higher resolution compared to traditional optical methods. However, gaining insights into the fast timescales governing translational and rotational diffusion necessitates spectroscopic techniques such as fluorescence correlation spectroscopy (FCS) and fluorescence anisotropy (FA). Because these techniques rely on fluorescence, they can leverage the same principles enabling super-resolution microscopy. An established example is STED-FCS. Recently, our lab introduced STARSS[1], extending time-resolved FA to large proteins. Expanding on these concepts, here, we propose the application of STED in FA for studying membranes.

[1] Volpato et al. Extending fluorescence anisotropy to large complexes using reversibly switchable proteins. Nat Biotechnol (2023). DOI: 10.1038/s41587-022-01489-7

BP 8.30 Mon 18:00 Poster C

The effect of aversive external conditions on the migration of small plasmodia of Physarum polycephalum — •Diana Lenski, Lucas Tröger, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Environmental conditions determine the behavior of living organisms: physical activities as well as internal processes can vary significantly in response to certain interventions in an organism's environment. In a favorable environment, the migration behavior of small plasmodia of the unicellular slime mold, *Physarum polycephalum*, shows a self-avoiding run-and-tumble movement. However, it is not yet clear if and how *P. polycephalum* adapts its migration behavior to aversive external conditions. In this study, we perform migration experiments under various aversive stimuli, in particular differently composed substrates - containing salts or altered pH - and substrates exposed to blue light. Statistical analysis of the cell trajectories and simulations based on data inferred parameters will lead to a deeper understanding of the central migration parameters that are adapted with respect to the environment in order to achieve a most efficient migration.

BP 8.31 Mon 18:00 Poster C

Unravelling the collective behavior of protrusions for directed migration — •Lucas Tröger and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Unlike bacteria, eukaryotic cells are large enough to sense a chemical gradient across their cell body. However, chemotaxis of an entire cell requires a mechanism for coordinating competing protrusions. The slime mold *P. polycephalum* is a giant unicellular organism built in the form of a fluid-filled tubular network. Its strong and large-scale cytoplasmic flows make it an ideal model organism to study the role of fluid flows in coordinating the collective behavior of competing protrusions during morphological changes during chemotaxis. We perform experiments, analyze trajectories and protrusion dynamics, and simulate fluid flows to elucidate the mechanism that coordinates the chemotaxis of this macroscopic cell.

BP 8.32 Mon 18:00 Poster C

Clutch Model for focal adhesions predicts perfect self-stablisation — •Anton Burnet[1,2] and Benedikt Sabass[1,2] — [1]Department of Veterinary Sciences, LMU München — [2]Department of Physics, LMU München

Cell-matrix adhesions connect the cytoskeleton to the extracellular environment and are essential for maintaining the integrity of tissue and

whole organisms. Remarkably, cell adhesions can adapt their size and composition to an applied force such that their size increases proportionally to the load. Recently, this group suggested a molecular mechanism that can explain adhesion growth under load for planar cell adhesions. The mechanism is based on conformation changes of adhesion molecules that are dynamically exchanged with a reservoir. Tangential loading drives the occupation of some states out of equilibrium, which for thermodynamic reasons, leads to the association of further molecules with the cluster, which is referred to as self-stabilisation. A variation of the latter model had been considered which linearly coupled the recruitment rate of the reservoir with the occupation number of the unfolded bound states. Simulation results found that a bifurcation occurs for a critical coupling value, where the system transitions from limited self-stabilisation to a perfect self-stabilisation regime where the system no longer undergoes rupture upon an ever increasing force. Moreover, a second regime was found where the system size exhibits exponential growth. In this work, we focus on quantitively understanding these results, starting with simpler coarse-grained models to shed light onto the qualitative behaviour observed from simulations.

BP 8.33 Mon 18:00 Poster C

Stochastic catch-bond model of cell-cell adhesion mechanics and turnover — •Antonella Di Concilio Moschen[1,2] and Benedikt Sabass[1,2] — [1]Department of Veterinary Sciences, LMU München — [2]Department of Physics, LMU München

Catenins are proteins that mediate the binding between transmembrane molecules called cadherins and intracellular actin filaments in cell-cell adherens junctions. Mechanical forces generated by cytoskeleton are directly transmitted via αE-catenin to the membrane-localized E-cadherin/β-catenin complex.

It has been proposed based on *in vitro* experiments that this mechanotransduction mechanism is well described by a two-state catch bond between αE-catenin and F-actin. We aim to understand how the catch bond affects the mechanics and structural dynamics *in vivo*. Specifically we focus on differences between two distinct states of the adherens junctions called zonula-adherens and punctate-adherens junctions. By implementing a Gillespie algorithm to the system's master equation, we construct a framework to quantitatively compare predictions from the above-mentioned two-state catch-bond model with results from FRET and FRAP experiments.

BP 8.34 Mon 18:00 Poster C

Studying cell-particle-interactions using blinking holographic optical tweezers — •David Gitschier, Wolfgang Gross, Manuel Eisentraut, Konrad Berghoff, and Holger Kress — Department of Physics, University of Bayreuth, Bayreuth, Germany

The corona pandemic underlined the importance of a healthy immune system. An indispensable part thereof are the interactions with infected cells and bacteria as well as their subsequent uptake. However, a complete mechanical characterization of this dynamic process still lacks. Here we show how to measure mechanical properties of immune cells during interaction with particles using the versatile technique of blinking holographic optical tweezers. This method enables us to obtain the binding kinetics and viscoelastic parameters of the cellular response. The latter are consistent with power law rheology. Using this, we determine the temporal evolution of the contact radius between particle and cell leading to the timescale of the binding kinetics. Regarding the material softness, addition of cytochalasin D resulted in an increase of the cellular compliance and fluidization of the cortex. Moreover, we visualize the influence of the cortical actin structure by fluorescence microscopy with Lifeact-GFP-transfected cells. Therefore the actin dynamics after initial cell-particle-contact are accessible. Our approach helps elucidating the biomechanical processes underlying this important part of innate immunity. Additionally it allows us to address important, yet unanswered questions like how different microplastic particles interact with cells.

BP 8.35 Mon 18:00 Poster C

Measuring viscoelastic properties in active, living systems through passive observations — •Till M. Muenker[1], Gabriel Knotz[2], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics, Universität Göttingen, Göttingen, Germany — [2]Institute of Theoretical Physics, Universität Göttingen, Göttingen, Germany

Accurately quantifying the viscoelastic material properties within active systems, such as cells, poses a challenging task. Due to the non-equilibrium nature of such systems, many powerful tools from statistical physics like the MSD fail to predict material properties from passive observation of a tracer particle. Instead, active methods such as optical- and magnetic tweezers are used where typically external forces are applied to measure the material response. Here, we introduce a new statistical method, termed mean back relaxation (MBR). By quantifying the mean displacement of a probe particle after having transitioned a specific distance in the immediate time history, this new quantity allows to detect breaking of detailed balance in confined systems. Firstly, we test this method in a well-controlled experimental model system where we are able to detect the level of non-equilibrium. Next, we turn to the most complex, but also highly relevant system, living cells. Strikingly, applying this novel approach not only allows us to measure the level of activity but also gives access to the viscoelastic material properties of a range of different cell types. This approach could drastically facilitate the quantification of intracellular mechanics, thus opening the door for many researchers who do not have access to elaborate experimental setups.

BP 8.36 Mon 18:00 Poster C

Analysis of traction stress of iPSC derived heart muscle cells — •Bastian Malte Winter[1], Fatemeh Abbasi[2], Karthika Annamalai[3], Karl Toischer[4], and Timo Betz[5] — [1]Drittes Physikalisches Institut, Göttingen, Deutschland — [2]Drittes Physikalisches Institut, Göttingen, Deutschland — [3]Department of Cardiology and Pneumology, Göttingen, Deutschland — [4]Department of Cardiology and Pneumology, Göttingen, Deutschland — [5]Drittes Physikalisches Institut, Göttingen, Deutschland

During the maturation of animal tissue, their heart, and in particular their myocardium typically undergoes a change of stiffness. Furthermore, it is known that conditions like hypertrophy can also change the stiffness of the myocardium. Generally, changes in stiffness have an effect on force generation of single cells but to which extent this can be also applied to single cardiomyocytes is not well studied. Our goal is to investigate the effect of different substrate stiffnesses on the environment on force generation of single iPSC derived cardiomyocytes. For that, we seed cardiomyocytes on Polyacrylamide-gel (PAA-gel) of different stiffnesses and use Traction Force Microscopy to locate the forces generated by single cardiomyocytes in magnitude and direction. We show that generally an increase in stiffness also results in an increase in force production of single cardiomyocytes.

BP 8.37 Mon 18:00 Poster C

Intracellular Mechanical Fingerprinting: Identifying the proteins controlling the intracellular active mechanics — •Noémie Veyret, Dorian Marx, Till Münker, and Timo Betz — Third institute of Physics, University of Göttingen, Germany

Over the past few years, the study of cell mechanical properties has allowed new insights on the understanding of biological processes and life complexity. According to previous work, intracellular mechanical properties can be narrowed down to a fingerprinting of only 6 parameters. Through the use of active and passive microrheology measurements via optical tweezers, frequency dependent viscoelastic properties and intracellular activity were found to vary for different cell types. The aim of this project is to find a correlation between changes in protein expressions and mechanical fingerprint of cells. To do so optical tweezers measurements will be performed during the differentiation process of induced Pluripotent Stem Cells (iPSC) into cell types derived from the three germ layers, namely neurons (ectoderm), skeletal muscles (mesoderm) and lung epithelia (endoderm). This measurement allows the characterization of the mechanics during the iPSC differentiation process. In parallel, the cell proteome will be studied using mass spectroscopy. Combining both, we hope to find the connection between proteins and their mechanical role, the intracellular "mechanome".

BP 8.38 Mon 18:00 Poster C

Microfluidic single cell study on protoplast fusion — •Ioannis Gkekas[1], Philipp J. Artmann[1], Dario Anselmetti[1], Thorsten Seidel[2], and Martina Viefhues[1] — [1]Experimental Biophysics, Bielefeld University — [2]Dynamic Cell Imaging, Bielefeld University

Plant cells are omnipotent and breeding of new varieties can be achieved by protoplast fusion. Such fusions can be achieved by treatment with poly(ethylene glycol) (PEG) or by applying an electric field. Microfluidic devices allow for controlled conditions and targeted manipulation of small batches of cells down to single cell analysis. To provide controlled conditions for protoplast fusions and achieve high reproducibility, we developed a microfluidic device to reliably trap few of *Arabidopsis thaliana* protoplasts and induced a cell fusion by controlled addition of PEG. Our results indicate that the following fusion

parameters had significant impact on the fusion efficiency and duration: PEG concentration, osmolarity of solution, and flow velocity. PEG concentration below 10% led to only partial fusion. Osmolarity of the PEG fusion solution was found to strongly impact the fusion process; complete fusion of two source cells sufficiently took part in slightly hyper osmotic solutions, whereas iso-osmotic solutions led to only partial fusion at 20% PEG concentration. We observed accelerated fusion for higher fluid velocities. Up to this study, it was common sense that fusion is one directional, i.e. once two cells were fused into one cell they stay fused. Here, we present for the first time reversible fusion of protoplasts. Our microfluidic device paves the way to a deeper understanding on the kinetics and processes of cell fusion.

BP 8.39 Mon 18:00 Poster C

Calcium-dependent flagellar adhessiveness of *Chlamydomonas* — •Marcel Schalling[1], Rodrigo Catalan[1], Marzieh Karimi[2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Calcium (Ca^{2+}) signalling influences several flagellar processes in flagellated microbes, namely maintenance of the flagella and the regulation of their waveform and beat frequency. The unicellular biflagellated microalga *Chlamydomonas reinhardtii* has been particularly used as a model organism to understand such processes. Interestingly, recent evidence shows that intracellular Ca^{2+} influences the adhesion of *C. reinhardtii* of their flagella to abiotic surfaces [1]. Additionally, *C. reinhardtii* exhibits light-switchable flagellar adhesion [2], such that they adhere to surfaces under blue light and detach under red light. Using single-cell micropipette force spectroscopy [3] in the presence of different concentrations of calcium in the medium, we study the effect of calcium on flagellar adhesiveness in different light conditions. Thereby, we aim at shedding light on the signal transduction pathway underlying light-switchable flagella adhesion.

[1] C. Fort *et al.*, *Journal of Cell Science* (2021)
[2] C. Kreis *et al.*, *Nature Physics* (2018)
[3] M. Backholm and O. Bäumchen, *Nature Protocols* (2019)

BP 8.40 Mon 18:00 Poster C

Nuclear mechanics across scales: from global deformation to local measurements — •Bart Vos[1], Yamini Vadapalli[2], Till Muenker[1], Ivan Avilov[2], Peter Lenart[2], and Timo Betz[1] — [1]Third Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Mechanics play a crucial role in a wide range of cellular processes, from differentiation to division and metastatic invasion. Additionally, mechanical signaling plays an important role in protein expression. Although the mechanical properties of the cytoskeleton, providing shape, motility and mechanical stability to the cell, have been extensively studied, remarkably little is known about the mechanical environment within the nucleus of a cell and the exact mechanisms of force transduction between the cytoplasm to the nucleus.

To address these questions, we apply external deformations to oocytes of different species to observe how cellular deformations can be transmitted to the nucleus, leading to nuclear deformations. We combine this with optical tweezers-based microrheology in the cellular nucleus, allowing a direct comparison between intracellular and intranuclear mechanics. We observe viscoelastic behavior of the nucleoplasm that is profoundly different from the cytoskeleton. In addition, we observe that the nuclear envelope plays an important role by providing stability to the nucleus.

BP 8.41 Mon 18:00 Poster C

Unravelling the action spectrum of light-switchable flagellar adhesion of *Chlamydomonas* — •Rodrigo Catalan[1,2], Antoine Girot[1,2], Alexandros Fragkopoulos[1,2], Olga Baidukova[3], Darius Rauch[3], Peter Hegemann[3], and Oliver Bäumchen[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen , Germany — [2]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [3]Humboldt University of Berlin, Institute of Biology, Invalidenstrasse 42, 10115 Berlin, Germany.

Most of the phenotypic repertoire of photoactive microorganisms is regulated by light-sensitive proteins called photoreceptors, which enable the organisms to adapt to alterations of their environment. The unicellular biflagellated microalga *Chlamydomonas reinhardtii* has been used as a model organism to study light-mediated phenotypes, such as phototaxis, the sexual life cycle, and the circadian rhythm. Recently, we discovered that *C. reinhardtii* can reversibly switch on and off the adhesiveness of their flagella in blue and red light, respectively [Kreis *et al.*, Nature Physics, 2018]. Using single-cell micropipette force measurements, we show that the action spectrum of flagellar adhesion forces in wild-type (WT) *C. reinhardtii* cells resembles the spectral sensitivity of cryptochrome (Cry) photoreceptors. Further comparison of the flagellar adhesion forces between WT and mutant *C. reinhardtii* cells lacking one or two known photoreceptors reveals that the deletion of both animal- and plant Cry completely disrupts the adhesion phenotype.

BP 8.42 Mon 18:00 Poster C

Modelling the impact of myosin IIA/IIB isoforms on cell migration — •Nils Winkler, Oliver M. Drozdowski, Falko Ziebert, and Ulrich S. Schwarz — Institute for Theoretical Physics and BioQuant, Heidelberg University, 69120 Heidelberg, Germany

Cell motility is one of the hallmarks of life. In mammalian cells, it is based on flow in the actin cytoskeleton, which in turn is driven by both actin polymerization and non-muscle myosin II motors. However, it is unclear how the different isoforms of this motor contribute to cell polarization and migration. Here we propose a one-dimensional active gel model with different myosin species to elucidate the role of non-muscle myosin IIA and IIB. Building on an established coarse-graining procedure [1], we start from binding kinetics and derive a model which can qualitatively explain experimentally found isoform concentration distributions. The model incorporates volume exclusion and cross-diffusion effects caused by the binding properties. Through numerical analysis we explore different migratory modes and the possibility of oscillatory motion driven by concentration differences both in length and velocity.

[1]: Drozdowski, Ziebert and Schwarz, Comms. Phys. 6, 158 (2023)

BP 8.43 Mon 18:00 Poster C

Mechanical fingerprint of the intracellular space — Muenker Till M., Vos Bart E., and •Betz Timo — University of Göttingen, Göttingen, Germany

Many important cellular functions such as organelle positioning and internal cargo transport are dependent on the viscoelastic intracellular mechanical properties of cells. A range of different mechanical models has been proposed to describe these properties. Whilst simple models such as Maxwell or Kelvin-Voigt models don't seem sufficient to capture the full complexity of cells, more elaborate models like generalized Kelvin-Voigt models require a huge number of parameters. This hinders the comparison and interpretation of experimental findings. Further, from a physics perspective, cells are systems out of thermodynamic equilibrium, permanently consuming metabolic energy to carry out mechanical work. The level of "non-equilibrium" can be proposed as an indicator for cell type, cell state or even diseases. To determine both, the viscoelastic properties and the cellular activity, we use optical tweezers based active and passive microrheology in a diverse group of 9 different cell-types. Surprisingly, despite differences in origin and function, the complex moduli of all cell types can be described using a 4 parameter based fractional Kelvin-Voigt model. Additionally, the frequency dependent activity can be described with a simple power law. This approach allows to reduce those complex and frequency dependent properties down to a fingerprint of 6 parameter. Further principal component analysis shows that only 2 of them may be sufficient to characterize the mechanical intracellular state.

BP 8.44 Mon 18:00 Poster C

Cell movement on the fast lane: how patterns can drive cell migration — •Annika A. Vogler, Sebastian W. Krauss, Florian Rehfeldt, and Matthias Weiss — Experimental Physics I, University of Bayreuth, 95447 Bayreuth, Germany

Cell migration is a fundamental process that is key in many physiological events, such as wound healing, embryonic development, or cancer metastasis. In living organisms cells often have to navigate through intricate and obstructed environments. Microstructured surfaces provide a versatile platform for mimicking such environments, and they allow for studying migration dynamics under controlled conditions.

Here, we have investigated the migration of MDA-MB-231 cells on microstructured surfaces, focusing on periodic stripe patterns of varying dimensions. Our results reveal a correlation between stripe width/periodicity and cell migration speed. Moreover, cells display

a unique behavior at the boundaries of the micropattern: Once they reach the edge, they tend to get stuck at these loci, akin to a migrate-to-capture dynamics that eventually leads to trapping in a confined state. Furthermore, the directionality and periodicity of the stripe pattern leads in general to an anisotropic movement, even though pattern features are roughly one magnitude smaller than cells. This finding highlights the ability of cells to sense even very small structures and to adapt their migration accordingly.

BP 9: Poster Session Ib

Cell Mechanics. Additional posters on Cell Mechanics in Poster Session Ia.

Time: Monday 18:00–20:30 Location: Poster D

BP 9.1 Mon 18:00 Poster D

Substrate functionalization reveals the electrostatic nature of flagellar adhesion to surfaces — •Lea Rupprecht[1], Rodrigo Catalan[1], Antoine Girot[1], Christian Kreis[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Am Fassberg 17, 37077 Göttingen, Germany

Elucidating the physical phenomena underlying the interactions between microorganisms and surfaces is crucial for the development of technologies that aim to control the formation of microbial biofilms. While most of the studies use bacteria as model organisms, the principles of microbial adhesion remain elusive for eukaryotic photosynthetic microorganisms. We recently discovered that the model unicellular microalga *Chlamydomonas reinhardtii* adheres to surfaces by means of its two flagella under specific light conditions [Kreis *et al.*, Nature Physics, 2018]. Using *in vivo* single-cell micropipette force spectroscopy, we characterized the adhesion forces on surface-functionalized substrates in order to dissect the influence of surface energy, hydrophobicity, long-ranged van der Waals and electrostatic interactions [Kreis *et al.*, Soft Matter, 2019]. We found that the flagellar adhesion of *C. reinhardtii* cells to surfaces is unspecific and predominantly governed by electrostatic interactions. Here, we present adhesion force measurements of *C. reinhardtii* on surfaces with tailored electrostatic interactions, e.g. poly-L-lysin-coated silicon wafers.

BP 9.2 Mon 18:00 Poster D

An analytical theory of the influence of a cell nucleus on cell deformation — •Clara Gremmelspacher and Stephan Gekle — Universität Bayreuth

We develop an analytical theory to investigate the influence of a nucleus on cell deformation under mechanical load. To do this, we use linear elasticity theory and compare the deformation of homogeneous and heterogeneous cells under different boundary conditions. From these calculations we aim at deriving effective elasticity moduli of these shell-nucleus systems. Our work is intended to give a theoretical background to the often used practice of simplifying cells with their complex internal structure as homogeneous cells in numerical simulations and experimental data analysis.

BP 9.3 Mon 18:00 Poster D

Investigation of cortex-membrane interactions forming cell stiffness — •Tim Kutz[1], Andreas Janshoff[2], and Timo Betz[1] — [1]Third Institute of Physics, Georg August Universität Göttingen, Göttingen, Germany — [2]Institute of Physical Chemistry, Georg August Universität Göttingen, Göttingen, Germany

Cellular stiffness, a critical aspect of cell mechanics, influences cellular functions, like migration or responses to external stimuli. However, the precise origin of cellular and in particular cortical stiffness remains a subject of intensive investigation. Deciphering whether the stiffness of the cell surface predominantly arises from the cell membrane, the actin cortex beneath the membrane, or a synergistic combination of both is essential for advancing our knowledge of cell mechanics. To address this challenge, we propose a comprehensive approach that combines atomic force microscopy (AFM), confocal spinning disk fluorescence microscopy (CSDFM), and micropipette aspiration. AFM allows for high-resolution topographical imaging, offering nanoscale insights into the mechanical properties of the cell membrane and the underlying actin cortex. Simultaneously, CSDFM provides dynamic 3D visualization of cellular processes, augmenting our understanding of the structural components influencing cellular mechanics. The integration of micropipette aspiration complements these techniques by directly manipulating mechanical forces applied to the cell. This multi-modal approach not only enhances the precision and depth of our biomechanical analyses but also enables the correlation of structural and dynamic information, providing a holistic perspective on cellular mechanics.

BP 9.4 Mon 18:00 Poster D

Spatially varying cell fitness induced by confinement geometry and alignment — •Patrick Zimmer[1,2], Yoav G. Pollack[1,2], Philip Bittihn[2], and Ramin Golestanian[2,3] — [1]University of Göttingen, Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, Germany — [3]University of Oxford, Oxford, UK

Competition of cell phenotypes for limited space plays a role in both development and in tumor progression (healthy-cancerous / cancerous-cancerous clones). We focus here on purely non-adversarial competition dominated by stochastic fluctuations, avoiding any 'killing' related advantage.

Predicting the outcome for competition of such growing active matter is non-trivial, as it depends on how cell turnover via growth, proliferation and the degradation of cellular matter is regulated by mechanosensing in confinement.

We show that in a circular confinement, fitness of clones varies in the edge compared to the center correlated with layering, polar order of cell alignment and pressure modulation.

BP 9.5 Mon 18:00 Poster D

Optimize Microfluidic Synthesis of Polymer Beads for In-Vivo Force Cell Sensing — •Jordan Dieter Groh, Alejandro Jurado Jiménez, and Timo Betz — Drittes Physikalisches Institut, Göttingen, Deutschland

Since the first use of deformable beads inside living tissue as force sensors some ten years ago, the technique has been refined with the introduction of new materials and methods to measure deformation. Specially in our lab, polyacrylamide beads have been extensively used to assess forces in all kinds of in-vivo an in-vitro systems such as developing embryos, cancer spheroids or reconstituted muscle tissue. However, using shear-induced emulsions as fabrication method still presents some limitations: a broad size distribution and small variations in polymer stiffness. This project aims to optimize the production of polyacrylamide beads in two ways. First, the adoption of flow-focusing. This microfluidics technique is commonly employed in diverse fields, including drug delivery and the food industry, for creating emulsions with precise control over droplet sizes. Secondly, the use of UV-light as polymerization initiator. These two approaches should massively improve the reproducibility of our experiments, creating more homogeneous batches for measurements.

BP 9.6 Mon 18:00 Poster D

Measuring Mean Back Relaxation with Dark-field Microscopy — •Julian Schulz — Georg August Universität, Göttingen, Germany

The measurement of mechanical properties in living cells presents significant challenges due to their non-equilibrium nature. Traditional methods, such as active rheology, assess the complex shear modulus and energy dissipation but require challengingly complex invasive experiments. In contrast, the "mean back relaxation" (MBR), a novel statistical measure introduced by Muenker, Knotz, Krüger & Betz in 2022, offers insights into the energy dissipation of a cell through purely passive observations. So far, MBR measurements have relied on optical tweezers-based particle tracking, a technique not readily accessible in many laboratories. In this work, we utilize broadly available dark-field microscopy to monitor the position of a tracer particle inside hydrogels or cells with high spatial and temporal resolution. By comparing the results from this method with simulations, we can align them with various viscoelastic models, thereby enabling the determination of

biomechanical properties of cells. Our approach significantly enhances the accessibility of MBR measurement, providing a high-throughput method suitable for a broader range of laboratories. Furthermore, we offer software tools for efficient data analysis, expanding the potential for MBR measurements in diverse research settings. This advancement allows more scientists to explore cellular mechanics with less specialized equipment and reduced overhead.

BP 9.7 Mon 18:00 Poster D

Using cell shape measurements to classify *in vivo* resident tissue macrophage morphology in health and disease — •Miriam Schnitzerlein[1,2], Anja Wegner[3,4,5], Stefan Uderhardt[3,4,5], and Vasily Zaburdaev[1,2] — [1]Department Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [3]Department of Medicine 3 - Rheumatology and Immunology, FAU und Universitätsklinikum Erlangen — [4]Deutsches Zentrum für Immuntherapie, FAU — [5]Exploratory Research Unit, Optical Imaging Competence Center Erlangen, FAU

Resident tissue macrophages (RTMs) are a type of immune cell present in essentially all tissues in the human body. One of their main functions is to keep the tissue in homeostasis by removing dead cells or resolving lesions, thereby preventing unnecessary inflammation. To find such incidents, RTMs show continuous sampling behaviour by extending and retracting their protrusions which changes their overall morphology accordingly. Thus, these morphology changes can act as an indicator of a specific activation state of RTMs. In this project, we have employed a high-resolution, intravital imaging protocol to generate dynamic data of murine RTMs *in vivo* in the peritoneum. Next we have built a custom image processing pipeline to assess RTM morphology and dynamics via a set of cell size and shape features. Our features can quantitatively distinguish differently activated RTMs induced by various chemical stimuli. Furthermore, we could use our quantifiers to improve the health of RTMs in different experimental settings *ex vivo*.

BP 9.8 Mon 18:00 Poster D

Adhesion-based active gel model for 1D cell migration — •Valentin Wössner, Oliver M. Drozdowski, Falko Ziebert, and Ulrich S. Schwarz — Institute for Theoretical Physics and BioQuant, Heidelberg University, 69120 Heidelberg

Active gel theory has demonstrated that actomyosin contractility is sufficient for polarization and self-sustained cell migration in the absence of external cues. However, in these models, the dynamic character of substrate adhesion is usually neglected, although it seems to play an important role in more complex migration modes and during motility initiation. Simple models based on bond dynamics have been suggested for the required adhesion dynamics, but these do not include intracellular flows. Here we show that, in a one-dimensional setting, active gel theory can be extended by such adhesion dynamics and that load sharing is the cooperative effect that is required to obtain symmetry breaking. For intermediate adhesiveness, symmetric actin polymerization then leads to robust motility in a bistable regime. Our model predicts adhesion and flow profiles in qualitative agreement with experimental results. We also study switching between sessile and motile states by applying nonlinear perturbations as well as cell behavior on adhesive pattern.

BP 9.9 Mon 18:00 Poster D

Metal Induced Energy Transfer for height analysis of actin architecture under shear stress — •Michelle Denise Schoft, Carolin Grandy, Jonas Pfeil, and Kay-Eberhard Gottschalk — Institut für Experimentelle Physik, Universität Ulm, Ulm, Germany

Cells interact with their environment by responding to mechanical and biochemical signals. The focal adhesion multi-protein complex provides a link between the extracellular environment and the actin cytoskeleton. Aside from adherence to the surface, focal adhesions are relevant in sensing and transduction of mechanical cues. This is initially mediated via integrins, the transmembrane proteins associated with focal adhesion complexes, linking the external environment to further internal force-sensitive proteins. To analyse the effect of mechanical stress on the actin architecture of 3T3 fibroblasts, a range of different shear stress levels was applied in a perfusion setup. Moreover, to determine the influence of integrins in mechanosignaling under fluid flow, the experiment was performed with fibroblasts expressing the fibronectin-binding $\alpha_5\beta_1$, $\alpha_v\beta_3$ and $\alpha_5\beta_1/\alpha_v\beta_3$ integrin variants. The height data of the actin organisation was aquired by Metal Induced Energy Transfer recorded with Fluorescent Lifetime Imaging Microscopy (FLIM) on a gold surface. We use this technique to achieve nanoscale resolution of the axial actin organisation.

BP 9.10 Mon 18:00 Poster D

Modeling durotaxis in living cells on alternating substrate stiffness: a boltzmann approach — •Mathis Grelier[1], Carlos Ureña martin[2], Mark Schvartzman[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Department of Materials Engineering and Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion University of the Negev, Beer-Sheva 84105, Israel — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Understanding cellular responses to substrate stiffness is crucial for unraveling fundamental principles of cell spreading and migration. Our study investigates durotaxis in HeLa cells by conducting experiments on substrates featuring alternating lines of distinct stiffness. To describe the cell spreading, we introduce a stochastic model grounded in a Boltzmann distribution. This comprehensive framework considers different energy contributions governing the stochastic spread of cells over line boundaries. We observe a higher alignment of cells along the lines when the width of the softest lines increases. This behavior arises due to the increasing energy expenditure incurred by the cell when attempting to bridge across the softer substrate. The model successfully captures the probability distribution of cell shapes and alignment of the experiments, providing a quantitative framework for predicting the biomechanics of cell migration over material of different stiffness.

BP 9.11 Mon 18:00 Poster D

Interpretation of cell mechanical experiments in microfluidic systems depends on cellular shape descriptors — •Bob Fregin, Doreen Biedenweg, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

Mechanical properties of cells are known to be linked to cell state, fate, and function. For identifying and tracking cells, as well as quantifying their deformations, it is crucial to accurately characterize cell shapes. While various shape descriptors have been explored for studying adherent cell morphology, their impact on rheological experiments involving suspended cells remains less understood. Here, we compared nine shape descriptors to quantify suspended cell deformation under extensional and shear flow in a microfluidic system using dynamic real-time deformability cytometry. Our findings reveal that while stress relaxation depends on stress amplitude and duration, steady-state deformation can be predicted from single-cell traces, even for short translocation times. By comparing data analysis strategies, we explored the balance between computational costs and experimental accuracy. Our results suggest that such measurements are feasible on an ensemble scale when the characteristic time matches the microfluidic system's dimensions. Additionally, we introduced a scoring method to evaluate shape descriptor-dependent effects on cell deformation after cytoskeletal modifications. We found that analyzing cells in extensional flow offers higher sensitivity, irrespective of shape parameterization, while inverse Haralick's circularity is more suited for studying cells in shear flow.

BP 9.12 Mon 18:00 Poster D

Virtual fluidic channels as liquid tweezer for mechanocytometry — •Karolin Melde[1], Doreen Biedenweg[1], Salvatore Girardo[2], Horst-Holger Boltz[1], Thomas Ihle[1], and Oliver Otto[1] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]Max Planck Institute for the Science of Light, Erlangen, Germany

Real-time deformability cytometry is a high-throughput method to study the mechanical properties of single cells. Utilizing hydrodynamic shear and normal stresses, micron-sized objects are deformed within a microfluidic channel of dimensions that have to match the cell size.
To overcome this limitation, we recently introduced virtual fluidic channels (VFCs) that enable tailoring the microfluidic geometry within seconds. VFCs are formed by co-flowing aqueous polymer solutions, where cells are confined between the corresponding liquid-liquid interfaces that act as a pair of tweezers. Interestingly, these liquid tweezers impose a normal stress on cells that cannot be understood from bulk interfacial tension, but that is sufficient to induce cell deformation.
Here, we aim to study the physics of this liquid-liquid interface by introducing calibration particles in the form of oil droplets and hydrogel

beads. While the latter possess a Young's modulus of 1.4 - 1.6 kPa, the surface tension of the oil droplets was characterized using a ring tensiometer. Preliminary experiments show that both particles can be deformed by the pair of liquid tweezers. We plan to build upon these initial results and examine the impact of different flow rates and polymer compositions on interfacial stability and stress.

BP 9.13 Mon 18:00 Poster D

Investigating the mechanical regulation of axon growth in three-dimensional matrices — •Niklas Gampl[1,2] and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Institute of Medical Physics and Microtissue Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

During brain development, neurons extend long axons, which grow along well-defined pathways to their destination. This axon pathfinding is known to be regulated by chemical guidance cues which are produced by neuroepithelial cells. However, Xenopus retinal ganglion cell axons have additionally been shown to actively probe their mechanical environment in vivo and when cultured on 2D substrates. To study this mechanical regulation in 3D environments with tunable stiffness, we developed a framework to culture Xenopus eye primordia in collagen-based hydrogels. We characterised the mechanical and topological properties of these matrices for different collagen concentrations and used them to mimic the mechanical environment neurons encounter in vivo during early embryonic development. We found that axon length was reduced in stiff (G' = 450 Pa) compared to soft (G' = 40 Pa) hydrogels and that growth cones, the motile tips of axons, exert contractile forces of up to 2 nN on their 3D environment. Further investigation of the mechanical and chemical regulation of axon growth in 3D environments could improve our understanding of the complex interplay between guidance cues and their integration by cells.

BP 9.14 Mon 18:00 Poster D

Investigating effective cell membrane tension and its dependence on substrate stiffness — •Julia Butzke[1], Tina Boric[1], Eva Kreysing[1,3], and Kristian Franze[1,2,3] — [1]Institute of Medical Physics and Microtissue Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

Cell membrane tension influences many important cell functions such as cell division or migration. It is further thought to contribute to transducing mechanical signals, such as the stiffness of the surrounding tissue, into intracellular responses via mechanosensitive ion channels embedded in the membrane. However, how a change in tissue stiffness activates mechanosensitive ion channels in the cell membrane is still not fully understood. In this project, we investigate the effective membrane tension of different cell lines using an optical tweezers setup for membrane tether pulling experiments. We examine cells cultured on glass as well as on polyacrylamide substrates of biologically relevant stiffnesses in order to illuminate how substrate stiffness affects the effective membrane tension. Furthermore, we analyze the correlation between the effective membrane tension and the expression and activity of mechanosensitive ion channels. Our work will contribute to understanding how mechanosensitive ion channels are gated, which may have important implications for drug design in the future.

BP 9.15 Mon 18:00 Poster D

Cellular-Matrix Interactions: The Impact of Cell Density on Fibroblast Contraction in Collagen Matrices — •Christin Heinrichs[1], Lydia Rebehn[1], Hans Kestler[2], Karin Scharffetter-Kochanek[3], and Kay-E Gottschalk[1] — [1]Institute for Experimental Physics, Ulm University, Ulm, Germany — [2]Institute for Medical Systems Biology, Ulm University, Ulm, Germany — [3]Department of Dermatology and Allergology, Ulm University, Ulm, Germany

Fibroblasts, a mesenchymal cell found in connective tissue, maintain the chemical and mechanical homeostasis of the extracellular matrix. To understand the mechanical implications of these cell-matrix interactions we investigate fibroblast contraction in collagen matrices via a 3D printed microscale device[1]. The microscale collagen gel contraction assay simplifies the contraction measurements to one dimension and utilizes a significantly smaller volume of cell-populated gel than a traditional collagen contraction assay. After validating the microscale devices use, we explore the contraction of cell-populated collagen gels with different cell densities reveal potential cooperative effects. Our results underline the need for further investigation into potential collective cell behaviors and the need to explore possible fibroblast transdifferentiation during the experiment.

[1] Zhang, Tianzi, et al. "Investigating fibroblast-induced collagen gel contraction using a dynamic Microscale platform." Frontiers in Bioengineering and Biotechnology, vol. 7, 2019

BP 9.16 Mon 18:00 Poster D

A Pump-Leak model can reproduce the biophysical properties of eukaryotic cell nuclei — •Omar Muñoz[1,2], Abin Biswas[1,3,4], Kyoohyun Kim[1,4], Johen Guck[1,2,4], Vasily Zaburdaev[1,2], and Simone Reber[3,5] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany. — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Max Planck Institute for Infection Biology, Berlin, Germany — [4]Max Planck Institute for the Science of Light, Erlangen, Germany — [5]University of Applied Sciences Berlin, Berlin, Germany

Biophysical properties of the cell nucleus are important for various cellular processes from migration to stress responses, but largely are still not well understood. One fundamental example is the mass density: we observed that the nuclear mass density consistently displays a lower value than its cytoplasmic counterpart for a wide range of species, which is surprising given that it contains the highly compacted genetic material. To understand the mechanisms behind this, we measured volume and mass density in two systems: growing nuclei reconstituted in Xenopus egg extracts and interphase HeLa cells. We propose a minimal theoretical description using the Pump and Leak model (PLM), which relies on a pressure balance. Based on our experimental results, we incorporate the most relevant contributions to the pressure balance, which we find to be the osmotic pressure and entropic polymer pressure exerted by chromatin. By taking into account relevant biological processes such as nucleocytoplasmic transport and its apparent coupling to chromatin, we are able to reproduce the experimental results.

BP 10: Computational Biophysics II

Time: Tuesday 9:30–12:45 Location: H 0112

BP 10.1 Tue 9:30 H 0112

Picosecond to Microsecond Dynamics of Aggregates of an Intrinsically Disordered Protein — •Saikat Chakraborty[1], Tatiana I. Morozova[2], and Jean-Louis Barrat[1,2] — [1]Université Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France. — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble, France.

Aggregates of intrinsically disordered proteins (IDPs) can exhibit multiple time scales of fluctuations because of the widely different relaxation times of their components. Neutron backscattering or neutron spin-echo spectra of such systems carry useful dynamic information on self- and pair-correlations at several spatio-temporal regimes. However, The motions of the different segments can be correlated and time scales can be entangled. Therefore, we employ explicit solvent molecular dynamics (MD) simulations with explicit solvent to disentangle the time scales at atomistic resolution with β-casein as the IDP. Microseconds-long simulations starting from different initial configurations of the protein retain the effect of conformational diversity on the dynamics. A Systematic study of the fluctuations of different parts of the aggregates reveals that the protein side chains show Rouse-like internal dynamics at the scale of picoseconds. Whereas, the motion of the proteins is primarily that of its center of mass. At the longest time regime diffusion of center of mass of the aggregate dominates.

BP 10.2 Tue 9:45 H 0112

Grand Canonical Simulations of Disordered Proteins — •Rodrigo F. Dillenburg[1], Hao Ruan[2,3], Edward A. Lemke[2,3], and Martin Girard[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Molecular Biology, Mainz, Germany — [3]Biocenter, Johannes Gutenberg University, Mainz, Germany

Investigations on Liquid-liquid phase separation (LLPS) have typically focused on intrinsically disordered proteins (IDPs), with theoretical support from polymer science. While great attention has been given to the study of large molecular condensates, little is known about non-deterministic smaller protein assemblies such as micelles. Such structures have been observed experimentally in artificially constructed sequences. We hypothesize that they could also arise in biologically relevant sequences. Coarse-grained force fields have provided an efficient framework for LLPS simulations with residue-level resolution and are remarkably accurate in reproducing phase diagrams of IDPs and the effects of residue mutations. Simulation methods designed for the study of molecular condensates must be modified to allow for simulations of microphases. The slab geometry devised to overcome slow diffusion times in highly dilute biological systems (~0.1% volume fraction), inhibits the formation of micelles. We implemented a Configurational Bias Monte Carlo algorithm based on the Rosenbluth-Rosenbluth method that allows for efficient LLPS simulations in a cubic simulation box and the investigation of microphase separation. We demonstrate the usefulness of this algorithm in the context of IDPs.

BP 10.3 Tue 10:00 H 0112

Structure of water molecules in FUS protein molecular condensate — •Daniel Chavez Rojas[1], Joseph Rudzinski[2], and Martin Girard[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany

There is evidence that molecular condensates of the FUS protein play a role in the development of some neurodegenerative diseases like ALS. For this reason, understanding the molecular mechanism by which these condensates form at an atomistic level is of therapeutic interest. However, the molecular structure and water-protein interactions of these condensates is poorly understood. In this work we investigate this structure with atomistic simulations, made possible by backmapping large condensates generated by a coarse grained model. We first use these simulations to explain the slowing of water dynamics of the protein condensate measured by 2D Infrared spectroscopy experiments, as highlighted In our recently accepted manuscript (*Liquid-liquid phase separation of the intrinsically disordered domain of the fused in sarcoma protein results in substantial slowing of hydration dynamic* J Phys Chem Lett). We then expand upon this analysis by comparing the network of protein and water contacts around individual amino acids in the condensate and in solution. Our results hint at a reduction of water tetrahedral structure in dense areas of the protein network. This analysis provides insights into the driving forces that promote the formation of these molecular condensates.

BP 10.4 Tue 10:15 H 0112

Determination of elastic moduli of lipid membranes with improved accuracy: a binning-free approach for lipid height and tilt fields. — •Jonas Paulus[1], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Department of Physics, Johannes Gutenberg University Mainz, Germany — [2]Faculty of Physics and Astronomy, Ruhr University Bochum, Germany

Lipid membranes play a pivotal role in various research domains. This study addresses the need for an improved measurement of the elastic properties of lipid membranes, which can be extracted from the fluctuation spectra of the height of lipids and their orientations. Traditional approaches involve binning the lipids onto a discrete evenly-spaced grid, average their positions and orientation in each bin, and then calculate the spectra by Fourier transform the binned data. However, this method introduces sampling errors and aliasing, due to the uneven distribution of lipids. Here, we first calculate the amplitude of the binning-related inaccuracies and a correction term to mitigate them. Then, we consider a binning-free approach for the fluctuation spectra based on least-square fitting the positions and orientations of lipids with a superposition of wave functions. We show how to cast it into a linear algebra problem involving the computation of a pseudoinverse matrix via singular value decomposition. We show that this approach improves the accuracy of the analysis over those based on data binning and apply it to the characterization of lipid formulations for nucleic acid delivery, computing the effect of pH on their elastic properties.

BP 10.5 Tue 10:30 H 0112

Condensate Coexistence in Gene Transcription: Molecular Dynamic Insights — •Arya Changiarath Sivadasan[1,2], Jasper J. Michels[3], Sonya M. Hanson[4], Jan Padeken[2], Friederike Schmid[1], and Lukas Stelzl[1,2] — [1]Johannes Gutenberg University, Mainz — [2]Institute of Molecular Biology, Mainz — [3]Max Planck Insitute for Polymer Research, Mainz — [4]Flatiron Institute, New York, USA

The formation of distinct phase-separated condensates of biological macromolecules underpins specific regulation in cells. Here we elucidate under what conditions phase-separated condensates can regulate biochemical processes by providing distinct chemical environments with particle-based multi-scale simulations. We study the disordered C-terminal domain of RNA polymerase II (CTD), which in experiments has been found to form condensates under both unphosphorylated and phosphorylated (pCTD) states. CTD condensates have been proposed to underpin transcription initiation, while pCTD condensates may support transcription elongation. A better understanding of the molecular driving forces of CTD phase separation will provide insights into how CTD and pCTD condensates can regulate transcription initiation and elongation. It has remained unclear whether CTD and pCTD condensates would mix when coexisting or remain as distinct chemical environments. Computing surface tensions from coarse-grained molecular dynamics simulations we establish under what conditions they remain coexist either as multi-phase condensates or by forming entirely distinct condensates.

BP 10.6 Tue 10:45 H 0112

Allosteric communication in PDZ3 studied by nonequilibrium simulations and Markov State Model — •Ahmed Ali, Adnan Gulzar, Steffen Wolf, and Gerhard Stock — Institute of Physics, University of Freiburg, Germany

While allostery is of paramount importance for protein signaling and regulation, the underlying dynamical process of allosteric communication is not well understood. PDZ3 domain represents a prime example of an allosteric single-domain protein, as it features a well-established long-range coupling between the C-terminal α3-helix and ligand binding. In an intriguing experiment, Hamm and coworkers employed photoswitching of the α3-helix to initiate a conformational change of PDZ3 that propagates from the C-terminus to the bound ligand within 200 ns. Performing extensive nonequilibrium molecular dynamics simulations combined with Markov modeling, the modeling of the experiment reproduces the measured timescales and reveals a detailed picture of

the allosteric communication in PDZ3. In particular, a correlation analysis identifies a network of contacts connecting the α3-helix and the core of the protein, which move in a concerted manner. Representing a one-step process and involving direct α3-ligand contacts, this cooperative transition is considered as elementary step in the propagation of conformational change.

15 min. break

Invited Talk BP 10.7 Tue 11:15 H 0112

RNA Contact Prediction by Data Efficient Deep Learning — Oskar Taubert[1], Fabrice von der Lehr[2], Alina Bazarova[3,4], Christian Faber[3], Philipp Knechtges[2], Marie Weiel[1,4], Charlotte Debus[1,4], Daniel Coquelin[1,4], Achim Basermann[2], Achim Streit[1], Stefan Kesselheim[3,4], Markus Götz[1,4], and •Alexander Schug[3,5] — [1]Scientific Center of Computing, Karlsruhe Institute of Technology — [2]Institute for Software Technology, German Aerospace Centre — [3]Jülich Supercomputing Centre, Forschungszentrum Jülich — [4]Helmholtz AI — [5]Faculty of Biology, University of Duisburg-Essen

On the molecular level, life is orchestrated via many biomolecules. To gain detailed understanding of biomolecular function, one needs to know their structure. Yet the structural characterization of many important biomolecules and their complexes remains experimentally challenging. For proteins, the richness of labeled training data enables highly successful deep-learning approaches. Deep learning on RNA, however, is hampered by the lack of such data. The limited data, however, can still be used to predict spatial adjacencies (*contact maps*) as proxy for 3D structure. Statistical physics based approaches such as direct coupling analysis can provide such contact maps. Going beyond such approaches, our recent model BARNACLE combines using unlabeled data through self-supervised pre-training and efficient use of the sparse labeled data. We observe a considerable improvement over both the established classical baseline DCA and other neural networks.

BP 10.8 Tue 11:45 H 0112

Next-Gen Protein Sequencing with Nanopores Empowered by Machine Learning — •Julian Hossbach and Christian Holm — Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany

In the last decade, the rise of DNA sequencing using nanopores has garnered significant attention within the scientific community, however, protein sequencing continues to pose substantial challenges. Recent investigations using the aerolysin nanopore have demonstrated that the discrimination of oligopeptides on a single amino acid basis is possible (Ouldali et. al, Nat. Biotechnol. 2020). Building on these advancements, our study showcases the use of machine learning to identify peptides that have thus far been undistinguishable. Our approach marks a pivotal step towards overcoming the complexities associated with protein sequencing, offering a pathway to more accurate and efficient analyses in the realm of molecular biology.

BP 10.9 Tue 12:00 H 0112

Enhancing protein-ligand binding affinity via optimal selection of water molecules — •Miljan Dašić, Jindřich Fanfrlík, and Jan Řezáč — Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, 166 10, Prague, Czech Republic

Accurate and fast determination of protein-ligand (P-L) binding affinity represents a foundational problem of computational biophysics. A promising solution is an universal physics-based scoring function **SQM2.20** based on semi-empirical quantum-mechanical computational methods. Its performance has been rigorously verified over a benchmark dataset **PL-REX** consisting of high-resolution crystal structures and trustworthy experimentally determined P-L affinities (10 diverse protein targets; 164 QM-optimized P-L complexes). Presence of water molecules has a significant impact on P-L binding affinity, via formation of hydrogen bond bridges. We have developed a computational tool which optimally selects waters enhancing the P-L binding affinity. Each of the ten protein targets comprises different crystals. Waters present in all of them represent the input for selection procedure. Such procedure includes clustering and comparison of waters contained in clusters with waters present in one selected reference crystal. Presence of optimally selected waters improves the correlation with experimental data. We investigated the sensitivity of scoring on the geometry of crystals. For each protein target, we determined the best reference crystal which maximizes the scoring results.

BP 10.10 Tue 12:15 H 0112

Transition intensities decomposition for $\pi-\pi$ interaction of X-ray absorption for proteins — •Carlos Ortiz-Mahecha[1], Lucas Schwob[2], Sadia Bari[2], and Robert Meissner[1,3] — [1]Technische Universität Hamburg — [2]Deutsches Elektronen-Synchrotron (DESY) — [3]Helmholtz-Zentrum Hereon

π-π stacking between aromatic side chains leads to structure stabilization in proteins, which could be studied by X-ray absorption spectroscopy (XAS) and quantum mechanical (QM) calculations. Access to such excited state calculations for proteins is quite challenging due to their computational cost. In order to decompose the XAS spectra of proteins into a sum of smaller constituents, we propose that the inner-shell transition intensities of aromatic amino acids can be correlated with the charge transfer occurring in the π-π^* interactions. We therefore propose a theoretical analysis to decompose the XAS spectra transition intensities into their atomistic contributions in order to derive distance thresholds for the core-to-valence transition between aromatic amino acid pairs in proteins.

We found that the intertransition intensities and the charge transfer energy can be correlated, enabling intermolecular properties to be associated with core-electron excited-state properties. We suggest that, for XAS in proteins, the electronic neighbourhood influence of the high conjugated electronic density of the aromatic amino acid interactions can be inferred by evaluating the charge transfer between them. This can be used as a criterion to define smaller constituents in a proteins by the charge transfer of the aromatic amino acid interactions.

BP 10.11 Tue 12:30 H 0112

Understanding the redshift of the absorption spectrum in ClCry4 protein — •Katarina Kretschmer, Anders Frederiksen, and Ilia A. Solov'yov — Universität Oldenburg, Germany

It is still a puzzle how some migratory birds utilize the Earth's magnetic field for biannual migration. The most consistent explanation so far roots on modulation of the biological function of the Cryptochrome 4 (Cry4) protein by external magnetic field. This phenomenon is closely linked with the FAD cofactor that is bound in the protein. The Cry4 protein with the bound FAD cofactor is activated by blue light, absorbed by the FAD cofactor. Through several transfers that trigger radical pair formation in Cry4, the protein can become sensitive to the geomagnetic field. An important redox state of the FAD cofactor is the signaling state, which is present after completion of the different electron transfers inside the protein. Recently it has been possible to crystallize the Cry4 protein from Columbia Livia (ClCry4) with the associated important residues needed for photoreduction. It is the most promising crystallization of the Cry4 protein so far, which also has great similarity with the Cry4 proteins of night migratory birds. The absorption spectrum of the FAD cofactor inside the ClCry4 protein was investigated experimentally in its different redox states during protein's activation. The absorption spectrum of the signaling state demonstrated a redshift if compared to the photoabsorption properties of the FAD cofactor in its signaling state in other Cry proteins. The aim of this study is to understand this redshift by employing the tools of computational microscopy, and in particular the QM/MM approach.

BP 11: Cell Mechanics I

Time: Tuesday 9:30–12:45 Location: H 2032

Invited Talk BP 11.1 Tue 9:30 H 2032

Mechanochemical regulation of epithelial barrier formation and function — •Carien Niessen — Department Cell Biology of the Skin and CECAD, University of Cologne

How cell shape and mechanics controls epithelial barrier morphogenesis and regeneration is still poorly understood. In the squamous stratifying epithelium of the skin, the epidermis, stereotypic changes in cell shape guide the differentiation and upward migration of cells to form a barrier that is robustly renewed in the face of multiple challenges including mechanical stress. Combining cell and mechanobiology, genetics and in collaboration with the Manning lab (Syracuse University) in silico modelling, my laboratory asks how cell shape, fate and position are coordinated to control the formation and renewal of spatially defined functional compartments within the epidermis. I will discuss how adhesive junctions and associated cytoskeletons control tissue mechanics and how dynamic changes in junctions and signalling locally alter cell mechanics to coordinate cell fate, shape and position in the epidermis that enable renewal while maintaining epithelial barrier function. I furthermore will touch how changes in these mechanochemical networks disturb tissue homeostasis and promote disease.

BP 11.2 Tue 10:00 H 2032

Passive viscoelastic response of striated muscles — •Fabio Staniscia[1] and Lev Truskinovsky[2] — [1]Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana SI-1000, Slovenia — [2]PMMH, CNRS UMR 7636, ESPCI, PSL, 75005, Paris, France

Muscle cells with sarcomeric structure exhibit highly non trivial mechanical response. The difficulty of its continuum modeling is due to the presence of long-range interactions transmitted by extended protein skeleton. To build a rheological model for muscle passive behaviour, relevant at time-scales of the order of the millisecond after a perturbation, we use a stochastic micromodel, and derive a linear response theory for a half-sarcomere, which can be extended to the whole fibre. Instead of the first order rheological equation, anticipated by Hill on the phenomenological grounds, we obtain a novel second order equation which shows that tension depends not only on its current length and the velocity of stretching, but also on its acceleration. Expressing the model in terms of elementary rheological elements, we show that one contribution to the visco-elastic properties of the fibre originates in cross-bridges, while the other can be linked to inert elements which move in the the sarcoplasm. We apply this model to explain the striking qualitative difference between the relaxation in experiments involving perturbation of length vs. those involving perturbation of force, and we use the values of the microscopic parameters for frog muscles to show that the model is in excellent quantitative agreement with physiological experiments.

BP 11.3 Tue 10:15 H 2032

Mechanical complexity of living cells can be mapped onto simple homogeneous equivalents — •Sebastian Wohlrab, Sebastian Johannes Müller, and Stephan Gekle — Biofluid Simulation and Modeling, Universität Bayreuth, Deutschland

Despite the complex composition of a biological cell with its constituents varying in both size and stiffness, experimental data analysis and numerical simulations often assume a strongly simplified homogeneous cell model. Accordingly, a single elastic modulus is assigned to the entire cell. This ad-hoc simplification has so far mostly been used without proper justification.

With our research we methodically demonstrate that indeed a mechanically heterogeneous cell can effectively be replaced by a homogeneous equivalent cell with a volume averaged elastic modulus. Using computer simulations we investigate a hyperelastic cell with a heterogeneous interior under compression and in shear/channel flow mimicking atomic force and microfluidic measurements, respectively.

We find that the homogeneous equivalent cell reproduces quantitatively the behavior of its heterogeneous counterpart, and that this equality is largely independent of the stiffness or spatial distribution of the heterogeneity. Our results thus validate in hindsight the simplifying approaches taken in many previous experimental and computational works, but also provide a solid basis on which future experimental data can be analyzed and physically reliable computer simulations can be constructed.

BP 11.4 Tue 10:30 H 2032

Shaping the embyo: a mechanical analysis of embryonal symmetry breaking — •Alejandro Jurado Jiménez[1], Leon Lettermann[1], Bernhard Wallmeyer[2], Lea Krüger[3], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Friedrich-Hund-Platz 1, University of Göttingen — [2]Institute of Cell Biology, ZMBE, Von-Esmarch-Str. 56, University of Münster — [3]Institut für Theoretische Physik, Wilhelm-Klemm-Straße 9, University of Münster

In this work we present a hydrodynamical analysis of early Zebrafish development which aims to understand the mechanical state of the tissue leading to its first symmetry breaking during epiboly: the shield formation. A full mechanical characterization of the blastoderm is achieved using a combination of Light-Sheet microscopy, state-of-the-art cell tracking of the cells nuclei and force measurements using polyacrylamide beads as in-vivo sensors. The analysis of our huge datasets required ad-hoc tools for embryo alignment, image segmentation, beads/nuclei detection and derivation of the forces from elastic deformations. All of them have proven to be very powerful when tacking similar experiments in living tissue, and we share them publicly in an online repository. Our experimental analysis is being supported and expanded by a NeuronalODE model, able to retrieve a full dynamical description of the blastoderm only using the velocity field of the embryo. Alltogether we expose a stress asymmetry prior and during the shield formation, form which we can learn more about the mechanical origin of embryonal symmetry breaking.

15 min. break

BP 11.5 Tue 11:00 H 2032

In-situ high-throughput analysis of mitochondrial membrane tension under pathophysiological conditions — •Eric Sündermann, Bob Fregin, Jan Maurice Wilder, Doreen Biedenweg, Stefanie Spiegler, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

The development of high-throughput methods for cell mechanical research is becoming increasingly important in biology, medicine and physics as the analysis of large samples increases the statistical robustness to identify rare cell populations and to transfer results from basic science into clinical applications. While most studies focus on 2D/3D cellular systems, little is known about how chemical and physical stress propagates inside the cell and impacts the mechanical properties of organelles.

Here, we applied membrane tension cytometry (MTC), a technology recently developed in our lab, to study the intracellular response of mitochondrial mechanics to hydrodynamic and oxidative stress. As a model system, HL60 cells have been chosen that were incubated with hydrogen peroxide to generate mitochondrial superoxide as reactive oxygen species. After staining cells with Mito Flipper-TR we took advantage of the fact that its fluorescence lifetime is proportional to the membrane tension of mitochondria. Preliminary experiments using MTC show that hydrodynamic stress propagates linearly to mitochondria inside the cytosol and that oxidative stress leads to their softening - in agreement with earlier results studying isolated mitochondria using real-time deformability cytometry.

