Biological Physics Division
Fachverband Biologische Physik (BP)

Gerhard Gompper
Theoretical Physics of Living Matter
Institute of Biological Information Processing
Forschungszentrum Jülich
52425 Jülich, Germany
g.gompper@fz-juelich.de

Frauke Gräter
Heidelberg Institute Theoretical Studies
Schlosswolfsbrunnenweg 35
69118 Heidelberg, Germany
frauke.graeter@h-its.org

Joachim Rädler
Fakultät für Physik
Ludwig-Maximilians-Universität
Geschwister Scholl Platz 1
80539 München, Germany
raedler@lmu.de

Overview of Invited Talks and Sessions

(Lecture halls H1 and H6; Posters P)

Invited Talks

BP 1.1	Mon	10:00–10:30	H1	**Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth** — •Robert Endres, Henry Cavanagh, Rob Lind, Andreas Mosbach, Gabriel Scalliet
BP 2.1	Mon	11:30–12:00	H1	**PINCH-1 promotes migration in extracellular matrices and influences the mechano-phenotype** — •Claudia Tanja Mierke
BP 3.1	Thu	10:00–10:30	H1	**SARS-CoV-2 induced membrane remodeling in infected cells revealed by in celullo cryo-ET** — Steffen Klein, Liv Zimmermann, Sophie Winter, Mirko Cortese, Moritz Wachsmuth-Melm, Christopher Neufeldt, Berati Cerikan, Megan Stanifer, Steeve Boulant, Ralf Bartenschlager, •Petr Chlanda
BP 6.1	Thu	13:30–14:00	H6	**How do lipids and proteins diffuse in cell membranes, and what do the diffusion experiments actually measure?** — •Ilpo Vattulainen
BP 7.1	Thu	15:00–15:30	H6	**Shaping embryos through controlled tissue phase transitions** — •Otger Campàs

Invited talks of the joint symposium Topological constraints in biological and synthetic soft matter (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert

SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium The Physics of CoViD Infections (SYCO)

See SYCO for the full program of the symposium.

SYCO 1.1	Mon	13:30–14:00	Audimax 1	**A Tethered Ligand Assay to Probe SARS-CoV-2:ACE2 Interactions** — Magnus Bauer, Sophia Gruber, Adina Hausch, Lukas Milles, Thomas Nicolaus, Leonard Schendel, Pilar Lopez Navajas, Erik Procko, Daniel Lietha, Rafael Bernadi, Hermann Gaub, •Jan Lipfert
SYCO 1.2	Mon	14:00–14:30	Audimax 1	**From molecular simulations towards antiviral therapeutics against COVID-19** — •Rebecca Wade
SYCO 1.3	Mon	14:45–15:15	Audimax 1	**The physical phenotype of blood cells is altered in COVID-19** — Markéta Kubánková, Martin Kräter, Bettina Hohberger, •Jochen Guck
SYCO 1.4	Mon	15:15–15:45	Audimax 1	**Extended lifetime of respiratory droplets in a turbulent vapor puff and its implications on airborne disease transmission** — •Detlef Lohse, Kai Leong Chong, Chong Shen Ng, Naoki Hori, Morgan Li, Rui Yang, Roberto Verzicco
SYCO 1.5	Mon	15:45–16:15	Audimax 1	**Beyond the demographic vaccine distribution: Where, when and to whom should vaccines be provided first?** — •Benno Liebchen, Jens Grauer, Fabian Schwarzendahl, Hartmut Löwen

Prize talks of the joint Awards Symposium (SYAW)

See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-1/2 antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt

SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Active nematics: From 2D to 3D (SYAN)

See SYAN for the full program of the symposium.

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik
SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

BP 1.1–1.4	Mon	10:00–11:15	H1	**Statistical physics of biological systems (joint session BP/DY)**
BP 2.1–2.4	Mon	11:30–12:45	H1	**Cytoskeleton**
BP 3.1–3.3	Thu	10:00–11:00	H1	**Protein Structure and Dynamics**
BP 4.1–4.11	Thu	11:15–12:15	P	**Posters Biological Physics**
BP 5.1–5.5	Thu	11:45–13:00	H2	**Active Matter (joint session DY/BP/CPP)**
BP 6.1–6.4	Thu	13:30–14:45	H6	**Membranes and Vesicles**
BP 7.1–7.4	Thu	15:00–16:15	H6	**Cell Mechanics, Cell Adhesion and Migration, Multicellular Systems**
BP 8	Thu	18:00–19:00	MVBP	**Annual General Meeting**
BP 9.1–9.5	Fri	11:15–12:30	H2	**Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)**

Annual General Meeting of the Biological Physics Division

Thu 18:00–19:00 MVBP

- Bericht
- Wahl
- Verschiedenes

BP 1: Statistical physics of biological systems (joint session BP/DY)

Time: Monday 10:00–11:15 Location: H1

Invited Talk BP 1.1 Mon 10:00 H1

Physics-Informed Deep Learning for Characterizing Perturbed Cell Growth — •Robert Endres[1], Henry Cavanagh[1], Rob Lind[2], Andreas Mosbach[3], and Gabriel Scalliet[3] — [1]Imperial College London, UK — [2]Syngenta International Research Centre, UK — [3]Syngenta Crop Protection AG, Switzerland

The morphodynamical analysis of cells can be a powerful and cost-effective way of understanding the phenotypic effects of perturbations, but current techniques often only work for stationary cell behaviour. Here, we introduce a novel framework that extends the morphodynamic analysis to nonstationary dynamics during early-stage growth of the soybean rust P. pachyrhizi. At its core, our approach learns the 2-dimensional feature space of cell shape using variational autoencoders from deep learning, and subsequently models how populations of cells develop over this space using two simple differential equations, each capturing complementary aspects of the dynamics with parameters depending on the perturbations. First, a Fokker-Planck model to describe the diffusive development on a Waddington-type energy landscape, providing a global perspective on the dynamics, and second, a cell-mechanical model describing local growth as a persistent random walk. Informative perturbation-dependent parameters are found by fitting simulations to the shape-space embeddings, representing a powerful tool for linking machine-learning and biophysical modelling.

BP 1.2 Mon 10:30 H1

Collisions increase self-diffusion in odd-diffusive systems — •Erik Kalz[1,2], Iman Abdoli[1], Hidde Derk Vuijk[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere, 01069 Dresden — [2]Technische Universität Dresden, Institut für Theoretische Physik 01069 Dresden

It is generally believed that collisions of particles reduce the self-diffusion coefficient. We show that in odd-diffusive systems, which are characterized by diffusion tensors with anti-symmetric elements, collisions surprisingly can enhance the self-diffusion. In these systems, due to an inherent curving effect, the motion of particles is facilitated, instead of hindered by collisions. We refer to this as an overdamped swing-by effect. Consistent with this we find that the collective diffusion remains unaffected. We demonstrate this counterintuitive behavior in a system of Brownian particles under Lorentz force. Using a geometric model, we theoretically predict a magnetic-field governed crossover from a reduced to an enhanced self-diffusion. The physical interpretation is quantitatively supported by the force-autocorrelation function, which turns negative with increasing magnetic field. Using Brownian dynamic simulations, we show that the predictions are also valid for active chiral particles as another odd-diffusive system.

