THIRD INFINITY

Physics of Biological and Complex Systems

21-23 September 2022

Max Planck Faßberg Campus, Göttingen

Third Infinity 2022: Beyond Scientific Borders
Abstract Booklet

September 19, 2022

Third Infinity 2022: Beyond Scientific Borders
Abstract Booklet
Göttingen, Germany, September 21 - 23, 2022
Editors: Sayedeh Hussaini, Jonas Dehning, and Venecia Chávez Medina

Göttingen, 2022

Cover and logo design: Sara Gabrielli
Alpaca picture: Irene Boettcher-Gajewski

Distributed free of charge

Preface

All of us, the organizing team, members of the Department of Physics of Biological and Complex Systems at the International Max Planck Research School, are pleased to welcome you to the fifth edition of the Third Infinity Conference: Beyond Scientific Borders. This conference is jointly organized by Ph.D. students and post-doctoral researchers at the MPI for Dynamics and Self-Organisation, the MPI for Multidisciplinary Sciences, and the University of Göttingen.

Third Infinity aims to provide an interdisciplinary platform for motivated young and experienced researchers from around the world to exchange ideas and promote scientific research in the field of physics of biological and complex systems. The goal is to provide participants with the latest advances in their fields through invited talks by high-profile speakers, and active, face-to-face interactions. Primarily, Third Infinity welcomes enthusiastic students who present and report on their latest findings and developments through student talks and poster sessions, with each session led by a renowned and experienced scientist and world leader in the field. One of the greatest benefits of a conference is the opportunity for scientists from around the world to meet and exchange ideas, hence at Third Infinity, our priority is to create a fruitful social environment in which new scientific collaborations and friendships can develop.

The conference will take place over three days and will cover three different scientific topics: *"Nonlinear dynamics and complex networks"*, *"Biophysics from experiments to computation"*, and *"Active matter and statistical physics"*. For each topic, we have invited at least two high-profile speakers. This year's scientific sessions are inaugurated by our keynote speaker Prof. Bjorn Stevens. In addition, a total of 20 oral contributions from Ph.D. students and postdocs will be presented. Two poster sessions will also be held on the first two days of the conference. Furthermore, five alumni from the research school will join us for two interactive sessions where we will learn from their experiences and the different paths that led them to their current positions: industry, academia, and start-up business. Finally, during the last day, in addition to the scientific lectures and the alumni presentations, we will have our sponsors on board with talks, a workshop, and booths. Their contribution has facilitated the organization of this conference, to which we are grateful.

With the title of the edition of this year's conference in mind, *Beyond Scientific Borders*, and our commitment to organize an environmentally sustainable conference, we would like to point out that, from day one of the organization, we have

done our best to make the most environmentally-friendly possible decisions and actions. On that note, the opening and closing scientific lectures respectively by our keynote Prof. Bjorn Stevens, and Prof. Marc Timme, will center around earth system models, and climate and energy in our planet. In addition, we targeted our selection of speakers and alumni to those based in Europe, making their accessibility to Göttingen more environmentally friendly always prioritizing train as the mean of transport. We have also dispensed with printing the brochure and made it available online for everyone. And lastly, small note in passing, our buffet for the conference dinner offers four out of five different vegetarian and vegan options. We hope that all these reflections will become a tradition in the organization of the Third Infinity Conference.

We look forward to three days of cutting-edge science during the 5th edition of the conference: *Third Infinity 2022: Beyond Scientific Borders*, here in Göttingen, *the city of science.*

Your Third Infinity 2022 Organizing Team

Organization

Third Infinity is a biennial conference organized by the graduate school for Physics of Biological and Complex Systems as a member of the International Max Planck Research School (IMPRS-PBCS).