BP 11.6 Tue 11:15 H 2032

Cellular Contraction of Fibroblast-Populated Collagen Gels Reveals Potential Cooperative Cell Behaviors — •Lydia Rebehn[1], Christin Heinrichs[1], Hans Kestler[2], Karin Scharffetter-Kochanek[3], Paul Walther[4], and Kay-E Gottschalk[1] — [1]Institute for Experimental Physics, Ulm University, Ulm, Germany — [2]Institute for Medical Systems Biology, Ulm University, Ulm, Germany — [3]Department of Dermatology and Allergology, Ulm University, Ulm, Germany — [4]Central Facility for Electron Microscopy, Ulm University, Ulm, Germany

Tissue homeostasis is maintained by a delicate balance of mechanical and chemical cues exchanged between the extracellular matrix and the incorporated cells. The mechanical properties of the matrix and the cells themselves cooperate to give tissues their structure and function. To understand the mechanical implications of these cell-matrix interactions we investigate fibroblast contraction in collagen matrices via a 3D printed microscale device [1]. We explore the contraction of

fibroblast-populated collagen gels with different cell densities for revealing potential cooperative effects. Furthermore, we use SEM and TEM imaging to expose the impact of cell density on contraction and matrix customization with by the embedded cells. The results highlight the necessity of further investigation into potential collective cell behaviors and the need to explore possible fibroblast transdifferentiation during the experiment. [1] Zhang, Tianzi, et al. "Investigating fibroblast-induced collagen gel contraction using a dynamic Microscale platform". Frontiers in Bioengineering and Biotechnology, vol. 7, 2019

BP 11.7 Tue 11:30 H 2032

Trade-offs in physiology and cellular stress determine lipid productivity in motile phytoplankton — •Narges Kakavand[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg

One of the long-standing challenges in our quest to produce biofuel sustainably is the negative correlation between lipid productivity and cell growth. Following our recent study on the role of nutrients in lipid generation [1], here we demonstrate how biomechanical cues could be used as an additional parameter to control lipid production without compromising biomass. By imposing hydrodynamic cues to stress motile phytoplankton at specific time points along the growth stages (indicating different nutritional states), we quantified the resulting cell growth, photo-physiological traits, and motility, in relation to the volume of lipid produced. Late induction of hydrodynamic stresses suppressed growth and photo-physiological traits, however, when applied at a relatively earlier time point after inoculation, flow-induced stresses allowed to significantly increase lipid content without observable changes in cell growth. Our findings indicate that hydrodynamic stress, coupled with physiology and motility may offer a controlling mechanism to tune lipid generation in diverse algal species. [Ref. 1] A. Sengupta,..., N. Kakavand, Science Advances 8, eabn6005, 2022.

15 min. break

BP 11.8 Tue 12:00 H 2032

Investigating single heart cell communication through TNTs using multi-mode ROCS microscopy — •arash felekary and alexander rohrbach — Lab for Bio- and Nano-Photonics, IMTEK, Freiburg, Germany

Cell-cell communication performs various biological functions, particularly in the heart. Among other communication pathways, tunneling nanotubes (TNTs) are of high interest due to their distinctive characteristics and functions. TNTs are dynamic, thin protrusions, up to 100μm long, and are not in contact with the substrate. To understand TNT functions in cardiac cell communication, we used Rotating Coherent Scattering (ROCS) microscopy, a label-free super-resolution imaging in different imaging modes. Using ROCS microscopy in total internal reflection (TIR), and dark-field (DF) modes, we quantified the growth of TNTs in Fibroblasts (FB) in the absence and presence of cardio-myocytes (CM), and we studied the influence of the Transforming Growth Factor beta (TGF-β) on TNT growth speed. After TNT establishment, we recorded and analyzed the dynamics of lamellipodia motion along TNTs using ROCS in Non-TIR and Bright field (BF) mode. Our findings revealed a linear relationship between TNT density and lamellipodia motion velocity. This suggests that TNTs facilitate cell-cell communication. Our findings also suggest that the interaction between FB cells undergoes distinct phases or steps, characterized by the spatial and temporal evolution of protrusions. We have developed a mathematical model to describe lamellipodia motion along TNTs and compare the results with those from experiments.

BP 11.9 Tue 12:15 H 2032

the role of the cytoskeleton for spatial and temporal control of cell mechanics studied using an average cell — •mohammad amin eskandari, bart vos, and till münker — Third institute of physics - Biophysics, Göttingen, Germany

Mechanical properties of cells have been shown to play a vital role in many biological functions such as migration, differentiation and division. While the cell mechanics has been largely studied at the cortex, hence the cellular interface to the environment, the intracellular mechanical properties are only recently within experimental reach. By doing active-passive microrheology using optical tweezers, we are able to directly measure the viscoelastic properties of the cytoplasm. The importance of intracellular mechanics for transport, organization, and even reaction kinetics is obvious, which suggests tight regulation by the cells. In contrast to this, we find that the viscoelastic shear modulus, which characterizes the intracellular mechanics varies over many orders of magnitude within a single cell type. To explain this discrepancy between expectations and measurement, we hypothesize that such heterogeneity arises from both, local and temporal variation cell compositions to test this we use micropatterns to create polarized cells in a well-defined way to achieve spatially registered microrheology experiments. Here I report on the challenge and present our solution for obtaining sufficient statistics, given that the probe particles used in the optical tweezers experiment are randomly distributed in the cytoplasm.

BP 11.10 Tue 12:30 H 2032

Multimodal quantum sensors for probing non-equilibrium thermodynamics at the nanoscale — •Sophia Belser[1], Louise Shanahan[1], Jack Hart[1], Qiushi Gu[1], David Jordan[2], Eric Miska[2], Mete Atatüre[1], and Helena Knowles[1] — [1]Cavendish Laboratory, University of Cambridge, JJ Thompson Avenue, Cambridge, CB3 0HE, United Kingdom — [2]Department of Biochemistry, University of Cambridge, 80 Tennis Ct Rd, Cambridge CB2 1GA, United Kingdom

Probing transient effects at the nanoscale enables us to understand living systems. However, challenges arise from small length scales, small signal amplitudes, and the risk of perturbing processes during observation. Thus, the isolation of a signal of interest in dynamic systems remains challenging. Due to their low cytotoxicity, amenability to surface functionalisation, and magneto-optical properties, nanodiamonds (NDs) have emerged as promising bio quantum sensors [1]. NDs enable real time *in vitro* and *in vivo* sub-degree thermometry and nanoscale rheometry [2]. We have developed a microfluidics compatible chip that allows for simultaneous local heating, on-chip and ND temperature readout. We have shown reliable quantum thermometry and rheometry in abiotic media and live cells with a temperature sensitivity of $2.3\,^{\circ}\mathrm{C}/\sqrt{\mathrm{Hz}}$ and a 3.7-nm spatial resolution with 9.6-ms update rate in living cells [2]. We demonstrate biocompatibility in cells and non-anaesthetized roundworms. Next steps include targeting organelles in biological organisms to gain insights into local metabolic activity. [1] Belser *et al.* APL (2023), [2] Gu *et al.* ACS Nano (2023)

BP 12: Active Matter II (joint session BP/CPP/DY)

Time: Tuesday 9:30–13:00 Location: H 1028

BP 12.1 Tue 9:30 H 1028

Disorder-induced cooperative behaviour in aligning self-propelled particle systems — •Eloise Lardet and Thibault Bertrand — Imperial College London, London, UK

In 1995, Vicsek et al. wrote a seminal paper describing a simple model that displays a transition from disorder to collective ordered behaviour. It describes a system of self-propelled point particles that align with their neighbours within a certain radius. This minimal model displays rich nonequilibrium behaviours such as flocking and banding. Inspired by the random couplings of spin glass models, I present numerical findings of introducing Gaussian distributed pairwise couplings into a self-propelled particle system. Through adding further disorder by increasing the standard deviation of the Gaussian distribution that the couplings are drawn from, we are able to observe the emergence of global polar order in systems where the majority of couplings are anti-aligning.

BP 12.2 Tue 9:45 H 1028

Swarming of self-steering and responsive active particles — •Rajendra Singh Negi, Roland G. Winkler, and Gerhard Gompper — Theoretical Physics of Living Matter, Institute of Biological Information Processing (IBI-5), Forschungszentrum Jülich, 52425 Jülich, Germany

The collective behavior of self-propelled agents emerges from the dynamic response of individuals to various input signals [1,2]. In our model of intelligent active Brownian particles (iABPs), information about the position and orientation of neighboring particles, obtained through directed visual and isotropic perception, respectively, is used to adjust the propulsion direction. The maneuverability due to visual signal and polar alignment determines the self-organization. Several non-equilibrium structures like worms, milling, compact, and dispersed clusters are obtained at different parameter sets [2]. As the strength of polar alignment increased compared to visual maneuverability, worm structures dominate over compact structures. Our results help to understand the collective behavior of cognitive self-propelled particles, like animal herds and micro-robotic swarms.

[1]. R. S. Negi, R. G. Winkler, and G. Gompper, Emergent collective behavior of active Brownian particles with visual perception, Soft Matter **18**, 6167 (2022).

[2]. R. S. Negi, R. G. Winkler, and G. Gompper, Collective behavior of self-steering particles with velocity alignment and visual perception, (2023) arXiv:2308.00670 .

BP 12.3 Tue 10:00 H 1028

Effect of cell-cell interactions on the collective behaviour of gliding *Chlamydomonas* populations — •Alexandros Fragkopoulos, Justin Nevells, Timo Völkl, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Cilia and flagella represent universal tools enabling cells and microbes to propel themselves in diverse environments. In the case of the unicellular biflagellated microbe *Chlamydomonas reinhardtii*, the flagella are used not only to swim in the surrounding medium, but also to adhere to surfaces. In this adhered state, a second flagella-mediated motility mode is observed, during which the cells glide along the surface. This is achieved by means of force transduction through an intraflagellar transport machinery. We recently showed that gliding *C. reinhardtii* cells form weak clusters, most likely assisted by mechanosensing of their flagella [1]. Here we show that *Chlamydomonas noctigama*, a close relative of *C. reinhardtii*, exhibits significantly stronger cell-cell interactions, resulting in pronounced cell clustering even at low densities. In addition, we observe that *C. noctigama* preferentially attach nearby other cells. Finally, we use morphological tools to quantify and compare the clusters to *C. reinhardtii*. By understanding the changes of the cell-cell interactions between the species, we aim to dissect their contribution to the observed cell clustering.

[1] Till et al., *Phys. Rev. Res.* **4**, L042046 (2022).

BP 12.4 Tue 10:15 H 1028

Magnetic colloidal crystals activated by light-driven bacteria — •Helena Massana-Cid[1], Claudio Maggi[1,2], Giacomo Frangipane[1], and Roberto Di Leonardo[1,2] — [1]Department of Physics, Sapienza University of Rome, Rome, Italy — [2]NANOTEC-CNR, Institute of Nanotechnology, Rome, Italy

Active solids, or self-propelling units elastically coupled on a lattice, are recently of growing interest and are predicted to show emerging out-of-equilibrium behaviour, while they can inspire the design of numerous applications. We show for the first time an experimental realisation of a large ordered active solid with activity and confinement tuneable in-situ and on-command. This two-dimensional active solid is composed of repulsive magnetic particles activated by a photokinetic bacterial bath. The bacteria induce active motion into the crystal by pushing its particles and, in a simplified picture, this can be described by an equilibrium state with a higher effective temperature. Nevertheless, this framework breaks down qualitatively because of the active fluctuations time correlations due to the persistent motion of bacteria. We explore the emerging dynamics of this active solid for different values of activity, controlled by the applied light, and repulsion strength, determined by the external magnetic field. Furthermore, we show how we can melt the crystal by increasing activity. Our findings pave the way to unveil the properties of a novel out-of-equilibrium system, an active colloidal solid, which presents questions vastly interesting from a statistical mechanics point of view.

BP 12.5 Tue 10:30 H 1028

Billiards with Spatial Memory — Thijs Albers, Stijn Delnoij, Nico Schramma, and •Mazi Jalaal — Institute of Physics, University of Amsterdam, Amsterdam, The Netherlands

It has been proposed that spatial memory can lead to more efficient navigation and collective behaviour in biological systems. This raises important questions about the fundamental properties of dynamical systems with spatial memory. We present a framework based on mathematical billiards in which particles remember their past trajectories and react to them. Despite the simplicity of its fundamental deterministic rules, such a system is strongly non-ergodic and exhibits highly-intermittent statistics, manifesting in complex pattern formation. We show how these self-memory-induced complexities emerge from the temporal change of topology and the consequent chaos in the system. We study the fundamental properties of these billiards and particularly the long-time behaviour when the particles are self-trapped in an arrested state. We exploit numerical simulations of several millions of particles to explore pattern formation and the corresponding statistics in polygonal billiards of different geometries. Our work illustrates how the dynamics of a single-body system can dramatically change when particles feature spatial memory and provide a scheme to further explore systems with complex memory kernels.

BP 12.6 Tue 10:45 H 1028

Chemical communication in suspensions of active particles — •Nils Göth and Joachim Dzubiella — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany

Chemical communication of bacteria plays an important role in their individual and collective behavior. Here, we study how a simple form of interparticle communication influences a system of colloidal particles. We employ two-dimensional Brownian dynamics simulations of a model of Responsive Colloids, in which the particle size and the internal proton concentration are explicit internal degrees of freedom. The communication between the particles is modeled as a chemical field around each particle to which the other particles respond by changes in their size. We find a rich behavior of structures, including pseudo-regular oscillations and longitudinal waves.

15 min. break

BP 12.7 Tue 11:15 H 1028

Structural Colour from Collective Gliding Bacteria Motion — •Junwei Wang[1], Marina Portoghese[2], Laura Caton[2], Colin Ingham[3], and Silvia Vignolini[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]University of Cambridge, Cambridge, UK — [3]Hoekmine BV, Utrecht, Netherland

We report a type of marine, non-pathogenic, gliding bacteria, Flavobacterium Iridescent 1 (IR1), that grows into a dense active liquid crystal colony, exhibiting structural colour. We demonstrate different crystalline phases arising from collective bacteria motility correlate

with varied optical appearances of the colony. We show the hierarchical collective motions of the rod-like bacteria that organize into clusters, monolayer, multi-layers and finally into large scale vortices. We also illustrate how the bacteria colony adapts to confinement of different geometries.

BP 12.8 Tue 11:30 H 1028

Chiral active molecules in traveling activity waves — •Bhavesh Valecha[1] and Abhinav Sharma[1,2] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, 01069 Dresden, Germany

Directed motion is crucial for the survival and maintenance of life-supporting functions of numerous biological systems, e.g., motion of sperms towards the egg during fertilisation or movement of immune cells to fight-off an infection. While systematic studies of chiral active molecules simulating crucial aspects of these systems in stationary activity gradients do exist [1-3], the majority of physical scenarios revolve around activity fields that vary with time. So, in this project we study the simplest possible case of an active molecule, the active dimer, in a propagating activity wave. We show that this simple molecule can show very rich emergent tactic behaviour using a cooperative mechanism between the two active chiral particles. In particular, this dimer can, on average, move along with the wave, against the wave motion or not move at all depending on the magnitude of chiral torque and the wave speed. We believe that this study can provide important insights into the design principles of hybrid bio-molecular devices of the future.

[1] P. L. Muzzeddu, H. D. Vuijk, H. Löwen, J.-U. Sommer, and A. Sharma, J. Chem. Phys. **157**, 134902 (2022)

[2] H. D. Vuijk, S. Klempahn, H. Merlitz, J.-U. Sommer, and A. Sharma, Phys. Rev. E **106**, 014617 (2022)

[3] H. Merlitz et al., J. Chem. Phys. **148**, 194116 (2018)

BP 12.9 Tue 11:45 H 1028

Physical principles of space allocation in an active biofluid — •Sebastian W. Krauss, Mithun Thampi, Pierre-Yves Gires, and Matthias Weiss — Experimental Physics I, Bayreuth, Germany

Living matter has the remarkable ability to self-organize into distinct cellular entities that ultimately form the building blocks of organisms. The organisation in multi-cellular systems emerges by replicating a single fertilized oocyte as template structure in multiple division cycles. In contrast, recent studies on Xenopus egg extracts have shown that an active biofluid that is devoid of template structures and genetic material can spontaneously self-organize into compartments in an ATP-driven fashion even when protein synthesis is blocked. The emerging compartments (protocells) are distinct, lack a confining membrane envelope, and vanish after all ATP has been consumed. Here, we show that protocell geometry is determined by a random-packing process with a coarse-graining dynamics that is similar to two-dimensional foams [Development 150, dev200851 (2023)]. Protocell sizes are seen to be tunable by altering the dynamics of microtubules while preserving geometric features of the pattern. Confining the self-organizing fluid in ellipsoidal microfluidic cavities, i.e. mimicking natural confinements like those in embryos, pattern formation is seen to adapt to the confinement, exhibiting a surprising similarity to spatial compartmentalization in early embryos. Further, we observe that an increasing aspect ratio of the chamber results in the formation of smaller protocells. Our results indicate that mechanical cues and simple self-organization principles are key ingredients in many developmental processes.

BP 12.10 Tue 12:00 H 1028

Foams Come to Life — •Ivan Maryshev[1], Filippo De Luca[1,2], and Erwin Frey[1] — [1]Ludwig-Maximilians-Universität München, München, Germany; — [2]University of Cambridge, Cambridge, United Kingdom

Recent experiments on active filament mixtures revealed a new non-equilibrium phase called active foam, consisting of a continuously reconfiguring network of bilayers [1]. The existence of similar structures was previously predicted in phenomenological models [2]. Here we introduce a microscopic model for microtubule-motor mixtures and rigorously derive a hydrodynamic theory that recapitulates the experimental observations. We explain the observed instabilities and associated mechanisms. Finally, we discuss various forms of foam that can be realized in different active matter systems and classify them according to the symmetry and order parameters involved. This research contributes to our understanding of the complex behavior exhibited by active foams and provides insights into their dynamics.

[1] B. Lemma, N. P. Mitchell, R. Subramanian, D. J. Needleman, and Z. Dogic (2022). Active microphase separation in mixtures of microtubules and tip-accumulating molecular motors. Phys. Rev. X 12(3), 031006.

[2] I. Maryshev, A. Morozov, B. Goryachev, and D. Marenduzzo (2020). Pattern formation in active model C with anchoring: bands, aster networks, and foams. Soft Matter 16(38), 8775-8781.

BP 12.11 Tue 12:15 H 1028

Modelling cancer metastasis with active nematics — •Josep-Maria Armengol-Collado[1], Luca Giomi[1], Oleksandr Chepizhko[2], Stephanie Alexander[3], Esther Wagena[3], Bettina Weigelin[3], Peter Friedl[3], Stefano Zapperi[4], and Caterina A.M. La Porta[5] — [1]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands — [2]Faculty of Physics, University of Viena, Boltzmanngasse 5, Viena, Austria — [3]Department of Medical Biosciences, Sciences, Radboud University Medical Centre, 6525 GA Nijmegen, The Netherlands — [4]Center for Complexity and Biosystems, Department of Physics, University of Milan, via Celoria 16, 20133 Milan, Italy — [5]Center for complexity and Biosystems, Department of Environmental Science and Policy, University of Milan, via Celoria 10, 20133 Milan, Italy

Tumor invasion is characterized by the coordinated movement of cancer cells through complex tissue structures. Here, we focus on recent in vivo experiments where metastasis is observed through the dermis of a living mouse, and low-cohesive modes of collective migration have been identified. Interestingly, local rotational patterns give rise to antiparallel flow tracks that deform the extracellular matrix and establish a sustained flow of cells. To model this phenomenon, we employ the framework of nematic liquid crystals in the so-called "active turbulence" regime. Analysing the effects of confinement and the role of topological defects we provide significant insights to better understand the underlying mechanisms of cancer cell migration.

BP 12.12 Tue 12:30 H 1028

Flow Localization on Active Ordered Surfaces — •Rushikesh Shinde[1], Raphael Voituriez[2], and Andrew Callan-Jones[1] — [1]Laboratoire de Matière et Systèmes Complexes, Université de Paris Cité and CNRS, Paris, France — [2]Laboratoire de Physique Théorique de la Matière Condensée, Sorbonne Université and CNRS, Paris, France

During morphogenetic processes, active flows occur in the plane of curved tissues. Tissues often exhibit orientational order, and topological defects arise during tissue development. We have studied the behavior of a +1 defect in a film of active ordered fluid on a curved axisymmetric surface. We find strikingly different physics compared with the flat-space variant of the problem, in which extensile activity causes vortex-like or aster-like integer defects to undergo spiral ordering and rotational motion. We focus in particular on the influence of extrinsic curvature in the elastic free energy, usually neglected in theories of ordered fluids on curved surfaces. We consider two biologically-relevant surfaces: a capped-tube-like rigid surface, similar to epithelial tubes; and a bump on an otherwise flat plane. In the first case, we find that the activity threshold for instability becomes independent of system size, and spontaneous rotational flows become localized. In the latter case, we find that an aster can be passively unstable towards a spiral state, and as a result, contractility-driven active flows are thresholdless and localized. High contractility extinguishes the flow and restores the aster. Surprisingly, for high enough saddle curvature, the spiral to aster transition shifts from continuous to discontinuous.

BP 12.13 Tue 12:45 H 1028

Self-Organization in Quorum-Sensing Active Matter: The Interplay between Nonreciprocity and Motility — •Yu Duan[1], Jaime Agudo-Canalejo[1], Ramin Golestanian[1,2], and Benoît Mahault[1] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Over the past years, the generation of interactions breaking action-reaction symmetry has emerged as new paradigm for active matter. The generalization of the Cahn-Hilliard theory of phase separation to nonreciprocal mixtures predicts the emergence of traveling states that break time reversal symmetry when intra-species attraction leads to demixing while chasing inter-species interactions are present. Here, we study a minimal model of active phase separation involving two species of particles regulating their self-propulsion speed via quorum-

sensing rules, and identify a mechanism for dynamical pattern formation that does not rely on the standard route of intra-species effective attractive interactions. Instead, our results reveal a highly dynamical phase of chasing bands induced only by the combined effects of self-propulsion and nonreciprocity in the inter-species couplings. Turning on self-attraction, we find that the system may phase separate into a macroscopic domain of such chaotic chasing bands coexisting with a dilute gas. We show that the chaotic dynamics of bands at the interfaces of this phase-separated phase results in anomalously slow coarsening.

BP 13: Statistical Physics of Biological Systems I (joint session DY/BP)

Time: Tuesday 9:30–13:00 Location: BH-N 334

Invited Talk BP 13.1 Tue 9:30 BH-N 334

Dynamics of genome replication — •Simone Pigolotti — Okinawa Institute of Science and Technology

The DNA replication program of an organism determines the timing at which different genomic regions are replicated, with fundamental consequences for cell homeostasis and genome stability. I will present a method to infer the DNA replication program, by combining stochastic modeling and deep sequencing experiments. Our approach can be applied to a vast range of organisms from bacteria to eukaryotes. Applied to E. coli, our method reveals regular variations of replication speed, that correlate with previously measured variations of the mutation rate. In budding yeast, our method is able to infer the location of replication origins with remarkable accuracy.

BP 13.2 Tue 10:00 BH-N 334

Theory for Adaptive Systems: Collective Robustness of Genotype-Phenotype Evolution — •Tuan Pham and Kunihiko Kaneko — Niels Bohr Institute, University of Copenhagen

Biological and neural networks are adaptive - their connections slowly change in response to the state of the coupled elements making up the systems. The dynamics of such adaptive networks are intriguingly complex, rendering it extremely difficult to answer the fundamental question of how the resulting collective states of biological and neural systems are functionally robust against environmental stochasticity. We tackle this problem by developing a new framework based on the path-integral formalism of non-equilibrium statistical physics. We demonstrate the wide applicability of our framework to various very high-dimensional dynamical systems on multiple timescales, often encountered in biological evolution and neural network learning. As a specific example of our theory, we apply it to biological evolution, where phenotypes are shaped by gene-expression fast dynamics that are subjected to an external noise while genotypes are encoded by the configurations of a network of gene regulations. This network slowly evolves under natural selection with a mutation rate, depending on how adapted the shaped phenotypes are. Here we find phenotypes with a robust high-valued mean gene-expression level within an intermediate level of noise. The emergence of such robustness can be characterised analytically within our framework as the onset of instability of the attractor state with zero gene-expression levels.

BP 13.3 Tue 10:15 BH-N 334

Modelling antibiotic killing and tolerance dynamics in tuberculosis treatment — •Miriam Clincy[1], Vijay Srinivasan[2], Rosalind J Allen[2], and Martin R Evans[3] — [1]Hochschule Esslingen, Esslingen, Germany — [2]Friedrich-Schiller-Universität, Jena, Germany — [3]University of Edinburgh, Edinburgh, UK

The bacterium Mycobacterium tuberculosis (Mtb), which causes tuberculosis, is the leading global cause of deaths from infectious disease. The antibiotic treatment regime for tuberculosis is very long, because Mtb can switch into tolerant physiological states that are only slowly killed by antibiotic. Here we introduce a stochastic two-species birth-death model for antibiotic treatment of an Mtb infection accounting for this switching.

Solving analytically for the probability generating function describing the treatment phase in which neither state proliferates allows 1) to recover the mean subpopulation dynamics from which numerical estimates for the birth, death and switching rates specifically for Mtb can be derived, and 2) the calculation of the extinction probability as a function of time. From the latter, a numerical measure for the extinction time of the bacterial population is defined. Studying this extinction time reveals distinct regimes in which the required treatment time is limited by either the rate of killing of tolerant bacteria, or the rate of switching out of the tolerant state.

BP 13.4 Tue 10:30 BH-N 334

Information theory of chemotactic agents using both spatial and temporal comparison — Julian Rode[1], Maja Novak[2], and •Benjamin M. Friedrich[1] — [1]Physics of Life, TU Dresden, Germany — [2]University of Zagreb, Croatia

Biological system process information despite noise-corrupted input, often operating at physical limits. A prime example is chemotaxis, i.e., active navigation of biological cells in spatial fields of chemical cues. Intriguingly, cells of different size use two different chemotaxis strategies, comparing concentrations in either space or time. Only heuristic arguments exist to explain this evolutionary choice. We present an information theory of an ideal agent that combines both strategies to quantify 'chemotaxis in bits' [1]. This enables us to predict when each strategy provides more information as function of a new powerlaw that combines agent size, motility noise and sensing noise. We demonstrate our theory with a bio-inspired search robot. [1] https://www.biorxiv.org/content/10.1101/2023.10.14.562229v1

BP 13.5 Tue 10:45 BH-N 334

Relaxation and first passage properties of boundary driven run and tumble particle — •Pritha Dolai[1,2] and Arghya Das[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]TIFR Centre for Interdisciplinary Sciences, Tata Institute of Fundamental Research, Gopanpally, Hyderabad, 500046, India

We study the spatio-temporal properties of boundary-driven noninteracting Run and tumble particles (RTPs) in one-dimension. We found exact results for the steady state density and current. The spatial and internal degrees of freedom, combined together, possess a symmetry, using which we have analytically obtained the full eigen-spectrum. The eigenvalues are arranged in bands around 0 and -2ω where ω is the tumble rate of the RTP. In the large system size limit, the steady state and dynamical properties are closely approximated by an effective passive-like dynamics with an effective diffusivity. Interestingly, we found that the genuine signatures of activity in the dynamics appear only as subleading correction in system size. Further, there is a crossover from the system size independent relaxation rate to the diffusive relaxation as the system size is increased. Along the lines of equilibrium, we explored the possibility of defining an effective temperature in the single active particle case. It turns out that the effective temperature not only depends on the details of the system parameters, but on the quantities through which it is defined as well as the boundary conditions. We also studied the first passage properties of an RTP in the presence of absorbing boundaries.

BP 13.6 Tue 11:00 BH-N 334

Single particle analysis of sorbing tracers — •Timo Doerries[1], Aleksei Chechkin[1,2,3], and Ralf Metzler[1,4] — [1]Institute of Physics & Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]Faculty of Pure and Applied Mathematics, Hugo Steinhaus Center, Wrocław University of Science and Technology, Wyspianskiego 27, 50-370 Wrocław, Poland — [3]Akhizer Institute for Theoretical Physics National Science Center "Kharkiv Institute of Physics and Technology", 61108 Kharkiv, Ukraine — [4]Asia Pacific Center for Theoretical Physics, Pohang 37673, Republic of Korea

Based on a simple switching diffusion process we describe tau proteins changing between a mobile (diffusive) and an immobile state, leading to strong non-Gaussian displacements. For long but finite observation times the time averaged mean squared displacements have a significant spread, of which we obtain the exact distribution. This behaviour is similar to the well known continuous time random walk, which has instantaneous jumps in contrast to our model. We discuss the role of the non-zero mobile duration in our model compared to the instantaneous jumps in the continuous time random walk.

15 min. break

BP 13.7 Tue 11:30 BH-N 334

Furutsu-Novikov theorem for shot-noise driven systems — •Jakob Stubenrauch[1,2] and Benjamin Lindner[1,2] — [1]Physics Department of Humboldt University Berlin, Newtonstraße 15, 12489 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, Philippstraße 13, Haus 2, 10115 Berlin, Germany

We consider an arbitrary system (later exemplified by a spiking neuron) that is driven by an intensity-modulated Poisson process with intensity $\lambda(t) = \lambda_0 + \varepsilon s(t)$. We derive an exact relation between the input-output cross-correlation in the spontaneous state ($\varepsilon = 0$) and the response function for a weak time-dependent modulation of the input intensity ($\varepsilon > 0$). This can be regarded as a variant of the famous Furutsu-Novikov theorem (FNT) for the case of shot noise. Neurons in networks fluctuate spontaneously and respond if stimulated. Spontaneous fluctuations and response properties are linked, in correspondence to the fluctuation-dissipation theorem, as has recently been shown (Lindner, 2022). Such relations constrain the signal-to-noise ratio, they can be used to fit models, and to advance theories. However, for the biologically relevant case of shot-noise driven neurons, such relations have not been reported yet. As we demonstrate, we can use the new FNT to obtain a fluctuation-response-relation between the spontaneous fluctuations of a neuron's output and its systematic response to a time-dependent stimulus, extending the approach of (Lindner, 2022) from Gaussian noise to shot noise. The relations are numerically tested and their limitation to Poissonian input exemplified for the important example of a leaky integrate-and-fire neuron with alpha synapses.

BP 13.8 Tue 11:45 BH-N 334

Mesoscopic dynamics of spiking neuron population with quenched randomness — •Nils Erik Greven[1,2], Jonas Ranft[3], and Tilo Schwalger[1,2] — [1]TU Berlin — [2]BCCN Berlin — [3]IBENS, Ecole Normale Supérieure & CNRS

To understand the neural mechanisms underlying the response and variability dynamics of neuronal populations in the brain, simple mean-field models at the mesoscopic scale are required that faithfully describe the fluctuations of population activities and recurrent synaptic inputs in network of spiking neurons. We derive a nonlinear stochastic mean-field model for a network of spiking Poisson neurons with random connectivity. The quenched disorder of the connectivity is treated by an annealing approximation leading to a simpler fully connected network with additional noise in the neurons. This annealed network enables a reduction to a mesoscopic model as a two-dimensional closed system of coupled Langevin equations for the mean and variance of the neuronal membrane potentials. Compared to microscopic simulations, the mesoscopic model well describes the fluctuations and nonlinearities of finite-size neuronal populations and outperforms previous mesoscopic models that neglected the recurrent noise effect caused by quenched disorder. This effect can be analytically understood as a softening of the effective nonlinearity. The mesoscopic theory also shows that, in the presence of synaptic transmission delays, quenched disorder can stabilize the asynchronous state. Furthermore, our theory correctly predicts the effect of connection probability and stimulus strength on the variance of the population firing rate.

BP 13.9 Tue 12:00 BH-N 334

Low-dimensional stochastic dynamics of finite-size, spiking-neuron populations via eigenmode expansion — •Tilo Schwalger[1,2] and Bastian Pietras[3] — [1]Technical University Berlin, 10623 Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin, 10115 Berlin, Germany — [3]Universitat Pompeu Fabra, Barcelona, Spain

Low-dimensional neural population models in the form of nonlinear Langevin equations provide an effective description of the collective stochastic dynamics of neural networks in the brain. However, existing population models are largely heuristic without a clear link to the underlying neuronal and synaptic mechanisms. Here, we derive a system of Langevin equations at the mesoscopic scale from a microscopic model of a finite-size, fully-connected network of integrate-and-fire neurons with escape noise. The theory is based on a stochastic integral equation for the mesoscopic dynamics of the neural network (Schwalger et al. PloS Comput Biol. 2017) and an eigenmode expansion of the corresponding refractory-density equation (Pietras at al., Phys. Rev. E 2020). Truncating the hierarchy of coupled spectral modes after the first M modes yields a $2M$-dimensional Langevin equation, permitting a systematic model reduction. Retaining only the dominant spectral mode, $M = 1$, already captures well oscillatory transients and finite-size fluctuations when compared to microscopic simulations. Our bottom-up theory thus connects biologically plausible spiking neural networks to the efficient firing-rate models often used in applcations.

BP 13.10 Tue 12:15 BH-N 334

The Effect of Temperature on Large Biochemical Networks — •Julian Voits[1] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, University of Heidelberg, Heidelberg, Germany — [2]BioQuant-Center for Quantitative Biology, University of Heidelberg, Heidelberg, Germany

An increase of temperature of a few Kelvin might seem modest on the absolute temperature scale, but it can have a dramatic impact on complex biosystems. Instructive examples are fever, when a rise in body temperature of 2-3K has strong effects on our immune system, or climate change, when even smaller temperature changes lead to dramatic shifts in ecosystems. From the physics point of view, the main effect of increased temperature should be the exponential acceleration of biochemical reactions (Arrhenius equation). However, it is unclear how this law plays out in the large biochemical networks of complex systems. We have developed a universal theory that describes the effect of temperature on large biochemical networks. We approach this problem with a graph theoretical interpretation of the mean first passage times of a biochemical master equation. We show that in the limit of large networks, one obtains quadratic forms of the Arrhenius plots, in excellent agreement with experimental data on developmental rates of Drosophila.

BP 13.11 Tue 12:30 BH-N 334

Tensile elasticity of multi-state flexible chains and loops — •Geunho Noh and Panayotis Benetatos — Department of Physics, Kyungpook National University, Daegu, Republic of Korea

Polymer loop structure commonly appears in biological phenomena, such as DNA looping and DNA denaturation. When a chain forms a loop, its elastic behavior differs from that of an open chain due to the loss of entropy. In the case of reversible loop formation, interesting behavior emerges related to the multi-state nature of the conformations. In this study, we model a multi-state reversible loop as a looping Gaussian chain which can bind to form a loop, or a zipping Gaussian loop which can zip to form a double-stranded chain. For each model, we calculate the force-extension relations in the fixed-force (Gibbs) and the fixed-extension (Helmholtz) statistical ensembles. Unlike the single Gaussian chain or loop, the multi-level systems demonstrate qualitatively distinct tensile elasticity and ensemble inequivalence. In addition, we investigate a Gaussian necklace consisting of reversible alternating blocks of the chain and loop, and obtain the temperature-force phase diagram. The phase diagram implies a force-induced phase transition from a completely looped (denatured) state to a mixed (chains and loops) state.

BP 13.12 Tue 12:45 BH-N 334

Manifestation of hidden degrees of freedom in dissipative self-assembly — •Seeralan Sarvaharman and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen 37077, Germany

Dissipative self-assembly is crucial for the development and healthy functioning of biological systems. By breaking time-reversal symmetry in either the binding or unbinding process of at least one of the components, living organisms are able to assemble structures with much more diverse compositions in a robust fashion. One such example that is of fundamental biological relevance are microtubules. Through a process called "dynamic instability" these microtubules, which are made up of several filaments, grow and shrink depending on the instantaneous compositions of the filaments. The observable that is often used to quantify such dynamic instability is the length of the assembled microtubule. However, the ability to infer the many-body effects underlying this instability from the projected length observable has remained elusive. Here we address this challenge by considering a stochastic Ising-type model of microtubule assembly with thermodynamically consistent driving. Using a mixture of analytical techniques and computational methods we uncover the manifestation of many-body physics encoded the time-ordering of the length of the assembly.

BP 14: Poster IIa

Bacterial Biophysics, Tissue Mechanics.

Time: Tuesday 18:00–20:30 Location: Poster E

BP 14.1 Tue 18:00 Poster E

Microfluidic Separation of Viable and Non-viable *Legionella* Cells by a Quantifiable Dielectrophoresis Approach — •Madeline Altmann[1], Anders Henriksson[1], Peter Neubauer[1], and Mario Birkholz[2] — [1]Laboratory of Bioprocess Engineering, Department of Biotechnology, Technische Universität Berlin, Ackerstr. 76, ACK24, D-13355 Berlin, Germany — [2]IHP Leibniz-Institut für Innovative Mikroelektronik, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Traditional pathogen detection methods, notably PCR, often fail to distinguish viable and non-viable cells. This distinction is crucial as non-viable cells hold limited pathogenic potential. To overcome this limitation, analytical methods must be able to separate between viable from non-viable cells. Dielectrophoresis (DEP) can non-invasively separate cells according to viability, allowing for increased accuracy in subsequent bioanalytic workflows. This study focuses on employing positive dielectrophoresis in a microfluidic system to separate viable *Legionella parisiensis* cells from non-viable cells rendered inactive via heat shock to refine the specificity of biosensors. Although separation in realistic inactivation conditions was difficult, discrimination of viable cells was achieved by a video-based, quantifiable DEP method, that evaluates the percentage of fluorescent cells in a region of interest around the electrodes. It was found that long heat shock inactivation times decrease the positive DEP-effect at higher frequencies, enabling a separation of viable *Legionella* above 25 MHz and 10 Vpp in both tap water and demineralized water.

BP 14.2 Tue 18:00 Poster E

Improving Sensitivity of Micro-Ring Resonators for Photonic Biosensors — •Philipp Schrenk[1], Anders Henriksson[1], Christopher Borgmeier[1], Peter Neubauer[1], and Mario Birkholz[2] — [1]Department of Bioprocess Engineering, Institute of Biotechnology, Technical University Berlin, Ackerstr. 76, ACK24, D-13355 Berlin, Germany — [2]IHP GmbH, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Silicon-based photonic biosensors represent a promising approach for the detection of various pathogens. Utilizing micro-ring resonator chips, assisted by dielectrophoresis and specific antibody coatings, enables label-free detection of a sample, such as Legionella pneumophila, already at concentrations below the limit value of 100 CFU/100 ml. In contrast to conventional methods for detecting Legionella cells, photonic biosensors are cost-efficient, have a small footprint of a few mm2, and notably, possess the capability to deliver real-time results. The measuring principle of photonic biosensors relies on the evanescent field and variations of the refractive index n associated with the sample adjacent to the waveguide. In this study, the sensitivities of five different micro-ring resonators were analyzed by employing solutions with varying NaCl concentrations. These solutions induce differences in n measured in refractive index units (RIU) and consequently affect the evanescent field. By variation of the chip architecture, the sensitivities could be increased from 3.6 up to 23.5 nm/RIU. These findings are crucial for further quantitative investigations in detecting Legionella pneumophila cells.

BP 14.3 Tue 18:00 Poster E

Drug interactions between antibiotics targeting translation and transcription — •Natawan Gadjisade and Tobias Bollenbach — University of Cologne, Institute for Biological Physics, Germany

Combining antibiotics has the potential to improve treatment efficacy and slow the evolution of resistance. When two antibiotics are combined, their effect on bacterial growth may be stronger or weaker than expected (i.e., synergistic or antagonistic). Recent work has shown that it is often possible to predict such interactions between ribosome-targeting antibiotics using a biophysical model based on bacterial growth laws. Here, we focus on establishing a new model that resolves the interplay between translation and transcription inhibitors. We classify drug interactions by measuring E. coli growth in two-dimensional concentration gradients of the transcription inhibitor rifampicin and several translation inhibitors. Our data indicate different types of interactions. We systematically quantify proteome allocation and individual protein regulation using mass spectrometry-based proteomics measurements optimized for absolute quantification of protein levels. Our preliminary data from single drug treatment with translation inhibitors confirm the known increase in ribosome concentration, whereas rifampicin led to a decrease. Our current aim is to quantify how the cells resolve the conflict of ribosome regulation by performing proteomics measurements in a two-dimensional concentration gradient of both drugs. This work may lead to a deeper understanding of the interplay of transcription and translation.

BP 14.4 Tue 18:00 Poster E

Tracing noisy gradients: chemotactic motion in fluctuating environments — •Thomas Suchanek — Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

We study the collective dynamics of chemotactically interacting agents in a system of two species coupled unilaterally via a chemical signaling field: a tracer species actively follows the paths of a target species, which itself moves purely randomly. We observe that fluctuations in the chemical field can have an important impact on the shape of the effective non-reciprocal interactions that determine the averaged dynamics of the two species. In particular, this results in interactions that deviate from the Predator-Prey scheme often considered in the literature [1]. We investigate the form of collective states that arise from interactions of this form and discuss the effects of additional self-interaction (autochemotaxis) of the tracer species.

[1] Liebchen, B., & Löwen, H. (2020). Modeling chemotaxis of microswimmers: From individual to collective behavior. In Chemical Kinetics: Beyond the Textbook (pp. 493-516).

BP 14.5 Tue 18:00 Poster E

Guiding Escherichia coli biofilm growth with textured surfaces — •Clémentine Ferrari[1], Marie-Ly Chapon[2], Laurent Pieuchot[2], Wei Wang[3,4,5], Weiwei Wang[3], Nan Ma[3,4], and Cécile M. Bidan[1] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam — [2]Université de Haute-Alsace, Mulhouse — [3]Helmholtz-Zentrum Hereon, Teltow — [4]Freie Universität Berlin, Berlin — [5]Jilin University, Changchun

Biofilms are complex 3D biological materials created by bacteria producing a protective matrix against adverse environments. These bacteria adapt their matrix in response to various chemical, biological or physical stimuli. This implies that the materials properties of biofilms can be influenced by the properties of their substrate. This project aims at regulating the growth and organization of biofilms by manipulating the geometry of their environment through structured surfaces. Therefore, we culture E. coli bacteria on agar plates to obtain 3D biofilms. The surface of the agar plate is previously shaped with different PDMS stamps. The patterns on these stamps consist of parallel periodic sinusoidal waves or an array of concave half-spheres. In both cases, different dimensions are tested to determine if there is a critical length range where biofilms respond to these modifications, and how this affect their growth and properties. First results indicate that microtopography can influence biofilm spreading. Quantitative methods based are now being established to characterize and measure these changes. Ultimately, textured surfaces may help to develop oriented biofilm-based materials with anisotropic properties.

BP 14.6 Tue 18:00 Poster E

Swimming motility and chemotaxis strategy of *Pseudomonas putida* in porous media — •Sönke Beier, Veronika Pfeifer, Robert Grossmann, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

The chemotaxis strategy of bacteria in liquids is well studied and can be explained in most cases by a run time bias. But how do they adapt their strategy in a porous environment, where there is only a small free path length?

By studying the population spreading and analyzing individual trajectories of the soil bacterium *Pseudomonas putida* in agar, we elucidate the effect of a porous medium on the swimming behavior of *P. putida*. For this purpose, we use a computer-automated event detec-

tion method to recognize the stop and turn events known from the movement pattern in liquid and characterize the trap events which occur in agar. By investigating the orientation of run phases, we found evidence that *P. putida* performs chemotaxis by adapting its swimming direction, similar to earlier report on the peritrichously flagellated intestinal bacterium *Escherichia coli*, suggesting that this could be a generally strategy in many bacterial species.

BP 14.7 Tue 18:00 Poster E

Antibiotic efflux-mediated interactions in a spatially structured bacterial population — •Silvia Vareschi[1], Valerie Jaut[2], Vijay Srinavisan[1], Marco Mauri[1], Frank Schreiber[2], and Rosalind J. Allen[1] — [1]Friedrich Schiller University Jena — [2]Federal Institute for Materials Research and Testing (BAM), Berlin

Multidrug efflux pumps are transmembrane protein complexes that use energy to pump antibiotic outside bacteria. Efflux pumps are among the most common mechanisms by which bacteria become antibiotic resistant. Moreover, mutations that increase efflux pump expression have been found within bacterial biofilms - dense, surface-attached communities that are notoriously difficult to treat with antibiotics. Therefore it is important to understand the role of efflux pumps in the development of antibiotic tolerance in spatially structured bacterial assemblies.

This is a complex problem: on the one hand the local antibiotic concentration alters the growth rate and, potentially, the effluxing capability of bacteria, on the other hand bacteria affect the local antibiotic concentration both by importing the antibiotic and pumping it out.

Our central hypothesis is that this interplay leads to the emergence of antibiotic-mediated interactions between bacteria. These interactions can impact the overall antibiotic response of the population and its spatial structure. We present preliminary experimental data and theoretical analysis, showing how efflux activity, together with antibiotic influx, has non-trivial implications for the structure of a bacterial colony, and its fate in the presence of antibiotic.

BP 14.8 Tue 18:00 Poster E

Modeling of antibiotic-induced perturbation in gut microbiome — •Rie Maskawa[1], Hideki Takayasu[1], Lena Takayasu[2], Wataru Suda[2], and Misako Takayasu[1] — [1]Tokyo Institute of Technology, Tokyo, Japan — [2]RIKEN, Yokohama, Japan

It is important to understand the fluctuation of microbiome due to external perturbations. However, detailed microbiome response to perturbations has not been quantitatively evaluated. We analyzed high-resolution time series of the gut microbiome of mice receiving different concentrations of the antibiotics using the extended Lotka-Volterra model. By modeling of the antibiotic change based on a pharmacokinetic model, detailed temporal changes of perturbation were incorporated into the model. As a result of identifying parameters that accurately describe the kinetics and extracting robustly estimated bacterial interactions between mice, we concluded that the interbacterial network may change depending on the antibiotic pharmacokinetics.

BP 14.9 Tue 18:00 Poster E

Traffic Slowdown by Antibiotics — •Johannes Keisers, Luca Ciandrini, and Phillippe Fuchs — Centre De Structurale Biologe (CBS), Montpellier, France

Bacteria adapt to environmental changes through significant protein expression changes. Despite the complexity of transcription and translation, quantitative growth laws link ribosome allocation and growth. Our focus is on sub-lethal antibiotic effects, reshaping cellular resources. Using a modified TASEP model, we study antibiotic-induced ribosome pausing states, reproducing the second growth law and quantifying active and inactive ribosomes. The approach interprets the ribosome allocation-growth rate relationship under sub-lethal antibiotic doses. It successfully predicts the acceleration of ribosomes under sub-lethal doses of antitbiotics, as observed in E. coli. Our model estimates active versus antibiotic-bound ribosomes and predicts antibiotic impact on charged tRNA concentration. This framework enhances understanding of sub-lethal antibiotic effects on bacterial dynamics, potentially informing future transcriptional perturbations.

BP 14.10 Tue 18:00 Poster E

Mechanical Properties of the Premature Lung — •Jonas Naumann[1], Nicklas Koppe[1], Ulrich Thome[2], Mandy Laube[2], and Mareike Zink[1] — [1]Research Group Biotechnology & Biomedicine, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Center for Pediatric Research Leipzig, Department of Pediatrics, Division of Neonatology, Leipzig University, 04103 Leipzig, Germany

Premature infants are often reliant on mechanical ventilation to survive. However, prolonged ventilation and associated mechanical stress may cause subsequent pulmonary diseases of the immature lung. To study the mechanical properties of fetal rat lungs on macroscopic scale, we performed rheology experiments under compression and tension using different velocities. Fetal lung tissue showed a hyperelastic behavior and became significantly stiffer with increasing deformation velocities. In fact, fetal lung tissue under compression showed clear viscoelastic features even for small strains. A higher Young's modulus of fetal lungs compared to adult controls clearly pointed towards altered tissue characteristics. In addition, the influence of a hydrostatic pressure difference on the electrophysiology of primary fetal distal lung epithelial cells was investigated on microscopic scale. We observed a strong impact of hydrostatic pressure on the activity of the epithelial sodium channel and the sodium-potassium pump. Vectorial sodium transport, crucial for alveolar fluid clearance, was significantly impaired.

BP 14.11 Tue 18:00 Poster E

Mechanical stress patterns instruct the division plane orientation and tissue morphology during radial growth in *Arabidopsis thaliana* — •Mathias Höfler[1], Xiaomin Liu[2], Thomas Greb[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Centre for Organismal Studies, Heidelberg University, Germany

Growing tissues requires coordination to morph functionally structured cell arrangements. Particularly, in plants, where cells cannot rearrrange spatially, coordination of cell division orientation is essential. Here, the radially growing tissue of the plant hypocotyl displays orchestrated cell divisions that pattern cell arrangements. In close comparison with experimental data we investigate how cell mechanics and emerging stress patterns may control cell division orientation and thereby emerging cell arrangement. Starting from reconstructed early hypocotyl cell pattern we model cell growth and follow the emerging mechanical stress pattern. Comparing mechanical stress guided cell division orientation with random cell division orientations we find that the well-ordered cell topologies of the hypocotyl only emerge when incorporating guidance by mechanical stress. Further, the instructive mechanical stress pattern is found to be robust against the cell division orientation. Finally, comparing changes to cell division patterns in experiment and model by mechanically pinching the hypocotyl confirm that mechanical stress instruct the cell division orientation, and thus organize radial growth and plant tissue arrangement.

BP 14.12 Tue 18:00 Poster E

Unraveling Morphogen Dynamics and Growth Mechanisms in Zebrafish Pectoral Fin through Mathematical Modeling — •Maximilian Kotz[1], Benjamin M. Friedrich[1], Lucas de Oliveira Petrocchi Ribas[2], and Rita Mateus[2] — [1]TU Dresden — [2]MPI-CBG, Dresden

During animal development and regeneration, morphogen gradients control tissue growth and patterning. Here, we study mechanisms of growth control using the pectoral fin of zebrafish as model system. A key open question is whether morphogen function similarly in development and regeneration. To address this question, we build data-driven mathematical models of morphogen dynamics coupled to growth. We quantitatively compare finite-element simulations of the models to time-lapse microscopy data provided by our experimental collaborators. For this, we use AI-based image analysis for nuclei segmentation, as well as curved coordinate systems to unwrap the curved 3D tissue geometry. Ultimately, we aim to delineate similarities and differences between development and regeneration, with respect to growth control by morphogens.

BP 14.13 Tue 18:00 Poster E

Small tissues, big opportunities: versatile applications of a new muscle tissue chamber — •Bruno Schmelz[1], Mattias Luber[1], Polina Malova[1], Till Münker[1], Arne Hofemeier[2], and Timo Betz[1] — [1]Third Institue of Physics, Göttingen, Germany — [2]University Medical Center, Göttingen, Germany

Tension and mechanical properties of skeletal muscle tissue are tightly related to its functionality, which makes experimental access to the biomechanics of muscle tissue a key requirement to advance our understanding of muscle function, development and diseases. Recently devised *in vitro* culture chambers allow for raising 3D muscle tissues

under controlled conditions and measuring the global tissue force generation. However, PDMS-based systems are inherently incompatible with high resolution microscopy used for fluorescence-based investigation methods for live and dynamic measurements and absorb small molecules, including many active substances that need to be applied in small yet specific amounts. A recently introduced chamber design blazed a trail for real-time high resolution 3D microscopy during muscle formation and, simultaneously, enabled non-invasive quantification of global contractile forces *via* post deflection analysis. Here we show the versatility of the chamber design by inhibiting the cellular contractility using Cytochalasin D and Blebbistatin. While this largely reduced the force generation, some electrical stimulation of the tissue remained in the Cytochalasin D situation. This suggests either partial protection of the actin from depolymerization or additional effects that lead to voltage-initiated post-deflection.

BP 14.14 Tue 18:00 Poster E

Understanding the stress generation and relaxation in model epithelium — •Madhura Ramani[1], Kevin Höllring[1], Maxime Hubert[1], Rudolf Merkel[2], and Ana Sunčana Smith[1,3] — [1]PULS, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]IBI-2: Mechanobiology, Institute of Biological Information Processing, Forschungszentrum Jülich,Germany — [3]Group for Computational Life Sciences,Ruder Bošković Institute, Zagreb, Croatia

Mechanical forces influence cells via a process known as mechanotransduction, in which cells within a tissue receive and respond to physical stimuli. Epithelia are constantly exposed to external mechanical stimuli, and compromised tissue morphology and architecture from the stress are associated with numerous pathological conditions such as cancer. It is crucial to understand the effect of stretch deformation on the maintenance of tissue structure and its function. We investigate the response of tissue by growing Madin-Darby canine kidney cells on a stiff PDMS substrate, which is later subjected to uniaxial stretch stress using a motorized stretch device. By subjecting the homeostatic tissue to uniaxial stretch stress, we investigate the stress relaxation responses in different time and length scales, providing insight into tissue remodelling, growth, and death. We present our in-house MATLAB code, which quantitatively measures the tissue remodelling, connectivity and cell growth upon tissue stretch. Our approach provides valuable insights into the mechanical feedback of tissue subjected to uniaxial stretch deformations, playing a crucial role in understanding the biophysical aspects of tissue response and disease progression.

BP 14.15 Tue 18:00 Poster E

Noninvasive measurement of tissue tension using low magnification brightfield microscopy — •Mattias Luber, Arne Hofemeier, and Timo Betz — Third Institute of Physics - University of Göttingen, Göttingen, Germany

The interplay of numerous biomechanical features is fundamental for proper tissue function. Therefore, having experimental access to biomechanics is crucial for advancing our understanding of the development of muscle and connective tissue, facilitating the identification of abnormalities and contributing to our understanding of disease mechanisms. Engineered in vitro tissues have proven to function as well-established disease models, allowing mimicking phenotypic conditions in a controlled environment. However, precise measurements of the relevant biomechanical features are still tedious and require specialized equipment as well as manual handling of the sensitive samples. To ease this burden, we present a platform to raise biomimetic tissue models under controlled conditions and measure the tissue tension (among others) noninvasively and throughout the full developmental lifecycle with low magnification brightfield microscopy only. Using this approach, we were able to identify tissue tension as a highly relevant readout for muscular disease like Duchenne Dystrophy, demonstrate the tension-regulating effect of certain compounds or, in context of connective tissues, to investigate fibrotic conditions.

BP 14.16 Tue 18:00 Poster E

Dense optical flow analysis to quantify spatiotemporal fluctuations during tissue growth — •Kai Lennard Fastabend[1], Tassilo von Trotha[2], Mario Christian Benn[2], Viola Vogel[2], and Philip Kollmannsberger[1] — [1]Biomedical Physics, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Laboratory of Applied Mechanobiology, ETH Zürich, Switzerland

The growth of fibroblast microtissues depends on the interplay between cell contractility, extracellular matrix and the geometry of the underlying substrate. Previous studies revealed gradients of cell phenotype and matrix stretch between growth front and tissue interior [1], but how these gradients emerge over time is not clear. We aim to better understand the dynamics of growth by quantifying spatiotemporal deformation patterns during growth. We first evaluated different strain mapping algorithms applied to phase contrast time lapse movies of growing tissues from [2] and found that the Farnebäck algorithm for dense optical flow showed the most robust results. Based on the resulting deformation fields, the time dependent divergence of motion was calculated to identify regions of stretching and compression. Spatial and temporal smoothing of the flow fields was employed to evaluate local tissue deformations at different scales. The presented framework is a promising approach to analyze the mechanical feedback regulation involved in the organization of tissue growth, enabling a more nuanced understanding of cellular responses to microenvironmental mechanical cues. [1] P Kollmannsberger et al., Science Advances 4(1) eaao4881 (2018) [2] MC Benn et al. Science Advances 9(13) eadd9275 (2023)

BP 14.17 Tue 18:00 Poster E

Dystrophin as a tension regulator in human skeletal muscles — •Mariam Ristau[1], Arne Hofemeier[1,2], Bart Vos[1], Till Münker[1], Mattias Luber[1], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University Göttingen — [2]Institute of Pharmacology and Toxicology - University Medical Center Göttingen

Skeletal muscles are associated with contraction, movement and force generation. They are important for maintaining posture, bone and joint stability. Muscular dystrophies such as Duchenne muscular dystrophy (DMD) result in progressive weakening and wasting of skeletal muscles. DMD is caused by the loss of the protein dystrophin which is thought to stabilize and protect muscle fibres from injury.

We have studied the contractile potential of reconstituted tissues derived from healthy and DMD patients, and found that DMD derived tissues exhibited an overall weaker contractility compared to healthy derived tissues. In contrast, DMD derived tissues showed an overall higher homeostatic tissue tension, suggesting that dystrophin may function as a tension regulator in skeletal muscles.

In order to rule out the possibility that these findings are due to patient variability, we established a DMD knockout model from healthy myoblasts by using the CRISPR/Cas9 system. Comparing the healthy tissues to the isogenic DMD tissues we could reproduce the same phenotype of increased homeostatic tissue tension in the DMD tissues, providing further evidence that dystrophin may regulate homeostatic tissue tension.

BP 14.18 Tue 18:00 Poster E

Mechanobiological response of an epithelial tissue under shear stress — •Narmin Abasova[1], Annemarie Wirth[1], Kevin Hoellring[1], Rudolf Merkel[2], and Ana-Sunčana Smith[1,3] — [1]PULS Group, Institute for Theoretical Physics, FAU Erlangen- Nurnberg (IZNF) — [2]Institute for Biological Information Processes (IBI), Forschungszentrum, 52428 Jülich, Germany — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epithelial cells endure a continuous array of mechanical stresses within the human body, from the rhythmic pulsations of blood circulation to the dynamic stresses induced by exercise. Understanding the mechanobiological aspects of stress generation in epithelial cells is crucial for unraveling the complex dynamics underlying cellular responses and tissue functionality. Hence, we employ stress-generating devices to investigate the effects of distinct stress types on the tissue.The influence of solid shear stress transmitted through the extracellular matrix (ECM) remains a less-explored frontier in tissue mechanics. This research employs a custom-made device capable of applying controlled shear stress to the substrate supporting epithelial cell cultures. Upon subjecting the studied cluster to solid shear stress, we systematically document the tissue's response to the applied stress under the microscope. Our investigation delves into the implications of solid shear stress on cellular behavior, encompassing analyses of cell elongation, proliferation, stress relaxation, and the T1 transitions at the cell membrane, where neighbor exchanges occur.

BP 14.19 Tue 18:00 Poster E

Thick elastic sheets and complex tissue shape: theory and modeling — •Wan Yee Yau[1,2,3] and Carl D. Modes[1,2,3] — [1]Max Planck Ins,tute for Molecular Cell Biology and Gene,cs (MPI-CBG), Dresden 01307, Germany — [2]Center for Systems Biology Dresden (CSBD), Dresden 01307, Germany — [3]Cluster of Excellence, Physics

of Life, TU Dresden, Dresden 01307 Germany

Folding formation in epithelial tissue can be driven by the deformation gradient, induced by cellular-scale or tissue-scale effects. In this study, we employ shape programmability in thick elastic sheets to investigate epithelial morphogenesis. This approach, with finite-thickness elastic sheets, allows the flexibility to select distinct deformation patterns on both surfaces, enabling the exploration of distinct apical and basal deformations in epithelia. Additionally, we examine the thickness effect of these competing patterns. Simulations within the spring-lattice model are conducted to predict shapes based on the initial deformation pattern. Subsequently, we analyze the relationships using the theory of elasticity.