BP 1.3 Mon 10:45 H1

How is anomalous diffusion compatible with thermodynamics in biophysical systems? — •David Hartich and Aljaz Godec — Mathematical bioPhysics Group, MPI-BPC, Göttingen, Germany

In a finite system driven out of equilibrium by a constant external force the thermodynamic uncertainty relation (TUR) bounds the variance of the conjugate current variable by the thermodynamic cost of maintaining the non-equilibrium stationary state. Here we highlight a new facet of the TUR by showing that it also bounds the time-scale on which a finite system can exhibit anomalous kinetics. In particular, we demonstrate that the TUR bounds subdiffusion in a single file confined to a ring as well as a dragged Gaussian polymer chain even when detailed balance is satisfied. Conversely, the TUR bounds the onset of superdiffusion in the active comb model. Remarkably, the fluctuations in a comb model evolving from a steady state behave anomalously as soon as detailed balance is broken. Our work establishes a link between stochastic thermodynamics and the field of anomalous dynamics that will fertilize further investigations of thermodynamic consistency of anomalous diffusion models.

[1] DH, A. Godec, Phys Rev. Lett. (in press), arXiv:2102.06678.

BP 1.4 Mon 11:00 H1

Maximum likelihood estimates of diffusion coefficients from single-particle tracking experiments — •Jakob Tómas Bullerjahn[1] and Gerhard Hummer[1,2] — [1]Department of Theoretical Biophysics, MPI of Biophysics, Frankfurt am Main, Germany — [2]Institute of Biophysics, Goethe University, Frankfurt am Main, Germany

Single-molecule localization microscopy allows practitioners to locate and track labeled molecules in biological systems. When extracting diffusion coefficients from the resulting trajectories, it is common practice to perform a linear fit on mean-squared-displacement curves. However, this strategy is suboptimal and prone to errors. Recently, it was shown that the increments between the observed positions provide a good estimate for the diffusion coefficient, and their statistics are well-suited for likelihood-based analysis methods. Here, we revisit the problem of extracting diffusion coefficients from single-particle tracking experiments subject to static noise and dynamic motion blur using the principle of maximum likelihood. Taking advantage of an efficient real-space formulation, we extend the model to mixtures of subpopulations differing in their diffusion coefficients, which we estimate with the help of the expectation-maximization algorithm. This formulation naturally leads to a probabilistic assignment of trajectories to subpopulations. We employ the theory to analyze experimental tracking data that cannot be explained with a single diffusion coefficient, and test how well the data conform to the model assumptions. https://doi.org/10.1063/5.0038174

BP 2: Cytoskeleton

Time: Monday 11:30–12:45 Location: H1

Invited Talk BP 2.1 Mon 11:30 H1

PINCH-1 promotes migration in extracellular matrices and influences the mechano-phenotype — •Claudia Tanja Mierke — University of Leipzig, Biological Physics, Leipzig, Germany

Cell migration performs a critical function in numerous physiological processes, including tissue homeostasis or wound healing, and pathological processes that include malignant cancer progression. The efficiency of migration appears to be based on the mechano-phenotype of the cytoskeleton. Cytoskeletal properties depend on intercellular and environmental factors. Thus, connections between the cell and its microenvironment are established by cell-matrix adhesion receptors. Upon activation, focal adhesion proteins such as PINCH-1 are recruited to sites where focal adhesions form. PINCH-1 specifically couples through interactions with ILK, which binds to cell-matrix receptors and the actomyosin cytoskeleton. However, the role of PINCH-1 in cell mechanics regulating cellular motility in 3D-collagen matrices is elusive. PINCH-1 is thought to facilitate 3D-motility by regulating cellular mechanical properties, such as stiffness. Therefore, PINCH-1 wild-type and knock-out cells were examined for their ability to migrate in dense extracellular 3D-matrices and cellular deformability. PINCH-1 wild-type cells migrated more numerous and deeper in 3D-matrices. PINCH-1 wild-type cells are less deformable (stiffer) compared to PINCH-1 knock-out cells. Migration and deformability were reduced by drug-dependent inhibition of Arp2/3 complex or actin polymerization. Finally, PINCH-1 appears to be essential for providing cellular mechanical stiffness, which regulates 3D motility.

BP 2.2 Mon 12:00 H1

A novel second PI(4,5)P_2 binding site determines PI(4,5)P_2 sensitivity of the tubby domain — Veronika Thallmair[1], Lea Schultz[1], Wencai Zhao[1], Siewert J. Marrink[2], Dominik Oliver[1], and •Sebastian Thallmair[2,3] — [1]Philipps-University Marburg, Germany — [2]University of Groningen, The Netherlands — [3]Frankfurt Institute for Advanced Studies, Frankfurt am Main, Germany

Phosphoinositides (PIs) are important signaling lipids multitasking in diverse cellular signaling pathways. They operate by recruiting proteins to the membrane surface by means of PI recognition domains.

One of the recognition domains for $PI(4,5)P_2$ lipids, which is the major PI species in the plasma membrane, is the tubby domain. It is conserved in the tubby-like protein (TULP) family and plays an important role in targeting proteins into cilia.

We used coarse-grained (CG) molecular dynamics (MD) simulations with the re-parametrized Martini 3 force field to explore the $PI(4,5)P_2$ affinity of the C-terminal tubby domain (tubbyCT). Our CG MD simulations revealed a novel second binding site consisting of a conserved cationic cluster at the protein-membrane interface. The simulations together with mutation experiments in living cells showed that the second binding site substantially contributes to the fine-tuned $PI(4,5)P_2$ affinity of tubbyCT. We will discuss the computational and experimental characterization of the novel binding site, its importance for the membrane targeting properties of tubbyCT, and for its ability to recognize distinct $PI(4,5)P_2$ pools in the plasma membrane.

BP 2.3 Mon 12:15 H1

Motor proteins generate the curved shape of the mitotic spindle — •Arian Ivec[1], Maja Novak[1], 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, Ruder Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

The mitotic spindle is a complex micro-machine made up of microtubules and associated proteins that are highly ordered in space and time to ensure its proper biological functioning. A functional spindle has a characteristic shape, which includes curved bundles of microtubules that are twisted around the pole-to-pole axis. An in-depth understanding of both how the linear and rotational forces define the overall shape of the mitotic spindle and how the twisted shapes arise as a result of interactions between microtubules and motor proteins is still unclear. To answer this, we introduce a model in which motor proteins generate forces at the poles and along the microtubule bundles, thereby regulating the shapes of microtubule bundles. The model provides predictions for forces in the spindle, including that the shape of the entire spindle is predominately determined by rotational forces, and that a difference in bending forces explains the disparity in the shapes of inner and outer bundles.

BP 2.4 Mon 12:30 H1

Bottom-up assembly of functional DNA-based cytoskeletons for synthetic cells — •Kevin Jahnke[1,2], Pengfei Zhan[3,4], Na Liu[3,4], and Kerstin Göpfrich[1,2] — [1]Max Planck Institute for Medical Research, Heidelberg, Germany — [2]Heidelberg University, Heidelberg, Germany — [3]Stuttgart University, Stuttgart, Germany — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany

Bottom-up synthetic biology aims at reconstructing a cell from biomolecular constituents. However, the combination of multiple elements and functions remained elusive, which stimulates endeavors to explore entirely synthetic bio-inspired solutions towards engineering life. To this end, DNA nanotechnology represents one of the most promising routes, given the inherent sequence specificity, addressability, and programmability of DNA. Here, we demonstrate functional DNA-based cytoskeletons operating in microfluidic cell-sized compartments and lipid vesicles. The synthetic cytoskeletons consist of DNA tiles self-assembled into filament networks. These filaments can be rationally designed and controlled to imitate features of natural cytoskeletons, including dynamic instability, ATP-triggered polymerization, and vesicle transport in cell-sized confinement. Also, they possess engineerable characteristics, including assembly and disassembly powered by DNA hybridization or aptamer-target interactions and autonomous transport of gold nanoparticles. This work underpins DNA nanotechnology as a key player in building synthetic cells.

BP 3: Protein Structure and Dynamics

Time: Thursday 10:00–11:00 Location: H1

Invited Talk BP 3.1 Thu 10:00 H1

SARS-CoV-2 induced membrane remodeling in infected cells revealed by in celullo cryo-ET — Steffen Klein, Liv Zimmermann, Sophie Winter, Mirko Cortese, Moritz Wachsmuth-Melm, Christopher Neufeldt, Berati Cerikan, Megan Stanifer, Steeve Boulant, Ralf Bartenschlager, and •Petr Chlanda — Heidelberg University Hospital, Heidelberg, Germany

Coronavirus replication in the host cell causes extensive remodeling of cellular membranes. To better understand the governing mechanisms of SARS-CoV-2 membrane remodeling during RNA replication and virus assembly we visualized hubs of virus replication and assembly using cryo-electron tomography of infected cells. Our data reveal the architecture of double-membrane vesicles which are associated with viral genome replication. Viral RNA filaments inside these compartments show a diameter consistent with double-stranded RNA and displayed frequent branching, likely representing secondary structures. Virion assembly sites were found at cisternae enriched in spike trimers and viral ribonucleoprotein complexes (vRNPs) at the cytoplasmic side. We further structurally analyzed the viral genome in newly assembled virions and revealed that the viral RNA is encased by multiple individual cylindrical vRNPs. We propose that this arrangement allows the incorporation of the unusually large coronavirus genome into the virion while maintaining high steric flexibility between the vRNPs during virion assembly.

BP 3.2 Thu 10:30 H1

Size-dependent deviations from the colloidal prediction: about the diffusion of proteins in a cellular environment — •Christian Beck[1,2], Felix Roosen-Runge[3], Tilo Seydel[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [2]Institut Laue-Langevin, 38042 Grenoble Cedex 9, France — [3]Department of Biomedical Science, Malmö University, Sweden

Diffusive properties are of fundamental importance for biological processes. For their quantitative understanding, the short-time diffusive properties are of huge interest. Previous studies investigated the volume fraction dependence of short-time diffusive properties for different pure proteins solutions [1] and recently in controlled poly-disperse cell-like environments [2]. In cooperation with the ILL life science group, we now investigated the diffusive properties of different sized proteins in the presence of deuterated lysate. In contrast to the previous study [2], the apparent global diffusion of the different proteins investigated does significantly deviate from the total volume fraction dependence of the pure protein solutions. While small proteins have a higher diffusion coefficient in the presence of lysate compared with the pure protein solution, big proteins, however, are slowed down. These results give a new insight into the diffusive properties of proteins in cells and might contribute significantly to a quantitative understanding of biological processes.

[1] M. Grimaldo, et al., Quart. Rev. Biophys. 52 (2019) e7, 1;
[2] M. Grimaldo, et al., J. Phys. Chem. Lett. 10 (2019) 1709

BP 3.3 Thu 10:45 H1

Scattering techniques: powerful tools to elucidate the molecular mechanisms of Wilson's disease — •Olga Matsarskaia — Institut Laue-Langevin, Grenoble, France

Copper (Cu) is an essential element for mammals and its metabolism is thus tightly regulated [1]. In the case of Wilson's disease, however, Cu metabolism is impaired, leading to abnormal Cu levels in the body [2]. Severe, often lethal, consequences ensue, such as liver and neurological damage [3,4] as well as the destruction of hemoglobin (Hb) and red blood cells (RBCs) [5]. The latter two symptoms are believed to be due to Cu-induced aggregation of Hb [6,7]. The current understanding of Wilson's disease is predominantly phenomenological. Thus, this project applies an interdisciplinary array of techniques including neutron and X-ray scattering to deepen the understanding of this highly complex condition. Scattering data recently obtained using human RBCs and purified human Hb will be presented, demonstrating real-time effects of Cu addition to these systems. The results obtained will be discussed in the broader context of medical research with the goal of inspiring an interdisciplinary dialogue between fundamental science and clinical applications.

[1] Löffler & Petrides, Springer Heidelberg (2007); [2] Riordan & Roger, J.Hepatol. (2001) 34, 433-48; [3] Ala et al., The Lancet (2007), 369, 397-408; [4] Gitlin, Gastroenterol. (2003), 125, 1868-77; [5] Ferenci, Metab. Brain Dis. (2004), 19, 229-39; [6] Rifkind, Blood (1965), 26, 433-48; [7] Jandl, Engle, Allen, J. Clin. Invest. (1960), 39, 1818-36

BP 4: Posters Biological Physics

Time: Thursday 11:15–12:15 Location: P

BP 4.1 Thu 11:15 P

Gelation dynamics upon pressure-induced liquid-liquid phase separation in a water-lysozyme solution — Marc Moron[1], •Ahmed Al-Masoodi[2], Clementine Lovato[2], Mario Reiser[3], Lisa Randolph[2], Göran Surmeier[1], Jennifer Bolle[1], Fabian Westermeier[4], Michael Sprung[4], Metin Tolan[1], Roland Winter[5], Michael Paulus[1], and Christian Gutt[2] — [1]Fakultät Physik / DELTA, TU Dortmund, 44221 Dortmund, Germany — [2]Department Physik, Universität Siegen, 57072 Siegen, Germany — [3]Department of Physics, Stockholm University, 10691 Stockholm, Sweden — [4]Deutsches Elektronen Synchrotron DESY, 22607 Hamburg, Germany — [5]Fakultät Chemie und Chemische Biologie, Physikalische Chemie, TU Dortmund, 44221 Dortmund, Germany