BP 15: Poster IIb

Bioimaging, Biomaterials and Biopolymers

Time: Tuesday 18:00–20:30 Location: Poster F

BP 15.1 Tue 18:00 Poster F

A Next-Generation qPlus-Sensor-Based AFM Setup: Resolving Archaeal S-Layer Protein Structures in Air and Liquid — Theresa Seeholzer, Daniela Tarau, Lea Hollendonner, Andrea Auer, Reinhard Rachel, Dina Grohmann, Franz J. Giessibl, and •Alfred J. Weymouth — Universität Regensburg, Regensburg, Deutschland

Surface-layer (S-layer) proteins form the outermost envelope in many bacteria and most archaea and arrange in two-dimensional quasicrystalline structures via self-assembly. We investigated S-layer proteins extracted from the archaeon Pyrobaculum aerophilium with a qPlus sensor-based atomic force microscope (AFM) in both liquid and ambient conditions and compared it to transmission electron microscopy (TEM) images under vacuum conditions. For AFM scanning, a next-generation liquid cell and a new protocol for creating long and sharp sapphire tips was introduced. Initial AFM images showed only layers of residual detergent molecules (sodium dodecyl sulfate, SDS), which are used to isolate the S-layer proteins from the cells. SDS was not visible in the TEM images, requiring more thorough sample preparation for AFM measurements. These improvements allowed us to resolve the crystal-like structure of the S-layer samples with frequency-modulation AFM in both air and liquid.

J. Phys. Chem. B 127, 6949 (2023)

BP 15.2 Tue 18:00 Poster F

High-resolution chemical imaging of model system Bacillus *subtilis* using mid-IR photo-induced force microscopy (PiF-IR) — •Selema Buzhala[1,2], Robin Schneider[1], Maryam Ali[2], Astrid Tannert[1,3], Sebastian Unger[1,2], Rainer Heintzmann[1,2], Ute Neugebauer[1,2,3], and Daniela Täuber[1,2] — [1]Leibniz Institute of Photonic Technology, Jena — [2]Friedrich Schiller University Jena — [3]Jena University Hospital, Center for Sepsis Control and Care, Jena, Germany

Mid-infrared photo-induced force microscopy (PiF-IR) offers high spectral resolution in combination with surface sensitivity and a spatial resolution in the range of a few nanometers. In a recent study, we demonstrated its ability to reveal local variations in the secondary protein structure of F-Actin on a scale of 5 nm [1]. Here we apply PiF-IR to individual cells of the well-known Bacillus *subtilis* treated with an antibacterial drug and to untreated controls. Cropped scans at high spatial resolution visualize variations in the sugar and peptide contents of the bacterial cell walls. Additional chemical information is provided from the analysis of hyperspectral images using home-written software. [1] J. Joseph, L. Spantzel, M. Ali, D.M. Joseph, S. Unger, K. Reglinski, C. Krafft, A.-D. Müller, C. Eggeling, R. Heintzmann, M. Börsch, A.T. Press, D. Täuber. Nanoscale chemical characterization of secondary protein structure of F-Actin using mid-infrared photoinduced force microscopy (PiF-IR). Spectrochimica Acta part A: Molecular and Biomolecular Spectroscopy, 306, 123612, 2024.

BP 15.3 Tue 18:00 Poster F

Robust and fast sorting of droplets in microfluidic devices by droplet size and droplet content based on bright field and fluorescent information — •Jonas Pfeil[1,2], Patricia Schwilling[1], and Othmar Marti[1] — [1]Universität Ulm, Ulm, Deutschland — [2]Sensific GmbH, Biberach, Deutschland

Droplet-based microfluidics is a promising tool to manipulate biological systems in small sample volumes down to single-cell level. Active sorting of droplets allows to enrich target configurations with high selectivity and selectivity.

We present methods and tools required to enrich droplets based on size and content in multiplexed bright-field and fluorescent microscopic imaging at sorting rates of 60 Hz. The PDMS-based microfluidic device uses a two electrode design with an high voltage AC field to sort droplets via dielectrophoretic forces.

BP 15.4 Tue 18:00 Poster F

Scanning small angle x-ray scattering of hydrated cells in flow environment — •Boram Yu[1], Mangalika Sinha[1], Rita Mendes da silva[1,2], Peter Luley[1], Manfred Burghammer[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Imaging biological cells using x-rays is a complementary approach to electron and fluorescence microscopy due to their high penetration depth and the possibility for label-free imaging. One such technique is scanning small angle x-ray scattering (SAXS), which provides both real space overview images with moderate resolution and reciprocal space information with high resolution, making it useful for obtaining structural information of ordered intracellular structures. However, imaging cells in an aqueous state, i.e., in a physiological environment, is challenging due to low electron density contrast, pronounced radiation damage, and radiation-induced gas formation. To overcome these challenges, we built a dedicated flow sample chamber, offering minimized thickness of the liquid layer in the beam path while continuously exchanging liquid during scanning. Using this technique, we conducted a study on fixed-hydrated mammalian cells with cytokeratin bundle networks. Despite the weak contrast and short exposure time, we were able to obtain distinguishable differences in strongly ordered cell components. It implies that scanning SAXS combined with the flow sample chamber offers structural information from fixed-hydrated cells in liquid flow.

BP 15.5 Tue 18:00 Poster F

Structure and mechanics of actomyosin contractility in hiPSC cardiomyocytes — •Mangalika Sinha[1], Boram Yu[1], Rita Mendes da Silva[1,3], Isabelle Refke[1,2], Manfred Burghammer[3], Ulrike Rölleke[1], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]University Medical Center, Göttingen, Germany — [3]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Cardiomyocytes derived from human induced pluripotent stem cells (hiPSC-CMs) are an interesting model system for studying heart activity and cardiovascular diseases in human. These cells contain sarcomeres, composed of actin-myosin, which is responsible for the contractility of cardiac muscles. Moreover, the contraction of these cardiac muscle cells depends on the geometry of these sarcomeres. In this study, we use complementary techniques, small angle x-ray scat- tering (SAXS) and traction force microscopy (TFM), to understand the relation between well-aligned sarcomeres and the contractile force generation of the actin-myosin complexes present in the muscle cells.Our SAXS results enable us to quantify the orientation of the sarcomeric structures. It correlates well with the fluorescence microscopy images of the actin filaments. The TFM data provide insights into contractile force generation. These findings play an important role in understanding the contractile nature of the sarcomeres and their behavior in healthy and diseased human heart.

BP 15.6 Tue 18:00 Poster F

Insights from live non-linear microscopy imaging: comparative analysis of temperature-induced mitochondrial morphology shifts using standard versus machine-learning method — •Marta Bukumira[1], Aleksandra Vitkovac[2], Tanja Pajić[2], Ma-

rina Stanić[3], Mihailo Rabasović[1], and Nataša V. Todorović[4] — [1]University of Belgrade, Institute of Physics, Belgrade, Serbia — [2]University of Belgrade, Faculty of Biology, Belgrade, Serbia — [3]University of Belgrade, Institute for Multidisciplinary Research, Belgrade, Serbia — [4]University of Belgrade, Institute for Biological Research "Siniša Stanković", Belgrade, Serbia

Using two-photon excited fluorescence (TPEF) modality of our home built nonlinear laser scanning microscope, we investigated, as a proof of principle, mitochondrial morphology adaptations in an eukaryotic cell in vivo, as a response to cooler ambient temperature during growth. The cells were stained with the vital mitochondrial dye Rhodamine 123 in order for mitochondria to exhibit TPEF. We compared cultures grown at two cooler and one control temperature. Acquired images show superior level of clarity and an optimal signal-to-noise ratio, allowing for the morphology differentiations of intricate subcellular structures influenced by subtle temperature variations. Two approaches for extracting parameters from TPEF images were juxtaposed: standard method of particle analysis in ImageJ and nonstandard method in Ilastik, a machine learning-based software. The latter demonstrated greater suitability for this type of analysis, showing increased efficiency in terms of time and reduced susceptibility to errors.

BP 15.7 Tue 18:00 Poster F

Functionalization of carbon nanoparticles for a cellular application — •Carla Sprengel, Lennard Fastabend, Cathrin Nollmann, and Thomas Heinzel — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

Nanoparticles as carriers in drug delivery systems are gaining in interest in the field of cancer therapies. Transporting drugs directly into targeted cells could enhance the efficiency and reduce side-effects in therapy. The carbon nanodots presented here show promise as potential carriers because of their low cytotoxicity and cellular uptake via endocytosis. Furthermore, the particles can be localized on a cellular level due to their fluorescence properties. Since an effective functionalization of our particles is crucial for the application in drug-delivery systems, we tested our particles as carriers by binding a polymer to them. Here we present the successful functionalization of our carbon nanoparticles and a cellular uptake into the lysosomes of MCF-7 cells.

BP 15.8 Tue 18:00 Poster F

Multifunctional Photoluminescent Quantum dots as Amplifiers for 1O2 Generation and Synergistic Enhanced Photodynamic Therapy — •Zahid Ullah Khan[1], Latif Ullah Khan[2], Hermi Felinto de Brito[1], and Paolo Di Mascio[1] — [1]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [2]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan.

The development of multi-functional nano-platform with integrated diagnostic and therapeutic features is highly desired for precise treatment. Here, we report the synthesis of CdSe/ZnS core-shell QDs by new method, which exhibited wide-range color-tunability (490-570 nm). The color tuning was achieved as result of interfacial alloying (predominantly exchange of Se2- by S2- anion) without changing the size of NCs. The QDs demonstrated efficient singlet molecular oxygen (1O2) quantum yields of 14, 12, and 18% for yellow-emitting CdSe/ZnS QDs (I), green-emitting CdSe/ZnS QDs (II), and blue-emitting CdSe/ZnS QDs (III), respectively. The 1O2 was produced by QDs via triplet-triplet energy transfer to dioxygen. The QDs were studied in macrophage cells that internalized the NCs via energy-dependent endocytosis predominantly macropinocytosis and other lipid raft-mediated endocytic pathways and manifested considerable amount in the intracellular regions without causing cytotoxicity3. In summary, the study will open new possibilities of band edge engineering and pathway-specific delivery of QDs-based theranostic into a site of interest for simultaneous bioimaging and photodynamic therapy.

BP 15.9 Tue 18:00 Poster F

In vivo Actin staining approaches validated using structured illumination and expansion microscopy — •Shangjun Cheng[1,2,3], Sara Gjeci[1,3], Aleksandar Rusevski[1,3], Patrick Then[1,4], Hans-Dieter Arndt[1], Rainer Heintzmann[1,2], Daniela Täuber[1,2], and Adrian T. Press[1,3] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]Jena University Hospital, Jena — [4]Microverse Imaging Center, Jena, Germany

Actin assembly and disassembly is essential for any type of cell mobility. Variations in Actin content in liver tissue have been found to be an indicator for animal survival in a recent study utilizing a mouse model for systemic infection [1]. In vivo imaging of Actin, thus, provides access to enhanced understanding of cellular behavior in various areas of research including the response to infection and therapy. We use structured illumination and expansion microscopy to evaluate several approaches for in vivo Actin staining. [1] P. Martinac, A.T. Press, A. Medyukhina, K.-J. Benecke, J. Shi, D. Täuber, S. Hoeppener, Z. Cseresnyes, I.G. Scheblykin, M.H. Gräler, I. Rubio, M.-T. Figge, U.S. Schubert. M. Bauer: Inhibition of phosphoinositide 3-kinase-y improves liver function in sepsis by preventing RhoA-mediated cholestasis in 9th International Congress "Sepsis and Multiorgan Dysfunction", Infection, 47, S6-S7, 2019.

BP 15.10 Tue 18:00 Poster F

Combining fluorescence lifetime imaging and expansion microscopy for investigation of Actin staining approaches — •Elza Sunil[1], Shangjun Cheng[1,2,3], Subham Adak[1], Sara Gjeci[1,3], Aleksandar Rusevski[1,3], Hans-Dieter Arndt[1], Adrian T. Press[1,3], Daniela Täuber[1,2], and Rainer Heintzmann[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]Jena University Hospital, Jena, Germany

Cytoskelettal Actin plays an important role in cell stability and mobility. In a previous study, an increased amount of aggregated F-Actin has been found in liver tissue from infected animals in a mouse model for systemic infection [1]. We combine fluorescence lifetime imaging and expansion microscopy to evaluate different Actin staining approaches aiming at enhancing our understanding of Actin aggregation in the context of infection and therapy. [1] P. Martinac, A.T. Press, A. Medyukhina, K.-J. Benecke, J. Shi, D. Täuber, S. Hoeppener, Z. Cseresnyes, I.G. Scheblykin, M.H. Gräler, I. Rubio, M.-T. Figge, U.S. Schubert. M. Bauer: Inhibition of phosphoinositide 3-kinase-y improves liver function in sepsis by preventing RhoA-mediated cholestasis in 9th International Congress "Sepsis and Multiorgan Dysfunction", Infection, 47, S6-S7, 2019.

BP 15.11 Tue 18:00 Poster F

Synchronisation of confocal laser scanning and single photon counting in a homebuilt Fluorescence lifetime imaging microscopy (FLIM) setup — •Subham Adak[1,2,3], Elza Sunil[1,2], Monalisa Goswami[1,2], Daniela Täuber[1,2], and Rainer Heintzmann[1,2,3] — [1]Leibniz Institute of Photonic Technology, Jena — [2]Institute of Chemical Physics, Friedrich Schiller University Jena — [3]Abbe Center of Photonics, Jena, Germany

Fluorescence Lifetime Imaging Microscopy (FLIM) is an attractive microscopy method in the life sciences, yielding information on the sample otherwise unavailable through intensity-based techniques [1]. In our homebuilt FLIM setup we combine a confocal laser scanning system from LaVison BioTec with a single photon counting system from picoQuant. The triggers for confocal scanning and for single photon acquisition are carefully synchronized. We tested (i) the accuracy of the determined lifetimes, and (ii) the time and spatial resolution of the instrument using fluorescent beads of different diameters. [1] A. Le Marois, S. Labouesse, K. Suhling, and R. Heintzmann, (2017), Noise-Corrected Principal Component Analysis of fluorescence lifetime imaging data. J. Biophoton., 10: 1124-1133.

BP 15.12 Tue 18:00 Poster F

Oxygen Measurements of single Red Blood Cells by Lightmicrospy — •Sarah Tabea Hermes, Agatha Belen Pinto Pino, Thomas John, and Christian Wagner — Campus E2.6 66123 Saarbrücken

The red blood cells in our body have a very high affinity for absorbing oxygen. In the lungs, they are loaded with oxygen and release it again in the body. The release of oxygen changes the light spectrum of the hemoglobin, thereby slightly altering its color. At selected wavelengths, this difference is significant and can be utilized to detect the O_2 content of individual cells using light microscopy. We are discussing various methods to prepare red blood cells in vitro without O_2. The objective is to investigate the oxygen release or uptake of individual cells under microfluidic conditions.

BP 15.13 Tue 18:00 Poster F

Monitoring the developmental dynamics of cysts with light sheet microscopy — •Ivana Jeremic, Paula Gironés Payá, Florian Rehfeldt, and Matthias Weiss — University of Bayreuth, Bayreuth, Germany

Proper epithelial morphogenesis is crucial for organ development and functioning. Understanding the mechanisms that guide morphogenesis is essential, not only for decoding the fundamental biology of organs but also for a better comprehension of the processes involved at the onset and progression of diseases. A key aspect of morphogenesis, e.g. in the kidney, is the formation of cell clusters that surround a hollow lumen. Development of the lumen depends on the interaction of epithelial cells with the extracellular matrix (ECM). So far, two primary mechanisms for lumen creation have been identified: cavitation and hollowing. During cavitation, cells in the center of spheroids undergo apoptosis, hence creating a hollow space. In contrast, during hollowing small endocytic vesicles are created that later fuse to produce a central lumen. Which of these two mechanisms is predominant depends on the interplay of various mechanical and chemical cues. In our project, we explore the influence of substrate composition and stiffness on the development of Caco-2 cell cysts. Monitoring of cyst development is facilitated by a custom-made light sheet microscope, designed for live-cell imaging of samples with a few hundred micrometers in diameter. Our preliminary data suggest that the mechanical properties of the surrounding matrix is key for the formation of a single lumen or multiple lumina in a given cell cluster.

BP 15.14 Tue 18:00 Poster F

Quantum optics meets microscopy - An ultra-sensitive resonator microscope for nano- and life sciences — •Florian Steiner, Rute Fernandes, Maerpreet Arora, and Thomas Hümmer — Ludwig-Maximilians-University Munich, Department of Physics, Munich, Germany

Isolated nanoscale systems provide only weak interaction with light due to their small size and therefore are often indirectly investigated via fluorescence microscopy. This limits insights into individual nanosystems and slows down research in the fields of nanotechnology, material science, drug design, and pharmaceutical diagnostics.

We can overcome these limitations by using of optical microresonators, a technology pioneered in quantum optics [1]. In these resonators, light strongly interacts with a sample and thereby enhances weak absorption for several orders of magnitude. The small mode waist in micro-cavities enables a scanning microscopy approach, i.e. ultra-sensitive spatially resolved absorption measurements near the diffraction limit, can be performed [2]. By optimizing the mechanical stability and by developing integrated electronics, extinction cross section of 1 nm2 can be imaged in real time. Different illumination energies allow sample characterization via their spectral profile.

The potential of the new microscope will be illustrated by examples including label free imaging of ultrathin human tissue sections [3].

1. D. Hunger et al., New J. Phys. 12, 065038 (2010) 2. M. Mader et al., Nat. Commun. 6, 7249 (2015) 3. J. Noe et al., Imaging & Microscopy 4 (2022)

BP 15.15 Tue 18:00 Poster F

MINFLUX allows measuring the Measuring Mean Back Relaxation in cells using fluorescent probes — •Tobias Deisel, Till Münker, Bart Vos, and Timo Betz — Third Institute of Physics, Georg-August Universität Göttingen, Göttingen, Germany

Living systems like cells exhibit dynamics far from thermodynamic equilibrium. In order to study such non-equilibrium systems, we need to use analytical methods beyond the classical methods developed in statistical physics. We have recently introduced the Mean Back Relaxation (MBR), which exploits a three-point probability function and is solely derived from passive measurements. A main hurdle in using the MBR is the requirement of particle trajectories with high temporal and spatial precision, that are sufficiently long to detect activity. In normal fluorescence microscopy, it is not possible to achieve this because of probe bleaching. To overcome this, we measure the MBR using MINFLUX nanoscopy, which is able to track fluorescent particles at a spatial-temporal resolution in the order of nanometers at a frequency in the order of a few kHz. This makes it an interesting tool to record detailed trajectories needed to evaluate the MBR, and paves the way to exploit the MBR even in single molecule imaging.

BP 15.16 Tue 18:00 Poster F

Motility of Salmonella Typhimurium above and within mucus — •Kevin Diestelhorst[1], Fereshteh Ghazisaeedi[2], Anton Klimek[3], Sebastian Braetz[2], Karsten Tedin[2], Marie Weinhart[1,4], Roland Netz[3], Marcus Fulde[2], and Stephan Block[1] — [1]Institute of Chemistry and Biochemistry, Freie Universität Berlin — [2]Institute of Microbiology and Epizootics, Freie Universität Berlin — [3]Department of Physics, Freie Universität Berlin — [4]Institute of Physical Chemistry and Electrochemistry, Leibnitz Universität Hannover

How do infectious agents like bacteria overcome protecting biohydrogels, such as the glycoalix or mucus? To address this question, the motion of GFP-labeled Salmonella Typhimurium in bulk solution and within hydrogels was recorded by fluorescence microscopy. A method is presented, which enables to correct the strong fragmentation of raw bacterial trajectories (caused by broad bacterial size distributions). In line with previous studies, random as well as ballistic bacterial motility is observed, the extent of which depends on the expression of key proteins. Analyzing random and deterministic features of the ballistic trajectories indicates that flagella-generated propulsion force is on the order of 100 fN per bacterium. To extend these investigations to 3D motion of bacteria across mucus, epithelial cells were cultured, leading to the formation of a native mucus layer on their apical side. The dynamics of bacterial penetration through mucus was followed by continuously recording fast 3D stacks of the cell culture. The experiments indicated that the invasion proceeded via tunnel-like structures.

BP 15.17 Tue 18:00 Poster F

Adapting your super-resolution microscope setup to the sample requirements — •Florian Schock[1,2] and Christoph Cremer[2,3] — [1]Institute for Physics, University of Mainz — [2]Kirchhoff Institute for Physics, University of Heidelberg — [3]Max Planck Institute for Polymer Research, Mainz

Several decades after the first development of super-resolution microscopy (SRM), methods to circumvent the Abbe limit of optical resolution, commercial devices have become almost standard equipment on the academical level. The introduction of commercial devices has many advantages for a wide range of users, but also means that the adaptive potential of devices developed in specialized microscopy groups is lost. Here we would like to give a brief overview of some of the possibilities and considerations necessary to serve different applications ranging from biology to materials science. In particular, we would like to point out that SRM is about methods. For example, circumventing the Abbe limit is possible even for small numerical apertures. An example of this is the SRM application in ophthalmology.

BP 15.18 Tue 18:00 Poster F

Electro-optic imaging for a lightsheet based fluorescence lifetime imaging microscope (FLIM) — •Nils Bode[1], Adam Bowman[2], Dara Dowlatshahi[3], Rose Knight[3], Soichi Wakatsuki[3], and Mark Kasevich[2] — [1]Physics Department, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 1, 91058 Erlangen, Germany — [2]Physics Department, Stanford University, 382 Via Pueblo Mall, Stanford, CA 94305, USA — [3]School of Medicine, Stanford University, 318 Campus Drive West, Clark Center, Stanford, CA 94305, USA

Electro-optic imaging enables fast fluorescence lifetime microscopy with throughputs that are $10^3 - 10^5$ times higher than those of typically used single photon counters. This enables the investigation of biological processes, like spatially resolved neuron activity and action potential propagation, that are beyond earlier systems capability. The presented electro-optic imaging setup utilizes a Pockels cell in combination with polarization splitting optics to acquire two distinct temporal gates per frame, whose ratio allows for lifetime calculation. For this work an electro-optical setup was built around a classical lightsheet microscope. This combination enables fast fluorescent lifetime imaging of volumetric samples. We used *Arabidopsis thaliana* seedlings, both labeled and label-free, as biological sample systems and performed spatial and lifetime calibration with fluorescent beads.

BP 15.19 Tue 18:00 Poster F

Visualizing Molecular Dynamics with High-Speed Tip-Scanning Atomic Force Microscopy — •Jörg BArner, Andre Körnig, Thomas Henze, and Heiko Haschke — JPK BioAFM Business, Bruker Nano GmbH, Am Studio 2D, 12489 Berlin, Germany

Biological systems exhibit very high structural and functional dynamics on molecular scales. Understanding the principles of the kinetics behind structural changes at that scale is of critical importance when studying samples ranging from single membrane proteins to complex macromolecular systems, in order to accurately develop novel therapeutic applications. We have used high-speed tip-scanning atomic force microscopy (AFM) with a kilohertz line-rate to visualize molecular dynamics by enabling temporal resolution on the sub-100-

milisecond scale. The use of a tip-scanning AFM, as compared to a sample-scanning system, enables high-resolution correlation experiments with advanced optical techniques. We will give two examples in which high-speed tip-scanning AFM was applied for studying of structural transitions and biomolecular dynamics in samples, containing triangular DNA origamis and photosensitive azobenzene-containing surfactants.

BP 15.20 Tue 18:00 Poster F

Virtual 3D Histology using Synchrotron Radiation: Present Status of GINIX, Outlook to PETRA IV — •Markus Osterhoff and Tim Salditt — Institut für Röntgenphysik, Uni Göttingen, Göttingen

We present the current state of the art of Synchrotron based phase-contrast tomography in a multi-scale setup.

In waveguide-filtered cone-beam geometry, high resolution scans (voxel sizes reaching 100 nm) reveal minute details of the specimen, at the scale of organelles. Conversely, the parallel beam geometry facilitates rapid acquisition, capturing a larger field of view, thereby integrating sub-cellular data within a broader physiological context. Thus, tomography scans with voxel sizes of 650 nm achieve a 2D in-plane resolution comparable to microscopic histology. However, as a non-invasive, fully three-dimensional technique, it eliminates the need for physical slicing of samples, resulting in isotropic 3D resolution.

We could image human lung tissue severely affected by Covid-19, and evidence diffuse alveolar damage with its prominent hyaline membrane formation. Extending conventional histopathological examination by a third dimension allows to analyse the delicate pathological changes of the vascular system of severe Covid-19 progressions.

In the future, with GINIX II we are aiming to improve biomedical x-ray tomography at better spatial resolution under physiological conditions. Notably, automated measurements and real-time analysis of raw detector images ensures balance between speed and accuracy for clinical diagnostics and research applications.

BP 15.21 Tue 18:00 Poster F

Infrared optical and thermal properties of snail shells — •Natanja Elliger[1], Bruno Gompf[1], Heinz-R. Köhler[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Physiologische Ökologie der Tiere, Institut für Evolution und Ökologie, Universität Tübingen, 72076 Tübingen, Germany

Land snails of arid habitats endure intense sunlight for months without overheating although their body is surrounded by a closed shell with its aperture sealed, minimising possible evaporative cooling. The thermoregulation process that enables land snails to withstand high temperatures is yet unknown. In a systematic investigation, we study the relationship between the optical and infrared optical properties and the thermodynamic properties to the underlying nano-/microstructures of the shells. We employ FTIR reflection measurements as well as absorption (photoacoustic) measurements in the Mid-IR to VIS spectral range on snails from different habitats. Additionally, we perform scatterometry in the NIR to VIS spectral range to investigate the diffuse reflection and possible Lambertian behaviour. With the combination of these techniques, we hope to gain a thorough understanding of how snails keep their houses up to 10°C colder than the stones nearby.

BP 15.22 Tue 18:00 Poster F

Rate-independent hysteretic energy dissipation in collagen fibrils — •Martin Dehnert, Paul Zech, Alexandra Bendixen, Andreas Otto, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

Nanoindentation cycles measured with an atomic force microscope on hydrated collagen fibrils exhibit a rate-independent hysteresis with return point memory. This previously unknown energy dissipation mechanism describes in unified form elastoplastic indentation, capillary adhesion, and surface leveling at indentation velocities smaller than $1\,\mu$m/s, where viscous friction is negligible. A generic hysteresis model, based on force–distance (FD) data measured during one large approach-retract cycle, predicts the force (output) and the dissipated energy for arbitrary indentation trajectories (input). While both quantities are rate-independent, they do depend nonlinearly on the indentation history and on the indentation amplitude. We present different types of cyclic FD measurements performed on native collagen fibrils in humid air. The energy dissipation is mainly caused by plastic deformation during tip indentation and it can be quantified with the plasticity index. The latter can be used for high-resolution mapping of connective tissues.

BP 15.23 Tue 18:00 Poster F

Haptic Perception of Nanomechanical Surface Properties — •Paul Zech, Martin Dehnert, Alexandra Bendixen, Andreas Otto, and Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

In the realm of analyzing and presenting scientific data, scientists heavily rely on their visual perception. Graphical representations of data, either as diagrams or tables, appear to be the standard approach. Here, we present a method for exploring nanomechanical properties on the human scale through haptic perception. This methodology opens up the possibility of utilizing multiple human senses simultaneously when analyzing data. We use a haptic device to translate the tip–sample interaction forces measured with an atomic force microscope (AFM) on the nanometer scale into forces perceivable by humans. In doing so, we introduce a generic rate-independent hysteresis model that describes sequences of mechanical phenomena occurring in AFM-based nanoindentation experiments, including plastic indentation, elastic response, capillary adhesion, and surface leveling. This model accurately describes the complex nanomechanical behavior of collagen fibrils in native tendon, and it is also applicable to other soft materials. As an example for human tissues, we demonstrate the interactive haptic exploration of gelatin droplets at different relative humidities. This allows to vary the mechanical properties of gelatin over a large range, from a stiff solid to a very soft gel.

BP 15.24 Tue 18:00 Poster F

Influence of water content on nanomechanical properties of native tendon tissue — •Mario Zerson, Martin Dehnert, Paul Zech, and Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Water is an essential component of natural tissues, providing elasticity to collagen fibrils and their interfibrillar matrix. Atomic force microscopy (AFM) in humid air enables high-resolution imaging of the nanomechanical properties of collagen fibrils in native tendons. Accurate control of humidity and temperature is essential for reproducible measurements of nanomechanical properties in AFM-based nanoindentation experiments. Here we report on the influence of relative humidity on the nanomechanical properties of native tendon tissue obtained from the calcaneus (Achilles) tendon of chickens. The sample is exposed to a flow of humid air with controlled relative humidity and force–distance data are measured. We use the same tip on the same collagen fibrils for different levels of relative humidity. This eliminates variation due to differences in tip shape and different tissue samples. Our data show the variation of effective indentation modulus and plasticity index as a function of relative humidity in the range of 40 to 95%. We compare these results with analogous experiments on gelatin films.

BP 15.25 Tue 18:00 Poster F

Triacylglycerides influence water content and nanomechanical properties of collagen fibrils — Martin Dehnert, •Tiberius Klose, Yang Pan, Dietrich R. T. Zahn, and Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Lipids are an essential component of connective tissue, which includes tendons, ligaments and cartilage. They act as lubricants in joints and tendons, with a major component being triacylglycerides. In cases of excess adiposity and other diseases, excess cholesterol is found in tendons, where it forms granular domains (xanthoma). However, the presence and effect of lipids in natural (healthy) collagen fibrils is poorly understood. Here, we show that collagen fibrils extracted from chicken calcaneal (Achilles) tendon contain triacylglycerides that influence the nanomechanical properties and water uptake of the fibrils. After extracting the lipids with organic solvents, we measure an increased swelling behavior and an increased indentation modulus in collagen fibrils using atomic force microscopy. With Raman spectroscopy, we identify triacylglycerides as the major lipid component. Our results demonstrate that triglycerides are an essential component of the natural collagen fibril structure, where they act as plasticizers and mediate the fibril's water content and mechanical properties. This methodology could be used to investigate the influence of lipids on the biomechanical properties of connective tissues during development, ageing, and diseases. In particular, the effect of nutrition, which has a major influence on lipid balance, could be studied.

BP 15.26 Tue 18:00 Poster F

Simulating synthetic, DNA-based systems across differ-

ent scales — •Aaron Gadzekpo[1], Xenia Tschurikow[1], Mai Tran[2], Rakesh Chatterjee[3,4], Vasily Zaburdaev[3,4], Kerstin Göpfrich[2], and Lennart Hilbert[1] — [1]Karlsruhe Institute of Technology — [2]Max Planck Institute for Medical Research — [3]Max Planck Zentrum für Physik und Medizin — [4]Friedrich-Alexander Universität Erlangen-Nürnberg

Molecular dynamics (MD) simulations at different scales can aid in the design and characterisation of synthetic biological systems. Combining coarse-grained MD-simulations with experiments allowed us to explain how the shape of droplets formed by self-interacting DNA-nanomotifs responds to adding increasing concentrations of amphiphilic nanomotifs. Currently, we are investigating how DNA-strands can serve as condensation surfaces for droplet formation at subsaturated nanomotif concentrations. To accurately simulate microscopic aspects of our DNA-based systems, such as transient hybridisation that underlies nanomotif interactions, we employ simulations at resolutions of one to a few nucleotides. Capturing macroscopic behaviour, such as phase separation, requires simulating larger systems sizes and time scales, for which we develop models averaging many nucleotides. We present ongoing research aimed at integrating simulations at different scales for model-guided design of synthetic, DNA-based systems.

BP 15.27 Tue 18:00 Poster F

How Crowding and Confinement change the Phase Behavior of Intrinsically Disordered Nuclear Proteins — •Janka Bauer[1], Dorothee Dormann[2,3], and Arash Nikoubashman[1,4,5] — [1]Institute of Physics, JGU Mainz, Germany — [2]Biocenter, Institute of Molecular Physiology, JGU Mainz, Germany — [3]Institute of Molecular Biology, Mainz, Germany — [4]Leibniz-Institut für Polymerforschung, Dresden, Germany — [5]Institut für Theoretische Physik, Technische Universität Dresden, Germany

The liquid-liquid phase separation of intrinsically disordered proteins plays an integral part for the formation of membraneless organelles in cells, which in turn have key functional and regulatory roles. Many studies on LLPS focus on in vitro experiments and bulk simulations in solution, but real-life systems are highly influenced by crowding within a cell as well as the confinement by the cell membrane. To mimic more closely conditions prevalent in cellular environments, we perform coarse-grained molecular simulations [1] of the low-complexity domains of heterogeneous nuclear ribonucleoprotein A1 (hnRNPA1) and Fused in Sarcoma (FUS) in spherical confinement, where we systematically vary the fraction of the crowding agent polyethylene glycol (PEG). We further elucidate how the elasticity of a PEG network influences and even limits size and mobility of the protein condensates.

BP 15.28 Tue 18:00 Poster F

Structural motif stability of bacteriophage MS2 RNA packaging signals upon changes in their flanking sequence — •Veronika Bukina[1,2] and Anže Božič[1] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]University of Ljubljana, Slovenia

The RNA motifs can be responsible for specific important functions. For instance, in bacteriophage MS2, they serve as packaging signals (PSs), which play a crucial role in binding viral coat proteins during capsid assembly. This work aims to analyze motif structural stability on the example of the well-studied MS2 virus. As a consequence of current experimental studies, which reveal the multiple putative PS sites across the MS2 RNA genome, we focus on 14 RNA motifs of the virus, including the most widely known TR hairpin. The study of motif stability involves manipulating the flanking sequences surrounding them and comparing various measures calculated from their secondary structure, such as structure probability, ensemble defect, and Shannon entropy. To verify the tertiary structures of these RNA segments, the oxDNA software is employed. Our results show the stability of certain motifs regardless of the presence or absence of sequences around them, even when the nucleotide content of flanking sequences is randomized. Conversely, other unstable motifs are stabilized by genome or flanking sequences that tell us about the importance of the particular structure as well as of the genome sequence. The outcome of this work is beyond viral PS structural stability, extending to applications in RNA binding protein (RBP) studies and more.

BP 16: Membranes and Vesicles II

Time: Wednesday 9:30–12:30 Location: H 0112

BP 16.1 Wed 9:30 H 0112

Structural changes in lipid monolayers induced by synapsin and vesicles investigated by X-ray reflectivity and GID — Hendrik Bruns[1], •Titus Czajka[1], Charlotte Neuhaus[1], Christian Hoffmann[2], Dragomir Milovanovic[2], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Georg-August-Universität Göttingen, Germany — [2]Laboratory of Molecular Neuroscience, DZNE, Berlin, Germany

Neurotransmitter release happens upon fusion of synaptic vesicles (SVs) carrying the neurotransmitter with the presynaptic membrane. SVs act as the trafficking organelles and are clustered in pools to facilitate the rapid release of neurotransmitters into the synaptic cleft. While the process of SV fusion mediated by SNARE complexes is well understood, the influence of the vesicle pool and its mediating protein, synapsin, on the membrane-vesicle interaction is less clear. To this end, we have carried out X-ray reflectivity (XRR) and grazing incidence diffraction (GID) experiments on lipid monolayers at controlled surface pressures in a Langmuir trough at ID10 (ESRF). Interaction between monolayer and SVs is measured in the monolayer plane by GID measurements, allowing the measurement of lipid molecule tilt angles. Density profiles modelled to fit the XRR data additionally reveal changes in the structure along the third dimension. We hypothesise that synapsin protein has a stiffening influence on the monolayer and also strengthens the interaction between monolayer and SVs, thus highlighting the importance of the protein not only to the clustering of SVs but potentially to the docking process as well.

BP 16.2 Wed 9:45 H 0112

Physics and slowerance of the erythrocyte sedimentation rate — •Alexis Darras, Thomas John, Lars Kaestner, and Christian Wagner — Saarland University, Saarbruecken, Germany

Red blood cells (or erythrocytes) sedimentation rate (ESR) is a physical parameter of blood which is often checked in medical diagnosis. It is indeed well known that in case of inflammation, the increase in fibrinogen and other proteins induces a higher ESR. A higher ESR is clinically established as a disease marker. Recently, we demonstrated that Red Blood Cells (RBCs), when left at rest and suspended at physiological volume fractions, form percolating aggregates as wide as the container. It follows that they sediment following a so-called " gel collapse", governed by the geometry of the percolating aggregate acting as a porous material. In this talk, by comparing physical models to experimental sedimentation curves, we show how this knowledge can help to quantify physically meaningful parameters that characterize the details of the collapse dynamics. Amongst others, we provide a dependency of the maximal sedimentation velocity as a function of the initial RBC volume fraction (i.e. the hematocrit), which was a long-sought correction for ESR measurements from anemic patients. We also review how those parameters make it possible to experimentally distinguish between healthy samples and some conditions where the ESR is slowed down. In particular, this opens new perspective to use the ESR as an objective marker to detect diseases where the RBCs are deformed and/or rigidified.

BP 16.3 Wed 10:00 H 0112

Origin of red blood cell slippers in confined geometries — •Berin Becic and Stephan Gekle — Biofluid Simulation and Modeling, Department of Physics, University of Bayreuth, Bayreuth, Germany.

Red blood cells flowing in confined geometries such as blood vessels or microchannels exhibit fascinatingly rich dynamics. The two main types of motion are a stationary parachute-like state and the so-called slipper state. The main characteristic of the latter is the steady rotation of its membrane. As a result the current understanding of this state relates it closely to the similarly rotating tank-treading state in pure shear flows.

Based on a numerical approach we here show that this analogy is inaccurate and that instead the slipper mode is more closely related to the tumbling mode in shear flows. In channel flow, tumbling be-

comes partly suppressed due to flow curvature thus creating the slipper mode. We obtain this insight by using a boundary-integral simulation technique which allows us to systematically dissect the contribution of different flow components (linear and/or parabolic in different directions) as well as the influence of the confining walls.

BP 16.4 Wed 10:15 H 0112

Molecular Origin of Plasma Membrane Heterogeneity and its Function — •Madhusmita Tripathy[1,2] and Anand Srivastava[1] — [1]Molecular Biophysics Unit, IISc Bangalore, India — [2]Department of Chemistry, TU Darmstadt, Germany

Plasma membrane(PM) heterogeneity has long been implicated in various cellular functions such as cell signaling and vesicle trafficking. However, their molecular origin and mechanistic principles governing their function are not well understood, as their nanoscopic and highly dynamic nature limit both direct experimental measurements and their interpretation. Toward this, we employ computer simulation to study model membranes with coexisting liquid ordered (Lo) and liquid disordered (Ld) phases. We characterize membrane heterogeneity using a non-affine deformation framework [1] and probe the three-dimensional lipid packing defects [2], both of which can be considered as conjugates. In doing so, we formalize the seemingly trivial connection between membrane packing and local membrane order. We use this connection to explore the mechanistic principles behind preferential localization of proteins in mixed phase membranes and membrane permeability of small molecules. Our observations suggest that heterogeneity in liquid membranes follow some generic features, where functions may arise based on packing-related basic design principles [3].

[1] S. Iyer, M. Tripathy and A. Srivastava *Biophys. J.***(2018)** 115, 117
[2] M. Tripathy, S. Thangamani and A. Srivastava *J. Chem. Theory Comput.***(2020)** 16, 12, 7800
[3] M. Tripathy and A. Srivastava *Biophys. J.***(2023)** 122, 13, 2727

BP 16.5 Wed 10:30 H 0112

Mesoscopic modeling for protein-membrane interplay with realistic kinetics — •Mohsen Sadeghi — Freie Universität Berlin

Biomembranes achieve their multitude of functions in an organized and collaborative interplay with membrane-associated proteins. Quantitative analysis of the dynamics of membranes interacting with a population of proteins in a consistent model that incorporates kinetics as well as protein structural information and flexibility is essential in fully describing these processes. Achieving this paves the way for understanding and potentially manipulating complex vital pathways. Here, we present our dynamic framework for modeling membranes and proteins [1, 2], which includes our novel approach to hydrodynamic coupling [3]. We present results on the dynamics of membrane-bound toxins [4,5,6], and the first computational model of the whole human cytomegalovirus particle, highlighting the organization of proteins in the viral tegument [7]. We make the case for how large-scale mesoscopic simulations offer unprecedented insight into the complex cellular dynamics, and provide access to spatiotemporal scales relevant to cell biology.

[1]. Sadeghi & Noé, Nat. Commun. (2020) 11:2951. [2]. Sadeghi, Weikl & Noé, J. Chem. Phys. (2018) 148:044901. [3]. Sadeghi & Noé, J. Chem. Phys. (2021) 155:114108. [4]. Sadeghi & Noé, J. Phys. Chem. Lett. (2021) 12:10497-10504. [5]. Sadeghi, Soft Matter (2022) 18:3917-3927. [6]. Sadeghi, bioRxiv (2023) 2022.11.09.515891. [7]. Bogdanow, et al. Nat. Microbiol. (2023) 8:1732.

15 min. break

BP 16.6 Wed 11:00 H 0112

Dense membrane packings: Predicting optimal configurations — •Stefanie Heyden[1] and Michael Ortiz[2] — [1]ETH Zurich, 8093 Zurich, Switzerland — [2]Caltech, Pasadena CA 91125, USA

In which way does a membrane fold to minimize its elastic energy? This question is directly tied to a better understanding of membrane packings encountered in nature, as well as facilitating the design of soft structures.

Here, we present a simple mathematical framework to predict optimal packing configurations of densely packed membranes. Membranes are represented by means of a director field and the corresponding boundary value problem is derived. Numerical solutions show foliations comprising many closed surfaces, based on which a distribution of cuts is introduced to minimize the total crease energy.

BP 16.7 Wed 11:15 H 0112

Coarse-grained Simulations of Fibril Formation on Local Structures of Two-Component Membranes — •Paul Louis Sonek and Friederike Schmid — Johannes Gutenberg University, Mainz, Germany

The cell membrane is one of the most essential parts of the cell. It consists of different components, such as phospholipids and cholesterol, forming local membrane domain structures. It has been hypothesized that many neurodegenerative diseases like Alzheimer's, Huntington's, and Parkinson's might be associated with a disturbance of the cell membrane induced by fibril formation of peptides.

In our research, we use generic coarse-grained lipid and peptide models to inspect the fibril formation near the local domain structures of our model membrane. The fibrils form primarily on top of the membrane for configurations with low amounts of our model cholesterol. However, we can observe that fibrils partly nucleate into the membrane for configurations with large amounts of cholesterol, seemingly forming an aggregate that disrupts the membrane structure. This observation correlates with the fact that membranes in the brain have larger amounts of cholesterol.

Our results may shed light on possible mechanisms responsible for the toxic effects of amyloids.

BP 16.8 Wed 11:30 H 0112

Quantification of mRNA and siRNA content of Lipid Nanoparticles — •Bernhard Kirchmair[1], Judith Müller[1], Thomas Kellerer[2], and Joachim Rädler[1] — [1]Ludwig-Maximilians-Universität München — [2]Hochschule München

Lipid Nanoparticles (LNPs) have been proven to be promising vectors to deliver mRNA to mammalian cells. Advanced strategies using multi-component nucleic acid motifs require a reliable quantification of the stoichiometric ratios. This project seeks to quantify the mRNA-content when varying the LNP size and surface composition. Employing Fluorescence Correlation Spectroscopy (FCS) measurements, assisted by Dynamic Light Scattering (DLS), both size and concentration of LNPs in solution can be estimated, allowing to obtain the average number of mRNA strands per particle. Based on this, using Fluorescence Cross Correlation, the stoichiometric ratio of short interfering RNA (siRNA) and mRNA, both fluorescently labeled, will be determined. Controlled co-formulation of siRNA and mRNA is expected to allow for regulated mRNA expression.

BP 16.9 Wed 11:45 H 0112

Interplay of phospholipids and saponins - why the application of complementary techniques is important — •Carina Dargel[1,2], Friederike Gräbitz-Bräuer[2], Lionel Porcar[3], and Thomas Hellweg[2] — [1]University of Münster, Institute of Physical Chemistry, Münster, Germany — [2]University of Bielefeld, Physical and Biophysical Chemistry, Bielefeld, Germany — [3]Institut Laue-Langevin (ILL), Grenoble, France

Scattering methods are a common tool to analyze structural changes in systems comprising, e.g., phospholipids mixed with natural surfactants such as saponins. Small-angle X-ray and neutron scattering (SAXS and SANS) have been extensively used to study the interaction of the saponins glycyrrhizin and aescin with the phospholipid 1,2-dioleoyl-*sn*-glycero-3-phosphoglycerol (DOPG), which carries a negatively charged head group. While for a small unilamellar vesicle (SUV) system prepared from the zwitterionic lipid 1,2-dimyristoyl-*sn*-glycero-3-phosphocholine (DMPC), membrane solubilization and thus bicelle formation was observed upon saponin addition[1], hardly any interaction could be detected for the DOPG-saponin mixtures[2,3]. Instead, DOPG SUVs coexist with saponin micelles/monomers. The investigated system clearly demonstrates the importance of using complementary techniques such as SAXS and SANS to avoid misleading conclusions from only a single method.

[1] Geisler *et al.* (2019), *Molecules*, 25(1), 117.; [2] Dargel *et al.* (2021), *Molecules*, 26(16), 4959; [3] Gräbitz-Bräuer & Dargel *et al.* (2023), *Colloid and Polymer Science*, 1-14

BP 16.10 Wed 12:00 H 0112

Application of Homogenization Techniques to Gas-Phase Deposited DPPC Films on Silicon Substrates: Unveiling Phase Transitions in Dry Environments of DPPC Bilayers — •Nicolás Moraga[1], Daniel Saavedra[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], María José José Retamal[3], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Universidad de Valparaíso, Chile — [3]Facultad de Ingeniería,

Universidad Finis Terrae, Santiago, Chile

The study investigates homogenization techniques for dipalmitoylphosphatidylcholine (DPPC) phospholipid bilayers deposited on single crystal silicon substrates through vapor phase deposition. Initial deposition employed physical vapor deposition (PVD) with controlled thickness and rate. Subsequent annealing, conducted in varied environments (in air and dry N2 at STP, vacuum), and temperature ramps in a dry N2 atmosphere (different pressures up to 1000 Torr) were explored as homogenization methods. The research emphasizes the critical role of precise and reproducible deposition rates during annealing in achieving homogeneity in DPPC bilayers. Different annealing conditions led to diverse effects on homogeneity, indicating distinct outcomes in air, nitrogen environments at different pressures, and high vacuum. The study revealed not only topographical changes but also documented phase transitions, suggesting the formation of lipid bilayers even in dry environments without the need for hydration. Acknowledgements: ANID Fellowships (NM, DS, NGV).

BP 16.11 Wed 12:15 H 0112

RNA adsorption dynamics onto membrane models for lipid nanoparticles — •Horacio V. Guzman — Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

RNA is a functionally rich molecule with multilevel, hierarchical structures and complex dynamics in the presence of different substrates. Much remains to be elucidated in terms of the RNA conformations and specific molecular interactions that modulate its adsorption to lipid membranes. Lipid nanoparticles (LNPs) are particularly promising as mRNA delivery medium due to their remarkable ability to transport genetic material to targeted cells. Yet, the design of LNPs remains challenging, owing to poorly understood mechanisms and factors that modulate RNA and LNP adsorption to membranous substrates. In our study, we perform an exhaustive modeling exploration of the influence of membrane composition on the adsorption behavior and conformation of an RNA fragment. Our approach is based on all-atom molecular simulations, including five distinct membrane models with lipid composition selected from commercially available LNPs. The membrane models account for crucial variables, such as surface charge, topological features, unsaturation degree of the fatty acid tails, and cholesterol content. Our results elucidate RNA adsorption modes and associated membrane response. We characterize adsorption dynamics in light of structural analysis for RNA, reorganization of membrane surface charge, as well as changes in the hydrophilic/hydrophobic interactions, which bear profound implications for enhancing their stability.

BP 17: Bioimaging

Time: Wednesday 9:30–12:45 Location: H 2032

BP 17.1 Wed 9:30 H 2032

X-ray tomography techniques for predicting medical implants performance — •Tatiana Akhmetshina, Robin E. Schäublin, Andrea M. Rich, and Jörg F. Löffler — Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland

Mg-based temporary implants that can be resorbed after fracture healing are beneficial for patients and necessary in certain clinical applications. However, since Mg reacts with body fluids and dissolves, we need reliable data to predict the implants performance in vivo. X-ray tomography techniques can provide valuable insights into the degradation behavior, but they also show limits in materials characterization. While absorption contrast works very well for some materials, in Mg-based alloys we often have features (second-phase particles) that cannot be resolved due to their low contrast. Additionally, the resolution required to characterize the material and understand the microstructure-property relationships is below 100 nm. In this study, we compare two distinct X-ray tomography techniques (Zernike and ptychography) to examine their advantages and disadvantages and present a case study focused on Mg-based alloys (WE43 and Mg-Ca: X0). Our results show that ptychographic tomography resolves features of less than 10% difference in their densities, such as a Mg2Ca phase in a Mg-Ca alloy, which is not possible with the Zernike. The 3D resolution reached is 23 nm, which allowed us to distinguish fine microstructural details. This illustrates the suitability of ptychographic X-ray computed tomography for the characterization of Mg alloys.

BP 17.2 Wed 9:45 H 2032

Helium Ion Microscopy for Morphological Analysis of Thrombi Extracted via Thrombectomy for Acute Stroke — •Michael Westphal[1], Natalie Frese[1], Clemens Sommer[2], Alkisti Kitsiou[3], Wolf-Rüdiger Schäbitz[3], André Beyer[1], and Armin Gölzhäuser[1] — [1]University Bielefeld — [2]Institut für Neuropathologie, Universitätsklinik Mainz — [3]Universitätsklinik für Neurologie, Evangelisches Klinikum Bethel gGmbH, Universitätsklinikum OWL

Strokes are one of the leading causes of death in the aging Western society. Especially in elderly patients, strokes are frequently recurring events. An essential component of stroke management after acute therapy is to diagnose the cause of the stroke forsecondary prevention. More than 50 thrombi extracted via thrombectomy were examined by chargecompensated helium ion microscopy to investigate possible correlations between their morphology and the origin.

BP 17.3 Wed 10:00 H 2032

The behaviour of vital mitochondria in response to nanoprobing using Scanning Ion Conductance Microscopy (SICM) — •Eric Lieberwirth[1], Christian Völkner[1], Regina Lange[1], Anja Schaeper[2], Magdalena Otte[2], Rica Waterstradt[2], Annett Kott[2], Ingo Barke[1], Simone Baltrusch[2], and Sylvia Speller[1] — [1]University of Rostock, Institute of Physics — [2]Rostock University Medical Center, Institute of Medical Biochemistry and Molecular Biology

The mitochondrial network maintains contacts with cell organelles such as the peroxisome, endoplasmic reticulum (ER) or cytoskeleton, but also undergoes constant remodelling of its structure and shape. In order to understand the processes further, we examine vital, metabolizing mitochondria extracted from HeLa cells using the non-contact Scanning Ion Conductance Microscope (SICM). The lateral resolution is approx. 50 nm - 100 nm and the resolution in the z-direction is approx. 1 nm. Besides the known diversity of shapes of the mitochondrial network, simple image processing techniques are sufficient to visualize structures, compatible with cristae folds. We observed a peculiar effect at the edges of mitochondria which decreases with time and which we interpret as a signature of vitality. An attempt of interpretation is based on the mistaking of the glass nanopipette probe as an organelle, e. g. as ER or microtubule.

BP 17.4 Wed 10:15 H 2032

High-resolution chemical imaging in mid-infrared photo-induced force microscopy (PiF-IR) — •Maryam Ali[1], Selema Buzhala[1,2], Sebastian Unger[1,2], Christoph Krafft[1,2], Rainer Heintzmann[1,2], and Daniela Täuber[1,2] — [1]Friedrich Schiller University, Jena — [2]Leibniz Institute of Photonic Technology, Jena, Germany

Non-contact force microscopy is able to report changes in the attractive Van-der-Waals (VdW) force between a metallic tip and a sample. In mid-IR photo-induced force microcopy (PiF-IR), thermal expansion due to absorption leads to a change in the VdW force, which is reported via a heterodyne detection scheme. This results in an unprecedented resolution < 5 nm for chemical imaging of surfaces including bacteria walls and cellular tissue[1]. In biomaterials, important chemical variations have to be identified above a rather heterogeneous background. Topological Data Analysis (TDA) is a promising approach for extracting signals of interests in hyperspectral PiF-IR images. We compare the analysis using TDA with other approaches including Principal Component Analysis (PCA), Hierarchical Clustering Analysis (HCA) and to a guided approach using known spectral components. [1] J. Joseph, L. Spantzel, M. Ali, D. Moonnukandathil Joseph, S. Unger, K. Reglinski, C. Krafft, A.-D. Müller, C. Eggeling, R. Heintzmann, et al., Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 2024, 306, 123612.

Invited Talk BP 17.5 Wed 10:30 H 2032

Red photocontrollable fluorescent proteins in nanoscopy — •Francesca Pennacchietti — KTH Royal Institute of Technology, Stockholm, Sweden

The observation of organelles dynamics and macromolecular complex interactions inside living cells and tissues, requires minimally invasive imaging strategies. In this context, photocontrollable fluorescent proteins (FPs) play a crucial role as tags in optical super-resolution microscopy and functional live cell imaging. To this end we have previously shown that reversibly switchable FPs enable fast (1 Hz for a 50 x 50 um2) and gentler (< 1 kW/cm2) nanoscopy (Masullo et al, Nat Comm, 2018). Additionally, irreversibly photoconvertible FPs can achieve photolabeling with high spatiotemporal precision. Nevertheless, their photophysical complexity poses some challenges in expanding such techniques toward multiplexing and in vivo imaging. Here, we explore novel photoswitching mechanism for fluorescent proteins in the red and near-infrared region of the spectra and assess their compatibility with live cell imaging at the nanoscale (Pennacchietti et al, Nat. Meth, 2018). Finally, we present strategies to combine the spectral and photophysical fingerprint of distinct photocontrollable FPs to achieve multiplexing in live cell imaging at the nanoscale and photolabeling studies (Pennacchietti et al, Nat Comm, 2023).

15 min. break

BP 17.6 Wed 11:15 H 2032

eSRRF: Super-resolution radial fluctuation is going 3D — R. F. Laine[1], •H. S. Heil[2], S. Coelho[2], J. Nixon-Abell[3], A. Jimenez[4], T. Wiesner[4], D. Martinez[2], T. Galgani[5], L. Régnier[5], A. Stubb[6], G. Follain[6], S. Webster[7], J. Goyette[7], A. Dauphin[5], A. Salles[8], S. Culley[1], G. Jacquemet[6], B. Hajj[5], C. Leterier[4], and R. Henriques[2] — [1]UCL, London, UK — [2]IGC, Oeiras, PT — [3]Cambridge University, Cambridge, UK — [4]CNRS-AMU, Marseille, FR — [5]Institut Curie, Sorbonne Université, Paris, FR — [6]University of Turku and Åbo Akademi University, Turku, FI — [7]University of New South Wales, Sydney, AU — [8]Institut Pasteur, Université de Paris, Paris, FR

Fluctuation-based image reconstruction extracts super-resolution details from brief wide-field image sequences, even under low light conditions (Gustafsson, Nat. Com. 2016). In the latest eSRRF version (Laine & Heil, Nat. Methods 2023, 10.1038/s41592-023-02057-w), reconstruction fidelity is significantly improved, with automated parameter optimization for image fidelity and resolution, crucial for avoiding artifacts (Culley, Nat. Methods 2018) and reducing user bias. While eSRRF excels in 2D super-resolution across microscopy techniques and biological systems, we've expanded its capability to 3D imaging.

For high-fidelity 3D live-cell nanoscopy with eSRRF, simultaneous detection of fluorescence fluctuations across multiple focal planes is crucial, achieved through a multifocus microscope (MFM, Hajj, PNAS 2014). This method allows volumetric super-resolution imaging of live cells at ~ 1 vol./s.

BP 17.7 Wed 11:30 H 2032

Quantitative visualisation immune cell interactions in complex three-dimensional environments — •Anna Schepers[1,2], Narain Karedla[1,2], Joannah Fergusson[2], Helena Coker[2], Kaitlyn Purdie[3], Robert Koechl[2], and Marco Fritzsche[1,2] — [1]The Rosalind Franklin Institue, Harwell, UK — [2]Kennedy Istitute of Rheumatology, Oxford, UK — [3]King's College London, UK

The intricate dynamics of the immune system, regulated by diverse cell interactions across tissues, present challenges for multiscale and real-time observation of the immune response, from tissues down to single cells and subcellular structures. A technological leap has been achieved with the introduction of lattice light sheet (LLSM) technology, allowing fast and gentle imaging of live samples while achieving subcellular resolution. By complementing LLSM-based volumetric imaging with advanced sample handling of biomimetic systems, *ex vivo* tissue samples, and custom-built fluidics, we provide a system that preserves critical physiological complexity. The perfusion system provides the necessary control over O_2 and nutrient supply while, at the same time, enabling imaging of the perfused samples. We show that in our setup, we can follow single cells and their interactions in volumes several cell layers deep in living samples within their environment, providing nuanced insights into the immune response.

BP 17.8 Wed 11:45 H 2032

Video-rate volumetric fluorescence lifetime imaging of living multicellular systems using single-objective lightsheet microscopy — •Valentin Dunsing-Eichenauer[1], Johan Hummert[2], Claire Chardès[1], Felix Koberling[2], Ivan Michel Antolovic[3], Léo Guignard[1], and Pierre-François Lenne[1] — [1]IBDM & CENTURI, Aix-Marseille University/ CNRS, Marseille, France — [2]PicoQuant GmbH, Berlin, Germany — [3]Pi Imaging Technology SA, EPFL Innovation Park, Lausanne, Switzerland

Fluorescence lifetime imaging microscopy (FLIM) is a widely used technique for functional and multiplexed bioimaging. It is commonly performed on confocal laser scanning microscopes equipped with time correlated single photon counting hardware. However, high excitation powers or long acquisition times are needed to obtain sufficient photon statistics, preventing applications on sensitive living specimen such as embryos or organoids. To overcome these limitations, we have combined single objective lightsheet microscopy with pulsed excitation and time-resolved detection on a 512x512 pixel gated SPAD array detector. We report excellent quantitative agreement with confocal FLIM at 100-1000-fold shorter acquisition times, down to 150 ms per image. We further demonstrate 3D FLIM on live embryonic organoids, lifetime unmixing of two spectrally overlapping fluorophore species, and time-lapse 3D FLIM of mechanosensitive tension probes. Our approach facilitates volumetric FLIM at unprecedented speed and throughput, providing a powerful tool for functional imaging of dynamic multicellular systems.

BP 17.9 Wed 12:00 H 2032

CRISPR screen to improve the optical properties of living tissues — •Susan Wagner, Venkat R. Krishnaswamy, Kaushikaram Subramanian, Heike Petzold, Benjamin Seelbinder, and Moritz Kreysing — Institute of Biological and Chemical Systems - Biological Information Processing, KIT, Karlsruhe

Optical microscopy has been massively advanced to deliver unprecedented resolution allowing discoveries down to the molecular level. Nevertheless, optical access of living biological samples by microscopes is usually restricted to the outer most surface owing to tissue-induced light scattering.

We successfully improved the optical properties of mammalian cells and found that evolved transparency frequently goes along with the reduction of nuclear granularity, while the gene expression profile reflects scattering properties of cells. To genetically clear living mammalian tissues, we are conducting a genome-wide CRISPR activation screen to find those genes which confer transparency.

As a next step, we are investigating how improved optical properties of individual cells influence the optical properties of 3D cell clusters, such as spheroids, using interspersed fluorescent microspheres to quantify imaging quality.

Understanding the full range of a tissue's optical plasticity will provide us with a broad toolkit, so that different genetic strategies can be applied depending on the specific nature of the various biological samples.

BP 17.10 Wed 12:15 H 2032

Illuminating Real-Time Plant Health: Optical Insights into Detecting Plant Stress and Metabolism Transitions — •Katarina Miletic[1], Marija Petković-Benazzouz[1], Sara Ristic[1], Dejan Jeremic[2], and Becko Kasalica[1] — [1]University of Belgrade, Faculty of Physics, Department of Metrology and Applied Physics, Studentski trg 12, 11000 Belgrade, Serbia — [2]University of Belgrade, Innovation Center of the Faculty of Chemistry, Studentski trg 12, 11000 Belgrade, Serbia

Global food security faces threats from plant stress caused by environmental factors. Traditional assessment methods are often invasive, time-consuming, and lack temporal resolution.

A novel developed nondestructive optical sensing method offers real-time insights into plant stress induced by light intensity, water scarcity, nutritional deficiency, and pathogen infection. This approach captures the values of the optical transmission coefficients, representing optical responses through the leaves of the plants, and presents them in graphs depicting the time dependence of circadian rhythms. The method, tested on various plants under diverse stressors, reveals distinct circadian rhythm changes, successfully detecting nutrient deficiencies, early pathogen presence, and metabolic shifts.

This innovative approach, providing continuous monitoring without causing harm to plants, holds significant potential for advancing plant research and improving agricultural practices.

BP 17.11 Wed 12:30 H 2032

Characterizing of complex random media and biologigal tissue with self-consistent quantum field theory — Andreas Lubatsch[1] and •Regine Frank[2,3] — [1]Physikalisches Institut, Rheinische Friedrich Wilhelms Universitaet Bonn — [2]College of Biomedical Sciences, Larkin University, Miami, Florida, USA — [3]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain

We present a quantum field theoretical method for characterizing disordered complex media with short laser pulses and (OCT). We introduce weighted essentially non-oszillatory solvers (WENO) for the analysis of highly nonlinear and discontinuous processes including interference effects and Anderson localization of light in time-of-flight (ToF) and pump-probe experiments. The results are a measure of the coherence of multiple scattering photons in passive matter as well as in soft matter and biological tissue.

[1] A. Lubatsch, R. Frank, Phys. Rev. Research 2, 013324 (2020) [2] D. Huang, et. al., Science 254, 1178 (1991) [3] K. C. Zhou, et. al., Nat. Photon. 13, 794 (2019)

BP 18: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Wednesday 9:30–13:00 Location: H 1028

Invited Talk BP 18.1 Wed 9:30 H 1028

Production and applications of artificial spider silk fibers and hydrogels — •Anna Rising — Department of Anatomy Physiology and Biochemistry Swedish University of Agricultural Sciences Uppsala 75007, Sweden — Department of Biosciences and Nutrition, Karolinska Institutet, Neo, Huddinge 14183, Sweden

Spider silk, nature's high-performance fiber, represents an attractive material for many different applications. However, production of the spider silk proteins (spidroins) is problematic due to their repetitiveness and propensity to aggregate.

We have developed a E.coli based production method that generates unprecedented amounts of correctly folded and soluble spidroins. A biomimetic spinning method combined with a protein engineering strategy, result in artificial spider silk fibers that match the toughness of native spider silk. The fibers have successfully been used to guide the extension of neurites in cell culture assays.

In addition, we have discovered that the recombinant spidroins rapidly form self-supporting and transparent hydrogels when incubated at 37 °C. The gelation is associated with the formation of nano-sized fibrils, and spidroin fusion proteins form hydrogels with intact functions of the fusion moieties. By varying the protein concentration, the compressive modulus of the hydrogels can be tuned to match that of skeletal muscle, myocardium and cartilage, respectively. In addition, human mesenchymal stem cells are viable after being encapsulated in the gels, and continuous release of biologics can be achieved as exemplified by an encapsulated cell line producing progranulin.

BP 18.2 Wed 10:00 H 1028

Understanding the molecular determinants of chitin-protein interactions in the arthropod cuticle - a single-molecule approach — •Ayesha Talib[1,2], Yael Politi[2], and Kerstin G. Blank[1,3] — [1]Max Planck Institute of Colloids and Interfaces, Mechano(bio)chemistry, Am Mühlenberg 1, 14476 Potsdam, Germany — [2]Technische Universität Dresden, CMCB, B CUBE, Tatzberg 41, 01307 Dresden, Germany — [3]Johannes Kepler Universität, Institute of Experimental Physics, Altenberger Straße 69, 4040 Linz, Austria

In the cuticle of arthropods, structural proteins and chitin fibers form a composite material with anisotropic mechanical properties. The molecular parameters that define the chitin-protein interaction are largely unknown. To answer the fundamental question of what controls cuticle mechanical properties, a molecular strategy is employed that integrates protein engineering with single-molecule force spectroscopy. Chitin binding domains (CBDs) from the spider Cupiennius salei have been identified and expressed recombinantly to compare the strength of the protein-chitin interaction. For CBD present in all spider tissues, we investigated three overlapping consensus motifs RR-1, RR-2 and CB-4. Pull-down assays and single-molecule force spectroscopy suggest that the RR-1 motif does not bind to chitin, whereas similar binding strength is observed for the RR-2 and CB-4. We observe a fast dissociation rate, suggesting that CBDs facilitate energy dissipation upon deformation. Our ultimate goal is to correlate molecular properties with the mechanical function of the composite and to synthesize artificial analogues with tunable mechanical properties.

BP 18.3 Wed 10:15 H 1028

Characterizing bursting spider silk coacervates with micropipette aspiration — •Isabell Tunn[1], Grégory Beaune[2], Jennifer Tersteegen[1], Jaakko V.I. Timonen[2], Francoise Brochard-Wyart[3], and Markus B. Linder[1] — [1]Department of Bioproducts and Biosystems, Aalto University, Finland — [2]Department of Applied Physics, Aalto University, Finland — [3]Institute Curie, Université Paris Sciences et Lettres, Sorbonne Université, Laboratoire Physico Chimie Curie, France

Hollow or core-shell coacervates composed of biomolecules have been reported to serve essential intracellular functions. Recently, numerous hollow and core-shell coacervates have been bioengineered in vitro opening new avenues for their application as drug delivery systems or vessels for chemical reactions. However, the relationship between the molecular structure and the biophysical properties of these coacervates remains largely unexplored. Thus, we characterized the biophysical properties of a set of five bioengineered spider silk protein coacervates using micropipette aspiration. Upon aspiration coacervates can burst like vesicles, demonstrating that protein forms a dense layer (shell) on the surface of the coacervate. To analyse the aspiration and bursting of the hollow coacervates we developed a model, which allows to calculate the surface and bulk viscosity and to estimate the thickness and viscosity of the shell. We anticipate that our model will aid in understanding the formation and properties of hollow coacervates and will facilitate their use as drug delivery systems, reaction vessels as well as material building blocks.

BP 18.4 Wed 10:30 H 1028

Connecting protein architecture to their emergent droplet properties — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz-Institut für Polymerforschung, Institut Theorie der Polymer, 01069, Dresden, Germany

Spatial organization is a fundamental characteristic of biological systems. Biomolecular condensates (droplets) is one class of spatial organization. Understanding how these droplets arise from molecular interactions remains a complex challenge. To address this, we focused on a specific model system consisting of two multivalent proteins with folded domains and disordered linkers which co-phase separate into droplets. We employed coarse-grained simulations to investigate how structural modularity impacts the phase diagram and material properties of these droplets. Our study focuses on the material properties: density, viscosity, and network architecture. The introduction of a coiled-coil domain substantially alters the phase behavior and material properties of the resulting droplets. The stiffness of this domain plays an important role in preventing self-loop closure and thus promoting phase separation, which enables a certain degree of orthogonal design across the various material properties we explored. Our research yields insights into the phase behavior of biomolecular condensates and provides guidelines for the modulation of droplet material properties.

BP 18.5 Wed 10:45 H 1028

Strain-Controlled Critical Slowing Down in the Rheology of Disordered Networks — •Abhinav Sharma[1,2], Jordan Shivers[3], and Fred MacKintosh[3] — [1]Mathematisch-Naturwissenschaftlich-Technische Fakultät, Universität Augsburg, 86159 Augsburg — [2]Leibniz Institute für Polymerforschung, Dresden — [3]Department of Chemical and Biomolecular Engineering, Rice University, Houston, Texas 77005, USA

Networks and dense suspensions frequently reside near a boundary between soft (or fluidlike) and rigid (or solidlike) regimes. Transitions between these regimes can be driven by changes in structure, density, or applied stress or strain. In general, near the onset or loss of rigidity in these systems, dissipation-limiting heterogeneous nonaffine rearrangements dominate the macroscopic viscoelastic response, giving rise to diverging relaxation times and power-law rheology. Here, we describe a simple quantitative relationship between nonaffinity and the excess

viscosity. We test this nonaffinity-viscosity relationship computationally and demonstrate its rheological consequences in simulations of strained filament networks and dense suspensions. We also predict critical signatures in the rheology of semiflexible and stiff biopolymer networks near the strain stiffening transition.

BP 18.6 Wed 11:00 H 1028

Mechanically biomimetic hydrogel suggests fundamental viscoelastic constraints in intracellular mechanics — •Dorian Marx, Bart Eduard Vos, Till Moritz Münker, and Timo Betz — Drittes Physikalisches Institut - Biophysik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The currently best fitting model for the viscoelastic mechanical properties of cellular cytoplasm lacks a connection to physical parameters. To establish this connection, we find and utilize a viscoelastic polyacrylamide-based hydrogel with cytoplasm-like mechanical properties. The variation of experimental parameters reveals the connection of their physical interpretations to the mechanical outcome of the measurement. The used viscoelastic hydrogel enables the comparison of different measurement methods spanning length scales of micrometers (optical tweezers) to centimeters (rheometer) and can serve as a calibration material that is neither ideally elastic nor ideally viscous. Furthermore, a detailed analysis of cellular and hydrogel data uncovers striking correlations of model parameters that closely match between the chemically and physically distinct materials. The results motivate further investigations into the theoretical reasons for the correlations and applications in building artifical cells.

15 min. break

BP 18.7 Wed 11:30 H 1028

Dynamic DNA origami nanopores — •Anna Baptist[1], Ze Yu[2], Sabina Caneva[2], and Amelie Heuer-Jungemann[1] — [1]MPI of Biochemistry, Martinsried, Germany — [2]TU Delft, The Netherlands

Nanopores are nanoscale structures that form channels across membranes and enable the translocation of molecules. Inspired by naturally occurring pore-forming proteins, different types of artificial nanopores have been created. The DNA origami technique allows for the fabrication of DNA nanostructures with precise control over shape and size that can be modified with a variety of functional molecules. Thus, DNA origami provides a platform for the customized design of nanoscale pores with different channel diameters that can be equipped with anchoring molecules for insertion into lipid membranes. Such nanopores have potential applications in single-molecule sensing, sorting of molecules depending on their sizes or for the fabrication of artificial cells. However, most nanopores created so far are static with a fixed pore diameter. Here, we present a large dynamic DNA origami nanopore that can be mechanically and reversibly switched between different conformations via strand displacement, offering three different pore sizes. After their successful insertion into the lipid bilayer, these nanopores form transmembrane channels with varying diameters depending on their conformation and can be used to control the transport of differently sized molecules across the lipid membrane. Such stimuli-responsive, actuatable nanopores are excellent mimics of complex natural occurring pores, while enabling a higher level of control and a more modular and easily adaptable design.

BP 18.8 Wed 11:45 H 1028

Nanotextured Surfaces Based on DNA — •Irina Martynenko and Tim Liedl — Faculty of Physics, Ludwig-Maximilians-University, 80539 Munich, Germany

A longstanding goal of material scientists is to fabricate functional materials in which nanoscale objects are precisely positioned on macroscale surfaces. This can be achieved by a combination of bottom-up techniques, such as molecular self-assembly of DNA origami, and top-down lithographic methods. Through DNA origami placement (DOP) on lithographically patterned surfaces a variety of nanoscale components such as organic dyes, proteins or nanoparticles, have already been patterned on large-scale arrays [1, 2]. However, any DOP methods developed so far were limited to two-dimensional DNA origami structures and thus resulted in flat patterns and arrays only. Here we extend DOP to the third dimension through positioning of three-dimensional DNA origami onto nanometer-precise patterns over micro- and even millimeter scales [3]. We demonstrate that our method can produce surfaces nanotextured with three-dimensional hybrid DNA-silica structures with controllable heights up to 50 nm and a feature size down to ~ 6 nm. We believe that the presented strategy can be used for the assembly of a wide range of materials from metals and semiconductors to functional biomolecules arranged in virtually any three-dimensional geometry on large-scale substrates. [1] R. Kershner, Nat Nanotechnol (2009) [2] A. Gopinath, et al., Nature (2016) [3] I. Martynenko et al., Nat Nanotechnol (2023)

BP 18.9 Wed 12:00 H 1028

DNA-Origami Diamond Crystal with photonic bandgap in the UV Range — •Xin Yin[1], Gregor Posnjak[1], Paul Butler[2], Oliver Bienek[2], Mihir Dass[1], Ian Sharp[2], and Tim Liedl[1] — [1]Ludwig-Maximilian-Universität München, Germany — [2]Walter Schottky Institute, Technical University Munich, Germany

Diamond lattice photonic crystals possess a broad complete photonic bandgap, although its manufacturing has proven challenging. [1] We showcase a DNA origami diamond crystal with 170 nm periodicity. [2] DNA origami is a technique that allows the rational design of complex geometries on the nanoscale, [3] which we apply to build tetrapod single units for the crystal. Pristine crystal formation requires careful control of interactions between the monomers. The thus-formed crystal undergoes silicification, via a wet chemistry method, for enhanced mechanical stability, followed by TiO2 coating via atomic layer deposition (ALD). The latter process is required to increase the refractive index and thus open the photonic bandgap. Optical measurement reveals a reflection band in UV range, with the peak red shifting as the coating thickness increases. These results align well with simulations predicting the structure's photonic properties. [1] R. K. Cersonsky, J. Antonaglia, B. D. Dice, & S. C. Glotzer. Nature communications, 12(1), 2543. [2] G. Posnjak, X. Yin, P. Butler, O. Bienek, M. Dass, I. D. Sharp, & T. Liedl, arXiv preprint arXiv:2310.10884. [3] P. W. Rothemund. Nature, 440(7082), 297-302.

BP 18.10 Wed 12:15 H 1028

Scaling properties of RNA as a branched polymer — Domen Vaupotič[1], Angelo Rosa[2], Luca Tubiana[3], and •Anže Božič[1] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]SISSA, Trieste, Italy — [3]University of Trento, Trento, Italy

Formation of base pairs between the nucleotides of an RNA sequence gives rise to a complex and often highly branched RNA structure. While numerous studies have demonstrated the functional importance of the high degree of RNA branching, its topology remains largely unexplored. We use the theory of randomly branching polymers to explore the scaling properties of RNAs by mapping their secondary structures onto tree graphs. Focusing on random RNA sequences of varying lengths, we determine the two scaling exponents related to their topology of branching. Our results indicate that ensembles of RNA secondary structures are characterized by annealed random branching and scale similarly to self-avoiding trees in three dimensions. We further show that the obtained scaling exponents are robust upon changes in nucleotide composition, tree topology, and folding energy parameters. Finally, we demonstrate how the scaling exponents can be obtained from the distributions of the related topological quantities of individual RNA molecules with fixed length. In this way, we establish a framework to study the branching properties of RNA and compare them to other known classes of branched polymers. By understanding the scaling properties of RNA structure we aim to improve our understanding of the underlying principles and open up the possibility to design RNA sequences with desired topological properties.

BP 18.11 Wed 12:30 H 1028

The role of receptor uniformity in multivalent binding — •Xiuyang Xia[1,2], Ge Zhang[3], Massimo Pica Ciamarra[1], Yang Jiao[4], and Ran Ni[1] — [1]Nanyang Technological University, Singapore — [2]Ludwig-Maximilians-Universität München, Munich, Germany — [3]City University of Hong Kong, Hong Kong, China — [4]Arizona State University, Tempe, USA

Multivalency is prevalent in various biological systems and applications due to the superselectivity that arises from the cooperativity of multivalent binding. Traditionally, it was thought that weaker individual binding would improve the selectivity in multivalent targeting. Here using analytical mean field theory and Monte Carlo simulations, we discover that for receptors that are highly uniformly distributed, the highest selectivity occurs at an intermediate binding energy and can be significantly greater than the weak binding limit. This is caused by an exponential relationship between the bound fraction and receptor concentration, which is influenced by both the strength and combinatorial

entropy of binding. Our findings not only provide new guidelines for the rational design of biosensors using multivalent nano-particles but also introduce a new perspective in understanding biological processes involving multivalency.

BP 18.12 Wed 12:45 H 1028

Salt Effects on Caffeine Across Concentration Regimes — Stefan Hervo-Hansen[1,4], Jakub Polák[2], Markéta Tomandlová[2], Joachim Dzubiella[3], •Jan Heyda[2], and Mikael Lund[4] — [1]Chem. Engineering Div., Osaka Uni., Toyonaka, Osaka 560-8531, Japan — [2]Physical Chem. Dpt., UCT Prague, Technická 5, CZ-16628 Praha 6, Czechia — [3]Physikalisches Inst., Albert-Ludwigs Uni. Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg im Breisgau, Germany — [4]Theoretical Chem. Div., Lund Uni., Lund SE 221 00, Sweden

This theoretical contribution is motivated by the early work of Charles Tanford, which led to the discovery that molecular surface motifs solvation is proportional to the solvent accessible surface area (SASA). Importantly, later studies have shown that the proportionality constant varies with salt *concentration* and *type*. Using multi-scale computer simulations combined with vapor-pressure osmometry on caffeine-salt solutions, we reveal that this SASA description captures a rich set of molecular driving forces in ternary solutions at changing *solute* and *osmolyte* concentrations.

Central to this theoretical work is a new potential energy function that depends on the instantaneous surface area, salt type, and concentration. Used in *e.g.* Monte Carlo simulations, this allows for a highly efficient exploration of many-body interactions and the resulting thermodynamics at elevated solute and salt concentrations.

This protocol opens the path to account for salt effects on the solvation thermodynamics of molecules of all sizes, including the *salting-in* or *salting-out* of aqueous bio(macro)molecules.

BP 19: Active Matter III (joint session DY/BP/CPP)

Time: Wednesday 9:30–13:00 Location: BH-N 334

Invited Talk BP 19.1 Wed 9:30 BH-N 334

Emergent chemotaxis in synthetic active matter — •Abhinav Sharma[1,2], Hidde Vuijk[1], Pierluigi Muzzeddu[3], Holger Merlitz[2], and Jens-Uwe Sommer[2] — [1]Universität Augsburg, 86159 Augsburg — [2]Leibniz Institute für Polymerforschung, Dresden — [3]SISSA, Trieste, Italy

Active particles with their characteristic feature of self-propulsion are regarded as the simplest models for motility in living systems. The accumulation of active particles in low activity regions has led to the general belief that chemotaxis requires additional features and at least a minimal ability to process information and to control motion. We show that self-propelled particles display chemotaxis and move into regions of higher activity if the particles perform work on passive objects, or cargo, to which they are bound. The origin of this cooperative chemotaxis is the exploration of the activity gradient by the active particle when bound to a load, resulting in an average excess force on the load in the direction of higher activity. In fact chemotaxis should emerge in all those structures which allow cooperative exploration of the activity landscape. We demonstrate this in simple assemblies of active molecules, which show robust chemotaxis both under static and dynamic activity landscapes.

BP 19.2 Wed 10:00 BH-N 334

Active particles interacting via phase-separating chemicals — •Dennis Schorn, Aritra K. Mukhopadhyay, and Benno Liebchen — Institut für Physik Kondensierter Materie, Technische Universität Darmstadt, Germany

Synthetic active particles self-propel by catalyzing a certain chemical reaction and moving up or down the resulting concentration gradient. In this talk, we present our study of the collective dynamics of chemotactic active particles which interact via self-produced chemicals that have an intrinsic tendency to phase separate. When the chemical interactions are attractive (chemoattraction), the particles aggregate to form a large cluster. In contrast, chemorepulsive particles exhibit two distinct patterns: a stationary foam-like structure and an oscillating stripe pattern. We explain the origins of these structures through a comprehensive linear stability analysis of our system. Our findings underscore that the intricate interplay between chemical phase separation and particle chemotaxis induces new instabilities, leading to the formation of unique patterns.

BP 19.3 Wed 10:15 BH-N 334

Towards the cybernetics of active matter — •Alexander Ziepke[1], Ivan Maryshev[1], Igor S. Aranson[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center and CeNS, LMU, Munich, Germany — [2]Dept. Biomed. Eng., Penn State University, University Park, PA, USA — [3]Max Planck School Matter to Life, Munich, Germany

Cybernetics describes the self-organized behavior of collectives of individual units in response to their environment, often taking inspiration from biological processes. Different organisms have developed various communication strategies to control such collective responses. For instance, social amoeba use chemical signaling to form localized aggregates in response to starvation, insects such as ants secrete pheromones for navigation, and bats and birds employ acoustic signals to form cohesive swarms. Our research focuses on how chemical and acoustic communication enables the formation of collective states with cooperative functionality, a targeted specification of the units, and the control of a coordinated response. In particular, we show that acoustic signaling of oscillatory agents leads to the formation of synchronized localized clusters and collectively propagating snake- and larva-like structures with distinct acoustic signatures. By emitting acoustic waves, these emergent structures are able to sense environmental changes, such as approaching reflective objects, and respond with a coordinated change in phenotype. This study provides insights into design principles for unsupervised microrobots, able to form adaptive, multi-functional structures with population-level cognitive capabilities (Ziepke, Maryshev, Aranson, Frey., Nat Commun 13, 6727 (2022)).

BP 19.4 Wed 10:30 BH-N 334

Active Spaghetti: Collective Organization in Cyanobacteria — •Jan Cammann[1], Mixon K. Faluweki[2,3], Lucas Goehring[2], and Marco G. Mazza[1] — [1]Loughborough University, UK — [2]Nottingham Trent University, UK — [3]Malawi Institute of Technology

Filamentous cyanobacteria can show fascinating examples of nonequilibrium self-organization, which, however, are not well understood from a physical perspective. We investigate the motility and collective organization of colonies of these simple multicellular lifeforms. As their area density increases, linear chains of cells gliding on a substrate show a transition from an isotropic distribution to bundles of filaments arranged in a reticulate pattern. Based on our experimental observations of individual behavior and pairwise interactions, we introduce a nonreciprocal model accounting for the filaments large aspect ratio, fluctuations in curvature, motility, and nematic interactions. This minimal model of active filaments recapitulates the observations, and rationalizes the appearance of a characteristic length scale in the system, based on the Péclet number of the cyanobacteria filaments.

Reference: M. Faluweki, J. Cammann, et al. Phys. Rev. Lett. 131, 158303 (2023)

BP 19.5 Wed 10:45 BH-N 334

Collective dynamics and pair-distribution function of active Brownian ellipsoids* — Stephan Bröker[1], •Michael te Vrugt[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

While the collective dynamics of spherical active Brownian particles is relatively well understood by now, the much more complex dynamics of nonspherical active particles still raises interesting open questions. Previous work has shown that the dynamics of rod-like or ellipsoidal active particles can differ significantly from that of spherical ones. In this work [1], we obtain the full state diagram of active Brownian ellipsoids depending on the Péclet number and packing density via computer simulations. The system is found to exhibit a rich state behavior that includes cluster formation, local polar order, polar flocks, and disordered states. Moreover, we obtain numerical results and an analytical representation for the pair-distribution function of active ellipsoids.

This function provides useful quantitative insights into the collective behavior of active particles with lower symmetry and has potential applications in the development of predictive theoretical models.

[1] S. Bröker, M. te Vrugt, and R. Wittkowski, arXiv:2307.15535 (2023)

*Funded by the Deutsche Forschungsgemeinschaft (DFG) under Project-IDs 525063330 (MtV) and 283183152 (WI 4170/3) (RW).

BP 19.6 Wed 11:00 BH-N 334

Flow and orientational properties of active nematic liquid crystals under an electric field — •Yutaka Kinoshita and Nariya Uchida — Department of Physics, Tohoku University, Sendai, Japan

Active nematic liquid crystals are materials where each constituent has nematic symmetry and produces dipolar flow along its axis. Examples include microtubule-kinesin suspensions and actomyosin networks. Because of the input of energy into the system, the state is driven out of thermodynamic equilibrium and shows a chaotic flow called active turbulence. The flow patterns are controlled by external field, confinement, and friction. An external field induces reorientation of the active elements and suppresses chaotic flow. Here we numerically simulate the effects of an electric field on the dynamics of two-dimensional active nematics [1].

We found transitions among three states that are characterized by the degree of flow anisotropy: the active turbulence, laning state, and uniformly aligned state. The average flow speed and its anisotropy are maximized in the laning state. We also found localization of vortices and topological defects associated with periodic shifts between active turbulence and laning state, which is similar to experimentally observed oscillations in a friction-controlled system. Our results might lead to a further understanding of the dynamical states of active nematics under an external field.

[1] Y. Kinoshita and N. Uchida, Phys. Rev. E **108**, 014605 (2023)

15 min. break

BP 19.7 Wed 11:30 BH-N 334

From Active Chiral Particles to the Active Model B + — •Erik Kalz[1], Abhinav Sharma[2,3], and Ralf Metzler[1,4] — [1]University of Potsdam, Germany — [2]University of Augsburg, Germany — [3]Leibniz-Institute for Polymer Research, Dresden, Germany — [4]Asia Pacific Centre for Theoretical Physics, Pohang, Republic of Korea

A first-principles approach for active chiral hard disks is presented, that explicitly accounts for steric interactions on the two-body level. With a handle on the full derivation, we explicitly point out the necessary assumptions to derive the field-theoretical description for Active Chiral Particles. By considering different regimes of the Péclet number, the well-known models in active matter can be obtained through our consideration. Explicitly, we derive the phenomenological Model B. By going to higher orders in the closure scheme, we show that this first-principles approach results in the recently introduced Active Model B +, a natural extension of Model B for active processes. Contrary to systems without chirality and to previous derivations, we find that chirality can change the sign of the characteristic activity parameters. This has profound consequences for the already shown effects in the Active Model B +. Finally, we draw a connection between Active Chiral Particles and Odd Diffusion, a phenomenon that has attracted considerable attention recently, and for which Active Chiral Particles are handled as an exemplary system.

Ref: E. Kalz, A. Sharma, and R. Metzler: *arXiv preprint arXiv:2310.16691*, 2023

BP 19.8 Wed 11:45 BH-N 334

Phase Behaviour of a Minimal Chiral Active Ising Lattice Model — •Boyi Wang[1,3], Frank Jülicher[1,4,5], and Patrick Pietzonka[2,1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom — [3]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [4]Center for Systems Biology Dresden (CSBD), Dresden, Germany — [5]Cluster of Excellence, Physics of Life, TU Dresden, Dresden, Germany

We introduce chiral activity into a lattice model with Ising interactions, achieved by locally rotating a random selected 2×2 neighbourhood of lattice site each time step only in clockwise direction. Monte Carlo simulations at low temperature reveal a path to condensate formation, marked by the evolution of the droplet's edge into a particular tilted orientation relative to the square lattice. This tilt angle depends on the local rotation direction, thus reflecting the chirality of the model on a macroscopic scale.

Furthermore, we investigate the stability of the chiral tilted angle in the droplet's lattice field. We identify a persistent edge current flowing along the droplet's interface. By an equivalent 1D model, we also quantify this current-angle dependence, allowing us to identify the angles that emerge in the stationary state.

Our findings provide a novel perspective on chiral non-equilibrium systems in a discrete and analytical framework, expanding our understanding of how chiral driving forces influence the formation and interface behaviour of active droplets.

BP 19.9 Wed 12:00 BH-N 334

Long-range fluctuation-induced forces in chiral active fluids — Hashem Fatemi[1], Hamidreza Khalilian[1], Jalal Sarabadani[1], and •Reza Shaebani[2] — [1]Institute for Research in Fundamental Sciences (IPM), Iran — [2]Department of Theoretical Physics, Saarland University, Germany

We study long-range fluctuation-induced (FI) interactions in chiral active matter systems. We show that the combination of self-rotation and self-propulsion can lead to large FI forces, depending on the elongation of active particles. Such strong forces can contribute to self-organization of chiral active matter into dynamic structures and patterns. We numerically measure the FI forces between intruders immersed in chiral active fluids and find that the influence of chirality depends on the particle elongation in the active bath. For round active objects, the FI force monotonically decreases with increasing chirality since the active bath structure gradually changes from rotating flocks and vortices to localized spinners. Contrarily, for elongated active objects there is an optimal chiral angle at which the magnitude and range of the FI interaction are maximized. We explain how the balance of collisions around the intruders varies with chirality and separation between the intruders.

BP 19.10 Wed 12:15 BH-N 334

Self-Solidifying Active Droplets Showing Memory-Induced Chirality — •Aritra K. Mukhopadhyay[1], Kai Feng[2], José Carlos Ureña Marcos[1], Ran Niu[2], Qiang Zhao[2], Jinping Qu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Huazhong University of Science and Technology, 430074 Wuhan, China.

Synthetic microswimmers have yet to achieve the autonomy and versatility of their biological counterparts, particularly in terms of energy supply and motion diversity. Here, we introduce an all-aqueous droplet swimmer that shows remarkable autonomy and rich dynamics without any external driving mechanism [1]. Comprising a surface tension-lowering polyelectrolyte mixture, the droplets undergo self-solidification on acidic water surfaces, gradually emitting polyelectrolytes into the surroundings. A spontaneous asymmetry of the emitted polyelectrolyte concentration along the droplet surface induces Marangoni flows, which causes the droplet to self-propel. The slowly diffusing polyelectrolytes form long-lived chemical trails creating memory effects that drive a dynamic transition from linear to chiral motion. This showcases the droplet's ability to navigate its environment in a persistent, directional manner requiring no externally imposed symmetry breaking. Practical applications are highlighted through the droplets' highly efficient uranium removal from wastewater. Our results provide a route to fueling self-propelled agents that can autonomously perform chiral motion and collect toxins.

[1] K. Feng et al., Advanced Science 10, 2300866 (2023).

BP 19.11 Wed 12:30 BH-N 334

Optimising transport of active magnetic particles with finite internal magnetic anisotropy — Andrey Kuznetsov[1], Ekaterina Novak[2], Vladimir Zverev[2], Tatyana Belyaeva[2], and •Sofia Kantorovich[1] — [1]University of Vienna, Vienna, Austria — [2]Ekaterinburg, Russia

In recent years, we have observed a rapid development in synthesis techniques that opens up new avenues for tailoring magnetic nanoparticles, including their size, shape, and internal anisotropy. The concept of creating magnetically controllable colloids with finely tuneable rheological properties on the nano- or micro-scale has sparked significant experimental and theoretical efforts but remains not fully realised. In this contribution, we employ molecular dynamics computer simulations to investigate the interplay between internal particle magnetic relax-

ation dynamics and particle self-propulsion. Our findings demonstrate that optimal transport can be achieved by selecting the strength of an applied magnetic field based on the particle's material and size. This, in turn, opens up an avenue for active magnetic particle sorting.

BP 19.12 Wed 12:45 BH-N 334

The Role of Anisotropy in Pulsating Active Matter — •Luca Casagrande, Alessandro Manacorda, and Etienne Fodor — University of Luxembourg, Department of Physics and Material Science

Contraction waves have been observed in different biological systems where contractile tissues are present. Some examples can be found in embryonic development, cardiac arrhythmogenesis and uterine contraction. Recently, a particle-based model reproducing the spontaneous emergence of contraction waves has been proposed. In this model, a dense system of active particles is considered, where each particle features isotropic repulsion with neighbors, and has an internal drive that periodically changes its size.*However, it is well know that cells in tissues are not isotropic. Therefore, we consider an additional degree of freedom which embodies the ability of particles to change their eccentricity. It enables us to investigate the role of particle anisotropy in pulsating collective dynamics. The resulting dynamics are studied through numerical simulations. Also an analytical hydrodynamics approach is used through coarse-graining methods. We present the full phase diagram that illustrates the stationary regime as a function of the control parameters of the model. Our model elucidates the interplay between nematic order and phase synchronization in pulsating active matter, and it paves the way towards studying how to control the emergence of contractile waves in biological tissues.

BP 20: Poster IIIa

Active Matter, Statistical Physics in Biological Systems, Systems and Network Biophysics

Time: Wednesday 11:00–14:30 Location: Poster B

BP 20.1 Wed 11:00 Poster B

Influence of Environmental Inhomogeneity on Active Particle Dynamics in Obstacle Parks: A Numerical Study — •Zeinab Sadjadi[1] and Heiko Rieger[1,2] — [1]Department of Theoretical Physics & Center for Biophysics, Saarland University, 66123 Saarbrücken, Germany — [2]Leibniz Institute for New Materials INM, 66123 Saarbrücken, Germany

Biological microorganisms have the ability to detect external fields and environmental signals, and they can adjust their dynamics accordingly. The redirected motion in response to a gradient of a stimulus, called taxis, is a vital navigation mechanism in many biological systems. Our focus lies on topotaxis, the ability of particles to sense the geometrical and topographical features of their surroundings. We numerically study the dynamic behavior of active particles moving in pillar parks. First, by introducing a disorder in the diameter size as well as the position of pillars, we investigate the influence of environmental inhomogeneity on particle dynamics. we also demonstrate how imposing a gradient in the disorder in geometrical characteristics could bias the direction of active agents and induce a topotaxis in the pillar park. Our results are of technological importance for design of efficient taxis devices.

BP 20.2 Wed 11:00 Poster B

Order from disorder: active particles with random alignment interactions — •Eloise Lardet and Thibault Bertrand — Imperial College London, London, UK

In 1995, Vicsek et al. wrote a seminal paper describing a simple model that displays a transition from disorder to collective ordered behaviour. It describes a system of self-propelled point particles that align with their neighbours within a certain radius. This minimal model displays rich nonequilibrium behaviours such as flocking and banding. Inspired by the random couplings of spin glass models, I present numerical findings of introducing Gaussian distributed pairwise couplings into a self-propelled particle system. Through adding further disorder by increasing the standard deviation of the Gaussian distribution that the couplings are drawn from, we are able to observe the emergence of global polar order in systems where the majority of couplings are anti-aligning.

BP 20.3 Wed 11:00 Poster B

Design and manufacture of self-propelled particles driven by light — •Jannis Fischer, Alejandro Jurado Jiménez, and Timo Betz — Third Institute of Physics, University of Göttingen, Göttingen, Germany

In all living things, biochemical processes take place on scales that are not visible to the naked human eye. However, when compared to forces we encounter in our daily lives, other forces tend to be more dominant: Frictional forces have a considerable influence on the movements of particles while inertial forces can often be neglected [1]. Therefore, it is of great interest and also a challenge to create particles that can actively move on such scales. Getting micrometer-sized particles to move in a controlled manner within living tissue would prove to be a great advantage for specific drug delivery or the design of micro-robots. A fundamental part of movement is propulsion. If the particles themselves can generate active movement, they are called self-propelled particles. One recently proposed method is to use homogeneous light illumination in conjunction with transparent particles that demonstrate a gradient of refractive index. Here the refraction of the light leads to a momentum transfer, which then drives the active movement. In this work, both a simulation and the production of the corresponding particles are used to investigate which particle shape leads to the greatest forces and thus to the highest velocities.

[1] E.M. Purcell, American Journal of Physics, 45(1) (1977).

BP 20.4 Wed 11:00 Poster B

Simulating a field-theoretic model of transcription condensates — •Kathrin Hertäg[1], Joshua Robinson[2,3], and Thomas Speck[1] — [1]ITP4, Stuttgart, Deutschland — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland — [3]H.H. Wills Physics Laboratory, University of Bristol

Phase separation of macromolecules has recently attracted substantial interest, in particular in the context of membrane-less organelles in the cell. These organelles are typically modeled as condensates. Instead of coarsening to a fully phase separated state, such protein condensates form stable droplets of finite size in vivo. Therefore, an important question is the role of non-equilibrium processes since the physical processes underlying stable droplet behavior are not yet resolved. Here we study active model B+, a scalar field theory developed in the context of motile active matter, and employ methods of active liquid theory to explore activity as the underlying mechanism for condensate stabilization.

BP 20.5 Wed 11:00 Poster B

Learning in slime molds? — Adrian Büchl, •Lisa Schick, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Learning and adapting to changing environments is crucial for the survival for living organisms. Generally, learning involves the formation of memory by gathering and storing information and applying this memory in novel contexts. In neuronal organisms, learning can be directly mapped to adaptations in the neuronal network. However, information processing and memory formation can also be found in non-neuronal organisms like slime molds that lack a central nervous system. The slime mold *Physarum polycephalum* is well known for its network adaption processes as a response to environmental cues. Can we consider this complex behavior learning? Using bright-field microscopy observations, we investigate how *P. polycephalum* networks react to repetitive negative blue light stimuli. We observe migratory behavior persisting much longer than network adaptation, and by this, establish memory of environmental stimuli in the slime molds migration dynamics. By looking at flow patterns and response times to different stimuli, we set out to unravel if learning exists in organisms without a nervous systems.

BP 20.6 Wed 11:00 Poster B

Mesoscopic hydrodynamic modeling of *Trypanosoma brucei* — •Zihan Tan, Julian Isaac Ufoma Peters, and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, 10623 Berlin, Germany

Trypanosoma brucei is notorious for causing African trypanosomiasis also known as sleeping sickness. Due to significant challenges in experimentation, a physical understanding of how *T. brucei* interacts with fluid environments and navigates through confinements, typically in blood vessels but also in tissue, remains largely elusive. To this end, mesoscopic hydrodynamic modeling can provide additional insights. Through elaborate comparison with experiments, our group has developed an in-silico *T. brucei* model coupled with a viscous solvent, simulated by multiparticle collision dynamics (MPCD). The *T. brucei* body is discretized into vertices and facets, allowing for adequate bending and torsion while satisfying surface and volume constraints. Moreover, a flagellum, starting from a pocket at the thicker posterior end of the body, is laterally attached. A sinusoidal bending wave is imposed along the flagellum. It deforms the whole cell body and through the interaction with the ambient fluid generates propulsion. Since the dynamics of MPCD solvents is independently computed inside each cubic collision unit, we could considerably accelerate our simulations using GPU parallel computing. Our model has been validated to exhibit realistic hydrodynamic and mechanical properties of *T. brucei*. In particular, we focus on how the model *T. brucei* navigates through a microchannel with constrictions or containing hard or soft obstacles.

BP 20.7 Wed 11:00 Poster B

Evaluating the cell-cell interactions of swimming flagellated microbes — •Henrik Groh[1], Alexandros A. Fragkopoulos[1], Colin-Marius Koch[2], Michael Wilczek[2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bayreuth, Theoretical Physics I, 95447 Bayreuth, Germany

In suspensions of living microorganisms individual cells often interact leading to larger-scale emergent effects. Such collective phenomena are studied more extensively than the single-cell behaviour and the interactions that lead to the overall effect. However, understanding their mutual interactions is necessary to fully understand the emergence of their collective behaviour. For example, the aggregation of *Chlamydomonas reinhardtii*, a swimming unicellular microbe, in the presence of self-generated oxygen gradients has been investigated [1], but the cell-cell interactions in this system have yet to be explored. Here, we investigate the mutual interactions of microswimmers in a quasi-2D suspension of *C. reinhardtii* with high temporal and spatial resolution. This involves the determination of an effective potential between two cells via the relationship between the incoming and outgoing cell motility of a collision event. A particular challenge in this context is to identify the influence of the flagella on the contact process. With our investigations we gain more detailed insights into the swimming behavior of *C. reinhardtii* and, thus, better understand their population-level properties.
[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).

BP 20.8 Wed 11:00 Poster B

Quantifying vascular morphology on a chip — •Leonie Karr, Fatemeh Mirzapour, and Karen Alim — Technische Universität München

Our human vasculature is dynamic, growing and re-organizing not only in development but continuously adapting its morphology. Yet, what determines vessel formation and branching in healthy and disease state seems complex given the multitude of contributing factors.

Our focus lies in growing a human vasculature within the controlled environment of a chip, with the goal of quantifying the flow properties of self-organized in vitro networks. Additionally, we are examining the interplay of various cell types on these self-organized morphologies. Employing image analysis techniques alongside flow simulation methods, our objective is to accurately quantify how flow and cell types determine network architecture. The results obtained from our analyses will significantly contribute to the development of next-generation therapeutics aimed at targeting vessel development.

BP 20.9 Wed 11:00 Poster B

Metabolically controlled bioconvection in suspensions of photoactive microbes — •Florian Böhme[1], Alexandros Fragkopoulos[1,2], Nicole Drewes[2], and Oliver Bäumchen[1,2] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany

Photosynthetic microbes have evolved and successfully adapted to environmental changes of their habitat. In the abscence of light, they can still sustain their biological functionality and metabolic activity through aerobic respiration. However, for the soil-dwelling microalga *Chlamydomonas reinhardtii*, their environment is often deprived of both oxygen and light, resulting in a significant reduction of their swimming velocity [1]. Here, we investigate the effect of these motility changes on the emergence of bioconvection, a collective phenomenon that arises due to the natural tedency of the bottom-heavy cells to move against gravity. We show that the motility change that is associated to the metabolic switch between photosynthesis and anaerobic respiration is sufficient to induce or prevent the formation of bioconvective plumes. Our experiments use a side-view perspective allowing us to extract the local cell density and flow fields of single bioconvection plumes, in addition to the wavelength and the spatiotemporal evolution of the pattern. In particular, we extract how these parameters depend on the single-cell motility.
[1] A.A. Fragkopoulos et al., *J. R. Soc. Interface* **18**, 20210553 (2021).

BP 20.10 Wed 11:00 Poster B

Effect of flagella length on the motility of confined microbes — •Tom Sosniok, Alexandros Fragkopoulos, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

Many microorganisms utilize flagella to propel and navigate through their surrounding liquid environment. Often times though, the natural habitats of such microswimmers comprise confined spaces, and therefore, cell interactions with boundaries play an important role on their navigation. *Chlamydomonas reinhardtii*, a biflagellated, green microalga that is commonly found in soil, typically swims in close proximity to curved boundaries [1]. We found that this near-wall swimming motility is controlled by gradients of wall curvature and steric interactions between the flagella and the surface [2]. Here we explore the effect of the flagella length on the motility and surface interactions of the cells using two different *C. reinhardtii* strains with different flagella lenghts in quasi-2D circular confinement. We extract information about their motion from their mean squared displacements and visualize the wall-guided swimming via relative and radial probability densities. By comparing the results for both strains we can directly analyse the influnce of the flagella lenght on their motility and find that steric interactions alone are insufficient to describe our observations.
[1] T. Ostapenko et al., *Phys. Rev. Lett.* **120**, 068002 (2018).
[2] J. Cammann et al., *PNAS* **118**, e2024752118 (2021).

BP 20.11 Wed 11:00 Poster B

Tracking and analysis of active droplet dynamics: from image processing to synthetic biology — •Roberto Menichetti[1,2], Matteo Scandola[1], and Raffaello Potestio[1,2] — [1]Physics Department, University of Trento, Trento, Italy — [2]INFN-TIFPA - Trento Institute for Fundamental Physics and Applications, Trento, Italy

Active matter can harness energy from its surroundings and propel itself away from equilibrium, with its constituents absorbing energy from the environment and dissipating it, e.g. through motion or the exertion of mechanical forces. The investigation of these systems offers promising new perspectives on the field of non-equilibrium statistical physics, further paving the way for the design of innovative life-like materials and devices. In this work, we analyse the behaviour of a synthetic active matter system consisting of liquid droplet surfers whose self-propulsion decays over time [1]. By relying on a synergistic combination of techniques, such as computer vision algorithms for accurate droplet detection and analyses grounded on non-equilibrium statistical mechanics and graph theory, we quantitatively characterise all the stages of the dynamic evolution of the system, from its initial diffusive regime up to the generation of large clusters of droplets that appear as the activity wanes. The presented work showcases a comprehensive analysis of an actively evolving system, offering not only a general pipeline for the investigation of analogous problems, but also a deep perspective at the intersection between physics and synthetic biology. [1] Tanaka, S. et al., Phys. Rev. E 91, 032406 (2015).

BP 20.12 Wed 11:00 Poster B

Entropy production of active crystals — •Connor Roberts and Gunnar Pruessner — Imperial College London, United Kingdom

We consider a two-dimensional triangular lattice of active particles

that interact with their nearest neighbours through a general pair potential. We study this "active crystal" as a means of characterising the dense phase of active matter at high packing fraction. By approximating the interactions to leading order, we obtain exactly the fully time-dependent two-point position correlation and position-self-propulsion cross-correlation matrices for an active harmonic crystal. Importantly, our approximation retains non-trivial terms that are often neglected despite capturing the essential geometry of a particle's local potential. From our expressions of the correlation matrices, we subsequently derive the entropy production, covariance, and mean square displacement. The entropy production is found to have a general form akin to that of non-interacting active particles in external potentials. This may suggest a universal expression for the entropy production that is valid for any system of active particles subject to linear forces, regardless of the forces' origins.

BP 20.13 Wed 11:00 Poster B

Quantification and model-based classification of the aging dynamics of single endothelial cells under confluent conditions — •Anselm Hohlstamm, Andreas Deussen, Stephan Speier, and Peter Dieterich — Institut für Physiologie, TU Dresden

Endothelial cells, which are grown into a two-dimensional, confluent layer, exhibit intricate movement patterns and aging processes. While maintaining dynamic cell-cell contacts, individual cells perform a continuous, correlated motion. It is the objective of this study to quantify and classify these dynamics. Therefore, we studied the migration of human umbilical vein endothelial cells. Their nuclei were marked using a fluorescent dye and observed for 48 hours, with data collected at 10-minute intervals. We were able to monitor several 10.000 cells in each of the 10 experiments. The mean squared velocity of the cells decreased as a function of time, which could be characterized with two temporal scales. In addition, the mean squared displacement revealed a temporal transition of scaling $\sim t^{\alpha}$ from more directional movements with $\alpha \sim 1.6$ for short times towards a subdiffusive behavior with $\alpha \sim 0.4$ for long times. Based on the analysis of the temporal velocity autocorrelation, we constructed different stochastic models as combinations of Ornstein-Uhlenbeck and fractional processes that were supplemented by aging contributions. Bayesian inference allowed selecting the best model given the experimental data. In summary, the movement of cells under confluent conditions can be characterized as an aging dynamics in a non-thermal environment.

BP 20.14 Wed 11:00 Poster B

Reinforcement Learning in Active Colloidal Reservoir Computing — •Jonas Scheunemann, Samuel Tovey, and Christian Holm — Institute for Computational Physics, Stuttgart, Germany

The capacity to process information through a physical system can be exploited and further understood by using the recently introduced framework of physical reservoir computing. The concept involves utilizing the dynamics of nonlinear physical systems for time series forecasting, speech recognition, or classification tasks. The characteristics of an effective reservoir are still under discussion, and we use reinforcement learning to delve deeper into this question. Our reservoir substrate consists of a swarm system of active matter colloids, which has recently been demonstrated to work using a modified Reynolds boids model. We train the swarm by rewarding the colloidal agents through a concentration field approach, inspired by the behaviour of E. coli, and tested by forecasting a chaotic time series with a Lorenz attractor input. As the swarm reservoir's memory depends on the colloids' correlation time, we employ the Langevin equation to set up the system at diverse temperatures. We identify a potential connection between temperature and prediction accuracy, opening up research on the advantages of temperature-induced noise in the reservoir.

BP 20.15 Wed 11:00 Poster B

Radius-Dependent Dynamics of Active Spot — •Arghavan Partovifard and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Active nematics exhibit distinctive behavior for a spatially varying activity [1,2]. Utilizing the Doi-Edwards theory supplemented by an active stress tensor [1], we investicate an active nematics solely confined to a circular spot by switching off activity outside of the spot. Depending on the spot radius, we observe different emerging dynamics. At very small radii, two +1/2 defects form a spiral and rotate synchronously, while the velocity field displays a single vortex. As the radius of the activity spot increases, the two +1/2 defects gradually separate from each other, while circling around each other. When the +1/2 defects approach the border of the spot, a third +1/2 defect forms. Subsequently, one of the original +1/2 defects leaves the spot, and the two remaining +1/2 In this regime, the velocity field exhibits two or three vortices moving within the spot. With further increase of the spot radius, pairs of ±1/2 defects are constantly generated and they annihilate with other defects. The corresponding velocity field consists of many vortices moving chaotically, similar to what is observed in active turbulence. We thoroughly investigate and classify the occuring dynamics.

[1] Partovifard *et al.*, submitted (2023).
[2] Rønning *et al.*, R. Soc. Open Sci. **10**, 221229 (2023).

BP 20.16 Wed 11:00 Poster B

Efficient Bayesian Inference of Active Brownian Motion using Reinforcement-learned Brownian Bridges — •Sascha Lambert and Stefan Klumpp — Georg-August-Universität Göttingen, Institut für Dynamik Komplexer Systeme

Active Brownian Particles (ABPs) describe microswimmers by a Langevin equation that combines stochastic fluctuations and deterministic forces, including the swimmer's active propulsion and the interactions with obstacles.

Full Bayesian inference of the parameters of the Langevin equation can be achieved within the framework of Particle Pseudo-Marginal Metropolis-Hastings algorithms (PMMH). These algorithms sample from the full posterior of the model parameters, conditioned on experimental observations. A key strategy in these algorithms is using a particle filter for resampling the trajectories between observations.

The sampling efficiency is largely determined by uncertainties of the experimental measurements, with lower uncertainties resulting in reduced acceptance rates of newly generated samples. The rotational degrees of freedom and the resulting memory of ABPs produce strong temporal correlations that are not easily resolved using particle filters, as they only filter based on individual observations. We construct an approximative Brownian Bridge to increase the particle swarm's coherence and to guide the swarm between the observations. This approach increases the resampling efficiency by several orders of magnitude.

The exact guidance parameters depend on the full non-linear system and can be learned through reinforcement learning.

BP 20.17 Wed 11:00 Poster B

Self-organized criticality in animal collectives: the effects of network topology and heterogeneities — •Bianca Pacini[2,4], Yunus Sevinchan[1,2], Carla Vollmoeller[1,2], David Bierbach[1,3], Jens Krause[1,3], and Pawel Romanczuk[1,2] — [1]Science of Intelligence, TU Berlin, Berlin, Germany — [2]Institute for Theoretical Biology, HU Berlin, Berlin, Germany — [3]Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany — [4]Department of applied science and technology, Politecnico di Torino, Torino, Italy

Large-scale collective biological systems – such as large animal groups – have been suggested to operate at or near so-called critical points, at which they show maximum sensitivity towards environmental signals [1]. We have studied large fish shoals of sulphur mollies (*Poecilia sulphuraria*) in Southern Mexico, which perform collective diving cascades as a response to predation. Through agent-based numerical simulations and analyzing videos and images, we investigated the structure and role of the underlying social interaction network. As changes in spatial structure are strictly local, the resulting network and its changes will strongly depend on the spatial wiring mechanism. Important question remain unanswered: How do local heterogeneities affect how behaviour spreads? What are the effects of changes in the network on the behavioural contagion and discrimination ability of the system? Our results contribute to a better understanding of mechanisms of self-organization and how collectives may self-tune their distance to criticality. [1]Gomez-Nava et al. *Fish shoals resemble a stochastic excitable system*, Nature Physics 19, 2023

BP 20.18 Wed 11:00 Poster B

Controlling Droplet Formation and Dissolution with Chemical Reactions — •Gerrit Wellecke, Jan Kirschbaum, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Droplets formed by phase separation are vital for intracellular organization and function. Chemical reactions can generally control the formation and dissolution of such droplets. To understand how cells can influence droplets in space and time, we here consider a ternary system that displays bistabilities between homogeneous and phase-separated states. We use a thermodynamically consistent approach to describe

the reactions, which allows us to quantify the energy dissipation during transitions in such a system. We identify optimal protocols for reaction-controlled droplet formation and dissolution in the bistable regime. Our model identifies plausible mechanisms for how cells control their droplets and suggests paths for controlling synthetic soft matter systems.

BP 20.19 Wed 11:00 Poster B

Clonal dynamics of surface-driven growing tissues — •Ruslan Mukhamadiarov[1,2], Matteo Ciarchi[1,2], Fabrizio Olmeda[1,2], and Steffen Rulands[1,2] — [1]LMU, München, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The self-organization of cells into complex tissues relies on a tight coordination of cell behavior. Identifying the cellular processes driving tissue growth is key for understanding the emergence of tissue forms and for devising targeted therapies for aberrant growth, such as in cancer. Inferring the mode of tissue growth, whether it is driven by cells on the surface or cells in the bulk, is possible in cell culture experiments, but difficult in most tissues in living organisms (in vivo). Genetic tracing experiments, where a subset of cells is labelled with inheritable markers have become important experimental tools to study cell fate in vivo. Here, we show that the mode of tissue growth is reflected in the size distribution of the progeny of marked cells. To this end, we derive the clone-size distributions using analytical calculations and an agent-based stochastic sampling technique in the limit of negligible cell migration an cell death. We show that for surface-driven growth the clone-size distribution takes a characteristic power-law form with an exponent determined by fluctuations of the tissue surface. Our results allow for the inference of the mode of tissue growth from genetic tracing experiments.

BP 20.20 Wed 11:00 Poster B

Measuring activity from particle trajectories — •Lukas Abegg[1], Till M. Muenker[1], Gabriel Knotz[2], Anna-Lotta Höper[2], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics, Georg August Universität Göttingen — [2]Institute of Theoretical Physics, Georg August Universität Göttingen

Is it possible to distinguish activity from thermal fluctuations just from observed trajectories? The newly introduced statistical quantity mean back relaxation aims to achieve exactly this by using three-point correlation functions. This non-dimensional function yields a measure for deviation from equilibrium within a confined system. It is calculated as the average displacement of a tracer particle under the condition of having moved the distance d in advance. For an equilibrium process this quantity results in a long time value of $\frac{1}{2}$. However, deviation from this value is a marker for broken detailed balance. To gain deeper inside into this new statistical measure, we investigate this quantity inside a controlled system, namely a viscoelastic polyacrylamide gel. This probe was tuned to imitate the mechanical properties of cells, containing polystyrene particles with size of one micron. To drive this system out of equilibrium, we use a movable optical tweezer to simulate active motion of the particle. The mean back relaxation is calculated for all trajectories and fitted with an analytical solution for a viscoelastic system. The results are used to quantify the diffusion coefficient of the trapping laser and thus, the activity of the system tuned by our experimental realisation. Additionally, we can calculate the shear modulus $G^\star$ from this result.

BP 20.21 Wed 11:00 Poster B

Phase separation on membranes with matter exchange and dimerization — •Riccardo Rossetto[1], Kueyoung Kim[2], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization — [2]Department of Chemistry, The Pennsylvania State University

Patterns form on membranes in a large variety of biological contexts. In many cases, the patterns are affected by material exchange between the membrane and the bulk. Moreover, the involved biomolecules often also form short polymers and interact unspecifically. We describe this situation with a thermodynamically consistent minimal model, which accounts for phase separation, dimerization, and material exchange between the membrane and the bulk. While these mechanisms are understood individually, interesting nonlinear effects emerge from their combination. We illustrate this by explaining experimental data from the PAR patterning system, which exhibits dimerization and membrane binding. The general conclusions from our model unveil fundamental mechanisms of pattern formation on membranes and will help us explain more biological observations in the future.

BP 20.22 Wed 11:00 Poster B

Unraveling the Role of Physical Interactions in Multicomponent Phase Separation — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Phase separation is a crucial phenomenon in soft matter and biophysics, e.g., for forming biomolecular condensates. Yet, our understanding of how the physical interactions between components affect phase separation remains limited, particularly in systems with many components. Investigations are often restricted to systems with very few species, are focused on pair interactions, or only consider the stability of the homogeneous state. We developed a powerful method to study coexisting phases in multicomponent fluids and used it to analyze two cases. First, we concentrate on the equilibrium behavior of a many-component system with pair interactions. We demonstrate that the number of coexisting phases can significantly differ from the number of unstable modes identified through stability analysis. Second, we explore the impact of higher-order interactions on phase separation. Our findings reveal that three-body interactions can trigger additional phases compared to pair interactions, underscoring the crucial role of higher-order interactions in phase separation. In summary, our study elucidates the nuanced role of physical interactions in phase separation, offering valuable insights for investigating biomolecular condensates in cells.

BP 20.23 Wed 11:00 Poster B

Probing Neuronal Dendrites by First-Passage Properties — •Fabian Hubertus Kreten[1,2], Ludger Santen[1,2], and Reza Shaebani[1,2] — [1]Department of Theoretical Physics, Saarland University, Saarbrücken, Germany — [2]Center for Biophysics, Saarland University, Saarbrücken, Germany

Probing Neuronal Dendrites by First-Passage Properties

Part of the neuronal signal transmission mechanism is the dendritic tree, an arborous structure of gradually thickening channels leading to the soma. Along these channels bulbous protrusions (spines) are located at which synapses can form.

Neurodegenerative diseases alter the structure of the dendritic tree and by that perturb this finely tuned machinery. Probing the structure of a patient's dendrites could thereby give insight into the progression of the disease in question.

Previously, studies of how the structural parameters of dendritic trees influence their transport properties and how these structural properties might be regained from measurements of tracer particles have been undertaken. [1,2] In the present work we extend these studies to hypothetical tracer particles which spontaneously enter the dendritic tree, perform a random walk on the dendritic tree and when reaching the soma spontaneously decay while emitting a signal.