Phase transitions in concentrated protein solutions have been in the focus of research for years. For example, many diseases can be attributed to protein aggregation or liquid-liquid phase separation in human cells. Lysozyme represents a well-studied model protein. We investigated the effect of hydrostatic pressure on concentrated lysozyme solutions in different environments and were able to show that besides temperature, protein concentration, cosolvents and ionic strength also the hydrostatic pressure modulates the protein-protein interaction. Up to now, only the static properties of the lysozyme solutions were characterized. In this work, we present first pressure dependent X-ray photon correlation spectroscopy (XPCS) measurements on concentrated lysozyme solutions to study the dynamics of pressure-induced liquid-liquid phase transitions.

BP 4.2 Thu 11:15 P

Nonlinear viscoelastic behavior and hysteresis in hydrated collagen fibrils — •Martin Dehnert, Paul Zech, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

We study the nanomechanical properties of hydrated collagen fibrils with AFM-based nanoindentation measurements. Force–distance (FD) data measured with tip velocities $< 1\,\mu$m/s and different indentation protocols (force relaxation, creep, and cyclic loading) display nonlinear viscoelastic and elastoplastic behavior: (a) stress relaxation with a time constant $\tau_R \sim 0.1$ s, (b) creep with a time constant $\tau_C \sim 5$ s, and (c) approximately rate-independent hysteretic behavior with return point memory at intermediate time scales. The main cause of the hysteresis is the elastoplastic deformation of collagen fibrils in the leathery regime. We explore the variations of these nanomechanical properties in sets of unfixed hydrated collagen fibrils isolated from native chicken achilles tendon and compare it with collagen fibrils embedded in the natural tendon. AFM imaging in air with controlled humidity preserves the tissue's native water content and allows for high-resolution imaging the assembly of collagen fibrils beneath an approximately 5 to 10-nm-thick layer of the fluid components of the interfibrillar matrix. This sheds new light on the role of interfibrillar bonds, the mechanical properties of the interfibrillar matrix, and the biomechanics of native tendon.

BP 4.3 Thu 11:15 P

Optical Stretcher for Adherent Cells — •Alexander Janik[1], Tobias Neckernuss[1], Nathalie Neffgen[2], Jonas Pfeil[1], Mika Lindén[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University — [2]Institute of Inorganic Chemistry II, Ulm University

We have demonstrated a method to stretch adherent cells with a parallel laser beam to probe their mechanical properties. This contribution focuses on improvements of the setup as well as on interactions between cells and the illumination light. Progress has recently been made in the detection of the z position of the upper cell membrane, which is now achieved by tracking fluorescent beads on the cell. This yields a high z resolution and eliminates artefacts resulting from laser induced aberrations, which affect mainly detection rays entering the objective at small angles.

BP 4.4 Thu 11:15 P

Identifying malignant tissue using fs-Laser Induced Breakdown Spectroscopy (LIBS) and Neural Networks — •Elena Ramela Ciobotea, Christoph Burghard Morscher, Cristian Sarpe, Bastian Zielinski, Hendrike Braun, Arne Senftleben, and Thomas Baumert — Kassel Universität, Kassel, Germany

The problem of differentiating cancerous tissue from a healthy one is currently solved in the diagnostic process through microscopic imaging of stained biopsy sections by pathologists. During surgical removal of cancerous tissue oncological safety margins must be established to ensure the complete removal of the tumor without affecting much of the neighboring healthy tissue. For this purpose, on-site pathological analysis is done on freshly frozen, stained cuts which is time consuming. We investigate a new approach of minimizing the time of discrimination between malign and benign tissue by an in situ, non-contact spectroscopic analysis. In a proof of principle experiment, a plasma is generated by focusing an 800 nm femtosecond laser on the pathologic postoperative sample. The spectrum of plasma radiation contains information on the element composition of the ablated tissue. Since the recorded spectra are complex and full of information, neural networks are employed to find differences between malign and benign tissue with a high speed and accuracy. In this contribution we present the experimental parameters that allow for the best possible differentiation of some biological tissues through fs-LIBS by minimizing deviations between the measurements.

BP 4.5 Thu 11:15 P

Epigenetic relevance of quantum phenomena in DNA — •Mirko Rossini and Joachim Ankerhold — Institute for Complex Quantum systems and IQST, Ulm University, Germany

The behaviour of excited particles along the DNA strand inside a cell has been a topic of foremost interest in the field of biophysics in the last 20 years. On one hand, understanding how the dynamics of such particles can affect the geometry and structural properties of the DNA, locally or globally, can lead to new insights in the field of epigenetics [1]. On the other hand, the DNA strand itself has been analysed to explore its potential as a molecular conducting nano-wire.
With this poster we provide a description of different tight-binding models with dissipative background, exploring their population dynamics and coherence properties. The choice of the parameters for the models is taken to mimic some specific DNA sequences which are relevant in the epigenetic field of research. We provide then some experimental results which justify our interest in this topic and in this methods. Apart from single charge dynamics, we also consider excitonic dynamics in various DNA sequences, in particular with respect to charge separation and localization.

[1] E. R. Bittner, J. Chem. Phys. **125**, 094909 (2006).

BP 4.6 Thu 11:15 P

Swimming vesicles propelled by flagellated bacteria in membrane tubes — •Lucas Le Nagard[1], Aidan Brown[1], Alexander Morozov[1], Angela Dawson[1], Vincent Martinez[1], Margarita Staykova[2], and Wilson Poon[1] — [1]The University of Edinburgh, United Kingdom — [2]Durham University, United Kingdom

Recent simulation studies have predicted that giant unilamellar vesicles submitted to a collection of local internal forces should display enhanced fluctuations and a fascinating diversity of shape changes, from the formation of membrane tubes to deformations leading to vesicle division. Experimental investigation of those phenomena, based on the encapsulation of self-propelled particles or swimming bacteria into giant lipid vesicles, has only recently started. Such minimal systems can be used to study the interactions between an active suspension and a confining (deformable) boundary. They should also help deepen the understanding of biological processes where membrane deformation under local forcing is important. In this work, we encapsulate motile *Escherichia coli* bacteria in low-tension giant lipid vesicles. We observe that the bacteria apply local forces on the membrane, deforming it to generate membrane tubes reminiscent of those seen in eukaryotic cells infected by *Listeria monocytogenes*. Strikingly, these bacteria-enclosing tubes can propel the vesicles. We show that the propulsive force arises from a tight coupling between the bacteria's well-bundled flagella and the membrane tubes, which become rotating helices turning the initially passive vesicles into active micro-swimmers.