[1] M. Reza Shaebani et al., Phys. Rev. E 98 (4 2018)

[2] Robin Jose, Ludger Santen and M. Reza Shaebani, Biophysical Journal 115.10 (2018)

BP 20.24 Wed 11:00 Poster B

Spherical harmonics and the morphology of red blood cells — •Thomas John, Felix Maurer, and Christian Wagner — Campus E26, 66123 Saarbrücken

Red blood cells are highly flexible and, at rest (without flow), exhibit a biconcave shape. Under flow conditions, altered environmental parameters, or due to diseases, this shape can deviate significantly from its resting state. Using 3D images obtained through confocal microscopy, we demonstrate how the shape, and thus the surface, can be represented as an expansion in spherical harmonics. This parameterization is rotationally invariant and can be utilized to distinguish between various cell shapes. This, in turn, can be done conventionally or through AI-based methods.

BP 20.25 Wed 11:00 Poster B

General motifs of flagella number control and cellular counting — •Richard Swiderski, Florian Rasshofer, and Erwin Frey — LMU, Munich, Germany

Monopolarly flagellated bacteria tightly control the flagellum assembly in order to construct only a single flagellum. Building upon models of the highly conserved C-ring assembly machinery, we present a theoretical study which identifies key motifs for number control in stochastic reaction networks. These findings not only help us to better understand the counting mechanism behind flagellum assembly, but can also be applied to more general processes which require the control of parti-

cle numbers. In the future this might be applied in medical treatments which rely on precise dosage on a cellular level.

BP 20.26 Wed 11:00 Poster B

Mean-filed theory for fibrillar aggregation and nematic-isotropic phase separation — •Kafa Alameh[1,2] and Christoph Weber[1] — [1]Mesoscopic Physics of Life, Institute of Physics, Universitätsstr. 1, Augsburg, Germany — [2]Center for Systems Biology Dresden, Pfotenhauerstr. 108, 01307 Dresden, Germany

Cells use droplet-like compartments to spatially organize their interior into sub-compartments, known as membrane-less organelles. Such organelles are liquid condensates and provide distinct physical environments for chemical processes. Recently, it has been shown that various proteins with beta-sheet structures, such as FUS, are involved in protein aggregation diseases such as ALS and Alzheimer's. Moreover, FUS-rich condensates were shown to undergo aberrant "phase transition," leading to fibrillar, solid-like aggregates. Several theoretical studies have focused on how phase-separated compartments affect the irreversible aggregation of dilute monomers; however, the interplay between aggregation and phase separation at non-dilute conditions remains elusive. Such conditions are particularly relevant at the condensate interface, where aggregates are often nucleated and enriched. Here, we propose a mean-field theory accounting for the interplay between aggregation, condensate formation, and phase transition at condensate interfaces. We find a rich phase behavior; three coexisting phases differing in density and the degree of order: disordered-dilute, disordered-dense, and nematic-dense phases. Our theory suggests the possibility of finding ordered membrane-less organelles in regulatory pathways of neurodegenerative diseases.

BP 20.27 Wed 11:00 Poster B

Tangential diffusion and motility-induced mixing transition in growing spheroidal cell colonies — •Torben Sunkel[1,2], Lukas Hupe[1,2], and Philip Bittihn[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Göttingen University, Göttingen, Germany

Growth is a known driver of cellular dynamics in a range of dense aggregates from bacterial colonies to developing tissues to tumors. Hence, universal physical principles underlying these dynamics are of great interdisciplinary interest. Here, we study the emergent dynamics arising from the interplay of growth, steric repulsion and motility in a minimal agent-based model of exponentially growing three-dimensional spheroids. Our results show that, without cell motility, deterministic motion caused by overall volume expansion dominates the dynamics of individual cells in the radial direction, while growth and division lead to cellular-scale diffusive motion in the tangential direction, whose magnitude is largely independent of expansion velocity. Despite this small-scale diffusion, we show that cell lineages are subject to confinement in their local environment, quenching weak cell motility. At higher motility, we find a transient regime of tangential superdiffusivity, accompanied by global mixing of cells. Reminiscent of glassy dynamics, we find a diverging mixing time scale at the transition. We also explore the influence of passive components like extracellular matrix. Our observations highlight the complex mechanical interaction between global expansion and local cell activity and may serve as a baseline to identify additional biological mechanisms in experiments.

BP 20.28 Wed 11:00 Poster B

A Study on Tradeoffs Induced Landscapes Model — •Muna Turki[1], Suman Das[2], Muhittin Mungan[3], Rotem Gross[4], and Joachim Krug[5] — [1]Institute of Biological Physics - University of Cologne — [2]Institute of Ecology and Evolution - University of Bern — [3]Institute of Biological Physics - University of Cologne — [4]Institute of Biological Physics - University of Cologne — [5]Institute of Biological Physics - University of Cologne

Effects mutations have on the fitness of a genotype are environment dependent. The endangering pressure of antibiotics directs bacterial cultures towards the selection of resistant mutants. These resistant mutants are equipped with mutations that increase the fitness of bacteria in the presence of antibiotics allowing for adaptation, however they come with a cost in the form of decreasing fitness in absence of antibiotics as the resistant mechanisms the mutant bacteria develop tend to be energy-costly, which is a tradeoff the mutant has to endure.

Tradeoff Induced Landscape (TIL) is a mathematical model that was motivated by antibiotic dose-response curves of Ciprofloxacin resistance in Escherichia coli strains which model evolution in a changing environment through adaptation-cost tradeoffs. The model assumes a non-epistatic accumulative effect of mutations on the fitness parameters, generating fitness landscapes with exceptionally smooth topology and high accessibility.

Recent experimental data on evolution of Escherichia coli in the context of β-lactam resistance are available through which the model could be tested and modified.

BP 20.29 Wed 11:00 Poster B

A Wang-Landau-based approach to sample the configurational space of complex biomolecules — •Camilla Spreti[1,2], Raffaello Potestio[1,2], and Roberto Menichetti[1,2] — [1]Physics Department, University of Trento, via Sommarive, 14 I-38123 Trento, Italy — [2]INFN-TIFPA - Trento Institute for Fundamental Physics and Applications,Trento, Italy

The Wang-Landau algorithm is a Monte Carlo (MC) method commonly employed to estimate the density of states (DoS) of a system through a random walk exploring the available energy space. This allows access to the thermodynamic properties of the system at all temperatures by means of a transformation from the microcanonical to the canonical ensemble. Although the algorithm was originally developed to study discrete systems, we propose a modified version of the method for sampling continuous systems, such as polymers, proteins and complex molecules. The implementation of the method is described and showcased with simple examples of liquid and polymeric systems.

BP 20.30 Wed 11:00 Poster B

Data-driven, ecosystem-based approach to cancer development — Alessandra Accettola, •Margherita Mele, and Raffaello Potestio — Physics Department, University of Trento, via Sommarive, 14 I-38123 Trento, Italy

Cancer cells exhibit a heterogeneous genetic and phenotypic landscape that evolves over time. Within this complexity lies the challenge of distinguishing critical driver mutations from less important ones.

Our approach, inspired by a minimalist model of microbial communities, explores hierarchically structured ecosystems to mimic the dynamics of resource competition. Using HiC data from different tumour stages, we model interactions to unravel the systematic differences that characterise evolutionary transitions from healthy to tumour cells.

Through this data-driven effort, we aim to achieve a dual goal: to delineate the systematic differences that drive evolutionary dynamics; and to identify critical features that drive such dynamics, ultimately providing the research community with a practical and useful instrument to comprehend and possibly hinder cancer development

BP 20.31 Wed 11:00 Poster B

Evolution on fitness landscapes with universal negative epistasis — •Daniel Oros and Joachim Krug — University of Cologne, Institute for Biological Physics, Germany

An approach to model evolution is by describing it as a process that selects viable genotypes from the space of all possible ones. Each genotype is assigned a fitness value, corresponding to its reproductive success. The search process then takes place in the landscape defined by the genotype and their corresponding fitness, referred to as fitness landscape. The notion of epistasis refers to the interaction between different mutations in the genotype and their effect on fitness. We investigate certain fitness landscapes that are structured [1]. The concept of universal negative epistasis (UNE) imposes short and long ranged effects on genotype interactions. A way to sample UNE landscapes and an analysis of them is presented together with a connection to the tradeoff induced landscapes (TIL) model [2]. This leads to a lower bound on the number of genotypes from which a peak is accessible from, already known from the TIL-Model. Recent experiments, see [1], highlight the importance of highly accessible landscapes. How their basins of attraction, meaning all genotypes from which a peak is accessible by increasing its fitness by mutations, differ is discussed along with general mathematical properties of UNE.

[1] Krug, J. and Oros, D. (2023) Evolutionary accessibility of random and structured fitness landscapes, https://arxiv.org/abs/2311.17432

[2] Suman G Das et al. Predictable properties of fitness landscapes induced by adaptational tradeoffs. In: eLife 9 (May 2020)

BP 20.32 Wed 11:00 Poster B

Modelling host-pathogen interactions: combining population dynamics with behavioural analysis — •Soham Mukhopadhyay[1], Jonathan Pollock[2], Ben Fabry[3], David Voehringer[2], and Vasily Zaburdaev[1] — [1]Max-Planck-Zentrum für

Physik und Medizin, Erlangen, Germany — [2]Department of Infection Biology, University Hospital Erlangen, Friedrich-Alexander University Erlangen, Germany — [3]Biophysics Group, Department of Physics, Friedrich-Alexander-University Erlangen

Helminth infections affect a large proportion of the world's population and cause significant morbidity. There are no vaccines against helminths, and the factors shaping how these parasites migrate through their hosts require further elaboration. To better understand the immune system response we develop a mathematical model describing the helminth load in different organs of the host as a function of time. We use the rodent helminth *N.brasiliensis* as a model to contrast migration dynamics in immunocompetent and susceptible mice during primary and secondary infection. We model the progression of infection as a system of coupled, time-delayed equations which allow us to link the initial infective dose to the number of eggs shed to the environment by adult worms and compare model predictions with experimental data. For a more microscopic insight into the behavior of larvae at different developmental stages, we carry out biophysical characterization of larval motility in in-vitro settings. Combining these results we aim to achieve a quantitative description of the infection progression in the host.

BP 20.33 Wed 11:00 Poster B

Mechanics of decision-making in light-trapped slime mold — •Lisa Schick, Emily Eichenlaub, Fabian Drexel, Siyu Chen, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

The human brain continuously makes conscious and unconscious decisions to navigate everyday life's complexity. Lacking a central nervous system, complex behavior and remarkable decision-making abilities have been reported for non-neuronal organisms like unicellular slime molds. Yet, decision-making is solely described as a response to processed information of the environment and focusing on the outcome rather than the decision-making process. We, here, trap the unicellular slime mold *Physarum polycephalum* in blue light shapes and follow its decision-making process to find an escape route. We find that decision-making is established by a dynamic adaptation of the flow pattern inside the tubular structure of the organism inducing a pressure buildup for overall mass reallocation.

BP 20.34 Wed 11:00 Poster B

Quantification of the network morphology of *Physarum polycephalum* under environmental effects — •Valentin Pauli, Lisa Schick, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

To fully understand an organism, one must consider both its intrinsic properties and its environmental interactions. Network-forming organisms, such as fungi and slime molds, continuously reorganize their networks. *Physarum polycephalum*, a unicellular slime mold, shows a remarkable adaptability in response to various environmental factors. In this study, we investigate environmental factors which lead to specific changes in network architecture and dynamics. By systematically altering the environment, we aim to decipher the factors that influence network adaptations in *Physarum polycephalum* and understand what functions underlie the observed adaptations. Understanding how the environment shapes *Physarum polycephalum* not only provides a better insight into the mechanisms of this extraordinary organism, but also contributes to a broader knowledge of adaptive behaviors in biological systems.

BP 20.35 Wed 11:00 Poster B

Periodic impulse response of ERK signaling in HeLa cells — •Stefan Köstler[1], Thoma Itoh[2], and Kazuhiro Aoki[2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]National Institute for Basic Biology, National Institutes of Natural Sciences, Okazaki, Japan

The Extracellular-signal Regulated Kinase (ERK) signaling pathway is one of the most important signaling pathways controlling the cell cycle and survival of most cells. Defects in this pathway are a critical step in the development of many cancers, making it a valuable target for treatment strategies. To gain insight into its response behavior, we activate ERK from different layers of the pathway by impulse stimulation. The ERK activity is quantified by using the fluorescent biosensor ERK-KTR-iRFP, which is exported from the nucleus upon phosphorylation. We show that impulse stimulation of two different layers of the pathway, either by EGF or the optogenetic tool Opto-RAF, both lead to a repeated activation of ERK with a characteristic period of about 65 minutes.

BP 20.36 Wed 11:00 Poster B

Dynamical Network Remodeling of Physarum polycephalum — •Mathieu Le Verge-Serandour and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Remodeling of a network is one of the hallmarks of biological flow networks, ensuring their optimal morphology. Due to limited building costs, the removal of vessels allows these networks to reallocate matter to minimize dissipation while ensuring maximum coverage,. *Physarum polycephalum* is a unicellular slime mold organized as a two-dimensional tubular network that evolves drastically over a few hours, evacuating a large zone of a few millimeters squared. Unfavorable competing parallel veins are first removed to form a tree-like structure, where veins prune sequentially until complete evacuation of the zone. Analyzing time-lapses of the slime mold, we find an exponential decrease in the number of tubes reproduced by our model based on the network hierarchy. We explore the dynamics of simulated networks by looking at the influence of the global outlets, tube length distribution, and network hierarchy. Our approach to flow networks may be generalized to pruning flow networks, as during embryonic development, stroke events, or information encoding.

BP 20.37 Wed 11:00 Poster B

Systematic Classification and Quantification of Microbial Interactions — •Timon Wittenstein, Gerrit Ansmann, Adriana Espinosa-Cantú, and Tobias Bollenbach — Institute for Biological Physics, University of Cologne, Germany

Microbial communities play a vital role in Earth's ecosystems, yet understanding how individual interactions shape the emergent properties of such communities remains a challenge. In a simplified laboratory system, we integrate theory and experiment to explore microbial interactions, focusing on a gut bacteria collection of the model organism *C. elegans*.

Informed by theoretical considerations, we employ a conditioned media approach to quantify pairwise interactions between individuals, aiming to differentiate various interaction types beyond just positive and negative classifications. We are able to identify trophic behaviours, such as resource competition or the exchange of nutrients, as well as more direct 'strong' interactions, like the transfer of toxins or vitamins.

The resulting interaction data unveils relationships among ecological interactions. For instance, competing populations exhibit more negative strong interactions, while more complex environments foster increased syntrophic interactions. Furthermore, these insights allow us to build a dynamical model and then quantitatively test its predictions in an experiment, offering a comprehensive approach for a deeper understanding of microbial ecology.

BP 21: Poster IIIb

Computational Biophysics, Protein Structure and Dynamics, Synthetic Life-like Systems and Origins of Life

Time: Wednesday 11:00–14:30 Location: Poster C

BP 21.1 Wed 11:00 Poster C

Contact Maps in RNA Structure Prediction — •Christian Faber, Utkarsh Upadhyay, Benjamin Kotton, and Alexander Schug — Forschungszentrum Jülich, Jülich, Germany

Predicting the spatial structure of non-coding RNA (*ncRNA*) is an important task for understanding fundamental processes in living nature. Physical force fields are used to infer the structure from a sequence using simulations on high-performance computers. However, the best results are obtained by incorporating evolutionary data via a binary mapping of contacts. The same phenomenon can be seen in protein structure prediction, where the groundbreaking *AlphaFold2* also incorporates this step. Much work has been done in the past to optimise the algorithms for simulations, but what are good contacts and why are these contacts important in the first place is an unsolved puzzle. To find answers, we tried different contact map topologies on a well-defined test set of *ncRNA*s. We also looked at using fewer, but wisely chosen contacts and how this can improve prediction. To obtain our results, we ran many simulations for comparison on the high performance cluster *JUWELS* with the RNA folding software *SimRNA* and used convolutional neural networks (*CNN*) to select contacts. Our results suggest that it is important to pay more attention to the selection of contacts, especially when developing machine learning algorithms. Furthermore, good contacts not only ensure faster folding in the simulation, they are actually essential for correct folding. It seems that it is the additional constraints that bring the physical force field into the more correct form.

BP 21.2 Wed 11:00 Poster C

Expanding the scope of bulk experiments by ensemble signal decomposition — •Nadin Haase, Simon Christ, and Sophia Rudorf — Institute of Cell Biology and Biophysics, Leibniz University Hannover, Germany

Compared to single-molecule experiments, ensemble or bulk methods are relatively time- and cost-efficient, and signal decomposition can help to expand their scope. Previously, we developed a detailed Markov model that incorporates the most central aspects of mRNA translation. Recently, we used our Markov model of translation to decompose fluorescent signatures of translating ribosomes in in-vitro ensemble experiments, revealing hidden kinetic information on the early phase of mRNA translation. Here, we investigate the limits of this method in terms of translation rates and the number of consecutive elongation cycles. Specifically, we show that the decomposition of a noisy ensemble signal generated by ribosomes translating mRNAs with more than just 5 codons represents already an ill-posed problem. We demonstrate that this problem can be treated with regularization to obtain translation state-specific information. Our results may aid in the extraction of information from bulk experiments to study the dynamics not only of translating ribosomes but also of other processive enzymes.

BP 21.3 Wed 11:00 Poster C

Implementation and Implications of a Lattice Model for the Understanding of Lipid Rafts in Membranes — •Simon Kellers, Fabian Keller, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstrasse 28/30, 48149 Münster, Germany

Based on comprehensive and extensive MD simulations of lipid bilayers, consisting of unsaturated, saturated lipids and CHOL [1], an existing lattice model [2][3] has been extended to incorporate the effects of CHOL on lipid ordering, relevant for the formation of lipid rafts. The MD simulation results suggest that interactions strongly depend on local CHOL concentrations. Furthermore, both lipids and CHOL are surrounded by four neighbors each, implying a square lattice model with a subgrid for CHOL.

The model relies solely on the enthalpic data from simulations and requires no phenomenological input. Additionally, as key variable it takes the order parameter of the lipids into account. The entropic contributions of the individual chains are adjusted through an iterative Boltzmann procedure, allowing for a clear separation and investigation of enthalpic and entropic effects. Due to the coarse-grained nature of the model, extensive and prolonged simulations of large systems will be feasible, allowing for the investigation of, e.g., the emergence of phase separation or phase transitions. [1] Keller, F; Heuer, A; *Soft Matter* **2021**, 25, 17 [2] Hakobyan, D; Heuer, A; *J. Chem. Phys.* **2017**, 6, 142 [3] Hakobyan, D; Heuer, A; *J. Chem. Theory Comput.* **2019**, 11, 15

BP 21.4 Wed 11:00 Poster C

Reversible formation of von willebrand factor platelet aggregates in blood flow — •Alper Topuz, Gerhard Gompper, and Dmitry A. Fedosov — Theoretical Physics of Living Matter, Institute of Biological Information Processing (IBI-5), Forschungszentrum Jülich, 52425, Jülich, Germany

Blood is a complex fluid that comprises of red blood cells, platelets, and various proteins suspended in plasma. Platelets and von Willebrand factor (vWF) proteins play a pivotal role in hemostasis (blood clotting). At high shear stresses, vWF molecules can stretch and become adhesive, so that they form bonds with encountered platelets, resulting in the formation of vWF-platelet aggregates. We employ hydrodynamic simulations together with explicit deformable cells and stretchable vWF polymers to model this aggregation-disaggregation process in blood flow. The aggregate formation is found to primarily occur near walls due to large wall-shear stresses. After reaching a critical size, the aggregates migrate away from the walls toward the vessel center. Under healthy conditions, vWF-platelet aggregates are reversible, as they dissociate again when the surrounding shear stresses become small. We explore different binding properties between vWF and platelets, which affect the reversibility of the aggregates and investigate the corresponding formation and disassociation characteristics of the aggregates. Understanding the aggregation process in blood flow is crucial in several pathologies such as thrombi formation and possible vessel blockage.

BP 21.5 Wed 11:00 Poster C

Modeling contraction of heart muscle tissue — •Michael Würriehausen[1], Volker Walhorn[1], Andreas Dendorfer[2], Hendrik Milting[3], and Dario Anselmetti[1] — [1]Bielefeld Univsersity — [2]Ludwig-Maximilians-University Munich — [3]Heart- and Diabetes Center Bad Oeynhausen

Computational modeling of heart muscle contractions is crucial for a better understanding of mechanical and electrical signals involved rhythmic dynamic of cardiac muscle dynamics. Two major groups of muscle models exist -the Hill-type and the Huxley-type muscle models, both of which are presented in this work. Hill-type models primarily use mechanical analogies such as an active force generating actuators, passive spring-like elements and passive viscous-damping elements to describe the whole muscle as a monolithic system. In contrast, Huxley models consider biophysical processes at the cellular level based on the actin myosin cross-bridge kinetics.

In the Huxley model we have designed, the muscle is divided into segments consisting of individual muscle cells, each of which has its own set of elements for reproducing muscle contraction. Both, Huxley and Hills models include the cardiac action potential and intracellular calcium concentration as key factors for a new approach in the muscle activation dynamics. The models can provide information about the relationship between heart muscle diseases and physiological parameters that are used in the numerical calculation to simulate muscle contraction.

BP 21.6 Wed 11:00 Poster C

Red blood cells adhesion and its Influence on capillary Flow in-vivo Microvasculature: A Simulation Study — •Mohammed Bendaoud[1,2], Alexis Darras[1], Yazdan Rashidi[1], Christian Wagner[1], and Chaouqi Misbah[2] — [1]Department of Experimental Physics, Saarland University, Saarbruecken 66123, Germany — [2]Université Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Red blood cells (RBCs) can aggregate and disassociate reversibly under normal physiological conditions. Cardiovascular diseases like hypercholesterolemia and diabetes have been associated with increased RBC aggregation. Fibrinogen is the main cause of this aggregation.

The normal range for human fibrinogen levels is 1.8 - 4 mg/ml. Diabetes can cause stable aggregates to form, leading to vessel blockages. This study aims to investigate the influence of adhesion between red blood cells and between RBCs and vessel walls on their behaviour in blood vessel networks. This encompasses RBC and plasma distribution, blood flow rate, and RBC lingering. Studying adhesion's impact on RBC behaviour is crucial for comprehending the intricate dynamics of blood flow in microvessels. We employ the lattice Boltzmann method in 2D to simulate RBCs behaviour with adhesion in a complex vascular network.

BP 21.7 Wed 11:00 Poster C

Simulating tumor-induced angiogenesis using Cells in Silico — •Eric Behle[1], Julian Herold[2], and Alexander Schug[1] — [1]NIC Research Group Computational Structural Biology, Jülich Supercomputing Centre, Jülich Research Center, Jülich, Germany — [2]Steinbuch Centre for Computing, KIT, Karlsruhe

Cancer remains an inadequately understood ailment affecting humanity. Its treatment poses a challenge due to tumor variability and a tumor's impact on the surrounding environment. Tumor-induced angiogenesis is a concerning aspect of the disease. Here, a hypoxic tumor secretes growth factors, which prompts nearby blood vessel branching and successive growth toward the tumor. To study this process on a computational level, we turned to Cells in Silico (CiS), a high performance framework for large-scale tissue simulation previously developed by us. Combining a cellular Potts model and an agent-based layer, CiS is capable of simulating tissues composed of tens of millions of cells, while accurately representing many physical and biological properties. Our ultimate objective is to construct a cellular digital twin of a tumor, and integrating a realistically evolving nutrient environment is crucial. Hence, we have implemented tumor-induced blood vessel growth into CiS, and have studied the behavior of tumors placed in different environments. With this we aim to explore questions regarding hot spots for tumor growth within the body.

BP 21.8 Wed 11:00 Poster C

Developing coarse graining RNA force fields via Machine Learning — •Anton Dorn[1] and Alexander Schug[1,2] — [1]Jülich Supercomputing Centre, Jülich, Germany — [2]Steinbruch Centre for Computing, Karlsruhe, Germany

In Protein structure prediction there have been massive improvements recently due to deep learning driven exploration of the rich experimental data. A direct transfer, however, of these methods to RNA structure prediction is impossible due to much sparser experimental data for RNA. Still, the combination of molecular force fields with constraints derived from statistical analysis of genomic data such as direct coupling analysis can lead to good quality structure predictions also for RNA. Here, we want to optimize the accuracy of the employed coarse-grained RNA force field for the molecular simulations by employing machine learning techniques. The data sparsity can here be alleviated by building on established atomistic RNA force fields. In a first step we show the viability of this approach by focusing on small RNA molecules in Molecular Dynamics simulations. We explore different bead numbers for the coarse graining to determine the best approximation.

BP 21.9 Wed 11:00 Poster C

Flexible patchy particles for modelling biomolecular condensates — •Alena Taskina[1,2], Simon Dannenberg[1], and Stefan Klumpp[1,2] — [1]Georg August Universität, Göttingen, Germany — [2]Max Planck School Matter to Life

Biomolecular condensates play a pivotal role in the spatial organization within cells. They form by liquid-liquid phase separation (LLPS), based on multivalent, non-specific interactions among proteins. The patchy particle model, comprising cores with isotropic repulsive potential and patches with attractive potential, captures the process of LLPS. In our study, we modify the current model by allowing patches to move laterally around the core. This refinement mimics the flexibility of protein domains. We investigated the phase behavior, connectivity, dynamics, and structural characteristics of the condensates. Increasing flexibility leads to a lower critical temperature, in gas-liquid coexistence curves, and thus a decreased stability of the condensate. The reason behind this decreased stability appears to be the dynamic nature of the bonds between patches, which results in fewer bonds being formed at certain temperatures. Furthermore, we observed that these more dynamic bonds contribute to an increased diffusivity of the condensates. Despite their reduced stability, condensates with more flexible patches were found to have a higher density that can be attributed to a less pronounced local ordering within the system, allowing for a more efficient packing of particles.

BP 21.10 Wed 11:00 Poster C

Free energy calculations of drug permeation through the bacterial outer membranes — •Vasily Unguryan and Jochen Hub — Saarland university, Saarbrücken, Germany

The development of bacterial resistance to antibiotics requires ongoing efforts to find new drugs. For the class of Gram-negative bacteria, their complex outer membrane represents a first and highly selective barrier on the cell-entering pathway for potential drug molecules. The outer leaflet of the membrane is mainly composed of lipopolysaccharides, whose chemical complexity leads to slow lateral diffusion and tight packing compared to phospholipid membranes, thus imposing poor uptake of many drug candidates.

Molecular dynamics simulations may, in principle, rationalize the low permeability of the outer membrane, for instance, by computing the free energy profile for drug permeation along the membrane permeation pathway. Unfortunately, common umbrella sampling simulations, widely used to compute free energy profiles, converge poorly for complex systems such as outer membrane models. In this project, we combine different enhanced sampling techniques to overcome such challenges, with the aim of deriving both free energy and diffusivity profiles for the permeation of bulky drug-like molecules across the outer membrane.

BP 21.11 Wed 11:00 Poster C

Dynamical and kinetic assessment of nucleic acid systems by CG simulations — •Lorenzo Petrolli, Manuel Micheloni, and Giovanni Mattiotti — Physics Department, University of Trento - via Sommarive, 14 I-38123 Trento, Italy

The in silico characterisation of nucleic acids at the molecular scale by Molecular Dynamics (MD) techniques has been extremely insightful in depicting the essential dynamics underlying a variety of biological activities. To relieve the numerical overhead associated with MD simulations of nucleic acids at the atomistic scale, coarse-grained (CG) force fields have been developed, such as oxDNA [1], that capture the global behaviour of nucleic acids, while keeping an appropriate level of resolution accounting for sequence-specific thermodynamic properties.

Here, we leverage the oxDNA force field and address two significant biological scenarios. On one hand, we characterise the equilibrium dynamics of a viral RNA fragment - and the evolution of the secondary and tertiary motifs thereof. On the other hand, we assess the kinetics of the DNA disruption by double strand breaks on circular DNA molecules, expanding on an earlier work [2], and describe the implications on the experimental characterization of the effects from cell irradiation.

[1] Snodin et al., J. Chem. Phys. 2015; [2] Micheloni et al., Biophys. J. 2023

BP 21.12 Wed 11:00 Poster C

A Bio-inspired Agent-based Model for Collective Shepherding — •yating zheng[1,2] and pawel romanczuk[1,2] — [1]Humboldt-Universität zu Berlin — [2]Research Cluster of Excellence 'Science of Intelligence'

Collective shepherding is a general control method for a swarm of intelligent agents to control other self-organized moving agents. The shepherding behaviour resembles prosperous animal behaviours, such as prey and predator, collective foraging and flocking behaviour and integrates their intrinsic qualities. However, most shepherding algorithms ignore the natural features of animal interactions and are limited to using one single shepherd. We propose an agent-based model to solve the shepherding problem with multiple shepherds. We first explore and compare different communication networks among sheep. Then we investigate the emerging coordination mechanism among shepherds and the related factors. Our model provides a potential method to control a heterogeneous swarm of robots.

BP 21.13 Wed 11:00 Poster C

Application of similarity measures to MD simulation data — •Fabian Schuhmann[1], Leonie Ryvkin[2], James D. McLaren[3], Luca Gerhards[3], and Ilia A. Solov'yov[3] — [1]University of Copenhagen, Copenhagen, Denmark — [2]Technische Universiteit Eindhoven, Eindhoven, Netherlands — [3]Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Biological processes involve movements across all measurable scales, which must be analyzed and understood to derive Nature's reasoning and understand the studied object's potential function. Especially in molecular dynamics simulations, considerable resources are allocated to get a picture of the motion of a protein.

While one can easily compare a protein structure to a reference employing tools like the Root Mean Square Deviation, methods need to become more involved to compare two whole trajectories. In a stop-motion movie, how does one spot the difference among thousands of atoms, all wiggling and moving?

We have gathered eight different similarity measures in an easy-to-use Python package called SiMBols. SiMBols includes the Hausdorff distance, the (weak) Fréchet distance, dynamic time warping, Longest Common Subsequence, a difference distance matrix approach, Wasserstein distance, and Kullback-Leibler divergence and combines them in a unified way.

Employing a case study, we will use the measures. We will find that the different similarity measures differ in their computation time and the research question they might answer.

BP 21.14 Wed 11:00 Poster C

Computational Approaches to Liquid-Liquid Phase Separation of Partially Disordered RS-Proteins — •Yannick Witzky[1], Arash Nikoubashman[1,2,3], and Friederike Schmid[1] — [1]Institute of Physics, JGU Mainz, Germany — [2]Leibniz-Institut für Polymerforschung, Dresden, Germany — [3]Institut für Theoretische Physik, TU Dresden, Germany

RS-proteins are RNA binding proteins that shape photomorphogenesis in plants by regulating alternative splicing events. Their light dependent appearance within nuclear speckles connects this alternative splicing function to their likely ability to induce or take part in liquid-liquid phase separation (LLPS). These divergent tasks of specific RNA binding and LLPS are reflected by the dual composition of RS proteins: folded domains, that contain the functionally important RNA binding sites, are complemented by intrinsically disordered regions (IDRs) which are common players in LLPS. To study the influence of the highly charged IDRs and the post translational phosphorylation of their amino acids on LLPS, we use replica exchange molecular dynamics with common IDP models [1,2] for enhanced sampling.

[1] Tesei et al. (2022) Open Research Europe, 2(94), 94. [2] Rizuan et al. (2022) J Chem Inf Model 62(18), 4474-4485.

BP 21.15 Wed 11:00 Poster C

Novel DNA-based nano force sensor to measure the clustering force of membrane-proteins — •Neda Rahmani and Weria Pezeshkian — Niels Bohr International Academy, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

Membrane-mediated clustering forces contribute to biological processes on cellular membranes, such as intracellular trafficking and signaling; they have their origin in a protein's ability to physically perturb the membrane's relaxed state. Clustering of extracellular ligands and proteins on the plasma membrane is required to perform specific cellular functions, such as signaling and endocytosis. Attractive forces that originate in perturbations of the membrane*s physical properties contribute to this clustering. The bacterial Shiga toxin (STxB) interacts with its cellular receptor, the glycosphingolipid globotriaosylceramide (Gb3 or CD77), as a first step to entering target cells. Previous studies have shown that toxin molecules cluster on the plasma membrane, despite the apparent lack of direct interactions between them. A membrane fluctuation-induced force generates an effective attractive force at separations around 1 nm, remains strong at distances up to the size of toxin molecules (several nanometers), and persists even beyond. This force is predicted to operate between manufactured nanoparticles providing they are sufficiently rigid and tightly bound to the membrane. In this project, we are going to design a nano force sensor to detect and calculate the clustering force between STxB bounded to a bilayer through GB3, and the suggested device is a DNA-based tweezer.

BP 21.16 Wed 11:00 Poster C

Using molecular dynamics simulation as a microscope of the peptide's translocation process through an aerolysin nanopore — •Michel Mom[1], Kumar Sarthak[2], Aleksei Aksimentiev[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany — [2]Beckman Institute for Advanced Science and Technology and Department of Physics, University of Illinois at Urbana- Champaign, Urbana, United-States

In recent years, a cost-effective method was developed to sequence DNA and RNA with high precision at the single-molecule level. This research project aims to extend this sequencing method to proteins and peptides which is still in the early stages. The method involves placing the analyte in an electrolyte solution separated by a lipid membrane which contains an implemented biological nanopore. An applied electrical voltage drives ion and analyte transport through the nanopore. The presence of the analyte in the nanopore results in a temporary reduction of the open-pore current, from which one can draw valuable conclusions about the structure of the investigated protein. To understand the effects of the analyte transport on the ionic flow at the atomic level, we conduct molecular dynamics simulations. Our results offer valuable insights into the translocation process of the peptide, revealing regions of resistance and predicting the residual ionic current. This poster demonstrates our application of molecular dynamics simulations to translocate peptides through a novel aerolysin nanopore variant, showcasing a proof of concept for future studies.

BP 21.17 Wed 11:00 Poster C

Reaction-diffusion models for growing skin patterns in cuttlefish — •Sigrid Trägenap, Feron Basoeki, and Matthias Kaschube — Frankfurt Institute for Advanced Studies

Cuttlefish exhibit unparalleled camouflage abilities supported by an array of chromatophores on their skin. These abilities persist throughout their lifespan, despite an at least 100-fold increase in body size and and chromatophore numbers. Recent advances (Reiter et al., Nature, 2018) allowed the identification and tracking of the chromatophore array over months. Their analysis revealed a typical distance between nearest neighbour chromatophores with unique local irregularities and that new chromatophores arise in gaps in the existing array. However, how this local irregularity arises and what local features predict chromatophore insertion remain unclear. Here, we address these questions by describing the development of the chromatophore array as an activator-inhibitor reaction-diffusion model on a growing domain. This can account for the experimentally observed distribution in distances between chromatophores, suggesting that a regular steady state is not reached due to the continuous growth. We find that chromatophores are inserted at the global inhibitor minima, predicting insertion locations for nonuniform growth. Additionally, such a model predicts an increased distance to the nearest neighbor chromatophore with development, explained by the overlapping ranges of Turing instabilities. This minimal model offers experimentally testable predictions and facilitates the identification of additional components necessary to fully describe chromatophore array development.

BP 21.18 Wed 11:00 Poster C

An order-disorder transition in cortical development — •Lorenzo Butti[1], Nathaniel Powell[2], Bettina Hein[1], Deyue Kong[1], Jonas Elpelt[1], Haleigh Mulholland[2], Matthias Kaschube[1], and Gordon Smith.[2] — [1]FIAS, Frankfurt am Main, Germany. — [2]University of Minnesota, Minneapolis, USA

How neural activity in cortex is shaped by the underlying neural circuitry remains poorly understood. Recent experiments in ferrets have shown that at an early stage in development, spontaneous activity exhibits a modular correlation structure that is similar to a quantitative degree across multiple cortical areas (including both sensory and higher association areas) [1].

In this work, we investigate how this correlation structure evolves over the course of development in different cortical areas. In all areas we observed a transition from an ordered, modular organization to a more fine-scaled, disordered organization.

To explain these results, we study a linear recurrent neural network model.* Assuming the recurrent interactions follow a local excitation and lateral inhibition (LELI) scheme, the model is able to reproduce the modular structure of spontaneous activity we observe in the early cortex[2]. We then analyse different scenarios of possible network changes and we find that an effective weakening of recurrent connections over development is a major factor affecting the degree of modularity and how it changes across development.

[1]https://www.world-wide.org/cosyne-22/universality-modular-correlated-networks-5a1134a0 [2]Smith et al., 2018

BP 21.19 Wed 11:00 Poster C

Stability of the Pore Structure of α-Latrotoxin and the Unusual Ion Transport Mechanism through a Synaptic Membrane — •Azadeh Alavizargar and Andreas Heuer — Institute

of Physical Chemistry, University of Muenster, Corrensstr. 28/30, 48149 Muenster, Germany

Latrotoxins (LaTXs) are presynaptic pore-forming neurotoxins found in the venom of Latrodectus spiders, known as black widows. Through the binding of LaTXs to specific receptors on the surface of neuronal cells, neurotransmitters are released by the formation of Ca2+-conducting tetrameric pores inside the membrane. The cryo-electron microscopy pre-pore and the pore structure of the α-LaTX has been resolved by the group of Christos Gastogiannis. However, the structure of the membrane part has not been characterized so far. Thus, the mechanism of ion transport through the membrane is still unclear.

Therefore, in this work we study the pore structure of α-LaTX, starting from the AlphaFold prediction, via molecular dynamics (MD) simulations also using Metadynamics. It turns out that the N-terminal is composed of a stable coiled-coiled bundle and a complex membrane-protein part. Specifically, we study the ion transport of Na+ and Ca2+ ions across the membrane. Surprisingly, the coiled-coiled region is not involved in the ion transport and the ions are attracted and finally crossed only through its membrane part. These results provide crucial insights towards the understanding of the mechanism of the LaTX family of neurotoxins.

BP 21.20 Wed 11:00 Poster C

Modelling contrast-variation SAXS experiments by explicit-solvent molecular dynamics — •Noora Aho and Jochen Hub — Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Small angle X-ray scattering (SAXS) has established its role in structural biology during the last decades, providing information on the shape, interactions and large-scale conformational transitions of biomolecules in solution. In addition, so called contrast-variation SAXS, where the scattering data is recorder at multiple solvent electron densities, adds the possibility to measure electron densities of biomolecular assemblies enabling the visualisation of distinct biomolecules. The interpretation of experimental SAXS data requires the accurate calculation of SAXS curves from structural models. To achieve this, explicit-solvent molecular dynamics (MD) is a powerful method, taking into account both the atomistic accuracy and correct thermal fluctuations in the scattering curve calculations.

In this work, our aim is to expand the application of explicit-solvent MD simulations from conventional SAXS to contrast-variation SAXS experiments. We model the ferrichrome membrane transporter protein FhuA in the presence of lanthanide contrast agents in explicit solvent and calculate corresponding SAXS curves using MD simulations. In addition to supplementing experimental SAXS data for the specific protein, our simulations serve as an example of the possibilities of explicit-solvent MD in interpretation of advanced SAXS experiments.

BP 21.21 Wed 11:00 Poster C

Machine Learning Guided RNA Structure Prediction — •Utkarsh Upadhyay[1], Oskar Taubert[2], and Alexander Schug[1] — [1]Jülich Supercomputing Centre, Germany — [2]Karlsruher Institut für Technologie, Germany

For around 50 years, the primary focus of genomic research has been the development of efficient and accurate methods to predict the structure of proteins, which led to the birth of better sequencing techniques and databases. About 98% of the human genome(RNA, DNA) during this action was overlooked. However, In the past few years, studies have revealed the existence of many non-coding RNAs which catalyse various biological processes; to understand these roles better, we require the appropriate structure of RNAs. Recent years have led to breakthroughs in protein structure prediction via Deep Learning. The scarcity of RNA structures, however, makes a direct transfer of these methods impossible. Here, we present machine-learning techniques that can work with limited training data. We predict contact maps as a proxy to understand and predict RNA structure, they provide a minimal representation of the structure. We have worked on methods that took accuracy from 47%(DCA)[1] to 77%(CoCoNet)[2] and now to 87%(Barnacle)[3] i.e. doubling accuracy while reducing false positives by five-fold. Further, we are working on developing language models that can make use of large sequence databases and provide more structural insights. We are confident that this remarkable progress will reduce the sequence-structure gap for RNA.

BP 21.22 Wed 11:00 Poster C

A NAP-XPS-study on X-ray radiation damage: Chemical changes to Gene-V Protein — •Dorothea C. Hallier[1,2,3], Jörg Radnik[2], Paul M. Dietrich[4], Harald Seitz[1,3], and Marc Benjamin Hahn[2] — [1]Fraunhofer Insitute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses, Potsdam, Germany — [2]Federal Insitute for Materials Research and Testing BAM Berlin, Berlin, Germany — [3]Univerity of Potsdam, Institute for Biochemistry and Biology, Potsdam Germany — [4]SPECS Surface Nano Analysis GmbH, Berlin, Germany

Single-stranded DNA-binding proteins such as Gene-V Protein (G5P/GVP) are involved in maintaining the DNA metabolism in cells. This is essential for cell viability, especially after exposure to ionizing radiation, i.e. after radiation therapy in cancer treatment. X-ray photoelectron spectroscopy (XPS) was used to analyze the chemical damage of ionizing radiation to G5P itself. Direct and indirect damage was detected through combined vacuum XPS and near-ambient pressure (NAP) XPS measurements under water atmosphere. A strong increase of protein damage was observed in water as compared to vacuum.

BP 21.23 Wed 11:00 Poster C

Length Scale Selection Through Mechano-Chemical Coupling — •Antonia Winter[1], Yuhao Liu[1], Alexander Ziepke[1], George Dadunashvili[1], and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoSciences, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 Munich, Germany — [2]Max Planck School Matter to Life, Hofgartenstraße 8, 80539 München, Germany

The formation of spatial and temporal patterns is an essential part of being a living organism. Control of the length scales of patterns is a key aspect of the robust and reproducible biological function of the organisms, which leads to the question of how this pattern length scale can be controlled. One possible mechanism is mechano-chemical coupling between curvature-inducing proteins and the deformation of membranes. We investigate a minimal system combining geometric membrane-mediated coupling and protein-protein interactions. In our theoretical framework, the dynamics of proteins are characterized by a Flory-Huggins energy capturing their interactions on a membrane manifold, while the fluid-elastic membrane is described by a Canham-Helfrich energy wherein proteins induce spontaneous curvature of the membrane. As a result, we obtain three different phases: A fully phase-separated system, a spatially homogenous regime, where the geometry suppresses the protein aggregation, and an interrupted coarsening regime, where the length scale of the resulting pattern is determined by the balance between the cost of protein mixing and the membrane curvature in the free energy.

BP 21.24 Wed 11:00 Poster C

Dramatic differences between the structural susceptibility of the S1 pre- and the S2 postfusion states of the SARS-CoV-2 spike protein to external electric fields revealed by molecular dynamics simulations — •Alexander Lipskij — Theoretical Physics and Center of Interdisciplinary Nanostructure Science and Technology, FB10

In its prefusion state, the SARS-CoV-2 Spike protein (S) is metastable, which is considered to be an important feature for optimizing or regulating their functions. Binding of its S1 subunit (S1) with the ACE2 receptor causes dramatic conformational change in the S protein where S1 splits from the S2 subunit, which then penetrates the membrane of the host cell, promoting the fusion of the viral and cell membranes resulting in the infection of the host cell. In a previous work, we showed using large scale molecular dynamics simulations that the application of external electric fields (EF) induce drastic changes and damage in the receptor-binding domain (RBD) of the wild type S protein, as well of the Alpha, Beta and Gamma variants, leaving a structure which cannot be recognized any more by ACE2. In this work we extend the study to Delta and Omicron and confirm the high sensitivity and extreme vulnerability of S to moderate EF, and we show that, in contrast, the postfusion state of the S protein does not suffer structural damage even if electric field intensities four orders of magnitude higher applied. As a consequence, these results provide a solid scientific basis for confirming the metastability roots of the SARS-CoV-2 S protein, which is susceptible to damage by EF, in the prefusion state.

BP 21.25 Wed 11:00 Poster C

Finding (Un)binding Pathways in Protein-Ligand Systems — •Miriam Jäger and Steffen Wolf — Biomolecular Dynamics, Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

Understanding dynamics and free energy landscapes of ligand association and dissociation from proteins is hampered by the slow timescales of these transitions. To enhance transition sampling we enforce ligand unbinding from a protein by applying dissipation-corrected targeted MD (dcTMD) simulations, which enforce a moving distance constraint along a pre-chosen reaction coordinate. Using a naive biasing coordinate, ligand unbinding occurs via different pathways, which need to be identified to carry out a dissipation correction. However, uncovering the different pathways along complex reaction coordinates presents a challenge. To address this challenge, we utilize the Streptavidin-biotin complex as test system. Employing various distance measures as input features to cluster similar unbinding trajectories, we aim to reconstruct unbinding pathways and connecting these pathways to internal coordinates.

BP 21.26 Wed 11:00 Poster C

AlphaFold-driven modeling of cytochrome bd-I: A structural approach to antibiotic design — •Noah Rickermann, Jonathan Hungerland, and Ilia A. Solov'yov — University Oldenburg, Department of Physics, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

In the pursuit of novel antibiotics, targeting proteins involved in the metabolic pathways of pathogens has emerged as a promising strategy. The terminal oxidase cytochrome bd-I, found exclusively in bacteria (e.g. E. Coli or M. tuberculosis), serves as a promising target for antibiotics. However, incomplete structural data due to limitations of electron microscopy hinders a comprehensive understanding of the protein's function. This study introduces a computational model of the cytochrome bd-I complex, reconstructed using the AlphaFold protein structure prediction program, in combination with experimental information for placement of the prosthetic groups. Model validation incorporated the mutation study of Mogi et al. [1], who examined substrate binding properties in cytochrome bd-I. To assess the accuracy of the derived protein model free energy perturbation simulations were employed. Additionally, efforts were carried out to identify potential inhibitors for Cytochrome bd-I, yielding promising drug candidates in the early stages of the investigation [2-3].

[1] Mogi et al. Biochem. 45.25 (2006) [2] Jacobsen et al. "Introducing the Automated Ligand Searcher". J. Chem. Inf. Model. (2023) [3] Korol et al. "Introducing VIKING: A novel misc platform for multiscale modeling". ACS Omega 5.2 (2020)

BP 21.27 Wed 11:00 Poster C

Binding Study of Beta-2-Glycoprotein I and Integrin-Containing Artificial Lipid Membranes — •Emma Weilbeer[1], Una Janke[1], Thomas McDonnell[2], and Mihaela Delcea[1] — [1]Biophysical Chemistry Department, Institute of Biochemistry, University of Greifswald — [2]Division of Medicine/ Biochemical Engineering, University College London, UK

Beta-2-glycoprotein I (β2GPI) is a highly glycosylated plasma protein and the most important antigenic target for autoantibodies in antiphospholipid syndrome. β2GPI circulates as a closed form but opens up under specific conditions. Although β2GPI has been found in blood clots, its physiological role is not yet fully understood. Therefore, it is of great importance to investigate the function and the dynamics of β2GPI in the coagulation cascade using for example, biophysical methods. Imaging of fluorescently labeled protein suggests that β2GPI binds to human embryonic kidney cells expressing αIIbβ3 integrin (i.e. the main platelet receptor essential for platelet aggregation and undergoing conformational dynamics). We have investigated the interaction of open and closed β2GPI with activated and non-activated integrin αIIbβ3-containing lipid bilayers mimicking the outer leaflet of platelet membranes. A combination of various biophysical methods (e.g. dynamic light scattering, circular dichroism spectroscopy, atomic force microscopy, surface plasmon resonance) have been used for protein characterization and protein-protein interactions. Our biomimetic model enables the specific analysis of disease relevant protein-protein interactions involving protein conformational dynamics.

BP 21.28 Wed 11:00 Poster C

Coarse-grained simulations of peptide Lge1(1-80) — •Agaya Johnson[1], Anton Polyansky[2], Sofia Kantorovich[1], and Bojan Zagrovic[2] — [1]Computational and Soft Matter Physics, University of Vienna, Kolingasse 14-16, 1090 Vienna, Austria — [2]Department of Structural and Computational Biology, Campus-Vienna-Biocenter 5, 1030 Vienna

Biomolecular condensates in cells such as p-bodies, nucleoli and stress granules play an important role in regulating biological processes like transcription, ribonucleic acid(RNA) metabolism and ribosome biogenesis. Studying of such biomolecular condensates will give insight into the molecular basis of diseases, like neurodegenerative diseases, cancer and diabetes. The main purpose of this study is to understand the main phenomenon, which leads to the formation of these bimolecular condensates such that we get a conclusion, whether is it phase separation, self assemble or an aggregation. We use Lge1(1-80) peptide as a model for study because Lge1(1-80) is mostly disordered, prone to form many cation-pi and pi-pi interaction(R, G and R rich sequence) and because of its alternating net charge which are the prerequisites for the phase separation. Due to the limitation of high-resolution experimental techniques, we are using molecular dynamics simulation with coarse-grained approaches, with the help of software ESPResSo. Our goal is to develop a coarse-grained model for the proteins that exhibit structural transitions and to understand the fundamental mechanisms under those transitions.

BP 21.29 Wed 11:00 Poster C

Non-Markovian friction dependence on intra-molecular reaction coordinates in protein folding — •Jonathan Remmert, Benjamin A. Dalton, and Roland R. Netz — Freie Universität Berlin, Berlin

Protein folding is commonly described using one-dimensional reaction coordinates. The dynamics of these coordinates depend on the free energy profile and on the effective friction. Experimental techniques to measure protein folding, such as FRET experiments, use distances between residues in the amino acid chain as reaction coordinates, which are known to exhibit strongly non-Markovian dynamics.

By applying novel methods to extract non-Markovian friction kernels from simulation data, we describe the dynamics of intra-molecular distance reaction coordinates by the Generalised Langevin Equation. We explore the dependence of the non-Markovian friction on the specific distance coordinate chosen, thereby enabling a detailed theoretical description and understanding of FRET experiments.

BP 21.30 Wed 11:00 Poster C

Electric field susceptibility of metastable proteins and implications for controlling viral propagation — •Claudia Arbeitman[1,2,3], Pablo Rojas[1], Alexander Lipskij[1], Pedro Ojeda-May[4], and Martin Garcia[1] — [1]Theoretical Physics, University of Kassel, Kassel, Germany — [2]GIBIO-UTN, Buenos Aires, Argentina — [3]CONICET, Buenos Aires, Argentina — [4]Umeå University, Umeå, Sweden

The internal motion and configuration of proteins are intimately related to their ability to perform functions. Their conformational changes and stability properties determine the molecular recognition capabilities and, ultimately, the set of interactions with other molecules. The thermodynamic stability and kinetic barriers that limit the kinetic accessibility of the conformational landscape of proteins are, though, not the same for all families of proteins.

In this work, we use molecular dynamics simulations to show that metastable proteins, such as the SARS-CoV-2 spike protein in the prefusion conformation, are susceptible to irreversible changes in their secondary and tertiary structures when exposed to moderate electric fields, orders of magnitude weaker than those reported for other proteins and for the same protein in the post-fusion conformation. Simulations of the docking with the host cell receptor ACE2 reveal that changes in the structure lead to impaired recognition. We explain the implications of these findings for the future study of metastable proteins and the development of inactivation technologies.

BP 21.31 Wed 11:00 Poster C

Role of Phase Separation in RNA co-evolution — •Samuel Santhosh Gomez, Gaetano Granatelli, and Christoph Weber — University of Augsburg, Augsburg, Germany

The PhD project, called 'Client Scaffold Model for Compartmentalized RNA Evolution', aims to create a theoretical framework that can account for RNA strand replication. From which, to then to study how compartments formed by scaffold phase-separation may be able to play a role in providing micro environments that might allow for the possibility for co-evolution of RNA replicators with RNA replicator parasites. The motivation for such a theoretical model comes from host-parasite RNA replicator experiments that suggested that droplet compartments might be able to provide an environment for co-evolution which is not possible in the well mixed homogeneous case.

BP 21.32 Wed 11:00 Poster C

Controlling transport for RNA enrichment in 2D-alkaline chimneys — •Mona Byberg Michelsen and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Alkaline vents at the prebiotic ocean floor are hypothesized as a setting for the emergence of life. These alkaline vents (AVs) produce chimneys with intricate hierarchical architectures and steep pH gradients. Under these conditions, intricate flow networks facilitate complex transport of organic molecules and other compounds. For the emergence of life, the enrichment and synthesis of organic molecules, in particular nucleic acids, need to be facilitated. Yet, the location within the AV chimneys and the necessary flow conditions to overcome the concentration problem are still unknown.

Our recently established microfluidic two-dimensional (2D) model of alkaline chimneys allows us to directly observe chimney architecture, fluid flow, and molecule transport and enrichment. By combining optical tracking with numerical methods, we aim to establish a quantitative model of transport through the AV chimney. Experimental 2D chimneys will be optimized using predictions from the quantitative model and tested for enrichment of organic compounds. Finally, the effects of a dynamic chimney environment will be probed by periodically changing inflow salt concentration and tracking the impact on denaturation and hybridization of nucleic acids. Through this combination of experiments and quantitative modeling, we aim to uncover the physical prerequisites for the enrichment of nucleic acids and the creation of dynamic environments facilitating replication at the origin of life.

BP 21.33 Wed 11:00 Poster C

Theory of RNA evolution in phase-separated systems — •Gaetano Granatelli, Samuel Santhosh Gomez, and Christoph Weber — Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Germany

Evolution is due to the error-prone replication processes of genetic material, DNA or RNA, performed by replication machinery translated from the same genetic material.

The aim of the project is to develop a theoretical framework that can account for RNA replication with and without a phase-separated droplet, to investigate how phase coexistence could play a role in providing spatially confined micro-environments which allow for the co-evolution with parasitic RNA replicators. We build our model upon a client-scaffold theoretical framework that decouples phase separation of scaffold molecules from the reaction kinetics of dilute clients.

The motivation for such a model comes from theoretical and experimental work on translation-coupled RNA replication systems within cell-like compartments, where the evolution of host and parasitic RNA species is analysed: hosts have the ability to translate a self-encoded RNA replicase, whereas parasites do not (having lost their replicase encoding region due to mutations). These studies suggest that compartmentalization might be necessary for co-evolution of host and parasite replicators, which instead is not observed in bulk conditions.

BP 21.34 Wed 11:00 Poster C

Cell-Free Gene Expression in Bioprinted Fluidic Networks — •Alexandra Bienau and Friedrich C. Simmel — Technical University Munich, Germany

Cell-free protein expression is a valuable tool to produce specific proteins in vitro without the need for a host organism. The reduced metabolic background activity enables high product concentrations and precisely controlled reaction conditions for prototyping genetic circuitry. Microfluidic devices instead of closed reactors were used in previous works to enable longer reaction times and out-of-equilibrium behavior.

In this work, we create fluidic networks in a diffusible hydrogel environment using extrusion-based bioprinting as a fast production tool. We print sacrificial structures of Pluronics F-127 and cast agarose around them to build channels within the hydrogel, mimicking natural fluid distribution networks. The channels can be filled with customized liquids, such as the cell-free reaction mixture, and the reactions are not limited to the channels but can extend into the surrounding gel by diffusion. The behavior of fluorescent protein production within the agarose hydrogels is investigated using an E. coli-based cell extract.

Implementing gene circuitry by cell-free reactions allows for adding another design layer using bottom-up self-organization. In the future, we aim to use this design strategy to create more complex, tissue-like objects. We envision the construction of biohybrid structures combining artificial and natural cells to develop smart soft-robotic materials.

BP 22: Bacterial Biophysics II

Time: Wednesday 15:00–17:15 Location: H 0112

BP 22.1 Wed 15:00 H 0112

Heterogeneous distribution of the adhesion capability across the cell envelope of *Staphylococcus aureus* cells — •Hannah Heintz[1], Christian Spengler[1], Erik Maikranz[2], Michael Klatt[1,3], and Karin Jacobs[1] — [1]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Department of Theoretical Physics, Saarland University, Saarbrücken, Germany — [3]Department of Physics, Princeton University, Jadwin Hall, Princeton, USA

Understanding how a bacterium attaches to a surface is particularly important for controlling biofilms. Bacterial adhesion is known to be mediated by thermally fluctuating cell wall macromolecules [1], but the distribution of these adhesive-supporting macromolecules across the cell envelope is still unknown. We apply single cell force spectroscopy to study the adhesion force of *Staphylococcus aureus*. As a new approach, a sinusoidal PDMS surface is used, and force-distance curves are recorded along a path perpendicular to the structured surface. This allows for probing contact points distributed over almost a hemisphere of an individual bacterium. The analysis of the adhesion strength data shows that some bacterial cells display particularly strong adhesion at certain locations [2]. To obtain a complementary picture, Monte Carlo simulations are used to interpret the resulting adhesion profiles. Simple geometric considerations couldn't explain the origin of all adhesion profiles. Therefore, angle-dependent molecule-substrate interactions must be considered. [1] Spengler, C, et al., Front. Mech. Eng., 7:661370 (2021). [2] Spengler, C., et al., Softmatter, D3SM01045G (2023).

BP 22.2 Wed 15:15 H 0112

Local decrease in cell wall mechanical stress as a possible trigger for cell splitting in *Staphylococcus aureus* — •Sheila Hoshyaripour[1,2,3], Marco Mauri[1,2], Abimbola F. Adedeji Olulana[4], David Owen[4], Jamie K. Hobbs[4], Simon J. Foster[4], and Rosalind J. Allen[1,2] — [1]Friedrich Schiller university, Jena, Germany — [2]Cluster of Excellence Balance of the Microverse, Jena, Germany — [3]Jena School of Microbial Communication, Jena, Germany — [4]University of Sheffield, Sheffield, UK

Staphylococcus aureus is a clinically important Gram-positive bacterium able to generate antibiotic-resistant strains. Cell division happens in few milliseconds without cell wall constriction and how the cell controls the initiation of division is not clear. Our observations using atomic force microscopy and fluorescence microscopy show that the mechanical and geometrical properties of the cell and the cell cycle timing change with genetic mutations and in the presence of antibiotics. In addition, it is observed that peptidoglycan hydrolase activity, which plays a key role in cell division, may be negatively stress dependent. Here, we created a theoretical model to show how mechanics and hydrolysis work together to regulate the cell cycle. Our modelling shows that, during the cell cycle, mechanical stress decreases around the division site. With the hypothesis of stress-dependent triggering of the enzymes, the model predicts the timing of the later phases of the cell cycle which is supported by microscopy data. The model provides new insights into the combined effects of mechanical forces and enzyme activity in cell cycle regulation and initiation of division in *S. aureus*.