BP 4.7 Thu 11:15 P

Effect of Liquid-Liquid Phase Separation of Pol II on gene regulation — •Arya Changiarath Sivadasan and Lukas Stelzl — Johannes Gutenberg University, Mainz

Liquid Liquid phase separation(LLPS) plays an important role in the regulation of cellular processes. In particular, LLPS underpins the formation of localized nuclear hubs of RNAP II during the transcription of genes. Recent experimental studies revealed that the disordered Carboxy terminal domain (CTD) of the largest subunit of RNAP II, has a very strong tendency to phase separate. In our research, we are trying to understand the molecular basis of phase separation of RNAP II using multiscale molecular dynamic simulations. Our initial preliminary studies show the effects of temperature on CTD phase behavior and the influence of polymer length on critical temperature of phase separation. The results show that critical temperature increases with polymer length as expected. As a next step, we are interested in studying the phase separation of phosphorylated RNAP II and the effect of noise in the biochemical signaling on phase behavior. Moreover, we are also keen to understand the phase separation of a complex mixture of biomolecules such as CTD and RNA binding protein FUS. This would give insights into how the LLPS of CTD and other biomolecules regulates the transcription process in cells and will enable us to elucidate how the regulation of genes by LLPS is affected by noise.

BP 4.8 Thu 11:15 P

Bio-inspired Magnetic Nanoprobes For Subcellular Manipulation Studies in Single Cells — •Andreas Neusch[1], Iuliia Novoselova[1], Julia-Sarita Brand[1], Marius Otten[1], Matthias Karg[1], Michael Farle[2], Ulf Wiedwald[2], and Cornelia Monzel[1] — [1]Heinrich-Heine-University, Düsseldorf — [2]University of Duisburg-Essen, Duisburg

Cellular signals rely on characteristic temporal and spatial distributions of signaling molecules, but hitherto it is unclear which patterns trigger which cellular response. In recent years, Magnetogenetics emerged as an approach where magnetic nanoparticles (MNPs) and magnetic fields are used to spatially manipulate molecules to trigger cellular processes in order to mimic and study natural signaling patterns [Monzel et al. (2017), DOI: 10.1039/C7SC01462G]. Here, we compared two MNPs regarding their use as nanoagents of cellular functions. First, a bio-inspired semisynthetic nanoparticle - Magnetoferritin (MFt) - was chosen, which consists of the iron storage protein ferritin and a synthetic magnetic iron oxide core. MFt is genetically equipped with mEGFP for microscopic observation and bio-orthogonal targeting [Lisse et al. (2017), DOI: 10.1002/adma.201700189]. Furthermore, synthetic iron-oxide MNPs (synomag, micromod, Rostock) were studied. After examining basic properties, we assessed methods of transfer into cells and probed MNP manipulation in the cytoplasm. Using external magnetic fields, MNPs were spatially redistributed and kinetically analyzed. Our magnetic manipulation approach bears the perspective to achieve an understanding of how cell signals evolve.

BP 4.9 Thu 11:15 P

On the adhesion-velocity relation and multistability of the motile state of MDA MB 231 cells on fibronectin lanes — Christoph Schreiber[1], Behnam Amiri[2], •Johannes Heyn[1], Joachim Rädler[1], and Martin Falcke[2,3] — [1]Ludwig-Maximilians-Universität München (LMU), Fakultät für Physik, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]Max Delbrück Center for Molecular Medicine in the Helmholtz Association, Robert Rössle Str. 10, 13125 Berlin, Germany — [3]Dept. of Physics, Humboldt University, Newtonstr. 15, 12489 Berlin, Germany

Migration of eukaryotic cells is a fundamental process for embryonic development, wound healing, immune responses, and tumour metastasis. A universal observation is the well-known biphasic adhesion-velocity relation. There is, however, little quantitative understanding of how adhesion and intracellular forces control cell velocity. We study the motion of MDA-MB-231 cells on microlanes with fields of alternating Fibronectin densities to address this topic and derive a mathematical model from the leading-edge force balance and the force-dependent polymerization rate. It reproduces quantitatively our measured adhesion-velocity relation. All motion-related forces are controlled by adhesion and velocity, which allows motion even with higher Fibronectin density at the rear than at the front. At transitions between different Fibronectin densities, steady motion is perturbed which changes the front and rear velocity. We then discuss the role of the biphasic relation between retrograde flow velocity and friction force for transitions of motile states.

BP 4.10 Thu 11:15 P

Exploring quantum features of the brain with MRI — •Christian Kerskens[1] and David Lopez Perez[1,2] — [1]Trinity College Institute of Neuroscience, Trinity College Dublin, Ireland — [2]Institute of Psychology, Polish Academy of Sciences, Warsaw, Poland

Recent proposals to explore quantum gravity have shown that if any physical system can mediate locally the generation of entanglement between two quantum systems, then it itself must be non-classical. Here, we adopted this idea to explore non-classicality in the human brain. Thereby, we considered an unknown brain function as the mediator which may or may not entangle the proton nuclear spins of free-diffusible bulk water. The challenge was to find a nuclear spin preparation that, together with a physiological condition, could facilitate the creation of quantum entanglement. For the spin preparation, we took the complementarity between magnetization and the likelihood of entanglement into account. As a result, we used a highly de-phased and saturated signal for our entanglement witness protocol, which was based on a hybrid multiple quantum coherence sequence. For the physiological condition, we assumed that some brain rhythms may influence the order at tissue level. Remarkably, we witnessed entanglement in the brains of our volunteers, if and only if, they were awake. Its temporal appearance showed a rhythm resembling heartbeat-evoked potentials. This link to conscious awareness underpins that the non-classical mediator may be used and manipulated in conscious-related computation, ergo we found indication that brain computation is non-classical.

BP 4.11 Thu 11:15 P

Revisiting the quantum brain — •Christian Kerskens — Trinity College Institute of Neuroscience, Trinity College Dublin, Ireland

More than 30 years ago, Penrose's published his pioneering ideas about the quantum brain, which was back then based on the knowledge at the time. This work, which marked an interim high in the field, received severe criticism. Meanwhile, many scientific areas relevant for the understanding of brain processes have evolved enormously. However, reservations remain. Here, we put some of those new jigsaw pieces together. We review findings from physics, quantum information, nematic, active matter, neuroscience, psychology, and philosophy which, we believe, could guide us towards a quantum brain theory. Thereby, we intend not to present a completed theory. We are aware that some direct translation from quantum physics to biology will, at the time, not hold a critical debate. However, we argue that the problem may be down to an insufficient understanding of physics, which needs to be solved. Biology may guide us (remember electrodynamics) once more to find in-depth insight into fundamental physics. Therefore, we divide the findings into those which resemble quantum computing but which can't be explained theoretically and into those which violate classicality in cognition and consciousness. We conclude that the brain may mimic a real brain quantum computer, which could potentially be based on topological quantum computing.