BP 22.3 Wed 15:30 H 0112

How Does a Riboswitch Differentiate Between Mg^{2+} and its experimental mimic Mn^{2+} for Specific Binding? — Kushal Singh and •Govardhan Reddy Patluri — Indian Institute of Science, Bangalore, India

Metalloriboswitches regulate metal ion homeostasis in bacteria. The aptamer domain of the Mn-sensing riboswitch (Mn-AD) binds to Mn^{2+} with high specificity in the presence of Mg^{2+}. However, Mn^{2+} can

substitute Mg^{2+} in the binding pockets of RNA structures and is exploited as an experimental probe. To understand the specificity of Mn-AD towards Mn^{2+} sensing in the presence of Mg^{2+}, we used computer simulations and RNA models with different resolutions. We find that the specificity of the binding pocket for Mn^{2+} binding is driven by kinetics as Mn^{2+} loses a water molecule from its first solvation shell and transitions to an inner-shell interaction with a phosphate oxygen in the binding pocket relatively faster compared to Mg^{2+}. The enhanced sampling simulations show that Mn^{2+} further consolidates its binding to the MB pocket via conformational rearrangements, facilitating hierarchical dehydration of the six water molecules from its solvation shell and transitions to inner-shell coordination. The free energy for Mn^{2+} to lose six water molecules for its solvation shell is downhill compared to Mg^{2+}. These results provide insight into how bacteria use RNA to sense specific metal ions from a pool of biologically relevant metal ions to maintain homeostasis.

BP 22.4 Wed 15:45 H 0112

Amyloid fibers in biofilms: structure adaptation to environmental cues — •Macarena Siri, Agustín Mangiarotti, Mónica Vázquez-Dávila, and Cécile Bidan — Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

E. coli biofilms consist of bacteria embedded in a self-produced matrix mainly made of protein fibers and polysaccharides. Not only the extracellular matrix plays a major role in achieving biofilm stability under different environmental conditions, but also is sensitive to their surroundings. The curli amyloid fibers found in the E. coli matrix determine the architecture and stiffness of their biofilms. They are promising versatile building blocks to design sustainable bio-sourced materials. To exploit their potential, it is crucial to understand how environmental cues during biofilm growth influence the molecular structure of these amyloid fibers, and how this translates at higher length scales. We studied the effect of water and nutrient content in the substrate on both biofilm materials properties and the structure and properties of curli amyloid fibers extracted from the biofilms. We used micro-indentation to measure the rigidity of the biofilms grown under different conditions, followed by microscopy and spectroscopy to characterize the amyloid fibers purified from the respective biofilms. The purified curli amyloid fibers present differences in the structure and functional properties upon different biofilm growth conditions. Our study highlights how E. coli biofilm growth conditions impact curli structure and functions contributing to macroscopic materials properties.

BP 22.5 Wed 16:00 H 0112

Global instabilities in maturing gonococcal colonies mediated by local type 4 pili interactions — •Marc Hennes[1], Kai Zhou[3], Benedikt Sabass[2], and Berenike Maier[1] — [1]Institute for Biological Physics, University of Cologne, Germany — [2]Institute of Infection Medicine and Zoonoses, Ludwig-Maximilians-University Munich, Germany — [3]Institute of Biological Information Processing, Forschungszentrum Jülich, Germany

Mechanical forces and interactions play a pivotal role in the outdifferentiation process of biofilm maturation. Active stresses in the form of swimming, growth pressure, and shear forces shape the three dimensional structure of bacterial aggregates and are linked to the metabolic activity of cells via underlying nutrient and metabolite fields. In the case of the pathogen *Neisseria gonorrhoeae*, initial aggregation is mediated by the short-range interaction of bound Type 4 Pili (T4P), filamentous appendages which cover the cell surfaces. Under load, pili connections continuously break, conferring dynamical and liquid-like properties to the proliferating colonies. As we discovered, the establishing nutrient gradients inside these growing aggregates entrain outdifferentiation of the local interaction frequency of T4Ps, and induce at a certain aggregate size a global mechanical instability which restructures the complete colony. We discuss the physical nature of the instability, identify the underlying nutrient trigger, and present possible advantages for the colonies in the form of increased cell dispersion.

15 min. break

BP 22.6 Wed 16:30 H 0112

Reciprocity of flagellar polymorphism and cell-body motion during tumbling of an *E. coli* — •Derek Cyrus Gomes[1], Holger Stark[2], and Tapan Chandra Adhyapak[1] — [1]Indian Institute of Science Education and Research (IISER) Tirupati, Tirupati, India — [2]Institut für Theoretische Physik, Technische Universität Berlin

The study of the dynamics of *E. Coli* has proven to be an extremely challenging problem due to the complex mechanisms underlying its motion. One such aspect of the dynamics involves *E.Coli's* abrupt change of swimming direction during the tumbling events. The event results from the reverse rotation of one of the flagella, making it leave the flagellar bundle and causing, at the same time, an overall change in the bacterium's motion. It has been shown experimentally that during the tumbling event, the reverse-rotated flagellum undergoes transitions among several of its stable structures known as the polymorphic forms. While polymorphic transitions accompany a tumbling event, their necessity and influence over the tumbling statistics are unknown. In this work, we numerically probe the interplay of the cell body dynamics and flagellar polymorphism during a tumbling event. We find a reciprocal response between the two: while the polymorphic transitions do affect the cell body's tumbling dynamics, in turn, the cell-body motion can arrest the growth of the polymorphic forms. We present our results in light of the observed tumbling statistics, revealing new insights to understand the experimental observations. We also investigate the role of hydrodynamic interactions and shear flow in the aforementioned phenomena.

BP 22.7 Wed 16:45 H 0112

Sensory adaptation in a continuum model of bacterial chemotaxis - working range, cost-accuracy relation, and coupled systems — •Vansh Kharbanda[1,2] and Benedikt Sabass[1,2] — [1]Department of Veterinary Sciences, LMU München — [2]Department of Physics, LMU München

Sensory adaptation enables organisms to adjust their perception in a changing environment. A paradigm is bacterial chemotaxis, where the output activity of chemoreceptors is adapted to distinct baseline concentrations via methylation. The range of internal receptor states limits the stimulus magnitude to which these systems can adapt. Here, we use a highly idealized, Langevin-equation based model to study how the finite range of state variables affects the adaptation accuracy and the energy dissipation in individual and coupled systems. Maintaining an adaptive state requires energy dissipation. We show that the steady-state dissipation rate increases approximately linearly with the adaptation accuracy for varying stimulus magnitudes in the so-called fully adaptative state. This result complements the well-known logarithmic cost-accuracy relationship for varying chemical driving. Next, we study linearly coupled pairs of sensory units. We find that the interaction reduces the dissipation rate per unit and affects the overall cost-accuracy relationship. A coupling of the slow methylation variables results in a better accuracy than a coupling of activities. Overall, the findings highlight the significance of both the working range and collective operation mode as crucial design factors that impact the accuracy and energy expenditure of molecular adaptation networks.

BP 22.8 Wed 17:00 H 0112

Photokinesis and phototaxis in light-driven E. coli — •Giacomo Frangipane[1,2], Claudio Maggi[2], Maria Cristina Cannarsa[1], and Roberto Di Leonardo[1,2] — [1]Department of Physics, Sapienza University of Rome, Italy — [2]NANOTEC-CNR, Soft and Living Matter Laboratory, Institute of Nanotechnology, Italy

Bacteria inherently possess signal-detection capabilities, altering their movement patterns accordingly. Today synthetic biology techniques allow us to engineer bacteria by introducing heterologous receptors so that they respond to new stimuli. In this work, we expressed the light-driven proton-pump proteorhodopsin in E. coli cells to control their flagellar motors with light. In this modified bacteria, light affects both speed (photokinesis) and tumbling rate (phototaxis). We study the phenomenology emerging from the interplay between these two effects and observe that, if we apply a sinusoidal light pattern, its spatial frequency affects the fate of the cells' density profile. For slowly changing patterns bacteria tend to behave as if photophilic, while for high spatial frequency modulation, the photokinetic mechanism is dominant and results in an higher concentration in dark regions. We develop a run-and-tumble model that includes both phototaxis and photokinesis and provides a robust description and aligns well with the observed experimental data. Furthermore, for small modulation of light, this organism behaves as microswimmer whose tumbling rate can be controlled with light. This represents a way to control the tumbling rate of microorganisms with light and thus a significant step forward in achieving comprehensive control over the motility of at the microscale.

BP 23: Focus Session: Inference Methods and Biological Data (German-French Focus Session) (joint session BP/DY)

Time: Wednesday 15:00–17:45 Location: H 2032

Invited Talk BP 23.1 Wed 15:00 H 2032

Inhibitor-induced transitions in pattern formation and their role to morphogenesis robustness — •Silvia Grigolon — Laboratoire Jean Perrin (UMR 8237), CNRS & Sorbonne Université, Paris, France

Development relies on the finely coordinated expression of morphogens, proteins driving cell differentiation and organ formation. Cell fate specification is achieved thanks to the establishment of morphogen patterns, which act as signals for cells in a concentration dependent manner. By the aid of reaction-diffusion systems, intense studies over the past decades were dedicated to the identification of the underlying microscopic processes leading to robust pattern formation and the classification of the emergent different mechanisms induced by these. In this work, we show that the presence of negative feedbacks in reaction-diffusion systems can lead to a transition in the modes of pattern formation during morphogenesis and induce memory and robustness. We apply this to the study of zebrafish early morphogenesis and show that the aforementioned mechanisms can indeed be found in this system.

BP 23.2 Wed 15:30 H 2032

Bayesian Model Inference for Biological Tracking Data — •Jan Albrecht[1], Lara S. Bort[1], Carsten Beta[1], Manfred Opper[2,3], and Robert Grossmann[1] — [1]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — [2]TU Berlin, Fakultät IV-MAR 4-2, Marchstraße 23, 10587 Berlin, Germany — [3]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

In order to understand and predict the motion patterns of microorganisms, robust methods to infer motility models from time discrete experimental data are required. Due to the internal complexity of the organisms, their movements appear to have random components which motility models need to account for. Bayesian statistical methods provide a way to efficiently extract information from the trajectory data and provide model parameter estimates together with a measure of uncertainty. We showcase that Bayesian methods are especially well suited when the models contain additional layers of stochasticity, for example population heterogeneity or temporal dependence of parameters. Furthermore, we demonstrate how challenges that arise when multidimensional dynamics is only partially observed, e.g. second order dynamics, colored noise or non-observed internal degrees of freedom, can be addressed.

BP 23.3 Wed 15:45 H 2032

Inference and modelling of the stochastic dynamics of cell shape during cellular state transition — •Wolfram Pönisch[1], Iskra Yanakieva[1], Belle Sow[1], Aki Stubb[2], Alex Winkel[1], Guillaume Salbreux[3], and Ewa Paluch[1] — [1]University of Cambridge, UK — [2]MPI for Molecular Biomedicine, Münster, Germany — [3]University of Geneva, Switzerland

The development of an organism involves a series of state transitions in which cells progressively specialize. Many state transitions coincide with changes in cell shape, with emerging evidence suggesting a strong crosstalk between shape and states. An example is epithelial-to-mesenchymal transition (EMT) which plays a crucial role in development and pathogenesis. Yet, there is very limited knowledge about cell morphodynamics during EMT. Here, we present a morphometric pipeline to analyse individual cell shapes in 3D as cells undergo EMT. By modelling the dynamics as a Langevin process, we infer the potential driving EMT and capture temporal dynamics of cell shape fluctuations during the transition. Our findings reveal a peak in cell shape fluctuations coinciding with the time of spreading during EMT. We hypothesize that downstream biomechanical mechanisms are controlling cell shape fluctuations during EMT and combine computational modelling of cell morphodynamics with molecular perturbation experiments. Overall, by combining morphometric approaches with stochastic inference and mathematical modelling, we create a comprehensive understanding of the biophysical basis of shape changes associated with state transitions.

BP 23.4 Wed 16:00 H 2032

From two to three cells: Are three-body interactions important in collective cell migration? — •Agathe Jouneau[1], Tom Brandstätter[2], Emily Brieger[1], Chase Broedersz[2], and Joachim Rädler[1] — [1]Faculty of Physics and Center for NanoScience, LMU Munich, Germany — [2]Department of Physics and Astronomy, VU Amsterdam, Netherlands

During collective cell migration, for example in embryo development or cancer invasion, cells coordinate their movement by actively interacting with each other. How cell-cell interactions shape the dynamics and emergent properties of the cell assembly is not fully understood. In recent work, we showed that the dynamics of two cells interacting on a dumbbell pattern can be captured by a particle model, including cell-cell interaction terms directly inferred from experimental data. However, we do not know if the collective dynamics of more than two cells can be described by pairwise interactions between cells, or if higher-order interactions come into play. To answer this question, we use time-lapse microscopy to record the dynamics of three cells interacting together in a tailored confinement. We collect a large number of cell trajectories and use them to infer the cell-cell interactions by adapting the framework of the two-cell study. Our work reveals that the pairwise interactions between cells appear to be preserved in the presence of a third cell. However, the superposition of the inferred pairwise interactions is not sufficient to fully capture the observed three-cell dynamics. This could indicate the presence of three-body interactions, with possible implications for large-scale collective behavior.

BP 23.5 Wed 16:15 H 2032

Model selection in stochastic dynamical systems — •Andonis Gerardos and Pierre Ronceray — Aix Marseille Univ, CNRS, CINAM, Turing Center for Living Systems, Marseille, France

Analyzing the dynamics of complex biological systems requires stochastic dynamical models; a common choice is stochastic differential equations (SDE). Given a time series, we developed a method that selects, among a class of SDE models, the one that best captures the dynamics and infers its parameters. This method corresponds to an adaptation of the Akaike information criterion (AIC) to SDE. We validated it using synthetic data generated with stochastic Lorenz and competitive Lotka-Volterra equation. Looking ahead, we envision applications of our data-driven method to unravel the hidden mechanisms of dynamical systems.

15 min. break

Invited Talk BP 23.6 Wed 16:45 H 2032

Bayesian inference of chromatin looping dynamics from live-cell measurements — •Christoph Zechner[1], Michele Gabriele[2], Hugo B Brandão[2], Simon Grosse-Holz[2], Asmita Jha[2], Gina M Daily[3], Claudia Cattoglio[3], Tsung-Han Hsieh[3], Leonid Mirny[2], and Anders S Hansen[2] — [1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]University of California, Berkeley, Berkeley, USA

Recent live-cell microscopy techniques allow the simultaneous tracking of distal genomic elements, providing unprecedented ways to study chromatin dynamics and gene regulation. However, drawing robust conclusions from such data is statistically challenging due to substantial technical noise, intrinsic fluctuations and limited time-resolution. I will present recent progress we have made in addressing some of these challenges; specifically, we developed a new statistical method to quantify CTCF/cohesin-mediated chromatin looping dynamics from two-point live-cell imaging experiments. The method combines a simple polymer model with a Bayesian filtering approach to infer loop lifetimes and frequencies. Its application to experimental data revealed that chromatin loops are surprisingly rare (~5% looped fraction) and short-lived (~20mins loop lifetime). I will discuss potential implications of these findings and outline future challenges.

BP 23.7 Wed 17:15 H 2032

Rigorous inference of stochastic reaction networks based on moment constraints via semidefinite optimisation — •Zekai Li, Barahona Mauricio, and Philipp Thomas — Imperial College London, London, United Kingdom

Stochastic reaction networks are used in many fields to model the behaviour of complex systems with uncertainty. Inference of the rate parameters has been an essential and challenging task for accurately understanding the network. While numerous inference methods have been proposed and implemented, the uncertainty measures associated with these methods often lack theoretical guarantees. Here, we propose a novel inference approach to obtain rigorous bounds on the parameters via convex optimisation over sets constrained by moment equations and moment matrices. Under the condition that the moment intervals, obtained through bootstrap from the original data, contain the true stationary moments, our bounds on the parameters are guaranteed to contain the true parameters. Our method is also capable in the case that there exists latent species or observation error, and in the former case, we can bound the stationary moments of the latent species.

BP 23.8 Wed 17:30 H 2032

Information rates of neural activity on varying time scales — •Tobias Kühn and Ulisse Ferrari — Institut de la Vision, Sorbonne Université, CNRS, INSERM

Evaluating electrophysiological recordings, time is normally discretized in bins. If one aims at determining the information rate, i.e. the mutual information per time, the time-bin size has to be chosen with care because the result will appreciably depend on it. The framework we suggest gives freedom in this choice because our single-neuron model is not restricted to a binary representation of neural activity - as is the case for Ising-like models of neural networks.

Our method allows to faithfully estimate the entropy of the neural activity and eventually the mutual information between neural activity and stimulus for a given time scale. Like in the Ising model, we restrict ourselves to pairwise interactions, so that we just need the mean activities and the covariances (across neurons or across time) to compute entropies. This estimate requires a number of measures growing only quadratically in the number of neurons, as opposed to the exponential growth associated to the estimate of the full probability distribution, which prohibits using the latter for real data. More concretely, to compute entropies, we use a small-correlation expansion, expressed in a novel diagrammatic framework (Kühn & van Wijland 2023), avoiding the explicit inference or even a concrete choice of a single-neuron model. Our approach enables studying the dependence of information rate on the time scale on which the information is registered, which is crucial to understand how dynamic stimuli are processed.

BP 24: Synthetic life-like systems and Origins of Life

Time: Wednesday 15:00–18:00 Location: H 1028

Invited Talk BP 24.1 Wed 15:00 H 1028

Steps towards the de-novo synthesis of life — •Sijbren Otto — University of Groningen, Groningen, the Netherlands

How the immense complexity of living organisms has arisen is one of the most intriguing questions in contemporary science. We have started to explore experimentally how organization and function can emerge from complex molecular networks in aqueous solution. We focus on networks of molecules that can interconvert, to give mixtures that can change their composition in response to external or internal stimuli. Molecular recognition between molecules in such mixtures leads to their mutual stabilization, which drives the synthesis of more of the privileged structures, amounting to self-replication. We have witnessed spontaneous differentiation (a process akin to speciation as it occurs in biology) in a system made from a mixture of two building blocks. When such systems are operated under far-from-equilibrium flow conditions, adaptation of the replicators to a changing environment can occur. Replicators that are able to catalyse reactions other than their own formation have been obtained, representing a first step towards metabolism. Rudimentary Darwinian evolution of purely synthetic molecules has also been achieved and the prospect of synthesizing life de-novo is becoming increasingly realistic.

BP 24.2 Wed 15:30 H 1028

Sequence self-selection by cyclic phase separation — •Philipp Schwintek[1], Giacomo Bartolucci[2], Adriana Calaca Serrao[1], Dieter Braun[1], Christof Weber[2], Alexandra Kühnlein[1], Yasha Rana[2], Philipp Janto[1], Dorothea Hofer[1], and Christof Mast[1] — [1]Ludwigs-Maximilian-Universität München and Center for NanoScience, Munich 80799, Germany — [2]Division Biological Physics, Max Planck Institute for the Physics of Complex Systems, Dresden 01187, Germany

The emergence of functional oligonucleotides on early Earth required a molecular selection mechanism to screen for specific sequences with prebiotic functions. Cyclic processes such as daily temperature oscillations were ubiquitous in this environment and could trigger oligonucleotide phase separation. Here, we propose sequence selection based on phase separation cycles realized through sedimentation in a system subjected to the feeding of oligonucleotides. Using theory and experiments with DNA, we show sequence-specific enrichment in the sedimented dense phase, in particular of short 22-mer DNA sequences. The underlying mechanism selects for complementarity, as it enriches sequences that tightly interact in the dense phase through base-pairing. Our mechanism also enables initially weakly biased pools to enhance their sequence bias or to replace the previously most abundant sequences as the cycles progress. Our findings provide an example of a selection mechanism that may have eased screening for auto-catalytic self-replicating oligonucleotides.

BP 24.3 Wed 15:45 H 1028

Thermal gradients drive separation of ions, naturally creating local niches for the OoL — •Thomas Matreux, Paula Aikkila, Almuth Schmid, Mechthild Rappold, Dieter Braun, and Christof B. Mast — LMU München, Deutschland

Rocks and their constituent phases provided a feedstock for the emergence of life. However, leachate concentrations, diluted by the ocean or retained by chelation processes, were too low to kickstart life and were mostly present in incompatible compositions. We are interested how physical non-equilibria can overcome this problem and offer unique opportunities for molecular selection on all levels.

Ions leached from mineral samples are selectively accumulated by heat flows through water-filled fractures. In contrast to upconcentration by dehydration or freezing, this actively alters the Magnesium:Sodium ratio to an extent that permits key ribozyme activities. Phosphate is liberated and made accessible at neutral pH by thermally driven separation starting from acid-dissolved Apatite, presumably the most abundant phosphorous mineral that is close to insoluble at physiological pH.

Even single ion species such as Na and Cl are fractionated to form pH gradients. In multi-ion systems, thermal gradients can drive the precipitation of otherwise unfavorable species such as Magnesium phosphates.

Heat flows thereby naturally provide local niches with optimized pH and salt conditions for key steps of nascent life.

BP 24.4 Wed 16:00 H 1028

A Mechanical-Electrical Model to Describe the Negative Differential Resistance in Membranotronic Devices — •Max Huber[1,2,3], Jörg Schuster[1,2,3], Oliver G. Schmidt[1,4,5], Harald Kuhn[3], and Daniil Karnaushenko[1] — [1]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), TU Chemnitz, Chemnitz, Germany — [2]Center for Microtechnologies, TU Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems ENAS, Chemnitz, Germany — [4]Material Systems for Nanoelectronics, TU Chemnitz, Chemnitz, Germany — [5]Nanophysics, Faculty of Physics, TU Dresden, Dresden, Germany

Membranotronic devices are artificial neural membranes designed to mimic the functionality of biological neural networks [*Adv. Funct. Mater.*, **32**(24), 2200233 (2022)]. Negative differential resistance (NDR) is essential for their function. We present a physical model of a membranotronic device which generates NDR. It consists of a deformable membrane with holes allowing ion currents, which are modulated by a deformation resulting from an applied voltage. A mechanical model for micro-electro-mechanical systems describes the deformable membrane including holes. We perform a parameter variation study and show that our model can reproduce the NDR for a wide and physically reasonable range of parameter combinations. In essence, our work bridges the gap between artificial membranotronic devices and biolog-

ical neural membrane by providing a robust physical model capable of emulating NDR, a key feature in the operation of such systems.

15 min. break

BP 24.5 Wed 16:30 H 1028

Protein Design for and with Synthetic Cells — •Béla P. Frohn and Petra Schwille — Max Planck Institute of Biochemistry, Martinsried, Germany

Bottom-Up Synthetic Biology creates cell-like systems from a minimal set of functional modules, such as purified proteins, membranes and DNA. This facilitates the study of biological systems under extremely well-defined conditions, where every parameter is known and can be controlled. Here we show that these systems provide an ideal screening platform to test designed proteins for complex biological functions, i.e., functions that only arise from interaction with the environment. On one hand, this can be used to build customisable minimal cells for medical and industrial applications. On the other hand, it allows to test fundamental principles of life under controlled conditions, via building systems from scratch that implement specific biophysical functions, enabling the field to move from post-hoc analysis of systems found in nature towards true hypothesis testing. As an example, we present a computational and experimental pipeline to design and screen proteins to test different theories of large-scale membrane deformation.

BP 24.6 Wed 16:45 H 1028

Networks of heat-flow chambers to trigger prebiotic reactions — Thomas Matreux, Paula Aikkila, and •Christof Mast — Systems Biophysics, Center for Nanoscience, LMU, Geschwister-Scholl-Platz 1, 80539 Munich, Germany

Prebiotic chemistry must achieve high yields to kickstart life, despite the complex conditions prevailing on the early Earth. While this is achieved in the laboratory through purification procedures and clearly timed process steps, the question arises as to how prebiotic chemistry can be successful in a homogeneous primordial pond. We investigate the influence of heat flows through networks of thin rock fractures numerically and experimentally. The physical non-equilibrium establishes a wide variety of compound compositions in the different pore sections, enabling different prebiotic chemistry. We test this hypothesis using the example of TMP-triggered glycine dimerization as well as nucleoside phosphorylation taking place in experimental pore systems and find a strong enhancement of yield. Our results show that even the simplest boundary conditions - ubiquitous heat flows and simple rock cracks - can create ideal conditions for prebiotic chemistry.

BP 24.7 Wed 17:00 H 1028

Persistent Motion of Liposomes Driven by a Mechanochemical Feedback Loop — •Tom Burkart[1], Meifang Fu[2,3], Petra Schwille[3], and Erwin Frey[1] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for NanoScience (CeNS), LMU München, Munich, Germany — [2]MPI of Biochemistry, Martinsried, Germany — [3]Shenzhen Institute of Advanced Technology (SIAT), Shenzhen, China

Can a living cell be synthesized de novo, and can we reconstruct features such as cell motility in their biomimetic analogues? Cell motion involves multiple chemical and mechanical processes that are coupled via feedbacks spanning a large range of time and length scales. Reconstitution of cell-like motion therefore is an extremely challenging yet rewarding way for us to better understand this basic property of life. We accomplish motion of liposomes by realizing a mechanochemical feedback loop between the E. coli MinDE protein system and the liposomes, controlled by protein reactions and membrane adhesion. Self-organized chemical gradients of membrane-binding Min proteins induce deformations of liposomes into asymmetric shapes. This asymmetry yields mechanical force gradients resulting in directional liposome movement, which in turn reorganizes the protein pattern. In-silico reconstitution of the protein reaction-diffusion dynamics and the dynamic liposome geometry show that a simple mechanochemical feedback loop - consisting of protein pattern formation sensitive to membrane geometries and membrane adhesion sensitive to protein concentrations - is sufficient to induce persistent liposome motion.

BP 24.8 Wed 17:15 H 1028

Speeding up chemical reactions - Precursor vs Wet dry cycle — •Pranay Jaiswal, Ivar Haugerud, and Christoph Weber — Institute of Physics, University of Augsburg, Augsburg, Germany

The coexistence of liquid and solid phases allows for localisation of key molecules and compounds. Solid surfaces can act as a catalyst and can adsorb and concentrate organic molecules, increasing their local concentrations and enhancing interaction and the likelihood of chemical reactions. This concentration effect is particularly significant in dilute environments, such as early Earth's oceans, where it would have been challenging for complex organic compounds to form without the aid of solid surfaces. Solid phases provide a protective shield for organic molecules against harsh environmental conditions. This protection is vital for the preservation and stability of early organic matter, enabling the development of more intricate and functional molecules. In this work we developed a theoretical model of liquid solid phase coexistence that provide diverse chemical landscapes. Different phases offer distinct chemical conditions and reactivity. Furthermore, we introduced non-equilibrium conditions of precursor cycles in contrast to wet-dry cycles. These cycles speed up chemical processes and leads to a resonance behaviour in the cycle frequency that maximises the chemical turnover, creating selective environments.

BP 24.9 Wed 17:30 H 1028

Polyplex formation process investigated by coarse-grained molecular dynamics simulations — •Jonas Lehnen[1], Friederike Schmid[1], and Giovanni Settanni[2] — [1]Institute of Physics, JGU Mainz, Germany — [2]Faculty of Physics and Astronomy, Ruhr University Bochum, Germany

Messenger RNA vaccines have proven invaluable in the fight against the COVID-19 pandemic. Among the vehicles for non-viral gene delivery Polyethylenimine (PEI) has attracted attention due to its high transfection efficiency. PEI binds to negatively charged mRNA forming polyplexes. The size and characteristics of these nanoparticles (NP) depend on the pH used for their assembly as well as salt, PEI and RNA concentration. Small NP have been shown to be critical for high transfection efficiency. We use coarse-grained molecular dynamics simulations with explicit ions to examine the effects of the various factors determining polyplex size and gain a better understanding of the processes involved in their formation. In agreement with available experimental data, our simulations show how small NP sizes are obtained when mixing RNA with an amount of PEI largely exceeding the requirement for RNA neutralization. Further, we present insight on the importance to focus not only on stoichiometric ratios of RNA and PEI but also on the overall concentration. Finally we present a kinetic and a thermodynamic mechanism which can explain the experimental results, and could be leveraged to reliably produce small NPs, minimizing the amount of necessary PEI, which, in large doses, can be toxic.

BP 24.10 Wed 17:45 H 1028

Coupling polymerization with droplet condensation simplifies forming protocells — •Xi Chen, Jens-Uwe Sommer, and Tyler Harmon — Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere 01069 Dsden

Macromolecules are essential building blocks of life, but how these long chains could be first synthesized in prebiotic conditions remains a mystery due to two major issues: the conditions are too dilute for robust chemical reactions and polymerization is expected to produce only short chains. Two independent solutions have been proposed for these two problems: droplet compartments could concentrate molecules for chemical reactions; autocatalytic templated assembly could produce polymers with medium lengths. We propose that coupling polymerization and liquid-liquid phase separation much more robustly solves both problems than either one individually. We use effective droplet model to investigate a minimal system with autocatalytic polymerization of a single monomer type. Small molecules form condensed droplets when polymerized into medium chains. These droplets further function as a reaction center that could significantly enhance the degree of polymerization to generate longer chains than templating alone. Additionally, the compartment is stable to much lower dilute concentrations.

BP 25: Members' Assembly

Time: Wednesday 18:15–19:15 Location: H 1028

All members of the Biological Physics Division are invited to participate.

BP 26: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Thursday 9:30–13:00 Location: H 0111

Invited Talk BP 26.1 Thu 9:30 H 0111

Self-organized protein/polysaccharide nano-assemblies for applications in biomedical and food sciences — •Aristeidis Papagiannopoulos — Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vass. Constantinou Ave. 11635 Athens, Greece

Multifunctional nanocarriers of drugs and nutrients are very important for applications in the food industry and pharmaceutics. Proteins and polysaccharides are extensively used in these fields as they are biodegradable, metabolizable, nontoxic and biocompatible. Nanostructures from these two biopolymer classes combine the multifunctionality of the proteins (hydropathy and pH-dependent charge surface distributions) with the hydrophilicity and hydrogen-bonding property of the polysaccharides. Our recent work on protein/polysaccharide nanoparticles by electrostatic self-organization and thermal treatment without the use of chemical reactions or toxic solvents will be presented. Examples will include fibrinogen-hyaluronic acid nanoformulations, bovine serum albumin-chondroitin sulfate or -xanthan nanoparticles, trypsin- and hemoglobin-based nanoparticles. The discussion will be focused on the stimuli-response, molecular interactions and hierarchical morphology of the protein/polysaccharide systems and the binding of bioactive compounds. Physicochemical characterization and optimization of the nano-assemblies by light scattering, small angle scattering and spectroscopy techniques will be analyzed. These works motivate the development of other novel protein/polysaccharide biomaterials.

BP 26.2 Thu 10:00 H 0111

Dichroic ATR-FTIR studies on thin bioinspired films of spider silk related peptide blends — Mirjam Hofmaier[1], •Thomas Scheibel[2], Andreas Fery[1], and Martin Müller[1] — [1]Leibniz Institute of Polymer Research Dresden (IPF), Institute of Physical Chemistry and Polymer Physics, 01069 Dresden, Germany — [2]University of Bayreuth, Chair of Biomaterials, 95447 Bayreuth, Germany

Bioinspired binary blends of a crystalline (C) and amorphous (A) peptide sequence were prepared addressing analogy to C-A multiblockcopolymer-like spider silk proteins. C/A blends were prepared in hexafluoroisopropanol for molar mixing ratios C/(C+A)=0, 25, 50, 77, 100%, deposited as thin films (d=31-44nm) onto silicon substrates and checked for secondary structure and orientation by dichroic transmission (T-) and ATR-FTIR spectroscopy. Amide I band analysis revealed little β-sheet (<15%) and much disordered (>79%) structure and dichroic ratios (R) of Amide I components indicating no β-sheet orientation for all C/(C+A) values. Whereas, after swelling in methanol vapor C/A blend films revealed increasing β-sheet up to 54% and decreasing disordered structure down to 42% with increasing C/(C+A). Furthermore, R values of Amide I components assigned to antiparallel beta-sheet were found by T-FTIR indicating no in-plane orientation, while ATR-FTIR revealed R values indicating significant out-of-plane orientation of β-sheet crystallites for blend films with C/(A+C)>0. SFM microscopy showed larger needle-like fibrillar structures for C/A blend films, while C-A copolymer films revealed smaller fibrillar or spherical structures correlating with the lower orientation obtained by ATR-FTIR.

BP 26.3 Thu 10:15 H 0111

Exploring deposition conditions for antibacterial thin films via GISAXS measurements — •Joanne Neumann[1,2], Maria J Garcia[1,3], Holger Sondermann[1,3], Matthias Schwartzkopf[1], and Michael Martins[2] — [1]DESY, Photon Science, Notkestr. 85, D-22607 Hamburg — [2]UHH, Physics Department, Luruper Chaussee 149, D-22607 Hamburg — [3]CSSB, Center for Structural Systems Biology, Notkestr. 85, D-22607 Hamburg

During the last decades, the rate of multiresistant microbes against antibiotics increased dramatically. Moreover, biofilm-based contaminations complicate cleaning procedures and require cost-intensive methods in industrial processes. In this context, Pseudomonas aeruginosa (PA) is one of those bacteria that forms biofilms at liquid/air interfaces as a protective shell, e.g. against antibiotics. To investigate the influence of nanostructured silver layers as antibacterial coatings on the initial bacterial growth, we employed micro-focused Grazing incidence Small Angle X-ray Scattering (GISAXS) as a very surface-sensitive X-ray-based method providing structural information about electron density distributions. In our experiments we characterized PA biofilms, grown under different deposition conditions at the P03 beamline at Petra III / DESY.

BP 26.4 Thu 10:30 H 0111

Colored CNC films reflect left and right circular polarized light. — •Silvia Vignolini — MPI Colloids and Interfaces Potsdam DE

The chiral self-assembly of nanoscale building blocks is a universal phenomenon that demonstrates the emergence of large-scale structures from the properties of individual sub-units. In many self-organising colloidal systems, such as cellulose nanocrystals (CNC), the emergence of chirality in the mesophase can be correlated to the properties of the building blocks and is therefore necessarily fixed. CNC chiral nematic suspensions are, in fact, always left-handed, giving rise when dried, to colored films reflecting only circular left-polarized light. In this talk, I will review some tricks that can be used to achieve CNC-colored films with circular right-polarized light reflection.

BP 26.5 Thu 10:45 H 0111

Tailoring morphologies of protein-templated titania nanostructures — •Linus F. Huber[1], Stephan V. Roth[2], Manuel E. Scheel[1], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany — [3]TUM, MLZ, 85748 Garching, Germany

Biotemplating is an effective technique for structuring hybrid inorganic-organic materials at the nano scale. This method facilitates the fine-tuning of material characteristics such as porosity and structure sizes. Therefore, parameters like the electronic conductivity can be adjusted for different applications. This work focuses on titania thin films with different structures, for their application in thermoelectric generators. Beta-lactoglobulin, a bovine whey protein, serves as a template in the sol-gel synthesis process. The Seebeck effect allows the conversion of waste heat into electrical energy. This research aims to address the scarcity, toxicity, and costliness of current state-of-the-art thermoelectric materials. To investigate the morphologies of titania, a combination of in situ GISAXS, GIWAXS, and SEM techniques are used. In particular, in situ GISAXS printing allows for a time-resolved exploration of the structure formation, domain sizes, and domain distances.These observed structural differences are subsequently correlated with measurements of the Seebeck coefficient, electrical conductivity and optical properties.

BP 26.6 Thu 11:00 H 0111

Sustainable photonic glass pigments from brush block copolymers — •Zhen Wang[1], Ruiting Li[2], Richard Parker[1], and Silvia Vignolini[1,2] — [1]Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK — [2]Department of Sustainable and Bio-inspired Materials, Max Planck Institute of Colloids and Interfaces, Am Mühlenberg 1, 14476 Potsdam, Germany

Growing societal concerns over microplastic pollution and resource sustainability is driving the pigment industry to search for sustainable alternatives. One promising avenue is block copolymer (BCP), which is known to self-assemble into structurally coloured materials. However, its real-world application has been hindered by limited exploration into the suitability of biocompatible and (bio)degradable monomers. In

this talk we will show that biocompatible BCPs can be self-assembled within emulsified microdroplets, which upon drying form microparticles with a porous photonic glass architecture. The colour from these pigments can be tuned by either the BCP properties or the fabrication conditions. Finally, the relationship between the microparticle morphology and its optical response was investigated for BCPs with similar composition but different thermal behaviour. This revealed the formation mechanism for the porous structure and allowed for a strategy to enhance colour purity.

15 min. break

BP 26.7 Thu 11:30 H 0111

Reservoir computing with organic fiber networks — •Richard Kantelberg, Anton Weissbach, Peter Steiner, Peter Birkholz, Hans Kleemann, and Karl Leo — Technische Universität Dresden, Dresden, Germany

Reservoir computing (RC) is a promising paradigm for machine learning that utilizes dynamic systems, known as reservoirs, to process and analyze complex temporal data. Organic mixed ionic electronic conductors (OMIECs) have emerged as a novel class of materials with intriguing properties, such as their ability to exhibit both electronic and ionic conductivity, as well as their biocompatibility, flexibility, and low power consumption. These features make OMIECs particularly suitable for the development of unconventional computing architectures. Conducting fiber networks grown by field-directed polymerization have been proven to be a suitable candidate for, e.g., heartbeat or image classification tasks. However, the dependency between classification accuracy and device parameters is still rather unclear. We present recent findings interlinking electronic conductivity, system nonlinearity and reservoir size with the neuromorphic functionality and RC performance. The recent progress in reservoir computing using organic mixed ionic electronic provides valuable knowledge for the targeted development of fiber reservoirs. Given these findings, we are confident to further increase the classification accuracy by adopting the system to specific application scenarios, paving the way to future commercialization.

BP 26.8 Thu 11:45 H 0111

Paper Fibers Beyond Saturation: μ-CT Analysis of Prolonged Structural Changes — •Maximilian Fuchs[1,2], Raimund Teubler[1,3], Daniel Kollreider[1,2], Maximilian Grillitsch[1,2], Ekaterina Baikova[1,2], and Karin Zojer[1,2] — [1]Institute for Solid State Physics, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper — [3]Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology, Austria

The uptake of water or dimethylsulfoxid (DMSO) by a cellulose-lignin based fiber network, in this case paper, is a complex interplay between capillary transport and sorption of these polar volatiles into the fibers. Microcomputed tomography (μ-CT) allows us to correlate this uptake with changes in the microstructure, with water and DMSO being offered either as a liquid or additionally via the gas phase to prevent capillary uptake. A pore network analysis of the 3D images shows that uptake from liquid and gas cause similar initial structural changes, although the fiber space and pore space between the fibers swells to different extents. Interestingly, fibers and pores continue to expand long after mass uptake from gas phase has ceased. This long-lasting expansion is most likely caused by an increasing amount of detached fibril bundles in the fiber wall.

BP 26.9 Thu 12:00 H 0111

Microgels for Enhanced Adsorption of Endothelial Cells on Artificial Networks — •Souraj Mandal and Regine von Klitzing — Soft Matter at Interfaces, Department of Physics, Technical University of Darmstadt, Darmstadt 64289, Germany

In human physiology, endothelial cells (ECs) form a lining inside blood vessels, which is essential for cell maturation and the development of capillary vessels. However, replicating this process ex vivo, especially ensuring the adequate adherence of ECs to the surfaces of 3D-printed artificial networks, presents a significant challenge. In this study, we focus on designing an effective mediator between the inner wall of the artificial network and endothelial cells that would remain mechanically stable against the flow of the nutrient solutions for cell maturation. Our strategy involves the use of Poly(N-isopropylacrylamide) (PNIPAM) microgels (MGs) as mediators for cell culturing surfaces. To enhance their attachment, we synthesized charged MGs and tested their adhesion on plasma-treated silicon (Si), glass, and 3D-printed polymeric surfaces. The MG particles were characterized based on their Zeta potential and hydrodynamic radius. To achieve rapid deposition, we employed spin coating to form a thin polymeric layer of MG particles on the substrates. We conducted atomic force microscopy (AFM) analyses and observed stable adhesion of MG particles on flat surfaces, even after water washing and exposure to mechanical stress. Moreover, we observed that these MG coatings yield superior endothelial cell adhesion and spreading compared to non-coated substrates.

BP 26.10 Thu 12:15 H 0111

A Computational Investigation into the Oxidation of Cytosine Epigenetic Modifications — •Vasilii Korotenko[1] and Hendrik Zipse[2] — [1]Forschungszentrum Jülich, IEK-9 — [2]LMU München, Fakultät für Chemie und Pharmazie

Studying the (aut)oxidation of 5-methylcytosine (5mC) is crucial for understanding the dynamic control of DNA methylation - a pivotal epigenetic modification linked to gene expression, cellular differentiation, and disease development. In this work, the oxidizing properties of oxygen-centered radicals and the reducing properties of epigenetically modified cytosines were studied. The O-H bond dissociation energies BDE(O-H) were calculated for various alcohols using selected theoretical methods. BDE(C-H) and pKa values have been calculated for various oxidation product of 5mC. Special attention was paid to the equilibrium of the hydration reaction of 5-formylcytosine (5fC), because the corresponding hydrate product can be very easily oxidized. All this together allowed us to propose and thermodynamically evaluate the mechanism of the 5mC (aut)oxidation reaction. The (aut)oxidation of 5mC is unlikely to occur through initiation by triplet dioxygen or through unimolecular decomposition of hydroperoxides. In the proposal mechanism, neural molecules react with free radicals, transferring hydrogen atoms to create products with higher BDE values. The thermodynamics of the presented mechanism agrees with the experimental kinetics. We assume that the protonation (pH $<$ 7) of oxidizable nucleic acids inhibits the (aut)oxidation process by increasing the BDE(C-H) values.

BP 26.11 Thu 12:30 H 0111

Arylazopyrazole Amphiphiles as New Candidates for Photo-Induced Drug Delivery — •Ipsita Pani, Michael Hardt, Dana Glikman, and Björn Braunschweig — Institute of Physical Chemistry, University of Münster, 48149 Münster, Germany

Photo-responsive materials have been extensively explored to meet the demands for high precision drug delivery. Azobenzene-based amphiphiles have been the focal point of research in photo-responsive drug delivery systems. However, most azo amphiphiles suffer from low thermal stabilities of the cis-isomer. Consequently, the drug carriers are subjected to prolonged and periodic UV irradiation of high intensity for the release of the encapsulated drug. Therefore, the design of nanocarriers for light-induced drug delivery demands innovations to achieve targeted release at low intensities and short exposure times of the UV irradiation. Arylazopyrazoles (AAPs) have emerged as novel photoswitches with superior thermal stability of the cis-isomer and photo-stationary states (>90%) for trans/cis photo-isomerization in both directions.[1,2] In this contribution, we report on the potential of an anionic AAP surfactant (octyl arylazopyrazole butyl sulfonate) as a micellar nanocarrier for doxorubicin which is the most widely used anti-cancer drug. Using surface specific tools such as surface tensiometry and vibrational sum-frequency generation (SFG) spectroscopy we demonstrate the UV-induced release of doxorubicin at the air-water interface, while the release of doxorubicin in aqueous solution is studied by UV-visible and fluorescence spectroscopy. [1] Hardt et al. *Langmuir* **2023**, 39, 5861 [2] Honnigfort et al. *Chem. Sci.* **2020**, 11, 2085

BP 26.12 Thu 12:45 H 0111

Untangling the stabilizing effects of proteins as foaming agents — •Kevin Gräff[1], Sebastian Stock[1], Luca Mirau[1], Sabine Bürger[1], Larissa Braun[1], Annika Völp[2], Norbert Willenbacher[2], and Regine von Klitzing[1] — [1]Soft Matter at Interfaces, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institute of Mechanical Engineering, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Foams appear in many applications such as in personal care products, firefighting and food technology. Macroscopic foams consist of air bubbles separated by foam films. Therefore, it is crucial to untangle electrostatic, steric and network stabilization effects in foam films

to understand macroscopic foam properties. We compare globular proteins (β - lactoglobulin and bovine serum albumin), a flexible protein (whole casein) and lupine protein isolate with varying solution pH. In a Thin Film Pressure Balance (TFPB) we use image intensity measurements to record spatially resolved disjoining pressure isotherms and to gain information about structure formation. We introduce feature tracking as a novel method to measure the interfacial mobility and stiffness of foam films. Around the isoelectric point, stable Newton Black Films (NBFs) for the globular proteins form in contrast to the unstable NBFs for the flexible proteins due to different characteristics of the network structures. To evaluate the foam films impact on macroscopic foams, we use a Bikerman cell to measure foam parameters (e.g. foamability). Small Angel Neutron Scattering (SANS) on macroscopic foams completes the picture.

BP 27: Single Molecule Biophysics

Time: Thursday 9:30–13:00 Location: H 0112

BP 27.1 Thu 9:30 H 0112

Metal-Induced Energy Transfer (MIET) for Live-Cell Imaging with Fluorescent Proteins — •Lara Hauke, Sebastian Isbaner, Arindam Gosh, Alexey I. Chizhik, Ingo Gregor, Florian Rehfeldt, and Jörg Enderlein — Third Institute of Physics, Biophysics, Georg August University Göttingen, Germany

Metal-Induced Energy Transfer (MIET) imaging has emerged as a versatile super-resolution technique, offering nanometer resolution along the optical axis in microscopy. While MIET has demonstrated its efficacy in various biological and biophysical studies, its potential for live-cell imaging using fluorescent proteins has yet to be fully realized. In this study, we explore the implementation of MIET imaging for live-cell studies across diverse cell types, including adult human stem cells, human osteo-sarcoma cells, and Dictyostelium discoideum cells. Our investigation encompasses a range of commonly used fluorescent proteins, such as GFP, mScarlet, RFP, and YPet. Our findings showcase the applicability and capabilities of MIET imaging in achieving nanometer axial mapping of living cellular and sub-cellular components. Importantly, we demonstrate MIET's ability to operate across multiple timescales, spanning from milliseconds to hours, while inducing negligible phototoxic effects. This work [10.1021/acsnano.2c12372] establishes MIET as a powerful and easy-to-implement tool for live-cell imaging, providing researchers with a valuable resource for non-invasive, high-resolution visualization of dynamic cellular processes in various biological contexts.

BP 27.2 Thu 9:45 H 0112

Imaging Mucin with Low Energy Electron Holography — •Moritz Edte[1,2], Ben Yang[1], Luigi Malavolti[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]École polytechnique fédérale de Lausanne, Switzerland

The glycosylated protein family of transmembrane mucins plays an important role in living cells [1,2]. Mucin molecules show different degrees of glycosylation in healthy and cancerous cells [1,2] associated with a possible structural change. Due to the high complexity and flexibility of these molecules, which challenges state-of-the-art methods, a single-molecule imaging technique is required to study how the degree of glycosylation affects the mucin structure. In our in-house custom-built low-energy electron holography (LEEH) setup, a low-energy electron beam in the 50-150 eV energy range allows high-contrast imaging of single biomolecules deposited by electrospray ion beam deposition (ES-IBD) [3,4]. Our method allows the mapping of conformational variability of single flexible molecules [3,4]. Here, I present LEEH imaging of single mucin molecules with varying degrees of glycosylation, and show that LEEH combined with ES-IBD is able to image these flexible molecules. This study demonstrates that LEEH can be used as a complementary method to study structural features associated with conformational changes in individual biomolecules. [1]*D.W. Kufe et al., Nature Review Cancer 9, 874-885 (2009) [2]*G.C. Hansson, Annual Review of Biochemistry 89, 769-793 (2020) [3]*H. Ochner et al., PNAS 118 (51), e2112651118 (2021) [4]*H. Ochner et al., scientific reports 13, 10241 (2023)

BP 27.3 Thu 10:00 H 0112

Label-free imaging and 3D single particle tracking in complex media via interferometric scattering microscopy (iSCAT) — •Kiarash Kasaian[1,2], Mahdi Mazaheri[1,2], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]FAU Erlangen-Nürnberg, Erlangen, Germany

Label-free imaging offers a distinct advantage over techniques employing fluorescent labels by eliminating concerns related to photobleaching and photo-toxicity. iSCAT is a highly sensitive tool for label-free microscopy [1]. However, imaging complex biological specimens with iSCAT remains challenging, as the scattering from multiple sources generates dynamic speckle patterns, which can obscure the signal of interest. Introducing a novel iSCAT modality termed "diffused-illumination iSCAT" (DI-iSCAT) [2], we engineer the spatial coherence of the illumination to mitigate the impact of dynamic speckle. We demonstrate high-speed imaging of live cells over a large field of view of 100 $\mu m \times 100\ \mu m$ and employ our newly developed 3D tracking algorithm [3] to perform 3D tracking of nanoparticles in cellular environment.

[1] Taylor, R. W.; et al. Interferometric scattering microscopy reveals microsecond nanoscopic protein motion on a live cell membrane. Nat. Photonics 13, 480 (2019)

[2] Mazaheri, M.; et al. Label-Free Imaging and Tracking with Speckle-Free Interferometric Scattering Microscopy (in preparation)

[3] Kasaian, K.; et al. Long-Range High-Speed 3D Tracking via Interferometric Scattering Microscopy (in preparation)

BP 27.4 Thu 10:15 H 0112

An optogenetic method for the controlled release of single molecules — P Kashyap[1], S Bertelli[2], F Cao[3], Y Kostritskaia[4], F Blank[1], N Srikanth[3], C Schlack[1], R Saleppico[5], D Bierhuizen[1], X Liu[6], W Nickel[5], RE Campbell[6], A Plested[2], T Stauber[4], MJ Taylor[3], and •H Ewers[1] — [1]Freie Universität Berlin — [2]Humboldt-Universität zu Berlin — [3]MPI Infection Biology — [4]Medical School Hamburg — [5]Heidelberg University — [6]University of Alberta

We developed a system for optogenetic release of single molecules in live cells. We confined soluble and transmembrane proteins to the Golgi apparatus via a photocleavable protein and released them by short pulses of light. Our method allows for the controlled delivery of functional proteins to cytosol and plasma membrane in amounts compatible with single molecule imaging, greatly simplifying access to single molecule microscopy of any protein in live cells. Furthermore, we could reconstitute cellular functions such as ion conductance by delivering BK and VRAC ion channels to the plasma membrane. Finally, we could induce NF-kB signaling in T-Lymphoblasts stimulated by IL-1 by controlled release of a signaling protein that had been knocked-out in the same cells. We observed light induced formation of functional inflammatory signaling complexes that could trigger IKK phosphorylation in single cells. We thus developed an optogenetic method for the reconstitution and investigation of cellular function at the single molecule level.

BP 27.5 Thu 10:30 H 0112

A single-molecule perspective on the RNA interactions of a Ser-Arg-rich splicing factor — •Marie Synakewicz[1], Sarah Habeler[1], Steffen Winkler[1], Lucia Franchini[1], Héloïse Bürgisser[2], Antoine Cléry[1], Frédéric Allain[2], Nina Hartrampf[1], and Benjamin Schuler[1] — [1]University of Zurich, Zürich, Switzerland — [2]ETH Zurich, Zürich, Switzerland

Boundaries between coding and non-coding regions within mRNAs are recognised by serine-arginine-rich splicing factors (SRSFs) that contain one or two structured RNA recognition motifs (RRMs) and a long intrinsically disordered domain consisting of many Arg-Ser repeats. Extensive phosphorylation of RS domains modulates SRSF conformation, cellular localisation and function. Using single-molecule techniques, we aim to understand the molecular detail of the SRSF1-RNA interaction, and how this is regulated by the RS domain and its phosphorylation pattern. We characterised the interaction of full-length SRSF1, the RRMs and the RS domain with ssRNAs using single-molecule Förster Resonance Energy Transfer (smFRET), before showing that an increase in phosphorylation of the RS domain correlates with a decrease in affinity. More recently, we started to explore protein-RNA inter-

actions in the context of a natural pre-mRNA construct. Using both smFRET and force spectroscopy we show that the conformational ensemble of the pre-mRNA consists of more than one structure, and that these are modulated by protein binding. Our results provide new insights into how SRSF1 can bind and modulate RNA structure, and therefore its capacity to regulate many cellular processes.

BP 27.6 Thu 10:45 H 0112

FRET-guided integrative modelling of (ribo-)nucleic acids — Fabio D. Steffen[1], Felix Erichson[2], and •Richard Börner[2] — [1]University of Zurich, Zurich, Switzerland — [2]Laserinstitut Hochschule Mittweida, Mittweida University of Applied Sciences, Mittweida, Germany

The functional diversity of RNA is encoded in their innate conformational heterogeneity. The combination of single-molecule spectroscopy and computational modeling offers new opportunities to map structural transitions within ribonucleic acid ensembles. Here, we describe a framework to harmonize single-molecule FRET measurements with molecular dynamics simulations and *de novo* structure prediction. Using either all-atom or implicit fluorophore modeling we recreate FRET experiments in silico, visualize the underlying structural dynamics and quantify the simulated reaction coordinates. Using multiple accessible-contact volumes (multi-ACV) as a post-hoc scoring method for fragment-assembly in Rosetta FarFar2, we demonstrate that FRET effectively refines *de novo* RNA structure prediction without the need of explicit dye labeling *in silico*. We benchmark our FRET-assisted modeling approach on double-labeled DNA strands and validate it against an intrinsically dynamic Mn(II)-binding riboswitch and a Mg(II)-sensitif ribosomal RNA tertiary contact. We show that already one FRET coordinate, i. e., describing the assembly of a four-way junction and the GAAA binding to a kissing loop, allows to recapitulate the global fold of both, the riboswitch and the tertiary contact, and to significantly reduce the *de novo* generated structure ensemble.

15 min. break

Invited Talk BP 27.7 Thu 11:15 H 0112

Integrative dynamic structural biology with multi-modal fluorescence spectroscopy and nanoscopy: From single molecules to live cells — •Claus Seidel — Heinrich-Heine-University Düsseldorf, Germany

Multimodal fluorescence spectroscopy and microscopy with multiparameter detection provide rich insights on biomolecular systems under ambient / live cell conditions, including spatial, structural and kinetic information. In a comparative single-molecule study, we assessed the accuracy of Förster Resonance Energy Transfer (FRET) measurements. We studied two protein systems with distinct conformational changes and dynamics and obtained an interdye distance precision of smaller than 2 Å and accuracy of smaller than 5 Å. Considering cellular studies, we introduced a framework for quantitative high throughput FRET image spectroscopy. We measured the time-evolution of pairwise homo- or hetero-interactions of the Guanylate binding proteins and the membrane receptor CD95 in live cells with 0.8% fraction precision. In this way, the next level of complexity is achieved by linking structural dynamics of biomolecules with their cellular function and localization.

BP 27.8 Thu 11:45 H 0112

Cavity-enhanced ultrafast sensing of single nanosystems — •Shalom Palkhivala, Larissa Kohler, and David Hunger — Karlsruhe Institute of Technology, Karlsruhe, Germany

The investigation of single unlabelled nanosystems is of interest in branches of science such as biophysics and chemistry, where sensors are needed which can detect nanosystems in aqueous environments. We demonstrate an open-access optofluidic platform for the high-speed label-free sensing of nanoparticles in aqueous suspension. The heart of the sensor is a fibre-based Fabry-Perot microcavity with high finesse (5×10^4 in water) integrated into a microfluidic system. By monitoring the cavity resonance as the optical field interacts with a nanoparticle, the particle can be detected and characterised. We have demonstrated three-dimensional tracking of a single diffusing nanoparticle by measuring the resonance frequency shifts of several transverse modes [1]. Now, our cavity-locked detection scheme allows measurement of fast nanoparticle dynamics with a temporal resolution ($\sim$ 10 ns) orders of magnitude better than most other techniques. Additionally, orthogonal polarisation eigenmodes of the cavity are interrogated to yield orientational information of anisotropic particles. Thus, the rotation of single nanorods 20 nm long could be tracked with high measurement bandwidth, and the diffusion dynamics used to determine the dimensions of individual nanorods. We shall report progress towards using our sensor to investigate the dynamics of biological nanosystems, such as the folding of DNA "origami".

[1] Kohler, L. *et al.* Nat Commun **12**, 6385 (2021).

BP 27.9 Thu 12:00 H 0112

Residue Size Dependency of the Geminate Recombination Dynamics of the Biologically Relevant Disulfide Moiety after UV-cleavage investigated by TRXAS — •Jessica Harich — Institute of Nanostructure and Solid State Physics, University of Hamburg and Center for Free-Electron Laser Science, Germany

The tertiary structure of proteins is stabilized by disulfide bonds formed from two spatially adjacent L-cysteinyl residues. These disulfide bridges are prone to UV radiation damage with potentially adverse effects. We employ time resolved X-ray absorption spectroscopy (TRXAS) to observe the UV photochemistry of the natural amino acid dimer L-cystine and the tripeptide Glutathione disulfide in aqueous solution to understand the photochemistry under physiological conditions. Furthermore, we have first exciting insights into the UV-photochemistry of the disulfide bridges within the protein hen egg white Lysozyme.

We find that upon UV irradiation, apliphatic disulfides immediately undergo S-S bond cleavage, leading to the formation of two identical thiyl radicals, followed by fast geminate recombination indicating a very effective recombination process for thiyl radicals to the ground state. This process is only possible in condensed phases and its speed increases with chain length. Our results show that L-cystine already captures the essence of the ultrafast photochemistry of the disulfide bridge, but that the size of the residue adjacent to the disulfide bonds has a strong influence on the immediate recombination dynamics of the photoproducts.

BP 27.10 Thu 12:15 H 0112

Direct imaging of single RNAs — •Shengpeng Huang[1], Klaus Kern[1,2], and Kelvin Anggara[1] — [1]Max Planck Institute for Solid State Research — [2]Institute de Physique, École Polytechnique Fédérale de Lausanne

Ribonucleic acid (RNA) plays key roles in many biological processes, including gene expression, protein synthesis, chemical catalysis, and cellular regulation. Despite its ubiquity, understanding flexible RNA structures remain challenging with ensemble-averaged methods, such as X-ray crystallography, cryo electron microscopy, and nuclear magnetic resonance.

We confront this problem by direct imaging of RNAs deposited on surfaces, which offers an interesting possibility to determine directly the RNA sequence and its consequent three-dimensional structures. We employ the Electrospray Ion Beam Deposition (ESIBD) technique to transfer intact RNA molecules in a solution onto a surface in vacuo, which are subsequently imaged by Scanning Tunnelling Microscopy (STM). Using our ESIBD+STM approach, we have successfully deposited and imaged single chains of intact 60-mer RNA, which allows individual RNA chains to be structurally characterized at the single nucleotide level. Single molecule imaging of RNA presents a new approach to structurally determine many interesting post-translational modifications (PTMs) of RNAs with important biological roles.