BP 5: Active Matter (joint session DY/BP/CPP)

Time: Thursday 11:45–13:00 Location: H2

BP 5.1 Thu 11:45 H2

Orientation-dependent propulsion of active Brownian spheres: from advection to polygonal clusters* — •Jens Bickmann[1], Stephan Bröker[1], Michael E. Cates[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Controllability of the collective dynamics of active Brownian particles is much desired for numerous potential future applications. In addition to the regular way of achieving control via external interventions, e.g., by traps, internal interventions in the dynamics of active Brownian particles become increasingly popular. Most often, internal intervention is achieved by a propulsion of the particles that depends on space, time, or orientation. Using field-theoretical modeling and particle-based simulations, we investigate systems of interacting active Brownian spheres in two spatial dimensions with an orientation-dependent propulsion. We show that different forms of orientation-dependent propulsion can give rise to advection, anomalous diffusion, and even the emergence of polygon-shaped clusters. **Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

BP 5.2 Thu 12:00 H2

The Anomalous Transport of Tracers in Active Baths — •Omer Granek[1], Yariv Kafri[1], and Julien Tailleur[2] — [1]Department of Physics, Technion-Israel Institute of Technology, Haifa, 3200003, Israel — [2]Université de Paris, Laboratoire Matière et Systèmes Complexes (MSC), UMR 7057 CNRS, F-75205 Paris, France

We derive the exact long-time dynamics of a tracer immersed in a one-dimensional active bath. In contrast to previous studies, we find that the damping and noise correlations possess long-time tails with exponents that depend on the tracer symmetry. For an asymmetric tracer, the tails lead to superdiffusion and friction that grows with time when the tracer is dragged at a constant speed. For a symmetric tracer, we recover normal diffusion and finite friction. However, when the symmetric tracer is small compared to the active-particle persistence length, the noise becomes anticorrelated at late times and the active contribution to the friction becomes negative: active particles then enhance motion rather than opposing it.

BP 5.3 Thu 12:15 H2

Forces on objects immersed in active fluids — Thomas Speck and •Ashreya Jayaram — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

Depending on their shape, objects immersed in active fluids may be subjected to a net force or net torque. We show that in a finite, periodic system, the force/torque on such an object is determined by the vorticity of the polarization of the surrounding active fluid which in turn is localized to regions close to the object where its curvature changes. We find that the system size L has a colossal influence on the magnitude of the force which grows as L^2 before saturating to a constant. We relate this force to the current away from the body and substantiate our theoretical results with numerical simulations of active Brownian particles.

BP 5.4 Thu 12:30 H2

Active Cooling in Inertial Active Matter — •Lukas Hecht[1], Suvendu Mandal[2], Hartmut Löwen[2], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

To cool down a target domain of an equilibrium system, the system must be coupled to an external bath to which heat can be transferred. However, active matter is intrinsically out of equilibrium and the active particles themselves do not obey the second law of thermodynamics. Therefore, we ask the question if we can actively cool down active particles in a target domain without transferring a significant amount of heat to particles in the environment.

In this work, we use the active Brownian particle (ABP) model with inertia to develop a route to cool down ABPs in a target domain without the need of an external bath. Such an active cooling requires two ingredients: First, we need the feature of inertial ABPs to undergo motility-induced phase separation into coexisting phases with different effective temperatures [1]. Second, a mechanism that localizes the phase-separated region in the target domain is required. We show several realizations of active cooling demonstrating how inertial effects in active matter can be utilized to actively cool down a target domain.

[1] S. Mandal, B. Liebchen, and H. Löwen, Phys. Rev. Lett. 123, 228001 (2019).

BP 5.5 Thu 12:45 H2

Arrested phase separation in nonreciprocally interacting colloids — •Sebastian Fehlinger and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Non-reciprocal interactions are wide spread in nature and can lead to a huge variety of phenomenons in many physical systems. For the specific case of a binary mixture of passive particles, the breaking of the action reaction principle can lead to formation of self-propelled dimers and other active molecules. For a small system size, these active molecules have already been realized in experiments based on phoretically interacting binary colloidal mixtures [1].

This work focuses on the numerical simulation of the Langevin equations describing many noninteracting colloids which we complement with a continuum theory. We find that the nonreciprocal attractions destabilize the uniform disordered phase and lead to clusters which grow in the course of the time. Surprisingly, for a wide parameter range, the clusters only grow up to a certain size such that coarsening is arrested. We attribute this to the spatiotemporal organization of the composition of the binary mixture within the cluster which essentially screens the phoretic attractions.

[1] F. Schmidt, B. Liebchen, H. Löwen, G. Volpe, J. Chem. Phys. 150, 094905 (2019).

BP 6: Membranes and Vesicles

Time: Thursday 13:30–14:45 Location: H6

Invited Talk BP 6.1 Thu 13:30 H6

How do lipids and proteins diffuse in cell membranes, and what do the diffusion experiments actually measure? — •Ilpo Vattulainen — Department of Physics, University of Helsinki

There are various techniques able to gauge diffusion in biomembranes. For instance, quasi-elastic neutron scattering measures diffusion in a non-perturbative manner over nanosecond time scales, yet sampling in space is in these experiments done over large distances. Meanwhile, single-particle tracking allows one to measure the dynamics of individual molecules in almost nanometer resolution, but these measurements are based on the use of markers that may interfere with the diffusion process. Here we discuss nanoscale simulation studies designed to explore the underlying molecular-scale diffusion mechanisms of lipids and membrane proteins. We also discuss the bases of single-particle tracking experiments by considering the effects of streptavidin-functionalized Au nanoparticle probes on lateral diffusion. The results show that lipids diffuse in a concerted fashion as clusters of lipids whose motion is highly correlated, and membrane proteins move as dynamical complexes with tens of lipids bound to the protein. Lipids linked to a streptavidin-nanoparticle complex also turn out to move in a concerted manner but as a complex with the linker protein and numerous non-labeled lipids, slowing down the motion of the probe by an order of magnitude. The results highlight that prior to using any technique, it is crucial to understand the physical basis of the diffusion process that one aims to measure. Otherwise, interpretation of experimental data can be a surprisingly difficult task.

BP 6.2 Thu 14:00 H6

Fusion of virus and host membranes - the role of virus geometry and matrix proteins — •Gonen Golani[1], Sophie Winter[2], Steffen Klein[2], Petr Chlanda[2], and Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics and BioQuant, Heidelberg University, D-69120 Heidelberg, Germany — [2]Schaller Research Groups, Department of Infectious Diseases-Virology, Heidelberg University Hospital, D-69120 Heidelberg, Germany

Many medically important viruses are enveloped by a lipid membrane, therefore, a crucial step in the infection process is the fusion of the viral and cellular membranes. The fusion pathway involves a series of non-bilayer intermediates configurations: First, the monolayers of the two opposing membranes merge to form a hemifusion connection, referred to as the stalk. Next, expansion of the stalk brings the distal lipid monolayers together into a hemifusion diaphragm. Lastly, opening and expansion of a fusion pore within the diaphragm completes the fusion process. The formation of the stalk and expansion of the fusion pore constitute the two major energy barriers in the process. While formation of the stalk is directly driven by the viral fusion proteins and was extensity studied in the last decades, pore expansion is less well understood. Here we compute the stresses in the diaphragm and the resulting energy barrier to fusion pore expansion. We analyze, for the first time, effect of the virus geometry and membrane-matrix interaction on viral fusion rate. We also suggest a model for the role of interferon-induced transmembrane proteins (IFITMs) in inhibition of fusion by increasing the energy barrier of fusion pore expansion.

BP 6.3 Thu 14:15 H6

Calponin-homology domain mediated bending of membrane associated actin filaments — Saravanan Palani[1,2], Sayantika Ghosh[1], Esther Ivorra-Molla[1], Scott Clarke[1], Andrejus Suchenko[1], Mohan Balasubramanian[1], and •Darius Köster[1] — [1]Centre for Mechanochemcial Cell Biology and Warwick Medical School, Division of Biomedical Sciences, CV4 7AL Coventy, UK — [2]Department of Biochemistry, Division of Biological Sciences, Indian Institute of Science, Bangalore-560012, India

Actin filaments are central to cell function and the actin cytoskeleton exhibits a variety of geometries. Here, we show that 'curly', the actin-binding calponin-homology domain and a C-terminal unstructured domain from the IQGAP family of proteins, stabilizes individual actin filaments in a highly curved geometry when anchored to lipid membranes. Whereas F-actin is semi-flexible with a persistence length of $10\mu m$, binding of mobile curly within lipid membranes generates actin filament arcs and full rings of high curvature with radii below $1\mu m$. Higher rates of fully formed actin rings are observed in the presence of the actin-binding coiled-coil protein tropomyosin and when actin is directly polymerized on lipid membranes decorated with curly. Strikingly, curly induced actin filament rings contract upon the addition of muscle myosin II filaments and expression of curly in mammalian cells leads to highly curved actin structures in the cytoskeleton. Taken together, our work identifies a new mechanism to generate highly curved actin filaments, which opens a range of possibilities to control actin filament geometries in vitro and in vivo.

BP 6.4 Thu 14:30 H6

Fission mechanisms of cylindrical membrane tubes — •Russell Spencer and Marcus Müller — Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

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) connecting the metastable starting and ending states of different membrane topology in order to determine the most likely pathway for the transition. Our results suggest that the free energy barrier to membrane fission, as well as the dominant pathway, can be controlled by the tension experienced by the membrane. At high tension, the inner tube partially collapses into a worm-like micelle, which then ruptures, resulting in two capped tubes. The outer membrane then follows similarly. This pathway is non-leaky, i.e. the solvent inside the inner membrane, between the membranes and outside the outer membrane never mix. At lower tension, the barrier to forming a worm-like micelle becomes prohibitive, and instead, the inner and outer membranes fuse. This pathway is leaky as pores form close to the fusion sites.

BP 7: Cell Mechanics, Cell Adhesion and Migration, Multicellular Systems

Time: Thursday 15:00–16:15 Location: H6

Invited Talk BP 7.1 Thu 15:00 H6

Shaping embryos through controlled tissue phase transitions — •Otger Campàs — Physics of Life Excellence Cluster, TU Dresden, Germany — University of California, Santa Barbara, USA

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 largely unknown, mainly because of a lack in methodologies enabling direct in vivo and in situ measurements of forces and mechanical properties within developing 3D tissues and organs. For similar reasons, understanding the fundamental physical nature of active multicellular systems has been very challenging. We have recently developed novel microdroplet-based techniques that allow direct quantitative measurements of mechanical forces and material properties within 3D multicellular systems, including developing embryonic tissues. Using these techniques and focusing on the elongation of the body axis, a hallmark morphogenetic process in vertebrate development, we reveal a new physical mechanism of tissue morphogenesis whereby spatiotemporally controlled fluid-to-solid (rigidity) transitions in the tissue physical state, rather than patterned mechanical stresses, guide tissue flows to shape functional embryonic structures. Moreover, combining computational and experimental data, we show that active tension fluctuations control tissue fluidization in vivo.

BP 7.2 Thu 15:30 H6

Traction force microscopy with invertible neural networks — •Johannes Blumberg[1], Timothy Herbst[1,2], Ullrich Koethe[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics and Bioquant, Heidelberg University — [2]Visual Learning Lab, IWR, Heidelberg University

In traction force microscopy (TFM), the mechanical forces of cells adhering to an elastic substrate are estimated from the substrate displacements as measured by the movement of embedded fiducial marker beads. While the direct problem of calculating displacement from forces is well-defined by elasticity theory, the inverse problem of reconstructing forces from displacements is ill-posed. Usually an estimate is obtained by minimizing the mean squared distance between experimentally observed and predicted displacements. The standard method in this regard is Fourier Transform Traction Cytometry (FTTC), whose superior efficiency is based on the convolution theorem in Fourier space. Here we explore if the performance can be improved by using machine learning methods, in particular invertible neural networks, which recently have emerged as powerful method to solve ill-posed inverse problems.

BP 7.3 Thu 15:45 H6

An active gel model for optogenetic control of cell migration — •Oliver M. Drozdowski[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany

Optogenetics has emerged as a new powerful experimental method to control cellular processes in space and time, including actin filament polymerization and contractility of myosin II molecular motors. Here we report on a mathematical analysis of spatiotemporal activation patterns in a simple one-dimensional variant of active gel theory with the aim to predict how optogenetics can be used to control cell migration [1]. We first show that the model can describe the symmetrical flow of the actomyosin system observed in optogenetic experiments but not the long-lasting polarization required for cell migration. Motile solutions, however, become possible if cytoskeletal polymerization is included through the boundary conditions. Optogenetic activation of contraction can then initiate locomotion in a symmetrically spreading cell and strengthen motility in an asymmetrically polymerizing one. If designed appropriately, it can also arrest motility even for protrusive boundaries.