BP 27.11 Thu 12:30 H 0112

Structure-Mechanics Relationships of Heterodimeric Coiled Coils — Zeynep Atris[1], Anna-Maria Tsirigoni[1], Melis Goktas[1], Patricia Lopez Garcia[1], Russell J. Wilson[1,2], Angelo Valleriani[1], Ana Vila Verde[3], and •Kerstin G. Blank[1,2] — [1]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany — [2]Johannes Kepler University, Linz, Austria — [3]University of Duisburg-Essen, Duisburg, Germany

Coiled coil (CC) structural motifs are found in diverse array of different proteins. Consisting of self-assembled alpha-helices that create helical superstructures, they serve as key elements of cytoskeletal and extracellular matrix proteins. Despite their widespread occurrence as mechanical building blocks, the fundamental structural factors governing their molecular mechanical properties have remained largely elusive.

We are applying AFM-based single molecule force spectroscopy and steered molecular dynamics simulations to determine the structure-to-mechanics relationship of de novo designed, synthetic CCs. When

comparing heterodimeric CCs of varying length and sequence, our findings reveal that higher thermodynamic and kinetic stability does not always correlate with higher rupture forces within the range of AFM-accessible loading rates. We further observe that a single sequence can exhibit diverse mechanical stabilities under different loading geometries. This knowledge is now utilized for the development of a library of CC-based mechanoresponsive hydrogel crosslinks for tissue engineering applications.

BP 27.12 Thu 12:45 H 0112

Visualizing and quantifying biomolecular interactions with fluorescence optical tweezers. — •Roman Renger, Philipp Rauch, and Nicholas Luzzietti — LUMICKS, Amsterdam, The Netherlands

Biological processes involving proteins interacting with nucleic acids, membranes or cytoskeletal filaments are key to cell metabolism and hence to life in general. Detailed insights into these processes provide essential information for understanding the molecular basis of physiology and pathological conditions. The next scientific breakthrough consists in direct, real-time observations and measurements of the most fundamental mechanisms and interactions involved in biology. Modern correlative single-molecule technologies offer a powerful opportunity to meet these challenges and to study dynamic protein function and activity in real-time and at unprecedented resolution. Here, we present our efforts to enable discoveries in biology and biophysics by combining optical tweezers with correlative fluorescence microscopy and advanced microfluidics. Our C-Trap allows to observe biomolecules while simultaneously measuring and controlling the generated forces and exposing the biomolecular system to different experimental conditions. We present examples in which our technology has enhanced the understanding of basic biological and biophysical phenomena, ranging from DNA repair to proteins dynamics to intracellular organization. Furthermore, we demonstrate how advances in hybrid single-molecule methods can be turned into an easy-to-use and stable instrument for tackling biophysical questions.

BP 28: Cytoskeleton

Time: Thursday 9:30–13:00 Location: H 2032

BP 28.1 Thu 9:30 H 2032

Actin waves as key functional structures of topological guidance and curvature sensing — •Cristina Martinez-Torres, Alexandra Faber, and Carsten Beta — Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany

The motility of cells in complex environments plays a crucial role in many biomedical processes such as wound healing or cancer metastasis. While the social amoeba *D. discoideum* is a well-known model organism to study pseudopod-based amoeboid motility, they can also move in a highly persistent motion reminiscent of keratocytes, where cells conserve a fan-shaped morphology. The occurrence of fan-shaped cells is intrinsically linked to the presence of actin waves, which are traveling wave patterns that propagate along the cortex, contributing to protrusion-driven cell motility. Here, we study the migration of single cells on micropillars of different geometries, and we investigate the interplay of topological guidance and curvature sensing. We show that when cells are able to form actin waves, the cells migrate preferentially along the edge of the pillar surface. This curvature-guided movement is persistent and occurs for curvatures comparable to the cell size, and also for different pillar geometries (circular, triangular, rectangular). However, when the preferred motility mode is that of an amoeboid cell without actin waves, the cells show no preference for tracking the edge of the pillar surface. Our results suggest that the topological guidance via actin wave formation is therefore critical for the edge-tracking migration.

BP 28.2 Thu 9:45 H 2032

Transient contacts between filaments bestow its elasticity to branched actin — Mehdi Bouzid[1,2], Cesar Valencia Gallardo[3], Magdalena Kopec[3], Giuseppe Foffi[4], Julien Heuvingh[3], Olivia du Roure[3], and •Martin Lenz[2,3] — [1]3SR, CNRS, Université Grenoble Alpes, France — [2]LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France — [3]Laboratoire de Physique et Mécanique des Milieux Hétérogènes, UMR 7636, CNRS, ESPCI Paris, PSL — [4]LPS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France

The biologically crucial elasticity of actin networks is usually understood as an interplay between the bending and stretching of its filaments. This point of view however fails when applied to the weakly coordinated branched actin networks found throughout the cell. Through experiments and theory, we show that their elasticity crucially involves reversible entanglements between their filaments. These entanglements can in turn be controlled during network growth to regulate the final properties of the network. These properties could be key to understanding how moving cells dynamically adapt their cytoskeleton to their environment.

BP 28.3 Thu 10:00 H 2032

Actin filament length is crucial in mesenchymal migration but not in amoeboid migration — •Carsten Baltes[1], Friederike Nolle[1,2], Kathi Kaiser[1], Erbara Gjana[1], Kristin Sander[1], Karin Jacobs[1,2], and Franziska Lautenschläger[1,2] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Center for Biophysics, Saarbrücken, Germany

The ability of cells to move is critical for a wide variety of cellular tasks inlcuding the search of immune cells for pathogens and the reorganization of cells in tissue development. The cytoskeletal protein actin is important for cellular migration as it is involved in its underlying mechanics. Alterations of the actin network therefore might have an impact on the migratory behaviour of cells.

Here, I present the effects of the stabilisation and elongation of actin filaments on migrating RPE-1 cells. I will show that mesenchymal migrating cells move at lower speed, while amoeboid migrating cells do not change their behaviour.

Cells with longer and more stable actin filaments have more but smaller focal adhesions. To test the effect on adhesion properties, we performed single-cell force spectroscopy. Cells with smaller focal adhesions showed lower adhesion strength and energy, suggesting that actin filament length is important for adhesion-based migration but negligible for friction-based migration.

This work emphasizes the different role of actin in mesenchymal versus amoeboid migration and adhesion and might help to influence all processes involving migration.

15 min. break

Invited Talk BP 28.4 Thu 10:30 H 2032

Quantifying the actin cortex of cells in different states — •Franziska Lautenschläger[1], Daniel Flormann[1], Christoph Anton[1], and Rhoda Hawkins[2] — [1]Saarland University — [2]AIMS Ghana, Accra

The actin cortex defines the shape of cells and is involved in a plethora of cellular functions. We aim to describe, predict and alter changes in cellular states by alterations of the actin cortex. I will show two examples of changes of a cellular states and their corresponding cortex alterations: An adhered cell compared with a suspended cell and a single cell compared with a cell in a monolayer. The parameters we chose to describe the actin cortex are the thickness, the mesh size, the bundling as well as the stiffness of the actin cortex. We compare our data of the actin cortex in cells with earlier theoretical and in vitro work and test theoretical predictions.

BP 28.5 Thu 11:00 H 2032

Cytoskeletal Networks in Cells Under Strain — •Ruth Meyer[1], Marie Tersteegen[1], Anna V. Schepers[1], Peter Luley[1], Ulrike Rölleke[1], Nicole Schwarz[2], Jonathan Bodenschatz[3], Amaury Perez Tirado[3], Andreas Janshoff[3], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]Institute of Molecular and Cellular Anatomy, RWTH Aachen University — [3]Institute of Physical Chemistry, University of Göttingen

The cytoskeleton of eukaryotes consists of three types of filaments: F-actin, microtubules and intermediate filaments (IFs). In contrast to microtubules and F-actin, IFs are expressed in a cell-type specific man-

ner, and among them keratins are found in epithelial cells. In certain cell types, the keratin IFs form a layer close to the membrane which may be referred to as an "IF-cortex". Furthermore, it is hypothesized that this IF-cortex arranges with radial spokes in a "rim-and-spokes" structure in epithelia. Based on this hypothesis, IFs and actin filaments might add complementary mechanical properties to the cortex. It was previously shown that single IFs in vitro remain undamaged even at high strains. We now ask the question of whether this unique force-extension behavior of single IFs is also relevant in the filament network within a cell. Here, we show the influence of equibiaxial strain on wild-type and keratin-deficient cells comparing the mechanical properties and the structure of actin and IF networks close to the cell membrane. We find an increase of cell stiffness and compressibility while fluidity and tension decrease during stretching.

BP 28.6 Thu 11:15 H 2032

The cytoskeleton positions protein condensates — •Thomas J. Böddeker[1,2], Roland L. Knorr[2], and Eric R. Dufresne[1,3] — [1]ETH Zürich, Zürich, Switzerland — [2]Humboldt-Universität zu Berlin, Berlin, Germany — [3]Cornell University, Ithaca, USA

Protein condensates inside human cells are liquid-like droplets composed of protein and RNA. These condensates interact with the heterogeneous, active and dense environment of the cytoplasm, crossed by various cytoskeletal filaments such as microtubules and actin. Capillary interactions with the cytoskeleton lead to stereotypical positioning of such protein droplets inside the cell. Using statistical physics approaches, we identified complementary functions of filamentous actin and microtubules for the positioning of such condensates: protein condensates couple to actin's native dynamics in the cell through steric interactions leading to directional motion towards the cell center. Microtubules (and their molecular building-blocks), on the other hand, act as Pickering agents and engage in energetically favorable wetting interactions that lead to a robust localization of protein condensates in microtubule-rich regions of the cell. Cytoskeletal filaments, in turn, deform in response to capillary forces, leading to network modulations centered on protein condensates. These mutual interactions are non-specific and ultimately arise from different affinities (contact angles) between condensate and filament, suggesting that similar mechanisms may impact localization of other liquid-like phases within the cell and structure formation within the cytoskeleton.

T.J. Böddeker, et. al. PRX Life, in press

BP 28.7 Thu 11:30 H 2032

Vimentin Secretion and its influence on macrophage functionality — •Divyendu Goud Thalla — Experimental Biophysics,Universität des Saarlandes, Saarbrücken, Germany

Macrophages play a vital role in the immune system by detecting and eliminating bacterial organisms through phagocytosis. Upon activation, macrophages expose vimentin cytoskeletal protein to the extracellular environment. Such extracellular vimentin can either remain bound to the cell surface or it can be released*into extracellular space. This phenomenon similarly occurs under circumstances like injury, senescence, and stress. However, the characteristics of the extracellular form of vimentin and its implications on macrophage functionality remain unclear. In this study, we demonstrate that vimentin is released from the back end of macrophages. Activation of macrophages further enhances this polarized secretion of vimentin. Our findings from migration and phagocytosis assays show that extracellular vimentin enhances macrophage functionality in terms of migration and phagocytosis. Through high resolution fluorescence microscopy and scanning electron microscopy techniques, we show that extracellular vimentin is released into extracellular space in the form of small fragments.Taken together, we propose a mechanism of vimentin secretion and its implications on macrophage functionality.

15 min. break

BP 28.8 Thu 12:00 H 2032

Lattice dynamics in microtubules: Revealing the dual effects of Tau in vitro — Subham Biswas[1], Rahul Grover[2], Cordula Reuther[2], Mona Grünewald[1], Karin John[3], Stefan Diez[2], and •Laura Schaedel[1] — [1]Saarland University, Saarbrücken, Germany — [2]TU Dresden, Germany — [3]LiPhy, CNRS/UGA, Grenoble, France

Microtubules are dynamic cytoskeletal filaments that grow and shrink by tubulin addition or removal at their tips. In contrast, the microtubule lattice far from the tips was long considered to be static. The discovery of tubulin loss and incorporation along the lattice far from the tips - termed lattice dynamics - led to a paradigm shift and revealed a new dimension of microtubule dynamics. Although lattice dynamics occur spontaneously, there is increasing evidence that microtubule-associated proteins (MAPs) are involved in their regulation. Here, we show that the neuronal MAP Tau, which typically decorates axonal microtubules, stimulates tubulin incorporation into the microtubule lattice in reconstituted in vitro systems. We uncover a dual effect of Tau: while it leads to an overall stabilization of the microtubule lattice in the absence of free tubulin, it also induces lattice turnover. Our data show how lattice dynamics are regulated by cellular factors, similar to the dynamics at their tips.

BP 28.9 Thu 12:15 H 2032

Lattice dynamics in microtubules: Theoretically exploring the dual effects of Tau — Subham Biswas[1], Rahul Grover[2], Cordula Reuther[2], Mona Grünwald[1], •Karin John[3], Stefan Diez[2], and Laura Schaedel[1] — [1]Saarland University, Saarbrücken, Germany — [2]TU Dresden, Germany — [3]Liphy, CNRS/Université Grenoble-Alpes, Grenoble, France

Microtubules are key structural elements of living cells that are crucial for cell division, intracellular transport and motility. They are dynamic polymers, which grow and shrink by addition and removal of tubulin dimers at their extremities. Within the microtubule shaft, dimers adopt a densely packed and highly ordered crystal-like lattice structure, which is generally not considered to be dynamic. Recent experiments have shown that microtubules exhibit a lattice dynamics far away from the extremities. This dynamics manifests itself as localized incorporation of free tubulin into the microtubule shaft. Tubulin incorporation into the microtubule lattice can occur either spontaneously or facilitated by microtubule associated proteins such as molecular motors and severing enzymes. The neuronal protein Tau is the latest addition to the growing number of molecules known to stimulate turnover of the MT lattice. However, the origin and underlying mechanisms of Tau stimulated lattice turnover is yet unknown, since Tau is rather known to stabilize the MT lattice. Here, we theoretically explore potential mechanisms of Tau stimulated lattice turnover, consistent with experimental observations.

BP 28.10 Thu 12:30 H 2032

Scanning small-angle X-ray scattering on single cardiomyocytes: high resolution in reciprocal space — •Hendrik Bruns[1], Titus Czajka[1], Michael Sztucki[2], Sören Brandenburg[3], and Tim Salditt[1] — [1]Institut for Xray physics, University of Göttingen, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]University Hospital Göttingen, Göttingen, Germany

Muscle contraction is driven by an ordered protein structure in the sarcomere which generates a macroscopic force by synchronized movement. The long-range order in the structure in combination with highly brilliant 4th generation synchrotron radiation enables measurements on single cardiomyocytes in an (ultra) small-angle X-ray scattering (USAXS, SAXS) geometry, with beam sizes comparable to the size of the cell. High spatial resolution in reciprocal space in combination with spatially resolved maps of cells helps to overcome the challenge that cardiac muscle tissue has so far been much less prone for diffraction studies compared to skeletal muscle or trabeculae. Our experiments reveal the structural organization of single cardiomyocytes. In particular, we are able to observe the myosin arrangement and the troponin spacing. The results open up a pathway to measurements of living cells during their contraction cycle, thus improving our fundamental understanding of cardiac muscle function.

BP 28.11 Thu 12:45 H 2032

Cytoskeleton flow-to-force — •Yoav G. Pollack, Nilay Cicek, Emily Klass, Pratima Sawant, Sarah Köster, Anne Wald, and Andreas Janshoff — University of Göttingen, Göttingen, Germany.

The cytoskeleton provides the cell with both structural integrity and the capability to continuously adjust shape to support functions such as crawling or squeezing through gaps. To gain insight into this process we study the motion of actin filaments driven by myosin motors. We aim to read active actin flow or contraction from reconstituted actomyosin networks in droplets and Giant Unilamellar Vesicles (GUVs) and solve the inverse problem to deduce the motion-generating force field. From the theory side, a solution to the inverse problem is obtained with some robustness to measurement noise via regularization. However, reading the flow from fluorescent images is an ongoing data

analysis challenge. We try to bridge this gap between experiment and mathematical theory using simulations. These can reveal both the necessary experimental parameters for reading the flow (e.g. frame rate and image resolution), as well as ascertain the minimal requirements of an experimental setup of showing a coherent flow, such as actin anchoring points and whether an induced anisotropy is needed.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), project-ID 449750155, RTG 2756, Projects A4, A6, A7.

BP 29: Statistical Physics of Biological Systems II (joint session BP/DY)

Time: Thursday 9:30–12:00 Location: H 1028

BP 29.1 Thu 9:30 H 1028

Coarsening model explains cross-species universality of crossover interference — •Marcel Ernst[1], Raphael Mercier[2], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]Max Planck Institute for Plant Breeding Research, Carl-von-Linné-Weg 10, 50829 Cologne, Germany

During meiosis, crossovers between female and male chromosomes mix genetic information. Experimental observations consistently produce two important results: First, the number of crossovers per chromosome is at least one and usually small, ranging from one to three. Second, there is crossover interference, which prevents nearby crossovers on a single chromosome. In this talk, I will present a novel quantification of crossover interference, which reveals a universal behavior across multiple species. This behavior is consistent with a recently proposed model, where biomolecular condensates that coarsen by exchanging material along chromosomes determine crossover positions. This process is disrupted in mutants lacking the axial structure connecting chromosome pairs, leading to strongly reduced interference. To explain that behavior, I will also present an extension of the coarsening model, which includes material exchange with the surrounding nucleoplasm. The modified coarsening dynamics provide a more detailed description of all experimental data and unveil the physical mechanism of crossover interference.

BP 29.2 Thu 9:45 H 1028

Designing phase coexistence in multicomponent mixtures: surface tensions and the Gibbs' rule — •Filipe Thewes and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Gibbs' phase rule constrains the maximum number of phases that can coexist in multicomponent mixtures. It relates the maximum number of phases to the number of components and the degrees of freedom. The phases formed in equilibrium depend directly on the interactions between the different components, opening the possibility for the inverse problem of designing a set of interactions that recover a desired phase behavior. This perspective has been explored recently in relation to phase separation in biological systems as a mechanism for cells to control their internal structure and function. Interestingly, recent approaches for such interactions design are able to retrieve in the grand-canonical setting a number of phases that is larger than predicted by a naive application of Gibbs' phase rule. In this talk, I will first revisit Gibbs' rule in the *grandcanonical* ensemble and show that designed interactions act as new degrees of freedom that do increase the number of possible phases. I then show that in a canonical setting the number of phases is determined by interfacial tensions; above the naive Gibbs limit we find long-lived metastable states in numerical simulations. In the second part, I will discuss which conditions on the interfacial tensions result in "super-Gibbs" canonical phase splits. These conditions lead to a second step in the design problem of multicomponent mixtures, namely that of controlling the interfacial properties.

BP 29.3 Thu 10:00 H 1028

Microscopic model for aging of RNA condensates — •Hugo Le Roy — EPFL, Lausanne, Switzerland

Biomolecular condensates are membrane-less comparments in the cell that are involved in a wide diversity of biological processes. These liquid-liquid phase-separated droplets exhibit a viscoelastic mechanical response. This behavior is rationalized by modeling the complex molecules that make up a condensate as stickers and spacers that can assemble into a network-like structure. The proper functioning of biocondensates requires precise control over their composition, size, and mechanical response. For example, several neurodegenerative diseases are associated with dysfunctional condensates that solidify over a long period of time (days) until they become solid. A phenomenon usually described as aging. The emergence of such a long timescale of evolution from microscopic events, as well as the structural reorganization that leads to aging remains mostly an open question. To explore the connection between the mechanical properties of the condensates and their structure, we use a simplified description of the condensates. In our framework, a condensate is considered as an associative gel made of polymers (RNA) and linkers (DEAD-box proteins), whose response time is related to the interaction time between the constituents. We show that the interaction between linkers and long polymers results in an attractive Casimir force between linkers. As a consequence, linkers tend to cluster over equilibration of the network. Such a clustering does not make the material stiffer but leads to an exponential increase of the relaxation timescale in agreement with experimental observations.

BP 29.4 Thu 10:15 H 1028

Are phases an appropriate description for cells? — •Martin Girard — Max-Planck-Institute für Polymerforschung

Phase separation has emerged as an important topic for cellular function. From lipid rafts to liquid-liquid phase separation, our current understanding is that it is crucial for organization. We putatively expect that rules extracted from simple systems, two component mixtures, extend to multicomponent systems. While this is true in the thermodynamic limit, I will discuss here the thermodynamic limit for multicomponent systems. Using a toy model, I will show that what we consider "large systems" is largely subjective and dependent on details in multicomponent systems. For "small" systems, rules are very different, and the system is dominated by fluctuations. Usual assumptions, such as equivalence of thermodynamic ensembles, are broken. Still, the system can be driven to exhibit behavior that is similar to a phase transition, for instance by changing the statistical ensemble. Practically, this means that observed phase behavior may be largely dependent on system preparation. This naturally leads to a fundamental question: is the traditional phase behavior an appropriate description for cellular behavior?

15 min. break

BP 29.5 Thu 10:45 H 1028

Complex and 3-dimensional RNA random walks: comparison and application to sequence data across biological taxa — •Jack Mortimer and Jens Christian Claussen — School of Computer Science, University of Birmingham, UK

The DNA random walk is a classical attempt to grasp long-range features of DNA (or RNA) sequences by mapping pairs of amino acids to ± 1 steps of a random walk, and interpret the resulting "time series" by scaling analysis [1]. But as four letters C,G,A,T comprise the DNA alphabet it is a straightforward idea to utilize complex numbers to exploit this information (rather than ignoring it). This direction has been investigated also elsewhere [2] but different definitions were used, and it is not yet conclusive how far biological data can be differentiated.

In this contribution, we attempt a comparison of different complex RW definitions together with a 3D RW, discuss their relations between each other, and apply them to a wide range of DNA sequences. While the various DNA RW's seem not to be directly disciminatory for each species, we find that they provide a wide spread across the datasets. In conclusion, complex and higher-dimensional DNA random walks are a promising tool to extract long-range features from DNA, although the biological interpretation of this method remains to be investigated.

[1] Peng, Buldyrev, Goldberger et al., Nature 356,168 (1992)
[2] Cattani, in: Bioinf Res Dev, Springer, p. 528 (2008)

BP 29.6 Thu 11:00 H 1028

Trajectory mutual information in biochemical systems: Gaussian vs. Poissonian fluctuations — •Anne-Lena Moor[1,2],

Christoph Zechner[1,2], and Pieter Rein ten Wolde[3] — [1]Max Planck Institute of Molecular Cell Biology and Genetics — [2]Center for Systems Biology Dresden — [3]AMOLF Amsterdam

Signal processing in biochemical networks relies on dynamic information transmission between time-trajectories of the respective molecular components. From a mathematical point of view, the transferred information can be described via the mutual information. Traditionally, this has been calculated using a Gaussian approximation. Our recent work suggests that this method is not always suitable for every biochemical networks which can lead to quantitative and qualitative mismatches to the exact solution. In this work, we explain the origin of these discrepancies and present a modified version of the Gaussian framework that aligns better with the characteristics of stochastic biochemical networks.

BP 29.7 Thu 11:15 H 1028

Geometry and epigenetic memory during ageing — •Matteo Ciarchi[1], Steffen Rulands[2], and Benjamin Simons[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Ludwig-Maximilians-Universität, München — [3]Department of Applied Mathematics and Theoretical Physics, Cambridge

Ageing is the decline of the physiological function of an organism over time. This process has been shown to be tightly correlated to changes in epigenetic modifications of the DNA. But how does the slow process of ageing over decades emerge from the fast molecular changes in the epigenome? Here, we show that the interplay between fluctuations and DNA geometry gives rise to memory that translates short-term molecular changes to a slow drift on the time-scales of aging. We draw on sequencing experiments that compare DNA methylation on the time scales of few cell divisions to longitudinal measurements over the much longer time scales of aging. We find that the drift of DNA methylation over time in both cases is highly nonlinear and cannot be explained by known biochemical processes. In order to understand these observations, we derive a field-theoretic framework that couples epigenetic processes along the DNA sequence with dynamic geometrical changes of the DNA in three-dimensional space. Using this theory, we show that the conformational changes in three-dimensional space allow for memory to form along the DNA sequence. Taken together, our work shows that epigenetic ageing is the accumulation of fast, intrinsic molecular processes over long time scales.

BP 29.8 Thu 11:30 H 1028

Exploring tumor karyotype evolution using the Macro-Karyotype concept — •Lucija Tomašić[1], Thomas van Ravesteyn[2,3], Geert J. P. L. Kops[2,3], and Nenad Pavin[1] — [1]Faculty of Science, University of Zagreb, Croatia — [2]Hubrecht Institute and University Medical Centre Utrecht, Utrecht, The Netherlands — [3]Oncode Institute, Utrecht, The Netherlands

Most tumors exhibit abnormal chromosome content (karyotype) resulting from errors in mitotic division. While tumors tend to manifest diverse karyotype aberrations, typically with gains of specific chromosomes, understanding the dynamics leading to these configurations is challenging due to the dimensionality of the karyotype space. To address this complexity, we introduce the 'Macro-Karyotype' concept,a novel framework for comprehensively exploring tumor chromosomal evolution. Combining in vitro organoid evolution with mathematical modeling, our study demonstrates that premalignant human organoids spontaneously undergo chromosome copy number alterations related to cancer. A gradual gain of specific chromosomes over time is observed, propelled by the enhanced fitness of these karyotypes. Additionally, some karyotypes undergo dramatic changes through whole-genome duplication and multipolar divisions, followed by normalization over time through the selection of karyotypes with lower mitotic error rates. Our findings uncover the selection of homogeneous karyotypes driven by cellular fitness, significantly constraining the available karyotype space. Our study deepens understanding of tumor karyotype evolution and informs factors influencing cancer related chromosomal changes.

BP 29.9 Thu 11:45 H 1028

How do particles with complex interactions self-assemble ? — •Lara Koehler[1], Martin Lenz[2], and Pierre Ronceray[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Université Paris Saclay — [3]Aix Marseille Université

In living cells, proteins self-assemble into large functional structures based on specific interactions between molecularly complex patches. Due to this complexity, protein self-assembly results from a competition between a large number of distinct interaction energies, of the order of one per pair of patches. Current self-assembly models however typically ignore this aspect, and the principles by which it determines the large-scale structure of protein assemblies are largely unknown. Here, we use Monte-Carlo simulations and machine learning to start to unravel these principles. We observe that despite widespread geometrical frustration, aggregates of particles with complex interactions fall within only a few categories that often display high degrees of spatial order, including crystals, fibers, and micelles. We then successfully identify the most relevant aspect of the interaction complexity in predicting these outcomes, namely the particles' ability to form periodic structures. Our results provide a first characterization of the rich design space associated with identical particles with complex interactions, and could inspire engineered self-assembling nanoobjects as well as help understand the emergence of robust functional protein structures.

BP 30: Active Matter IV (joint session DY/BP/CPP)

Time: Thursday 9:30–13:00 Location: BH-N 334

Invited Talk BP 30.1 Thu 9:30 BH-N 334

Flocking by turning away — •Ricard Alert — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Flocking, as paradigmatically exemplified by birds, is the coherent collective motion of active agents. As originally conceived, flocking emerges through alignment interactions between the agents. Here, I will show a new mechanism of flocking based on interactions that reorient agents away from each other. Combining simulations, kinetic theory, and experiments, we demonstrate this mechanism of flocking in self-propelled Janus colloids with stronger repulsion on the front than on the rear. We show that, unlike for alignment interactions, the emergence of polar order from turn-away interactions requires particle repulsion. The polar flocking state is stable because particles achieve a compromise between turning away from left and right neighbors. These findings could help to reconcile the observations that cells can flock despite turning away from each other via contact inhibition of locomotion. Overall, our work shows that flocking is a very robust behavior that arises even when the orientational interactions seem to prevent it.

BP 30.2 Thu 10:00 BH-N 334

Metastability of ordered phase in discretized flocking — •Swarnajit Chatterjee[1], Mintu Karmakar[2], Matthieu Mangeat[1], Raja Paul[2], and Heiko Rieger[1] — [1]Center for Biophysics & Department for Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany. — [2]School of Mathematical & Computational Sciences, IACS, Kolkata – 700032, India.

Polar flocks are observed in a large class of active matter systems and have been considered robust to fluctuations. However, recent studies have argued that liquid polar flocks are metastable to the presence of small obstacles [1] or to the nucleation of opposite-phase droplets [2]. In this work, we study the stability of the ordered phase in flocking models with q-fold symmetry under the influence of counter- or transversely-propagating droplets. We observe that the liquid phase is more susceptible to a transversely-propagating droplet than a counter-propagating droplet. Also, for droplet counter-propagation, system morphology is dominated by a novel *"sandwich state"* of the liquid state and the droplet state rather than a reversal of the liquid phase. Here spatial anisotropy plays a crucial role. Metastability of the liquid phase in a discretized Vicsek model shows a strong dependency on the noise strength where the anisotropy parameter q does not significantly affect the reversal dynamics. Our study further investigates the influence of droplet size, density, and other control parameters on liquid stability.

[1] Codina et al., PRL 128, 218001 (2022).
[2] Benvegnen et al., arXiv:2306.01156 (2023).

BP 30.3 Thu 10:15 BH-N 334

Emergent Metric-like States of Active Particles with Metric-free Polar Alignment — Yinong Zhao[1], Cristian L. Huepe[2], and •Pawel Romanczuk[3,4] — [1]Shanghai Jiao Tong University, Shanghai, PR China — [2]Northwestern University, Chicago, USA — [3]Department of Biology, Humboldt Universität zu Berlin, Germany — [4]Excellence cluster "Science of Intelligence", Berlin

We study a model of self-propelled particles interacting with their k-nearest neighbors through polar alignment. By exploring its phase space as a function of two nondimensional parameters (scaled alignment strength g and Peclet number Pe), we identify two distinct order-disorder transitions. One appears to be continuous, occurs at a low critical g value independent of Pe, and resembles a mean-field transition with no density-order coupling. The other is discontinuous, depends on a combined control parameter involving g and Pe, and results from the formation of small, dense, highly persistent clusters of particles that follow metric-like dynamics. These dense clusters form at a critical value of the combined control parameter Pe/g^{α} , with $\alpha \approx 1.5$, which appears to be valid for different alignment-based models. Our study shows that models of active particles with metric-free interactions can produce characteristic length-scales and self-organize into metric-like collective states that undergo metric-like transitions.

BP 30.4 Thu 10:30 BH-N 334

Strong Casimir-like Forces in Flocking Active Matter — •Giuseppe Fava[1,2], Andrea Gambassi[3], and Francesco Ginelli[1,2] — [1]Dipartimento di Scienza e Alta Tecnologia and Center for Nonlinear and Complex Systems, Università degli Studi dell'Insubria, Como, Italy — [2]INFN sezione di Milano, Milano, Italy — [3]SISSA International School for Advanced Studies and INFN, via Bonomea 265, 34136 Trieste, Italy

Confining in space the equilibrium fluctuations of statistical systems with long-range correlations is known to result into effective forces on the boundaries.

In this work we demonstrate the occurrence of Casimir-like forces in the non-equilibrium context provided by flocking active matter. In particular, we consider a system of aligning self-propelled particles in two spatial dimensions, which are transversally confined by reflecting or partially reflecting walls. We show that in the ordered flocking phase this confined active vectorial fluid is characterized by extensive boundary layers, as opposed to the finite ones usually observed in confined scalar active matter. A finite-size, fluctuation-induced contribution to the pressure on the wall emerges, which decays slowly and algebraically upon increasing the distance between the walls.

We explain our findings which display a certain degree of universality within a hydrodynamic description of the density and velocity fields.

Ref: "Strong Casimir-like Forces in Flocking Active Matter", arXiv:2211.02644

BP 30.5 Thu 10:45 BH-N 334

Collective Dynamics in Dense Systems of Active Polar Disks — •yating zheng[1,2], weizhen tang[3], amir shee[4], pawel romanczuk[1,2], and cristian huepe[4] — [1]Humboldt-Universität zu Berlin — [2]Research Cluster of Excellence 'Science of Intelligence' — [3]Beijing Normal University — [4]Northwestern University

We study a general model of a dense system of active polar disks with repulsive linear interactions, confined by a circular boundary. Each disk advances with a preferred self-propulsion speed and changes heading by turning around an axis of rotation located at a distance R behind its barycenter. We characterize the emerging phases and collective states as a function of R, density, and noise, for disks with isotropic and anisotropic damping disks, and a smooth or rough boundary. We find a rich phase space that combines transitions from solid to fluid states with novel R-dependent transitions from a collective state displaying localized disk rotation to a milling state around a common centre of rotation. These transitions are related to the formation of vortices that follow simple or complex dynamics depending on the boundary properties and system size. Our results demonstrate generic collective states that are expected to be observed in experimental dense systems of natural or artificial active agents in confined spaces.

BP 30.6 Thu 11:00 BH-N 334

Cooperative resetting exhibits a delocalisation phase transition — •Felix J. Meigel and Steffen Rulands — Arnold Sommerfeld Center for Theoretical Physics, Department of Physics, Ludwig-Maximilians-Universität, München, Germany

In the realm of biology, many non-equilibrium systems are inherently noisy, while their proper functioning relies on the adept control of fluctuations. Stochastic resetting processes, where the state of a system is reset to its initial condition at random times, provide a framework for the control of the accumulation of fluctuations over time. Yet, in this framework, resetting is externally imposed. Here, we demonstrate that a constraint of fluctuations can also be achieved in a self-organized manner by cooperative resetting in many-particle systems. Specifically, we demonstrate that many-particle systems, wherein pairs of particles are reset to their respective average positions, exhibit a second-order phase transition as a function of the resetting rate. This transition delineates a regime where particles localize, thereby controlling fluctuations, and another regime where particle positions become unbounded. Our research showcases that cooperative resetting enables adaptation to external perturbations and enhances the optimization of search tasks compared to extrinsic resetting. We showcase the versatility of self-organized fluctuation control through cooperative resetting, with applications ranging from biological systems, such as intracellular vesicle dynamics and the fitness advantages of genetic recombination, to technical domains like the optimization of shared mobility services.

15 min. break

Invited Talk BP 30.7 Thu 11:30 BH-N 334

Growth and division as drivers of complex dynamics in dense cellular matter — •Philip Bittihn — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Cells in systems such as tissues, bacterial aggregates, embryonic development or tumors self-organize on large scales to fulfil their biological functions. Many such collective behaviors have been studied in the broader context of active matter, where they emerge from the intrinsic non-equilibrium activity of the constituent particles. Growth and division as drivers of activity have received less attention, although they are defining features of life and often play indispensable roles.

Here, I will describe some of our recent theoretical efforts in characterizing their effects in dense cellular matter. Using minimal models of mechanically interacting particles, we investigate scenarios in which growth and division either lead to large-scale flows and volume expansion or total volume is conserved. By developing statistical descriptions suited for non-conserved particle numbers, we find that certain components of particle motion follow simple scaling laws that can be related to macroscopic flows or to classical active particle models. Other features of the dynamics reveal new phenomena and transitions due to growth-induced pressure, confinement and anisotropic particle shapes. If time permits, I will outline interactions with motility or chemical activity. Overall, our results aim to establish universal physical principles as a baseline for experimental observations and provide design strategies for bio(technological) applications or artificial systems.

BP 30.8 Thu 12:00 BH-N 334

Motility-induced clustering of active particles under soft confinement — •Timo Knippenberg[1], Ashreya Jayaram[2], Thomas Speck[2], and Clemens Bechinger[1] — [1]FB Physik, Universität Konstanz, Deutschand — [2]Institute for theoretical physics IV, Universität Stuttgart, Deutschland

In the field of active matter, motility-induced phase separation (MIPS) is one of the most widely studied subjects. This phenomenon, characterized by a phase transition from a homogeneous phase into a densely clustered state with a gaseous surrounding, occurs at sufficiently high density and active particle (AP) velocity. However, most of these studies focus on APs in bulk or near hard walls, while research on APs in soft confinement is scarce. The latter promises insights into the dimensionality-dependent aspects of MIPS, as gradually increasing the confinement strength provides a way to approach the 1-dimensional limit, where MIPS is known to be absent.

To address this topic, here we experimentally investigate the structural and dynamical properties of APs confined in a soft annulus-shaped channel. Depending on the strength of the confinement and the AP velocity, we observe a novel re-entrant phase behavior. We can explain our measurements by the strong coupling between velocity and the effective confining dimensionality in such soft systems.

In addition to highlighting the important influence of soft boundaries on APs, our research has implications for future applications in micro-robotics.

BP 30.9 Thu 12:15 BH-N 334

Emergent memory from tapping collisions in active granular matter — •Lorenzo Caprini, Anton Ldov, René Wittmann, Christian Scholz, and Hartmut Löwen — Heinrich-Heine University of Düsseldorf

In an equilibrium thermal environment, random elastic collisions between the background particles and a tracer establish the picture of Brownian motion fulfilling the Einstein relation between diffusivity and mobility. In nature, environments often comprise collections of autonomously moving objects, termed active matter, which exhibit fascinating phenomena. We investigate experimentally the impact of an active environment on a passive tracer by using active granular particles, i.e. vibrationally excited inertial self-propelled units termed vibrobots. They display multiple correlated tapping collisions with the tracer, by bouncing and sliding on its surface. As a consequence, the tracer displays a persistent memory and is described by a generalized active Einstein relation that constrains fluctuations, dissipation, and effective activity due to the tracer memory. Since the resulting persistence can be tuned by the environmental density and motility, our findings can be useful for engineering properties of various active systems in biomedical applications and swarm robotics.

BP 30.10 Thu 12:30 BH-N 334

Stationary particle currents in sedimenting active matter wetting a wall — •Matthieu Mangeat, Shauri Chakraborty, Adam Wysocki, and Heiko Rieger — Saarland University, Saarbrücken, Germany

Recently it was predicted, on the basis of a lattice gas model, that scalar active matter would rise against gravity up a confining wall in spite of repulsive particle-wall interactions [PRL 124, 048001 (2020)]. We confirm this prediction with sedimenting active Brownian particles (ABPs) in a box and elucidate the mechanism leading to the formation of a meniscus rising above the bulk of the sedimentation region. The height of the meniscus increases algebraically with the activity, and the formation of the meniscus is determined by a stationary circular particle current centered at the base of the meniscus. The origin of these vortices can be traced back to the confinement of the ABPs in a box: already the stationary state of non-interacting ABPs without gravitation displays highly symmetric circular currents. Gravitation distorts this vortex configuration downward, leaving two major vortices at the two side walls, with a strong downward flow along the walls. Repulsive interactions between the ABPs change this situation only as soon as motility induced phase separation (MIPS) sets in and forms a dense, sedimented liquid region at the bottom, which pushes the center of the vortex upwards towards the liquid-gas interface. Self-propelled particles therefore represent an impressive realization of scalar active matter that forms stationary particle currents being able to perform visible work against gravity, which we predict to be observable experimentally.

BP 30.11 Thu 12:45 BH-N 334

Velocity-density scaling for active particles in an external field — •Colin-Marius Koch and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Germany

Active particles in external fields can show diverse aggregation phenomena. The emerging collective phenomena and their statistics can thereby depend on microscopic details of active constituents' interactions. Here, we investigate how different steric interactions and self-propulsion mechanisms affect the aggregation of active particles in an external field. While density and velocity profiles individually differ between the studied cases, they consistently scale inversely with each other, when the instantaneous velocity projected onto the particle orientation is considered. The observed velocity-density scaling is robust for relatively dilute systems in which no strong aggregation, i.e. motility-induced phase separation, is present. We conclude that different microscopic details can result in the same statistics of collective behaviour in systems that are dilute enough.

BP 31: Protein Structure and Dynamics

Time: Thursday 15:00–18:00 Location: H 0112

BP 31.1 Thu 15:00 H 0112

BCL11B CCHC Zinc Finger Domain and Its Potential for Cancer Therapy — •Anne Susemihl[1,3], Lukas Schulig[2], Norman Geist[1], Piotr Grabarczyk[3], Felix Nagel[1], Christian Andreas Schmidt[3], and Mihaela Delcea[1] — [1]Institute of Biochemistry, Greifswald, Germany — [2]Institute of Pharmacy, Greifswald, Germany — [3]University Medicine, Greifswald, Germany

B Cell Lymphoma/Leukemia 11B (BCL11B) is a transcription factor, exerting a bi-directional role in cancer. BCL11B KO in vitro lead to T cells acquiring properties of natural killer cells, suggesting BCL11B*s role as an emerging cancer target. Previous FACS-FRET experiments and extensive enhanced sampling simulations indicated that BCL11B forms dimers, with this being a prerequisite for its functionality. New simulations and size exclusion chromatography data suggest the formation of not only dimers but tetramers. Multimerization is mediated by an atypical CCHC zinc finger (ZF) motif within the N-terminal region of the protein. Understanding the nature of BCL11B*s multimerization and its zinc binding properties may enable the use of BCL11B in targeted cancer therapy. We show here that zinc coordination is essential for the oligomerization of the N-terminal domain. Zinc binding properties of the CCHC ZF domain were determined using UV-Vis spectroscopy and isothermal titration calorimetry. BCL11B mutations within the tetramer interface led to insufficient zinc binding and incomplete ZF formation, resulting in monomerization. Other mutants showed monomerization but tetramer formation with the wild type zinc finger, with the physiological relevance yet to be elucidated.

BP 31.2 Thu 15:15 H 0112

Electric-field induced ultrafast protein changes — •Karsten Heyne, Clark Zahn, and Ramona Schlesinger — Freie Universität Berlin, Fachbereich Physik, Berlin, Deutschland

Light absorption activates photoreceptors and triggers a cascade of structural changes leading to the biological function. The time span of these processes ranges from femtoseconds to seconds. The fastest process is the absorption of a photon on a time-scale of a few fs. It is a long-standing debate whether excitation of the chromophore impacts the protein structure immediately or if the protein response is delayed until the photoproduct is formed. Here, we show direct response of the protein prior to chromophore isomerization. The vibrational fingerprint region of bacteriorhodopsin (bR) studied with polarization-resolved fs VIS-pump IR-probe spectroscopy reveals protein restructuration before and after photoisomerization. Transient protein signals were identified prior to and after photoisomerization with 500 fs. A proton continuum band, amide I band, and carboxylic acid groups, essential elements for the function of the bR proton pump, are altered by the excited chromophore. These groups have distances up to 10 Å to the chromophore. Therefore, we propose that an impulsive electric field change at the chromophore in the excited state perturbs polar groups throughout the protein. The ensuing reorganization prepares the protein for the down-stream processes.

BP 31.3 Thu 15:30 H 0112

New insights into the structural dynamics of intrinsically disordered proteins by high-field NMR relaxation experiments — Tobias Stief[1,2], Katharina Vormann[1,2], and •Nils-Alexander Lakomek[1,2] — [1]Forschungszentrum Jülich, Structural Biochemistry (IBI-7), 52425 Jülich, Germany — [2]Heinrich Heine University Düsseldorf, Institute of Physical Biology, 40225 Düsseldorf Germany

Intrinsically disordered proteins (IDPs) compose about 30% of the human proteome and are highly dynamic entities. Nuclear magnetic resonance (NMR) spectroscopy can provide insights into their structural dynamics at residue-specific resolution. Recently available higher magnetic field strengths, up to 28 Tesla (corresponding to 1.2 GHz 1H Larmor frequency), offer substantially improved resolution, with particular benefits for studying IDPs. We have derived an improved set of 15N NMR relaxation experiments suited for operation at high-field magnets and applicable to fully protonated proteins. Here, we used SNARE proteins as a model system. SNARE proteins play a crucial role during neuronal exocytosis by eliciting the fusion of the synaptic vesicle membrane with the presynaptic plasma membrane. In their pre-fusion state, the membrane-anchored SNARE proteins are disor-

dered. To assess the internal dynamics of the SNARE protein SNAP25, we recorded NMR relaxation experiments at different magnetic field strengths, between 14 and 28T. The field-dependent NMR measurements reveal novel insights into IDP dynamics at the ps-ns timescale.

Invited Talk BP 31.4 Thu 15:45 H 0112

Polarizing nuclear spins at the interface between ESR and NMR spectroscopy — •Marina Bennati — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — Institute of Physical Chemistry, University of Göttingen, Göttingen, Germany

Latest developments in magnetic resonance spectroscopy are aimed at increasing sensitivity for nuclear spin detection, which is limited by the small energy splitting at the available polarizing magnetic fields. A powerful approach is taking advantage of the larger magnetic moment of unpaired electrons and uses hyperfine couplings to transfer their polarization to nuclear spins.

The talk will illustrate recent progress in polarization transfer experiments using electron-nuclear double resonance techniques, either with ESR or NMR detection. In ESR spectroscopy, we detect nuclear spins up to the second ligation sphere of a paramagnetic center. We have recently demonstrated that at high electron Larmor frequencies (263 GHz) nuclear chemical shift tensors as well as quadrupolar nuclei can be resolved. In conjunction with 19F spin labelling, our techniques can be employed for measuring inter-spin distances in biomolecules in the angstrom to nanometer range. Moreover, we are developing dynamic nuclear polarization for enhanced NMR detection in the liquid state. Progress and strategies for future applications will be discussed.

15 min. break

BP 31.5 Thu 16:30 H 0112

NAP-XPS analysis of X-ray radiation damage to Proteins in Water — •Dorothea C. Hallier[1,2,3], Jörg Radnik[2], Paul M. Dietrich[4], Harald Seitz[1,3], and Marc Benjamin Hahn[2] — [1]Fraunhofer Insitute for Cell Therapy and Immunology, Branch Bioanalytics and Bioprocesses, Potsdam, Germany — [2]Federal Insitute for Materials Research and Testing BAM Berlin, Berlin, Germany — [3]Univerity of Potsdam, Institute for Biochemistry and Biology, Potsdam Germany — [4]SPECS Surface Nano Analysis GmbH, Berlin, Germany

X-ray photoelectron spectroscopy (XPS) was used to analyze the chemical damage of ionizing radiation to the single-stranded DNA-binding protein Gene-V Protein (G5P/GVP) and its most abundant amino acids. This protein plays a crucial role in maintaining the DNA metabolism, especially DNA replication, recombination and repair. XPS vacuum measurements were combined with near-ambient pressure (NAP) XPS measurements under water atmosphere to detect both direct and indirect radiation damage and to identify corresponding damage pathways. The exposure of proteins and aminoacids to x-rays leads to degradation i.e. via dehydrogenation, decarboxylation, dehydration and deamination. A strong increase of protein damage was observed in water as compared to vacuum.

BP 31.6 Thu 16:45 H 0112

What is the structure of a biomolecular condensate? — •Charlotta Lorenz[1,2], Takumi Matsuzawa[1], Etienne Jambon-Puillet[3], Teagan Bate[1], Kaarthik Varma[1], Harsha Koganti[1], Gianna Wolfisberg[1], Aleksander R. Rebane[4], and Eric R. Dufresne[1] — [1]Cornell University, Ithaca, NY, US — [2]ETH Zürich, CH — [3]LadHyX, CNRS, Ecole Polytechnique, Paris, FR — [4]New York University Abu Dhabi, AE

Biomolecular condensates are important for a variety of cellular functions, such as biochemical regulation, structural organization, and RNA metabolism. While the properties and physiology of these condensates depend on their structure, this important aspect has received little experimental consideration. On the other hand, recent simulations of disordered proteins with interactions based on the sticker-and-spacer suggest fascinating structures in the bulk and surface of condensates. We aim to reveal the structure of biomolecular condensates using X-ray scattering. Here, we will present results for a simple model system consisting of a stable protein that forms a condensate due to crowding by addition of small molecules. With these results, we aim to establish methods to probe the structure of a wide variety of biomolecular condensates made of intrinsically disordered proteins.

BP 31.7 Thu 17:00 H 0112

Enzymatic phosphorylation of intrinsically disordered proteins in coarse-grained simulations — •Emanuele Zippo[1], Lukas Stelzl[1,2], Thomas Speck[3], and Friederike Schmid[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [2]Institute of Molecular Biology (IMB), Mainz, Germany — [3]Institüt für Theoretische Physik IV, Universität Stuttgart, Stuttgart, Germany

Understanding the condensation and aggregation of intrinsically disordered proteins (IDPs) in a non-equilibrium environment is crucial for unraveling many biological mechanism. We can now address this with residue-level coarse-grained Molecular Dynamics simulations, integrating Metropolis Monte Carlo steps to model chemical reactions. We investigate TDP-43 phosphorylation by CK1d enzyme in simulations, examining patterns of phosphorylation and assessing its preventive role in chain aggregation, possibly associated with neurodegenerative diseases. We find that the degree of residue phosphorylation is determined by sequence preference and charges, rather than the position in the chain. Depending on the sequence context, phosphorylation stabilizes or de-stabilizes condensates. For TDP-43, our simulations show condensates dissolution through phosphorylation, in accordance with experiments. The disordered tail of the kinase Ck1d drives recruitment to the condensates. To further explore the dynamics of non-equilibrium steady-state systems, like our target system, we apply Markov state modelling (MSM). We used MSM to verify the thermodynamic consistency of the phosphorylation step.

BP 31.8 Thu 17:15 H 0112

Memory-dependent friction in protein folding — •Benjamin Dalton and Roland Netz — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin, Germany

When described by a low-dimensional reaction coordinate, the folding rates of many proteins are determined by an interplay between free-energy barriers, which separate folded and unfolded states, and friction. While it is commonplace to extract free-energy profiles from molecular trajectories, a direct evaluation of friction is far more elusive and typically relies on fits of measured reaction rates to memoryless reaction-rate theories. Here, using memory-kernel extraction methods founded on a generalized Langevin equation (GLE) formalism, we directly calculate the time-dependent friction acting on a variety of well-known reaction coordinates for eight fast-folding proteins, taken from a published set of large-scale molecular dynamics protein simulations. We show that memory decay times are typically of the same order as folding times and are much longer than transition-path times. Furthermore, we show that folding times are significantly faster than predictions made by standard Markovian models. This memory-induced reaction speed-up effect is a hallmark of non-Markovian systems, confirming that non-Markovian models are, in general, suitable for describing protein folding dynamics.

BP 31.9 Thu 17:30 H 0112

Log-periodic oscillations as real-time signatures of hierarchical dynamics in proteins — •Emanuel Dorbath, Adnan Gulzar, and Gerhard Stock — Institute of Physics, University of Freiburg, 79104 Freiburg, Germany

The time-dependent relaxation of a dynamical system may follow a power law that is superimposed by log-periodic oscillations. This behavior can by explained by a discrete scale invariance of the system, which is associated with discrete and equidistant timescales on a logarithmic scale. Recent time-resolved experiments and molecular dynamics simulations suggest that this also holds for hierarchical dynamics in proteins, where several fast local conformational changes are a prerequisite for a slow global transition to occur.

An entropy-based timescale analysis and Markov state modeling is applied to a simple one-dimensional hierarchical model and biomolecular simulation data of the achiral peptide helix Aib9, showing that hierarchical systems in fact give rise to logarithmically spaced discrete time scales [arXiv:2311.11839 (2023)]. Introducing a one-dimensional reaction coordinate, the free energy landscape exhibits a characteristic staircase shape with two metastable states, which causes the observed log-periodic time evolution of the system. The period of these oscillations reflects the effective roughness of the energy landscape and can in simple cases be interpreted as the energy barriers of the staircase.

BP 31.10 Thu 17:45 H 0112

IP_3 affinity of Tubby reveals cooperativity mechanism for membrane binding — •Sebastian Thallmair — Frankfurt Institute for Advanced Studies (FIAS), Germany

We recently showed by means of coarse-grained (CG) molecular dynamics (MD) simulations and life cell experiments that two cooperative binding sites of the C-terminal domain of the Tubby protein determine its $PI(4,5)P_2$ affinity. Notably, the $PI(4,5)P_2$ concentration sensitivity of the Tubby protein is more pronounced than the one of the well-known $PI(4,5)P_2$ binding Pleckstrin homology (PH) domain of phospholipase C (PLC)-δ1.

Here, I will show that surprisingly the IP_3 affinity of Tubby is comparably to the one of the PLCδ1-PH domain using CG MD simulations with the Martini 3 force field. This is in contrast to the pronounced affinity difference between both proteins to a single $PI(4,5)P_2$ lipid embedded in a POPC membrane. In addition, I will compare both affinities to a single $PI(4,5)P_2$ lipid in water. Taken together, my results indicate that the recently discovered second $PI(4,5)P_2$ binding site of Tubby not only preferably interacts with $PI(4,5)P_2$, but also disfavors the interaction with zwitterionic lipids such as POPC. I will discuss how this increases the $PI(4,5)P_2$ concentration sensitivity of Tubby compared to the PLCδ1-PH domain.

BP 32: Tissue Mechanics II

Time: Thursday 15:00–17:45 Location: H 2032

BP 32.1 Thu 15:00 H 2032

Letting cells off the Hook: A non-mechanistic vertex model predicts inverse stress-strain relation in epithelial tissues by statistical inference. — •Zoë Lange and Franziska Matthäus — Frankfurt Institute for Advanced Studies, Goethe-Universität, Frankfurt am Main, Germany

Disordered epithelial cell packings are considered to be a result of cell mechanics, cell-cell interaction and proliferation (Farhadifar et al. 2007). A recent vertex model proposes remodeling of cell-cell junction length and tension as a proliferation-free alternative explanation (Pérez-Verdugo & Banerjee 2023). Despite the mechanical basis of vertex models it remains poorly understood how stress and strain in epithelial tissues relate to each other on the cell scale. We use a non-mechanistic vertex model to estimate effective forces in different epithelial tissues by statistical inference (Ishihara & Sugimura 2012). We obtain an inverse relation between tension and cell shape in both proliferating and non-proliferating epithelial tissues. We show that the modulus of the relation is exclusively negative even when tissue is not stretched. We find that the cell perimeter alone is not correlated with tension. Our work highlights how the power of statistical inference will contribute to unravelling different contributions of subcellular processes on macroscopic properties of tissues by extracting empirical laws from experimental data.

BP 32.2 Thu 15:15 H 2032

Agent-based model for active nematics of cellular tissues — •Mathieu Dedenon[1,2], Carles Blanch-Mercader[3], Karsten Kruse[1,2], and Jens Elgeti[4] — [1]Department of Biochemistry, University of Geneva, 1211 Geneva, Switzerland — [2]Department of Theoretical Physics, University of Geneva, 1211 Geneva, Switzerland — [3]Laboratoire Physico-Chimie Curie, Institut Curie, Université PSL, Sorbonne Université, CNRS UMR168, Paris, France — [4]Theoretical Soft Matter and Biophysics, Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany

Biological cellular tissues often exhibit domains of orientational order, separated by topological defects where orientation is ill-defined. Those regions concentrate active stresses generated by cell force dipoles and give rise to spontaneous flows. This interplay of nematic order and activity has been explored based on two-dimensional continuum theory, but more complex geometries remain unexplored theoretically.

Based on a two-particle agent-based model, we describe cells as multi-particle filaments with controllable aspect ratio. We incorporate mechanical activity in terms of individual cell force dipoles. This framework is designed to capture hydrodynamic modes at large scales.

In agreement with the continuum theory of active nematics, we recapitulate the active flow transition beyond a critical activity threshold for two-dimensional simulations. In addition, we confirm the influence of activity on the onset of nematic order and identify a fluidization effect. In the future, we plan to explore active nematic features in more complex geometries.

BP 32.3 Thu 15:30 H 2032

Cell divisions imprint long-lasting shear strain on epithelial tissue — •Ali Tahaei[1], Romina Pisticello-Gómez[2,3], Suganthan S[1], Greta Cwikla[3], Jana Fuhrmann[2,3], Natalie Dye[3], and Marko Popović[1,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Cluster of Excellence Physics of Life, Technische Universität Dresden

Biological tissues exhibit complex dynamics, with mechanical behaviors that vary across different timescales. They flow on long timescales and exhibit more solid-like characteristics on short timescales. In this work, we use experiments and linear elasticity theory to show that fruit fly wing epithelial behave as two-dimensional linear elastic solids. To this end, we measure the strain field in the epithelium generated by a linear laser ablation and we find that we can describe them as a linear combination of elastic stress propagators. This allows us to determine the relative magnitudes of force dipoles generated by the laser ablation. Motivated by this discovery we next analyzed the strain patterns in the tissue generated by cell divisions. As before, by accounting for the observed strain using linear elasticity propagators, we find that cell divisions generate an isotropic force dipole transiently during the division process, which subsequently vanishes soon after the cell division. However, cell divisions exert a pure shear force dipole that imprints a long-lasting elastic strain pattern in the tissue. In summary, we have developed a method that allowed us to describe in detail the dynamics of forces generated during cell divisions.

BP 32.4 Thu 15:45 H 2032

Topological Transformations in Graph Vertex Model — •Urban Železnik, Tanmoy Sarkar, and Matej Krajnc — Jožef Stefan Institute, Jamova cesta 39, SI-1000 Ljubljana, Slovenia

Vertex Model (VM) shows its reliability in modeling confluent biological tissues in two dimensions (2D). However, its application in three dimensions (3D) has been constrained by computational complexities, primarily stemming from managing topological changes during cell rearrangements. In the talk, I will demonstrate how the recently introduced Graph Vertex Model (GVM) successfully addresses the challenges posed by VM. GVM achieves this by exclusively storing topological data of cell networks within a Knowledge Graph (KG). The unique data structure of KG enables cell rearrangements and divisions to be equivalent to elementary graph transformations, which are also represented by graphs. Furthermore, cell rearrangements in 3D consist of graph transformations that correspond to more fundamental T1 transitions, thereby unifying topological transitions in both 2D and 3D space-filling packings. This implies that the GVM's graph data structure may be the most natural representation for cell aggregates and tissues.

BP 32.5 Thu 16:00 H 2032

Vertex Model Challenges Meet Knowledge Graph Solutions — •Tanmoy Sarkar and Matej Krajnc — Jožef Stefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

Vertex model (VM) shows its credibility in modeling confluent biological tissues in two dimensions. However, due to computational complexities, only a few studies have been reported since the introduction of the first three-dimensional (3D) vertex model almost two decades ago. Most of the challenges lie in handling the changes in topology during dynamic cell rearrangements, which justifies the absence of a proper algorithmic form of topological transformations so far. This issue is often viewed in the community as a complex engineering problem. In the talk, I will demonstrate a possible solution to this outstanding problem using a new approach called the Graph Vertex Model (GVM). GVM is founded on the concept of representing the topology of the cell network using a Knowledge Graph (KG), effectively rendering topological transformations both intuitive and mathematically well-defined. Furthermore, I will highlight the enhanced credibility and utility of the KG by introducing the GRAPh Embryo project (GRAPE). GRAPE is an online database designed to facilitate interactive analyses of an entire fly embryo, showcasing the practical applications and benefits of this approach.

15 min. break

BP 32.6 Thu 16:30 H 2032

Growth arrest and scaling during axolotl limb regeneration — •Natalia Lyubaykina[1,2], Pietro Tardivo[3], Dunja Knapp[4], Tatiana Sandoval-Guzmán[4], Elly Tanaka[3], and Benjamin M Friedrich[1,2] — [1]Cluster of Excellence 'Physics of Life', Technical University Dresden, Dresden, Germany — [2]Center for Advancing Electronics, Technical University Dresden, Dresden, Germany — [3]Research Institute of Molecular Pathology, Vienna Biocenter (VBC), Vienna, Austria — [4]CRTD/Center for Regenerative Therapies, Technical University Dresden, Dresden, Germany

Axolotl can regenerate lost limbs even as adults, posing the question of how a regenerating limb matches animal size, which can differ up to five-fold between juvenile and adult axolotl. Two key morphogens, SHH and FGF8, are known to regulate proliferation and growth. Yet it remains unclear how these morphogens control growth arrest once a correct target size of the wound tissue (blastema) is reached. Inspired by this biological example, we theoretically investigate growth arrest during blastema growth and address the question of proportional growth matching animal size. Using a minimal reaction-diffusion model, we describe SHH and FGF8 dynamics during regeneration and formulate French flag-like growth rules to discern conditions for robust growth arrest during tissue growth. We also explore how a putative scaling of SHH or FGF8 morphogen gradients with either blastema or animal size impacts growth arrest and proportional growth. Finally, we compare theory predictions to recent quantifications of SHH and FGF8 morphogen gradients.

BP 32.7 Thu 16:45 H 2032

A mechano-chemical model of Hydra regeneration — •Suganthan Senthilkumar[1], Yonit Maroudas-Sacks[2], Kinneret Keren[2], and Marko Popović[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden — [2]Technion University, Haifa, 3200003, Israel

Hydra is a freshwater animal with extraordinary regeneration properties making it an excellent model organism to study morphogenesis. It has a simple body plan, with a double layered epithelium enclosing a fluid-filled lumen. Hydra epithelia contain long actin muscle fibres that are highly organized with an aster point defect positioned at the head. Starting from an excised tissue fragment Hydra can fully regenerate, however, it is unclear how the fibre pattern self organizes. The regeneration of the fibre pattern is inhibited by perturbing either tissue strain or production of Wnt, which is a morphogen relevant for head regeneration. We propose a mechano-chemical feedback between tissue mechanics, nematic fibre pattern and morphogen dynamics, as a mechanism of Hydra regeneration. For this we have developed a vertex model of curved epithelia that incorporates the feedback mechanism. In the model, each cell contains a nematic, representing the orientation of actin fibres, that generate stress upon activation, and a morphogen concentration. We implement the mechano-chemical feedback such that the morphogen production depends on cellular strain, with morphogen gradients guiding nematic orientation, which in turn focusses the tissue strain. We find that this mechanism can robustly reproduce experimentally observed dynamics of Hydra tissue and nematic fibres.

BP 32.8 Thu 17:00 H 2032

Continuum mechanics of apical constriction — •Chandraniva Guha Ray[1,2,3], Marija Krstic[2,3], and Pierre Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Apical constriction, the contraction of apical cell sides, is a common mechanism driving deformations of biological tissues during development. It is associated with the geometric singularity in which cell cross-sections become triangular and hence the cell sides are maximally bent, splaying the cells and thus bending the cell sheet.

Here, we explore the mechanical consequences of this geometric singularity in what is perhaps the simplest problem of tissue buckling: Under external compression, a monolayer of cells buckles, and, as the compression is increased further, fans of triangular cells expand from the crests and troughs of the buckled shape. Taking a continuum limit of a "differential-tension model" describing the cell mechanics [1], we show how these expanding fans lead to a strong increase of the resistance of the tissue to further compression. We reveal an intriguing secondary bifurcation beyond the onset of triangular cells: The buckling amplitude of a thin monolayer increases with increasing compression until the cells touch sterically, but, surprisingly, the buckling amplitude of a thick monolayer decreases with increasing compression. We develop a scaling argument to describe this bifurcation, and discuss its consequences for tissue development.

[1] P. A. Haas and R. E. Goldstein, Phys. Rev. E 99, 022411 (2019)

BP 32.9 Thu 17:15 H 2032

Mechanotransduction in Lateral Root Initiation: A Model Integrating Growth Mechanics and Auxin Signaling — •João R. D. Ramos[1], Karen Alim[1], and Alexis Maizel[2] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]Centre for Organismal Studies, University of Heidelberg, Germany

Plant development relies on the precise coordination of cell growth, which is influenced by the mechanical constraints imposed by rigid cell walls. The hormone auxin plays a crucial role in regulating this growth by altering the mechanical properties of cell walls. During the post-embryonic formation of lateral roots, pericycle cells deep within the main root are triggered by auxin to resume growth and divide to form a new root. This growth involves a complex interplay between auxin, growth, and the resolution of mechanical conflicts, that is still not well understood. We propose a model that integrates tissue mechanics and auxin transport, revealing a connection between the auxin-induced relaxation of mechanical stress in the pericycle and auxin signalling in the endodermis. We show that the growth of pericycle cells is initially limited by the endodermis. However, the resulting modest growth is sufficient to redirect auxin to the overlying endodermis, which then actively accommodates the growth, allowing for the subsequent development of the lateral root. Our model uncovers the mechanical parameters that underlie endodermal accommodation and how the structure and shape of the endodermis influence the formation of the new root. These findings emphasize the vital role of the endodermis in shaping root development through mechanotransduction and auxin signalling.

BP 32.10 Thu 17:30 H 2032

Cytoplasmic streaming induces nuclear trafficking and signalling in Physarum polycephalum — •Johnny Tong[1], Kaspar Wachinger[1], Siyu Chen[1], Nico Schramma[2], and Karen Alim[1] — [1]School of Natural Sciences, Technical University of Munich, Germany — [2]University of Amsterdam, The Netherlands

Syncytial organisms and organs house hundreds of thousands of nuclei within a single cell, are often shaped into a complex network architecture. How are nuclei able to efficiently exchange signals over long distances? To understand how syncytia coordinate gene expression, intracellular transport within these networks is key. Here, we investigate how communication is achieved by flow-driven behaviours of nuclei functionally different regions of the network in Physarum polycephalum. Using microinjection of fluorescent dsDNA markers, followed by image-based methods such as tracking and velocimetry, we analyze the dynamics of nuclei and cytoplasm flow.

This dynamics of nuclei allows us to formulate a potential framework of how Physarum utilizes the two-phase flow profile and distribution of nuclei, which it enables a relay-like model for long-range signal propagation, where flowing nuclei act as carriers and trapped nuclei act as waypoints. Our findings could lead to a better understanding of the mechanisms of long-range genetic communication within network-shaped systems like fungi and placenta.

BP 33: Focus session: Physics of organoids

Time: Thursday 15:00–17:30 Location: H 1028

Invited Talk BP 33.1 Thu 15:00 H 1028

Symmetry breaking in early embryonic organoids: bridging networks, mechanics and metabolism — •Vikas Trivedi — EMBL Barcelona, Spain — EMBL Heidelberg, Germany

How can tissue shapes and patterns emerge reproducibly and robustly in multicellular systems like animals? Despite more than 100 years of embryology, it still remains unclear how gene networks, forces and mechanical properties and the metabolic state of the cells integrate together to self-organize complex structures. This is due to our inability to disentangle the combined action of these factors (biophysical properties, gene networks and metabolic activity) within populations of genetically equivalent cells. We address this challenge within the context of the establishment of body axes in animals using aggregates of embryonic stem cells (ESCs) that recapitulate hallmarks of early embryonic development in vitro and probe the first symmetry breaking event that establishes anteroposterior polarity. By means of quantitative live imaging, mechanical measurements, molecular perturbations and mathematical modelling, we show how mechanochemical coupling between cells controls tissue rheology and metabolic activity controls the proportions of different cells types by acting upstream of signalling. Altogether, our results allow us to investigate how differentiation trajectories in vivo and in vitro can converge onto similar cell fates through coordinated changes in signaling, metabolic states and biophysical properties.

BP 33.2 Thu 15:30 H 1028

Mechanisms of pattern formation and self-organization in embryonic organoids — •Valentin Dunsing-Eichenauer, Alice Gros, Sham Tlili, Jules Vanaret, Leo Guignard, and Pierre-François Lenne — IBDM & CENTURI, Aix-Marseille University/ CNRS, Marseille, France

The emergence of asymmetries within a mass of equivalent cells is a key event in embryonic development, resulting in formation of the main body axes. We investigate symmetry breaking in gastruloids, an in vitro model of early mammalian embryogenesis. Upon Wnt activation, polarized gene expression patterns emerge from an initially homogenous state, followed by elongation and formation of germ-layer-like tissues. Interestingly, robust symmetry breaking occurs only in aggregates of a certain size, smaller or larger aggregates do not polarize. To understand this phenomenon, we investigate the underlying patterning mechanism. To this aim, we have developed a quantitative imaging pipeline using in toto 2-photon imaging and deep learning based cell segmentation. For aggregates of different size, we quantify i) overall shape, ii) coarse grained spatiotemporal distribution of differentiation, iii) relative proportions of emerging heterogenous cell populations. Our results indicate that cell differentiation emerges first in outer and subsequently propagates to inner cell layers. Concomitantly, the initially continuous adhesion protein network fragments and cells sort into different domains. We next plan to incorporate these findings into a cell-based model to test whether such propagation mechanism and fluctuations in aggregate shape are sufficient to break symmetry.

BP 33.3 Thu 15:45 H 1028

Dynamical systems theory of self-organized collective cell fate patterning — •David Brückner — Institute of Science and Technology, Am Campus 1, 3400 Klosterneuburg, Austria

A key feature of many developmental systems is their ability to self-organize spatial patterns of functionally distinct cell fates. A spectacular example of this ability are artificial stem cell assemblies, which are paving the way towards a quantifiable self-organization of biological systems. However, while the relevant molecular processes are increasingly well understood, we lack conceptual theoretical frameworks for the dynamics and statistics of self-organized patterning. Specifically, it is unclear how to generically quantify the patterning performance of biological self-organizing systems, and how to identify the dynamical systems motifs that optimize this performance. Here, we develop an information-theoretic framework and use it to analyze a wide range of models of self-organization. Our approach can be used to define and measure the information content of observed patterns, to functionally assess the importance of various patterning mechanisms, and to predict optimal operating regimes and parameters for self-organizing systems. I demonstrate the application of our framework using experimental gene expression data of gastruloid and intestinal organoid symmetry breaking. This framework represents a unifying mathematical language to describe biological self-organization across diverse systems.

BP 33.4 Thu 16:00 H 1028

Morphological instability at topological defects in spherical epithelial shells — •Oliver M. Drozdowski and Ulrich S. Schwarz — Institute for Theoretical Physics and BioQuant, Heidelberg University, 69120 Heidelberg, Germany

Spherical epithelial shells like cysts or intestinal organoids are model systems for developmental biology and have large potential for biomedical applications. They also lead to highly interesting physics questions: due to Euler's polyhedron theorem, they must contain at least 12 topological defects in the network of neighbor relations, similar to viral capsids. Topological defects have mainly been studied in a hydrodynamic context. Here we study them in the elastic context of spherical epithelial shells. We start from a three-dimensional vertex model and perform a rigorous coarse-graining procedure to a continuum model. We predict stretching and bending moduli in excellent agreement with computer simulations of the vertex model. For large spherical shells we find a generic morphological instability to an icosahedral shape at topological defects, at a length scale similar to budding events in organoids. This instability can be explained by our continuum theory and might be used by organoids to change shape during development.

15 min. break

BP 33.5 Thu 16:30 H 1028

Quantification of mechanical relaxation in retinal organoid tissues across scales — •Elijah Robinson Shelton[1], Michael Frischmann[1], Achim Theo Brinkop[1], Rebecca James[1], and Friedhelm Serwane[1,2] — [1]Faculty of Physics and Center for NanoScience, LMU Munich, Germany — [2]SyNergy, LMU Munich, Germany

Quantifying mechanical properties is critical for understanding how forces shape tissues during retinal development. Organoids recapitulate retina composition and morphology, providing physicists with a platform to study the mechanics underlying this self-organization. While retina mechanical properties have been investigated with various technologies, such probing has been restricted to timescales of seconds or less. Using retina organoids as in vitro models and ferrofluid droplets as force actuators, we probe retina rheology over a range of timescales. After we inject ferrofluid droplets (30 microns), we live-image organoids on a confocal microscope. We introduce homogenous magnetic fields to actuate the droplets and the tissue. Using linear viscoelastic models, we find a mean elastic modulus of 0.63 kPa when probed at a second timescale. We find viscosities of 4.5 to 15.1 kPa s for strain responses over 5 to 20 minutes, indicating stress relaxation over a range of timescales. To describe this rheology across scales, we employ fractional viscoelastic models and discuss their application to retinal organoid tissue mechanics. This modeling combined with our experimental observations provide mechanical insights for how the retina is shaped during development in vivo and in vitro.

BP 33.6 Thu 16:45 H 1028

DNA microbeads for spatio-temporally controlled morphogen release within organoids — •Tobias Walther[1,2], Cassian Afting[3], Joachim Wittbrodt[3], and Kerstin Göpfrich[1,2] — [1]Max-Planck-Institut für medizinische Forschung, Jahnstraße 29, 69120 Heidelberg — [2]Zentrum für Molekulare Biologie der Universität Heidelberg, INF 329, 69120 Heidelberg — [3]Centre for Organismal Studies Heidelberg, INF 230, 69120 Heidelberg

To this day, organoids across types and species fail to reach full maturity and function. A key reason for this is that current organoid culture methods lack spatial organization of the biochemical cues provided to guide organoids. Here, we introduce stiffness adaptable DNA microbeads as a novel tool for implementing spatio-temporally controllable sources of morphogen into organoids at any point in their life cycle. Employing medaka retinal organoids, we show that DNA microbeads can be integrated into organoids via microinjection and be non-invasively erased by light-triggered breakdown. Coupling a recom-

binant surrogate Wnt to the DNA microbeads nanostructure allowed its temporally controllable release from the microinjection site. We were thus able to bioengineer retinal organoids more closely mirroring the cell type diversity of in vivo retinas. While this work presents a first application, this technology is straightforward to adapt to other organoid applications and does not require specialized equipment for usage

BP 33.7 Thu 17:00 H 1028

Multi-cellular rosette formation guides cellular rearrangement initiating lumen opening in PDAC organoids — •Marion K. Raich[1], Tamara Müller[1], Fridtjof Brauns[3], Samuel J. Randriamanantsoa[1], Ann-Caroline Heiler[1], Maximilian Reichert[2], and Andreas R. Bausch[1] — [1]Chair for Cellular Biophysics, TUM, Garching, Germany — [2]Klinik und Poliklinik für Innere Medizin II, Klinikum rechts der Isar der TUM, Munich, Germany — [3]KITP, UCSB, Santa Barbara, California 93106, USA

Organ development and tissue growth is regulated by morphogenetic programs driven by molecular motors, such as non-muscle myosin II, acting on cytoskeletal crosslinked filaments, like F-actin as well as adherens junctions proteins, e.g E-cadherin. Pancreatic ductal adenocarcinoma (PDAC) organoids, forming branched structures, were used to investigate the contribution of these protein species during distinct morphogenetic growth phases, that result in the emergence of a lumen.

Live-cell imaging of PDAC organoids showed a transformation from an elongated cell shape to an epithelial-like structure. These alterations were marked by the presence of three-dimensional rosette formations, characterized by a wedge-like geometry of the cells, with a minimum of six cells converging at a single point. Rosettes appeared periodically within the branch, having a constant distance based on its diameter. The accumulation of non-muscle myosin II and F-actin at the center of the rosette indicated that stochastically distributed actomyosin dependent force generation was required for cellular rearrangement preceding lumen formation.

BP 33.8 Thu 17:15 H 1028

Rheology in 3D confined spaces: PANC-1 spheroids on polyHEMA-coated substrates using atomic force microscopy — •Isis do Vale Meira Lima, Shruti Kulkarni, Mènie Wiemer, and Manfred Radmacher — Institut für Biophysik, Universität Bremen, Bremen, Germany

Understanding biomechanical properties of living cells and tissues is a relevant foundation in advancing knowledge related to physiological and pathological processes, such as the effects of vascularization in tumor development and metastatic processes. In addition, considering that all types of biological tissues are viscoelastic materials, it becomes necessary to delve into the mechanical response of tissues at multiple time scales. From this point of view, in this work, we have developed a protocol to assemble PANC-1 cells in order to obtain spheroids and quantify their rheological properties using atomic force microscopy (AFM) technique. We used force curves to measure the relaxation response of cell aggregates, extracting the respective Young's modulus, storage and loss modulus from each force curve. PANC-1 cells are originated from a human pancreatic carcinoma. These cells are known to form aggregates, generating a structure which resembles a tumor. To achieve a three-dimensional structure which mimicks the tumor environment, we coated our supports with polyHEMA except at small depressions. Cells will not adhere to the support and aggregate in the depressions. Because of the three dimensional confinement of aggregates it is easy to investigate the tumor-like cell clusters by AFM.

BP 34: Statistical Physics of Biological Systems III (joint session BP/DY)

Time: Friday 9:30–13:00 Location: H 2032

BP 34.1 Fri 9:30 H 2032

The Sun within: active processes from two-temperature models — •Faezeh Khodabandehlou and Christian Maes — Department of Physics and Astronomy KU Leuven, Leuven, Belgium

We propose an embedding of standard active particle models in terms of two-temperature processes. One temperature refers to an ambient thermal bath, and the other temperature effectively describes "hot spots," i.e, systems with few degrees of freedom showing important population homogenization or even inversion of energy levels as a result of activation. As a result, the effective Carnot efficiency would get much higher than for our standard macroscopic thermal engines, making connection with the recent conundrum of hot mitochondria. Moreover, that setup allows to quantitatively specify the resulting nonequilibrium driving, useful in particular for bringing the notion of heat into play, and making easy contact with thermodynamic features. Finally, we observe that the shape transition in the steady low-temperature behavior of run-and-tumble particles (with the interesting emergence of edge states at high persistence) is stable and occurs for all temperature differences, including close-to-equilibrium.

BP 34.2 Fri 9:45 H 2032

Irreversibility across a nonreciprocal PT-symmetry-breaking phase transition — •Henry Alston[1], Luca Cocconi[2], and Thibault Bertrand[1] — [1]Imperial College London, London, UK — [2]Max Planck Institute for Dynamics and Self-Organization, Gottingen, Germany

Nonreciprocal interactions are commonplace in continuum-level descriptions of both biological and synthetic active matter, yet studies addressing their implications for time-reversibility have so far been limited to microscopic models. We derive a general expression for the average rate of informational entropy production in the most generic mixture of conserved phase fields with nonreciprocal couplings and additive conservative noise. For the particular case of a binary system with Cahn-Hilliard dynamics augmented by nonreciprocal cross-diffusion terms, we observe a non-trivial scaling of the entropy production rate across a parity-time symmetry breaking phase transition. We derive a closed-form analytic expression in the weak-noise regime for the entropy production rate due to the emergence of a macroscopic dynamic phase, showing it can be written in terms of the global polar order parameter, a measure of parity-time symmetry breaking.

Invited Talk BP 34.3 Fri 10:00 H 2032

Bacterial transport in dilute and porous environments — •Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Unraveling the motion of microorganisms in dilute and porous media is important for our understanding of both the molecular basis of their swim gait and their survival strategies in microbial habitats. First, I will show that by using renewal processes to analyze experimental measurements of wild-type E. Coli, we can provide a quantitative spatiotemporal characterization of their run-and-tumble dynamics in bulk [1]. We further demonstrate quantitatively how the persistence length of an engineered strain can be controlled by a chemical inducer and characterize a transition from perpetual tumbling to smooth swimming. Second, I will address how this run-and-tumble gait evolves towards a hop-and-trap motility pattern of agents moving in a porous environment [2]. Using computer simulations, we discover a geometric criterion for their optimal spreading, which emerges when their persistence lengths are comparable to the longest straight path available in the porous medium. Our criterion provides a fundamental principle for optimal transport in densely-packed biological and environmental settings, which could be tested experimentally by using engineered cells and may provide insights into microbial adaption mechanisms.

[1] arXiv:2212.11222 (2022) [2] Nat. Commun. 12, 7088 (2021)

BP 34.4 Fri 10:30 H 2032

Signature of (anti)cooperativity in the stochastic fluctuations of small systems: application to the bacterial flagellar motor — •María-José Franco-Oñate[1], Andrea Parmeggiani[2], Jérôme Dorignac[2], Frédéric Geniet[2], Jean-Charles Walter[2], Francesco Pedaci[3], Ashley Nord[3], John Palmeri[2], and Nils-Ole Walliser[2] — [1]MPI Physics of Complex Systems, Dresden, Germany — [2]Laboratoire Charles Coulomb (L2C), Montpellier, France — [3]Centre de Biologie Structurale (CBS), Montpellier, France

The cooperative binding of molecular agents onto a substrate is pervasive in living systems. To study whether a system shows cooperativity, one can rely on the fluctuation analysis of quantities such as the number of substrate-bound units.

Using a general-purpose grand canonical Hamiltonian description of

a small one-dimensional (1D) lattice gas with nearest-neighbour interactions as a prototypical example of a cooperativity-influenced adsorption processes, we elucidate how the strength of the interaction potential between neighbouring bound particles on the lattice determines the intensity of the fluctuations of the mean occupancy at steady state.

We then employ this relationship to compare the theoretical predictions of our model to data from single molecule experiments on bacterial flagellar motors (BFM). In this way, we find evidence that cooperativity controls the mechano-sensitive dynamical assembly of the torque-generating units, the so-called stators, onto the BFM.

BP 34.5 Fri 10:45 H 2032

A power-law growth model of pancreatic cancer precursor lesions — Ashley L. Kiemen[1], Denis Wirtz[1], and •David Zwicker[2] — [1]Departments of Pathology, Johns Hopkins University School of Medicine, Baltimore, MD, USA — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Pancreatic cancer often originates from microscopic precursor lesions in the pancreatic ducts. Recent evidence showed that even healthy people possess more and larger lesions than previously believed. A better understanding of the growth of these lesions may thus improve our ability to understand how a minuscule fraction transitions to invasive cancer. Using advanced imaging, we quantified >1,000 lesions and found that lesion size is distributed according to a power law with a fitted exponent of -1.7 over more than three orders of magnitude. To explain these data, we analyze several models of lesion growth and fit the predicted size distributions to the observed data. Our analysis suggests that lesions either (i) grow sub-exponentially and frequently seed new lesions or (ii) grow super-exponentially and frequently merge. Independent genomic mapping of lesions supports both alternatives, suggesting both are relevant. Our work demonstrates how combining experimental measurements of human tissues with dynamic modeling can improve understanding of cancer tumorigenesis.

15 min. break

BP 34.6 Fri 11:15 H 2032

Exclusion model of mRNA translation with collision-induced ribosome drop-off — Johannes Keisers[1] and •Joachim Krug[2] — [1]Centre de Biologie Structurale (CBS), Université de Montpellier, 34090 Montpellier, France — [2]Institute for Biological Physics, University of Cologne, 50937 Köln, Germany

The translation of messenger RNA transcripts to proteins can be modeled as a one-dimensional totally asymmetric exclusion process with extended particles. In this contribution we focus on the effects of premature termination of translation through the irreversible detachment of ribosomes. We consider a model where the detachment is induced by the unsuccessful attempt to move to an occupied site [1]. The model is exactly solvable in a simplified geometry consisting of the translation initiation region followed by a single slow site representing a translation bottleneck. In agreement with a recent experimental study, we find a non-monotonic dependence of the protein production rate on the initiation rate, but only if the leading particle in a colliding pair detaches. The homogeneous version of the model is related to an asymmetric reaction-diffusion model with a localized input of particles. We exploit this connection to show that, for long transcripts, the ribosome density decays asymptotically as the inverse square root of the distance to the initiation site.

[1] J. Keisers, J. Krug, J. Phys. A 56 (2023) 385601

BP 34.7 Fri 11:30 H 2032

Boundary geometry drives three-dimensional defect transitions in a polar fluid — •Pamela Guruciaga[1], Takafumi Ichikawa[2], Takashi Hiiragi[2,3], and Anna Erzberger[1,4] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Kyoto University, Kyoto, Japan — [3]Hubrecht Institute, Utrecht, The Netherlands — [4]Heidelberg University, Heidelberg, Germany

Motivated by observations of an interplay between apico-basal polarity and boundary geometry in mouse embryo morphogenesis, we develop a minimal model to address the role of boundaries—with emphasis on their geometry—in the surface-induced ordering of a 3D polar fluid. We find that, although material parameters are responsible for the creation of defects in the order parameter field, their location and structure are determined by the system geometry. We test our results in the experimental context of the mouse epiblast, where cells gradually align along their apico-basal axis and eventually form a fluid filled cavity (lumen) at their apical sides. Since field defects represent regions where the apical sides of the cells meet, changes in defect position can be relevant to lumen formation in the biological system. We compare our predictions with imaging data of the morphogenetic process for wild-type and genetically perturbed mice, finding a remarkable quantitative agreement without any fitting parameters. Our work provides insights into luminogenesis and embryonic viability, while paving the way for defect control by geometry manipulation in more general settings.

BP 34.8 Fri 11:45 H 2032

Optimal Memoryless Chemotaxis — •Jacob Knight[1], Paula García-Galindo[2], Johannes Pausch[1], and Gunnar Pruessner[1] — [1]Department of Mathematics, Imperial College London, South Kensington, London SW7 2BZ, UK — [2]Department of Chemical Engineering and Biotechnology, University of Cambridge, Philippa Fawcett Drive, Cambridge CB3 0AS, UK

A wide array of biological systems can navigate in shallow gradients of chemoattractant with remarkable precision. Whilst previous models approach such systems using coarse-grained chemical density profiles, we construct a model consisting of a chemotactic cell responding to *discrete* cue particles, giving rise to novel phenomenology. For a cell without internal memory, we derive an effective velocity with which the cell approaches the source. This effective velocity is independent of the chemoattractant diffusivity, which can be tuned such that the cell can navigate in arbitrarily shallow chemical gradients. The effective velocity becomes negative beyond some homing radius, which represents an upper bound on the distance within which chemotaxis can be reliably performed.

BP 34.9 Fri 12:00 H 2032

Two-stage adaptive evolution in a rugged yet highly-accessible fitness landscape model with delayed commitment — •Muhittin Mungan[1], Suman G. Das[2], and Joachim Krug[1] — [1]Institute for Biological Physics, University of Cologne, Köln, Germany — [2]Institute of Ecology and Evolution, University of Bern, Bern, Switzerland

We study an empirically-motivated theoretical fitness landscape model of antibiotic-resistance evolution in bacteria [1]. The fitness of a genotype at any concentration depends on two parameters, the resistance level and the drugless growth rate, with a tradeoff between these. For intermediate concentrations fitness landscapes are rough while the fitness peaks are nevertheless highly accessible. Adaptation on such landscapes occurs in two stages. At first there is rapid accumulation of mutations and fast growth of fitness and resistance level along with a decrease in the drugless growth rate. Next there is slow growth of fitness and resistance level, and recovery of the drugless growth rate through the reversion of some of the mutations. We numerically demonstrate a robust pattern of evolution with qualitative features that are largely independent of specific model assumptions. The basins of individual fitness peaks overlap strongly, so that commitment to a peak is delayed substantially. An analytically tractable special case reproduces our findings rather well, shedding light on the nature of adaptive evolution, basins of fitness peaks and delayed commitment.

[1] S.G. Das et al. eLife 9:e55155 (2020)

BP 34.10 Fri 12:15 H 2032

Optimal memory with niche construction — •Edward Lee[1], Jessica Flack[2], and David Krakauer[2] — [1]Complexity Science Hub Vienna, Vienna, Austria — [2]Santa Fe Institute, Santa Fe, USA

Adaptation to changing environments is a universal feature of life and can involve the organism evolving or learning in response as well as actively modifying the environment to control selection pressures. The latter case couples the organism and environment together. Then, how quickly should the organism adapt in response to the changing environment? We formulate this question using a simple model of adaptive costs that considers timescales of memory and environment. We derive a general, sublinear scaling law for optimal memory as a function of environmental persistence, which encapsulates the trade-off between remembering vs. forgetting. The scaling holds for finite memory but a wide range of mediating factors. We then explore strategic game dynamics, uncovering a ratcheting mechanism that promotes reducing environmental volatility when niche constructors can monopolize benefits; conversely, niche destructors can dominate by degrading a shared environment. Finally, we compare the results with metabolic costs to predict that adaptive costs matter more for smaller organisms. Taken together, we predict stabilizing niche construction will evolve when

environments are volatile and niches are separable, possibly enriching the behavioral repertoire of social organisms.

BP 34.11 Fri 12:30 H 2032

Interfaces as a probe for interactions in biological systems — •Nirvana Caballero — University of Geneva

Controlling cells, either individually or as a proliferating cell front, remains elusive because the plethora of interactions at widely varying lengthscales present in these systems leads to highly complex dynamical and geometrical properties. Interfaces separating regions of heterogeneous composition, or domains, can encode critical information about these systems' underlying physics. I will show how physical theories describing interfaces can be used to capture the microscopic interactions dominating a system. I will give examples at different scales from cell membranes [1], where the heterogeneous domain composition is key to biological function, to migrating colonies of cells, where interfaces reveal the main interactions present in a colony [2].

[1] NC, K. Kruse, T. Giamarchi. Phase separation on surfaces in the presence of matter exchange. Phys. Rev. E 108, L012801 (2023)

[2] Roughness and dynamics of proliferating cell fronts as a probe of cell-cell interactions. G. Rapin*, NC*, I. Gaponenko, B. Ziegler, A. Rawleight, E. Moriggi, T. Giamarchi, S. A. Brown, and P. Pruch, Sci. Rep. 11, 8869 (2021)

BP 34.12 Fri 12:45 H 2032

Heterogenity in Mucus by statistical analysis from particle tracking — •Thomas John, Sten Leipnitz, Enkeleda Meziu, and Christian Wagner — Campus, University Saarland, Saarbrücken, Germany

In the respiratory tract, cells constantly produce mucus that transports tiny dust particles out of the lungs. It's a protein solution that consists of more than 95% water. It's believed that the proteins form a heterogeneous network, but this cannot be resolved with light microscopy. We are investigating the diffusion behavior of nanoparticles (multi-particle tracking) in mucus and comparing it to glycerol-water mixtures with comparable viscosity. We show that the probability density function of individual particle diffusion coefficients D_i in mucus is significantly broader than expected from a homogeneous solution. The spatial autocorrelation of D_i also declines more slowly in mucus compared to glycerol-water mixtures. Experiments are compared with numerical simulations of Brownian motion. With these statistical analysis methods, we can support the model of a heterogeneous structure of mucus.

BP 35: Active Matter V (joint session BP/DY)

Time: Friday 9:30–13:00 Location: H 1028

BP 35.1 Fri 9:30 H 1028

Noise reduction with droplets of many components — •Tyler Harmon — Leibniz Institute for Polymer Research, Dresden, Germany

Noise control is critical for cell homeostasis and decision making. We previously showed that phase separation could be used to robustly reduce noise in phase separating systems. Others have suggested that noise buffering has the strongest suppression of noise parallel to the coexistence tie lines. They proposed that correlations from features such as coupled transcription could align the noise with the tie lines, significantly reducing the noise. Here we show how the kinetics associated with phase diagrams naturally aligns the noise to the tie lines. This helps optimize the noise reduction in systems with many components.

BP 35.2 Fri 9:45 H 1028

Pulsatile Control of Actomyosin Contraction — •James Clarke and José Alvarado — Department of Physics, The University of Texas at Austin, Austin, Texas, USA

Cells are always under control and tightly control their mechanics. The actomyosin cytoskeleton is one important cellular structure which receives control signals and turns that into contraction. Existing research has investigated the mechanical properties of actomyosin materials. However, these are usually in terms of responses to external stresses, which may be absent in living systems. Here we instead measure response to biochemical control signals. We apply a control-theoretical framework and investigate quasistatic actomyosin contractility in response to external pulsatile signals of UV light that release ATP molecules from light-sensitive NPE-cages. Across all experimental conditions, we report statistically indistinguishable maximum strains achieved by the gel. We find that the coupling from energy input to contractile strain is weakly nonlinear, with a s^{-2} dependence in Laplace space. Our novel characterization is not only an essential first step in a better understanding of how cells control cytoskeletal contractions via internal control signals. It is also an essential first step towards using biomimetic actomyosin active gels for microrobotic applications.

BP 35.3 Fri 10:00 H 1028

Self-assembly of myofibrils in muscle cells — Francine Kolley[1], Ian D. Estabrook[1], Clara Sidor[2], Clement Rodier[2], Frank Schnorrer[2], and •Benjamin M. Friedrich[1] — [1]Physics of Life, TU Dresden, Germany — [2]IBDM, Marseilles, France

Voluntary motions and heartbeat in animals is driven by contractions of myofibrils, millimeter-long acto-myosin bundles with characteristic periodic patterns of micrometer-sized sarcomeres. Yet, the physical mechanisms that drive the self-assembly of these "cytoskeletal crystals" are not understood. Here, we report data demonstrating that myosin molecular motors and actin-crosslinking Z-disc proteins form sarcomeric patterns first, while actin becomes polarity-sorted only hours later [1]. This data informs mathematical models of sarcomere self-assembly that are able to replicate periodic sarcomeric patterns, either through (i) non-local interactions between spatially-extended myosin filaments and Z-disc proteins, which bind to an actin scaffold, or (ii) catch-bond behavior of the prominent Z-protein α-actinin in response to active myosin forces. Both models are robust to small-number fluctuations for a wide parameter range in agent-based simulations, providing plausible mechanisms of early sarcomere self-assembly.

Next, even after the establishment of sarcomeric patterns, new sarcomeres are added to myofibrils, despite these being under mechanical tension. We report a new mechanism of controlled "self-rupture" in which a mother sarcomere divides into two daughter sarcomeres by splitting its myosin stack, and establishing a new Z-disc in between.

[1] https://www.biorxiv.org/content/10.1101/2023.08.01.551279v1

BP 35.4 Fri 10:15 H 1028

Size-coordination trade-off in Trichoplax adhaerens, an animal lacking a central nervous system — Mircea R. Davidescu[1], •Pawel Romanczuk[2,3], Thomas Gregor[4], and Iain D. Couzin[5,6,7] — [1]Dept. of Ecology and Evolutionary Biology, Princeton University, USA — [2]Dept. of Biology, Humboldt Universität zu Berlin, Germany — [3]Excellence cluster "Science of Intelligence", Berlin, Germany — [4]Lewis-Sigler Institute for Integrative Genomics, Joseph Henry Laboratories of Physics, Princeton University, USA — [5]Dept. of Collective Behaviour, Max Planck Institute for Animal Behavior, Konstanz, Germany — [6]Dept. of Biology, Chair of Biodiversity and Collective Behaviour, University of Konstanz, Germany — [7]Centre for the Advanced Study of Collective Behavior, University of Konstanz, Germany

Coordination with increasing size is a fundamental challenge affecting collective systems from biofilms to governments. The earliest multicellular organisms were decentralized, with indeterminate sizes and morphologies, as exemplified by Trichoplax adhaerens, arguably the earliest-diverged and simplest motile animal. We investigated the coordination in T. adhaerens by observing the degree of collective order in locomotion across animals of differing sizes and found that larger individuals exhibit increasingly disordered locomotion. We reproduced this effect using an active elastic cellular sheets model and show that this relationship is best recapitulated across all body sizes when the simulation parameters are tuned to criticality. We discuss possible implications of this on the evolution hierarchical structures such as nervous systems in larger organisms.

BP 35.5 Fri 10:30 H 1028

SwarmRL: Lowering the entry barrier to reinforcement learning for active matter research — •Samuel Tovey, Christoph Lohrmann, and Christian Holm — Institute for Computational

Physics, University of Stuttgart, Stuttgart, Germany

As scientists learn to better design and control devices at a microscopic scale, so too must the tools used to control these devices develop. Multi-agent reinforcement learning (MARL) is a powerful machine learning paradigm for learning control strategies in agents at all scales. Recent work has applied MARL to controlling microscopic agents, whether in learning chemo-taxis behaviour, object manipulation, or swarming.

This talk introduces SwarmRL, a powerful open-source library for applying MARL to microscopic environments. We demonstrate how SwarmRL is used in our group to control micro-scale agents in simulation and experiments and how to interpret the learned policies. The talk introduces the library broadly before looking into results from our recent work using SwarmRL, including a better understanding of the role of temperature on learned strategy and the emergence of chemotactic behaviour in unstable regimes. Finally, we discuss our vision for the future of the library and its integration into experiments and simulations.

BP 35.6 Fri 10:45 H 1028

Sensitive shape dependence in agent-based simulations of growth — •Jonas Isensee[1,2], Lukas Hupe[1,2], Ramin Golestanian[1,2,3], and Philip Bittihn[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Faculty of Physics, University of Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

We consider purely sterically interacting particles that grow and divide in two-dimensional confinement. Such models have been used to study cell dynamics in tissues and bacterial aggregates. A common feature in these is the rich emergent orientation dynamics due to anisotropic shapes, directed growth, and confinement. By introducing continuously tuneable tip variations around a common rod shape and characterizing the resulting orientation dynamics in space and time, we identify trends in the collective dynamics caused by certain shape features. In particular, we find a strong effect of small deviations from the traditional rod shape. Our results separate the effects of aspect ratio and particle shape, contribute to the characterization of the effective dynamics at large and intermediate length scales, and thereby also provide strategies for the design of future artificial systems.

15 min. break

Invited Talk BP 35.7 Fri 11:15 H 1028

Large scale collective dynamics of bacteria suspensions — •Eric Clement[1], Benjamin Perez Estay[1], Anke Lindner[1], Carine Douarche[2], Jochen Arlt[3], Vincent Martinez[3], Wilson Poon[3], and Alexander Morosov[3] — [1]PMMH-ESPCI, Sorbonne University, Paris , France — [2]FAST, University Paris-Saclay — [3]School of Physics & Astronomy, University of Edinburgh

Fluids laden with swimming micro-organisms have become a rich domain of applications and a conceptual playground for the statistical physics of active matter. Such active bacterial fluids display original emergent phases as well as unconventional macroscopic transport properties, hence leading to revisit standard concepts in the physics and hydrodynamics of suspensions.

Here, I will present and discuss some recent advances on the spontaneous emergence of a "critical fluid" state for dense bacteria suspensions, characterized by a vanishing viscosity and and a divergent "active turbulence" scale controlled by the confinement. Close to the transition I will also describe a novel collective state leading to very large scale coherent motion of the bacteria.

BP 35.8 Fri 11:45 H 1028

Analysis techniques for active matter simulations — •Lukas Hecht, Kay-Robert Dormann, Aritra Mukhopadhyay, Kai Spanheimer, Mahdieh Ebrahimi, Suvendu Mandal, and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany

Simulations of active matter systems provide a promising route to understand collective phenomena and the non-equilibrium physics of active matter. Prominent models for active matter systems comprise particle-based models such as the active Brownian particle model and continuum models such as the active model B+. To analyze the data obtained from the numerical solution of these models, currently, many researchers develop in-house code. Here, we present the Active Matter Evaluation Package (AMEP), a unified framework to analyze active matter simulations. This Python library is easy to use and provides a powerful and simple interface for handling large data sets. The package features various methods for calculating observables, visualizing results, and analyzing data from molecular-dynamics, Brownian-dynamics, and continuum simulations. These features allow the user, for example, to easily calculate spatial and temporal correlation functions, to perform cluster analyses, to visualize simulation results, and to study phase separation, pattern formation, and critical phenomena in active matter systems.

BP 35.9 Fri 12:00 H 1028

Unveiling Active Fluctuations in Cellular Aggregates through Derivation of Hydrodynamic Transport — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

The biological functionality of cellular aggregates is a collective result of the activities and displacements of individual constituent cells. The theoretical characterization of this activity involves hydrodynamic transport coefficients, such as diffusivity and conductivity. Motivated by the clustering dynamics in bacterial microcolonies, we propose a model for active multicellular aggregates on 1D lattice. Employing macroscopic fluctuation theory, we derive a fluctuating hydrodynamics framework for this model system. Both semi-analytical theory and microscopic simulations reveal that non-equilibrium microscopic parameters exert a significant influence on the hydrodynamic transport coefficients, causing a notable decrease within the clusters. Additionally, we illustrate how the active nature of intercellular interactions disrupts the conventional Einstein relation that establishes a connection between transport coefficients and fluctuations. This study not only provides a comprehensive understanding of the hydrodynamic transport in bacterial microcolonies but also offers valuable tools for experimental investigations in other systems involving active cellular aggregates, such as tumor spheroids and organoids.

BP 35.10 Fri 12:15 H 1028

Expansion-flow driven orientation patterns in systems of growing rods — •Lukas Hupe[1,2], Jonas Isensee[1,2], Ramin Golestanian[1,2,3], and Philip Bittihn[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Faculty of Physics, University of Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

In densely-packed two-dimensional systems of growing rods, such as bacteria, a number of experimental and numerical studies report long-range nematic alignment in the presence of confinement. In some geometries, spatially heterogeneous preferred orientations are observed. So far, these effects have been qualitatively explained using continuum theories of growing active nematics adapted to the specific geometry under investigation.

Here, we first show how the shear rate tensor of the expansion flow alone can be used to qualitatively predict time-averaged orientation patterns from the geometry of the confinement. We apply this method to a series of example geometries and compare with results from agent-based simulations. To quantitatively describe alignment strength, we then develop a simple model which takes into account advection and explore its potential for cross-prediction across different geometries.

Our results provide a unifying theoretical framework and highlight the role of domain geometry in shaping nematic order of growing systems.

BP 35.11 Fri 12:30 H 1028

Walking the Road to Active Nematic Turbulence — •Malcolm Hillebrand[1,2] and Ricard Alert[1,2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzerstr 38, Dresden 01187 — [2]Center for Systems Biology Dresden, Pfotenhauerstr 108, 01307 Dresden, Germany

Active matter, where internal energy consumption drives motion, exhibits a richly complex array of behaviours. In particular, the appearance of turbulent-like flows at very low Reynolds number, termed active turbulence, provides possibilities for chaotic fluid motion at scales as small as the surface of a cell. Here, in a hydrodynamic model of an active nematic, we thoroughly investigate the transition from smooth shear flow all the way to fully developed active turbulence. We utilise tools from dynamical systems theory, including Lyapunov exponents

and time series analysis of velocity fields, as well as energy spectra and scaling laws, to describe the series of changes in dynamics that occur as we increase the activity. We find a sequence of increasingly unpredictable rearrangements between steady flow states that eventually give rise to continuously unstable chaos via a regime of apparent multistability. In addition, intermittent flow characteristics of fully active turbulent flows from simulations are compared to data from kinesin-microtubule experiments.

BP 35.12 Fri 12:45 H 1028

Activation fronts, fluctuations and criticality in the initiation of collective motion — •Parisa Rahmani[1], Hadrien-Matthieu Gascuel[2,3], Richard Bon[2], and Fernando Peruani[1,3] — [1]LPTM, UMR 8089, CY Cergy Paris Universite, 95302 Cergy-Pontoise, France — [2]CNRS, Centre de Recherches sur la Cognition Animale, F-31062 Toulouse Cedex 9, France — [3]Universite Cote d'Azur, Laboratoire J. A. Dieudonne, UMR 7351 CNRS, F-06108 Nice Cedex 02, France

Collective motion is generally not a continuous process, and collectives display repeated transitions from static to moving phases. The initiation of collective motion – of an initially static group – is a crucial process to ensure group cohesion and behavioral synchrony that remains largely unexplored. Here, we investigate the statistical properties of the initiation of collective motion. We find that the information propagates as an activation wave, whose speed is modulated by the velocity of the active agents, where both, the magnitude and direction of the agents' velocity play a crucial role. The analysis reveals a series of distinct dynamic regimes, including a selfish regimes that allow the first informed individuals to avoid predation by swapping position with uninformed individuals. Furthermore, we unravel the existence of a generic and intimate connection between the initiation of collective motion and critical phenomena in systems with an absorbing phase, showing that in a range of agents' velocities the initiation process displays criticality. The obtained results provide an insight in the way collectives distribute, process, and respond to the local environmental cues.

BP 36: Cell Mechanics II

Time: Friday 10:00–13:00 Location: H 0112

BP 36.1 Fri 10:00 H 0112

Optical Cavities for Biology — •Maerpreet Kaur Arora[1,2], Florian Steiner[1,2], and Thomas Hümmer[1,2,3] — [1]Ludwig-Maximilians-University Munich, Department of Physics, Munich, Germany — [2]Qlibri GmbH, Munich, Germany — [3]Max-Planck-Institut für Quantenoptik, Garching, Germany

Label-free imaging of bio-molecules in combination with absorption spectroscopy is essential for observing mechanisms in real time. Analysis of absorption properties for sub-cellular structures is challenging due to their weak interaction with light. Fiber-mirror optical cavities strongly enhance this interaction and enable direct imaging and absorption characterization of nano-scale samples.

To this end, the analysis of cavity properties in the natural environment of these biological samples is crucial. We observe the parameter changes of the cavity in water and air and compare them to simulated data.

BP 36.2 Fri 10:15 H 0112

Electromagnetic field stimulation (EMS) rescues defects in axonal organelle trafficking, regeneration and DNA damage response (DNA-DR) in amyotrophic lateral sclerosis (ALS) — •Arun Pal, Jens Pietzsch, and Thomas Herrmannsdörfer — Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

Cellular events benefit from EMS with alternating fields (AC). Our in vitro experiments on cultured compartmentalized iPSC-derived spinal motoneurons from familiar ALS patients aim to reveal the optimal magnetic field configuration with respect to the AC frequency, amplitude and orientation. Following EMS, we analyzed its impact on axonal organelle trafficking, regeneration after axotomy and DNA-DR in the nucleus by live-cell imaging. All three readout assays are clinically relevant for neurodegeneration and revealed clear defects in our ALS neurons. Beyond a critical threshold of field strength, we found a sustained rescue of the motility of axonal mitochondria and lysosomes along with increased outgrowth speed of growth cones after axotomy and a re-activated DNA-DR through AC sine waves at perpendicular field orientation to the axonal plane with a special frequency optimum. Our results point to a powerful non-invasive and non-pharmacological novel therapeutic method. Thus, we are prototyping a patient stretcher with multiple arrayed built-in magnetic coils to expose all body parts to vectorized magnetic fields of any spatiotemporal modulation for the treatment of neurodegenerative diseases. The coils can be operated either in a continuous AC mode or with repetitive pulses by discharging a capacitor bank.

BP 36.3 Fri 10:30 H 0112

Coordinated poleward flux of sister kinetochore fibers drives chromosome congression — •Domagoj Božan[1], Jelena Martinčić[2], Patrik Risteski[2], Nenad Pavin[1], and Iva Tolić[2] — [1]Department of Physics, Faculty of Science, University of Zagreb, Bijenička cesta 32, 10000 Zagreb, Croatia — [2]Division of Molecular Biology, Rudjer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

Chromosome congression and alignment at the spindle equator promote proper chromosome segregation and depend on pulling forces exerted at kinetochore fiber tips together with polar ejection forces. However, kinetochore fibers are also subjected to forces exerted by motor proteins that drive their poleward flux. Here we introduce a flux-driven centering model that relies on flux generated by forces within the overlaps of bridging and kinetochore fibers. This centering mechanism works so that fewer longer kinetochore fibers fluxes faster than the greater number of shorter ones, moving the kinetochores towards the center. We compare this model with the results of speckle microscopy performed by our collaborators and obtain good correspondence with the experiment. Thus, length-dependent sliding forces exerted by the bridging fiber onto kinetochore fibers promote chromosome congression and alignment.

BP 36.4 Fri 10:45 H 0112

An oblique plane light-sheet microscope for volumetric imaging of neural signals and *in situ* sample manipulation — •Achim Theo Brinkop[1], Stefan Stöberl[1], Florian Schorre[1], Rebecca James[1], Lena Glanz[1], and Friedhelm Serwane[1,2,3] — [1]Faculty of Physics & Center for NanoScience, LMU Munich, Germany — [2]Munich Cluster for Systems Neurology (SyNergy), Germany — [3]Graduate School of Systemic Neuroscience (GSN), Munich, Germany

Many biophysical applications require high-speed volumetric imaging with open top access, e.g. long-term imaging of living organisms and sample manipulation. Existing microscope set-ups, however, are complex or tailored to specific applications. To investigate both mechanical and electrical properties of neural organoids, we designed and built a high-speed oblique plane microscope using one objective for illumination and detection. The set-up allows for imaging genetically encoded calcium and voltage indicators. At the same time, it is compatible with the use of magnetic actuators which can be mounted above the sample to probe the tissue's mechanical properties *in situ*. First measurements show a signal-to-noise ratio on the order of 10 for Ca^{2+}-imaging inside neural organoids at a single-cell level for exposure times of milliseconds. With this set-up, we aim to gain a deeper understanding of 3D organoid neuronal network formation and function.

BP 36.5 Fri 11:00 H 0112

Electron UHDR and FLASH radiation biology studies at PITZ, DESY — •Yuliia Komar[1,2], Anna Grebinyk[1,2], Marcus Frohme[1], Frank Stephan[2], Zakaria Aboulbanine[2], Namra Aftab[2], Zohrab Amirkhanyan[2], Aida Asoyan[2], Prach Boonpornprasert[2], Paul Borchert[1], Hakob Davtyan[2], Dmytro Dmytriiev[2], Georgi Georgiev[2], Matthias Gross[2], Andreas Hoffmann[2], Mikhail Krasilnikov[2], Xiangkun Li[2], Max Liebel[2], Zahra Lotfi[2], Frieder Mueller[2], Anne Oppelt[2], Aleksandar Radivoievych[1], Chris Richard[2], Felix Riemer[2], Houjun Qian[2], Grygorii Vashchenko[2], and Daniel Villani[2] — [1]Technical University of Applied Sciences Wildau, Wildau, Germany, — [2]Deutsches Elektronen-Synchrotron, Zeuthen, Germany

The Photo Injector Test facility at DESY in Zeuthen (PITZ) together with the Technical University of Applied Sciences Wildau are going to study ultra-high dose rate (UHDR) cancer radiation therapy (RT) at FLASHlab@PITZ. FLASH RT is based on UHDR irradiation (40-10^9 Gy/s) and was shown to have a higher sparing effect on normal tissue in comparison to conventional dose rate (0.05 Gy/s) applied in clinics. The unique parameter space of the PITZ beam allows to deliver dose rates in the range between 0.05 Gy/s and 10^14 Gy/s, providing a unique possibility to investigate the effect of dose rate escalation and contribute to widening of the RT therapeutic window. For that matter, the in vitro effect of UHDR was studied at FLASHlab@PITZ. The obtained data demonstrated ROS generation, DNA damage and cell proliferation decrease at increasing doses for both UHDR 10^5 Gy/s and conventional 0.05 Gy/s. The obtained first results highlighted the potential to explore UHDR further for cancer RT.

BP 36.6 Fri 11:15 H 0112

Electrohydraulics of electrically polarized spherical organoids — •Amit Singh Vishen[1], Ahandeep Manna[1], Jacques Prost[2], and Frank Julicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Laboratoire Physico-Chimie, Institut Curie, Paris, France

Cells and tissues in many contexts are electrically polarized. We develop a three-dimensional electro-hydraulic model that simultaneously solves for the electric potential, ion concentration, and hydrodynamic flows and stresses inside and outside a spherical water-filled cavity enclosed by an epithelium. We analyze two sources of electric asymmetry in the system: (i) heterogeneous ion transporter along the surface of the sphere and (ii) organoid in an external electric field. We show that inho- mogeneous ion transport leads to an organ-scale electric current and water flux. Consistent with recent experimental observation we find that a constant electric field leads to isotropic swelling of the organ.

15 min. break

BP 36.7 Fri 11:45 H 0112

Light-Induced Chloroplast Morphodynamics in a Single Celled Algae — •Nico Schramma, Gloria Casas Canales, and Maziyar Jalaal — Van der Waals-Zeeman Institute, University of Amsterdam, Amsterdam, Netherlands

Photosynthesis is essential for all life on Earth. However, the ever-changing light conditions in the environment of immobile organisms are continuously challenging the photosynthetic performance. A vast amount of photosynthesis takes place in the ocean and even simpler forms of life, such as the non-motile single-celled marine algae Pyrocystis lunula, can adapt to changes of light by moving their chloroplasts. As this process occurs in confinement by the rigid cell wall, the drastic intracellular re-arrangement needs "smart" logistics strategies. Here we uncover that the cell exploits meta-material properties to efficiently adapt to such environmental changes. Exposing the cell to different physiological light conditions and applying temporal illumination sequences shows that the morpho-dynamics follow simple rules. This kind of dynamic testing allows us to extract the coarse-grained equations of motion to describe this biological system. Our study shows how topologically complex metamaterials are applied in critical life-sustaining processes in nature and that simple dynamical rules can account for complex material transport in a crowded intracellular environment.

BP 36.8 Fri 12:00 H 0112

Band pattern formation in a suspension of red blood cells during centrifugation in a Percoll density gradient — •Felix Maurer, Thomas John, Christian Wagner, and Alexis Darras — Saarland University, 66123 Saarbrücken, Germany

Percoll is a suspension of silica nanoparticles often used to establish density gradients and separate biological matter in centrifugation protocols. When red blood cells (RBCs) sediment in a Percoll medium, they form patterns of discrete bands. While this is a popular approach for RBC age separation, the mechanisms involved in band formation were unknown. In a series of experiments we could show that the formation of those patterns could be explained by cell aggregation. We developed a new continuum model to describe the volumetric RBC density under the influence of attractive pair interaction. Our numerical solutions are characterized by pattern formation and transitions between the equilibrium states depending on aggregation energy and initial volumetric RBC concentration.

BP 36.9 Fri 12:15 H 0112

Unraveling the dynamics of *Trypanosoma brucei*: a microfluidic approach — •Hannes Wunderlich[1], Sebastian W. Krauss[1], Lucas Brehm[2], Marinus Thein[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth, Germany — [2]Molecular Parasitology, University of Bayreuth, Germany

Trypanosoma brucei is a unicellular parasite that causes the African sleeping sickness after transmission by tsetse flies. These microswimmers use a single microtubule-driven flagellum for their helical forward motion, which is essential for the virulence and survival of the parasite. A highly ordered subpellicular microtubule array equips the cell with a considerable bending elasticity. However it is unclear how this elasticity relates to the cell's propulsion.

Using microfluidic devices, we have studied the swimming of wild-type trypanosomes and mutant strains in which post-translational modificiations of microtubules have been altered. First, trypanosomes were allowed to move freely in 2D chambers, from which a run-and-tumble motion and the effective velocities of individual cells were extracted and compared. When encapsulating single trypanosomes in droplets of similar size, a purely rotational motion emerged. While each cell showed a mostly persistent (counter-)clockwise rotation, no directional preference was seen on the ensemble level. Monitoring the angular motion over extended periods revealed again a run-and-tumble behavior. The planar and angular velocities depended on the cell's elasticity. Our results suggest that an effective propulsion requires a distinct elasticity of the subpellicular microtubule array.

BP 36.10 Fri 12:30 H 0112

Red blood cell lingering: impact on microcirculation hematocrit distribution and differences in rigid versus healthy cells — •Yazdan Rashidi[1], Selina Wrublewsky[2], Felix Maurer[1], Khadija Larhrissi[1], Thomas John[1], Lars Kaestner[1], Matthias W. Laschke[2], Michael D. Menger[2], Christian Wagner[1], and Alexis Darras[1] — [1]Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Institute for Clinical and Experimental Surgery, Saarland University, 66421 Homburg, Germany

The distribution of red blood cells (RBCs) in the microcirculation determines how the oxygen is delivered to tissues and organs. This process relies on the partitioning of RBCs at successive microvascular bifurcations. Usually, downstream of a microvascular bifurcation, the vessel branch with a higher fraction of blood flow receives a higher fraction of RBC flux. However, both temporal and time-average deviations from this phase-separation law have been observed in recent works. Here, we quantify how the microscopic behaviour of RBCs lingering (i.e. RBCs temporarily residing near the bifurcation apex with diminished velocity) influences their partitioning, through combined in vivo experiments and in silico simulations. We developed an approach to quantify the cell lingering at highly confined capillary-level bifurcations and demonstrate that it correlates with deviations of the phase-separation process from established empirical predictions by Pries et al. Furthermore, we shed light on how the bifurcation geometry and cell membrane rigidity can affect the lingering behaviour of RBCs, and show rigid cells tend to linger less than softer ones.

BP 36.11 Fri 12:45 H 0112

Lightmicroscopy of Red Blood Cells — •Agatha Belén Pinto-Pino, Sarah Tabea Hermes, Thomas John, and Christian Wagner — Campus E2.6 66123 Saarbrücken

The observation of cells in liquids under a conventional light microscope is a common practice in research. Because the refractive index within the cells is greater than in the medium, refraction also takes place in addition to absorption. The resulting microscope image is therefore a composition of absorption and refraction as a function of the set focal plane. This is very important for the detection of the cell edges and thus the cell morphology [1]. Using the example of red blood cells, we show how refraction leads to "ghost edges" and compare this with numerical simulations of the light paths. Surprisingly, the optimal focus is not the position with the highest contrast. We give further hints for the optimal observation of red blood cells.

[1] Yoon at. al., Flickering Analysis of Erythrocyte Mechanical Properties, Biophysical Journal **97, 1606, (2009)**

BP 37: Closing Talk (joint session BP/CPP/DY)

Time: Friday 13:15–14:00 Location: H 0104

Invited Talk BP 37.1 Fri 13:15 H 0104

Virus traps and other molecular machines of the future — •Hendrik Dietz — Technische Universität München, Garching b. München, Deutschland

Our interest is in learning how to build molecular devices and machines that can execute user-defined tasks. To this end, we investigate how to adapt the physical principles underlying the formation of natural macromolecular assemblies such as viruses or molecular motors for our purposes. Programmable molecular self-assembly with DNA origami is an attractive route toward implementing these principles to create synthetic molecular machinery. We combine computational design and cryo electron microscopy to learn how to construct synthetic molecular objects with increasing accuracy and increasing complexity.

For example, we have learned from viruses how to program DNA blocks to self-assemble into icosahedral shells with specific geometry and apertures, which led to an interesting application: the virus trap, which we hope to develop into a programmable antiviral drug to neutralize viruses. We have also learned how to design DNA origami so that genetic instructions included within them can be read by mammalian cells.

We also have recently learned how to control the movement of nanoscale assemblies. For example, we have built autonomous, power-generating rotary DNA motors driven by AC fields and also turbines that can be driven by ion flux across membranes. With these new machines, opportunities are created to accomplish user-defined, energy-consuming tasks in various contexts.