[1] https://arxiv.org/abs/2104.14636, to appear in Phys. Rev. E

BP 7.4 Thu 16:00 H6

Defect-mediated morphogenesis — •Ludwig A. Hoffmann, Livio N. Carenza, Julia Eckert, and Luca Giomi — Universiteit Leiden, The Netherlands

Growing experimental evidence indicates that topological defects could serve as organizing centers in the morphogenesis of tissues. We provide a quantitative explanation for this phenomenon, rooted in the buckling theory of deformable active polar liquid crystals. Using a combination of linear stability analysis and computational fluid dynamics, we demonstrate that confined cell layers are unstable to the formation of protrusions in the presence of disclinations. The instability originates from an interplay between the focusing of the elastic forces, mediated by defects, and the renormalization of the system's surface tension by the active flow. The post-transitional regime is also characterized by several complex morphodynamical processes, such as oscillatory deformations, droplet nucleation and active turbulence. Our findings offer an explanation of recent observations on tissue morphogenesis and shed light on the dynamics of active surfaces in general.

BP 8: Annual General Meeting

Time: Thursday 18:00–19:00 Location: MVBP

Annual General Meeting

BP 9: Machine Learning in Dynamical Systems and Statistical Physics (joint session DY/BP)

Time: Friday 11:15–12:30 Location: H2

BP 9.1 Fri 11:15 H2

Tayloring Reservoir Computing Performance via Delay Time Tuning — •Tobias Hülser, Felix Köster, and Kathy Lüdge — Institut für Theoretische Physik, TU Berlin

Reservoir Computing is a versatile, fast-trainable machine learning scheme that utilises the intrinsic information-processing capacities of dynamical systems. In recent years delay-based reservoir computing emerged as a promising, easy to implement alternative to classical reservoir computing. Previous work showed that a mismatch between input time and delay time enhances computational performance significantly[1]. For delays much higher than the input time, it was shown that certain inputs cannot be recalled by the network which lead to gaps in the memory capacity[2]. Via manipulating the delays in a system of ring-coupled Stuart-Landau oscillators, we show that some of the gaps can be closed. Moreover, we can tune the range of previous inputs the reservoir can memorise. Consequently, we find a significant increase in performance for nonlinear memory tasks and the NARMA10 task.

[1] S. Stelzer et al., Neural Networks 124, 158-169 (2020)
[2] F. Köster et al., Cogn. Comput. (2020)

BP 9.2 Fri 11:30 H2

Employing artificial neural networks to find reaction coordinates and pathways for self-assembly — •Jörn Appeldorn, Arash Nikoubashman, and Thomas Speck — Inst. für Physik, Universität Mainz, Germany

We study the spontaneous self-assembly of single-stranded DNA fragments using the coarse-grained oxDNA2 implementation [1]. A successful assembly is a rare event that requires crossing a free energy barrier. Advanced sampling methods like Markov state modeling allow to bridge these long time scales, but they require one or more collective variables (order parameters) that faithfully describe the transition towards the assembled state. Formulating an order parameter typically relies on physical insight, which is then verified, e.g., through a committor analysis. Here we explore the use of autoencoder neural networks to automatize this process and to find suitable collective variables based on structural information. For this step, one still needs to map configurations onto structural descriptors, which is a non-trivial task. Specifically, we investigate the latent space of EncoderMap [2] and how it changes with the amount of information contained in the descriptor. With this approach, we were able to determine the free energy landscape, the locations of the (meta)stable states, and the corresponding transition probabilities.

[1] - Snodin et al., J. Chem. Phys.(2015), 142, 234901 [2] - T. Lemke and and C. Peter,J.Chem.TheoryComput.(2019), 15, 1209-1215

BP 9.3 Fri 11:45 H2

Efficient Bayesian estimation of the generalized Langevin equation from data — •Clemens Willers and Kamps Oliver — Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Corrensstr. 2, 48149 Münster, Germany

A recent topic of research attracting broad interest is the modeling of stochastic time series whose dynamics includes memory effects. To cover this non-Markovian case, the Langevin equation, which is frequently used in many fields of science, is extended by a memory kernel, yielding the generalized Langevin equation (GLE). Since a direct derivation of the GLE from basic mechanisms through the well known Mori-Zwanzig formalism is not accessible in many cases, it is a relevant question how to estimate the model solely based on measured data.

In our work we develop a realization of Bayesian estimation of the GLE. The Bayesian approach allows for the determination of both estimates and their credibility in a straightforward manner. To facilitate this method, we consider the GLE with white noise. Although

this is an approximation, we still deal with a very general model class representing systems with memory.

Importantly for applications, we realize the method in a numerically efficient manner through a piecewise constant parameterization of the drift and diffusion functions of the model, a reformulation of the likelihood, and an effective initial guess for the estimate.

We illustrate our method by an example from turbulence. Here we are able to reproduce the autocorrelation function of the original data set, which is an essential characteristic of a turbulent flow.

BP 9.4 Fri 12:00 H2

Master memory function for delay-based reservoir computers — •Felix Köster[1], Serhiy Yanchuk[2], and Kathy Lüdge[1] — [1]Institut für Theoretische Physik, TU Berlin, Hardenbergstraße 36, 10623 Berlin — [2]Institut für Mathematik, TU Berlin, Str. des 17. Juni 136, 10587 Berlin

The reservoir computing scheme is a versatile machine learning mechanism, which shows promising results in time-dependent task predictions in comparable fast-training times. Delay-based reservoir computing is a modification in which a single dynamical node under the influence of feedback is used as a reservoir instead of a spatially extended system.

We show that many delay-based reservoir computers considered in the literature can be characterized by a universal master memory function (MMF). Once computed for two independent parameters, this function provides linear memory capacity for any delay-based single-variable reservoir with small inputs. Moreover, we propose an analytical description of the MMF that enables its efficient and fast computation. Our approach can be applied not only to the reservoirs governed by known dynamical rules such as Mackey-Glass or Ikeda-like systems but also to reservoirs whose dynamical model is not available.

BP 9.5 Fri 12:15 H2

Investigating the role of Chaos and characteristic time scales in Reservoir Computing — Marvin Schmidt[1,2], Yuriy Mokrousov[1,3], Stefan Blügel[1,3], Abigail Morrison[2,3,4], and •Daniele Pinna[1,3] — [1]Peter Grünberg Institute (PGI-1), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Institute for Theoretical Neuroscience Institute of Neuroscience and Medicine (INM-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [3]Institute for Advanced Simulation (IAS-6), Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [4]Computational and Systems Neuroscience & JARA-Institut Brain structure-function relationships (INM-10), Wilhelm-Johnen-Straße, 52428 Jülich, Germany

Reservoir Computing (RC) dynamical systems must retain information for long times and exhibit a rich representation of their driving. This talk highlights the importance of matching between input and dynamical timescales in RC systems close to chaos. We compare a chain of Fermi-Pasta-Ulam-Tsingou anharmonic oscillators and a sparsely connected network of spiking excitatory/inhibitory neurons. The first is toy model for magnetic spin-wave reservoirs while the latter that of a biological neural net. Both systems are shown to rely on a close matching of their relaxation timescales with the driving input signal's frequency in order to memorize and make precise use of the information injected. We argue that this is a general property of RC systems. We acknowledge the HGF-RSF project TOPOMANN for funding.