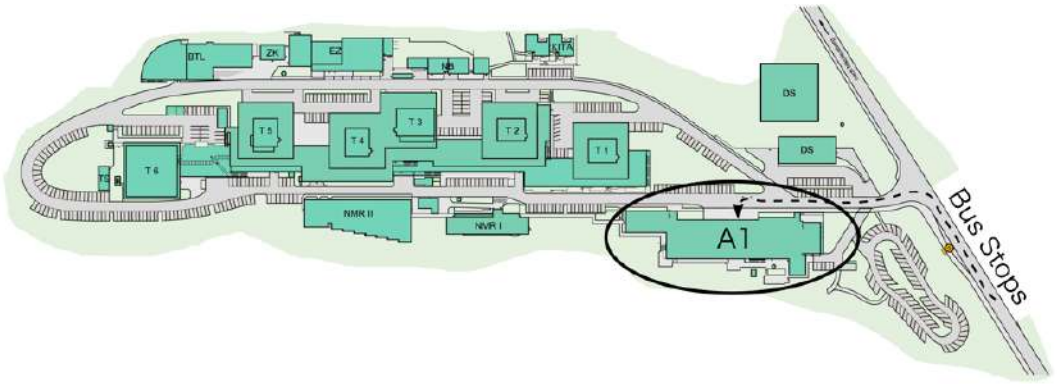
Organization committee

In the first row from left to right: Sara Gabrielli, Rodrigo Catalan, Birte Thiede and Sayedeh Hussaini. In the second row, from left to right: Tina Abbasi, Justine Wolter, Venecia Chávez Medina, and Nick Scholand. Not in the picture, but in all of our hearts: Jonas Dehning. In the background: the actual organization committee.

General Information

Venue

The conference will take place at the Max Planck Campus in Göttingen (Am Fassberg 11, 37077 Göttingen, Germany) in building A1. This building is home to the Manfred Eigen lecture hall in which all talks will be given, the Prandtl lecture hall in which the poster sessions will be held, the foyer in which registration and all coffee breaks will take place and the cafeteria (downstairs) in which lunch will be served.



Public transportation

To get to the campus, there are three bus lines: 21, 22 and 23. You can take line 22 if your accommodation is in the city center, but lines 21 and 23 also have stops near the city center and both have a stop at the train station. The ticket can be bought directly from the bus driver and only with cash or in the ticket shops (e.g. GöVB Service Center, Groner str 40, 37077, Göttingen), where you can also pay with a credit card. If you would like to buy an online ticket, please visit this website: **https://www.goevb.de/fahrkarten/luftlinientarif**

Registration

The registration desk is in the foyer of building A1, just left of the main entrance. Registration will begin on Wednesday, September the 21st, 2022 at 08:30 and officially remains open until 09:30. For attendees who are not able to register during that time, our committee members will attempt to staff the registration desk throughout the period of the conference. If you find yourself at the registration desk

with no one to help you, please contact a member of the committee for assistance. You will easily recognize us by a volunteer badge and T-shirts with the Third Infinity logo.

Identification badge

You will be given a conference badge when you register. Please wear your badge at all times so that you can be easily recognized by the other conference participants and the organizing team. Use the QR code on the badge to connect to our website and quickly access the booklet and all relevant information.

Coffee breaks

Coffee breaks will be held in the foyer in between sessions. Coffee, tea, water, and snacks will be available for all. We respectfully but firmly ask our guests to stick to these times so that the schedule for the presentations can be adhered to.

Poster sessions

The poster sessions will take place on Wednesday the 21st and Thursday the 22nd of September. The session on Wednesday will take place from 17:00 to 18:30, while the one on Thursday will start at 17:10 and will last until 20:00. **On Wednesday all odd-numbered posters are scheduled, and on Thursday the even-numbered**. Poster numbers can be found on the left/right side of the corresponding abstract. During both poster sessions, juice and snacks will be provided. In addition, pizza will be provided during the second half of the poster session on Thursday.

Color code

The following color code is used in the conference booklet to identify the different subjects of each session:

Nonlinear dynamics and complex networks

Biophysics from experiments to computations

Active matter and statistical physics

Photo Policy

Please note that we will be taking photos and/or films during the conference, which may be used afterward for reporting on this event and for other non-commercial purposes, e.g. website, press releases, social media, etc. If you do not agree to this, please contact the photographer(s) and/or filmmaker(s) directly.

Social Media

During the conference we will post pictures, announcements and important communications on Twitter, Instagram and LinkedIN. Follow us and/or join the LinkedIN group to stay posted and live the full Third Infinity experience!

Internet

For those who are eligible, the Eduroam WiFi network should suffice for those wishing to connect to the Internet during the conference. Otherwise, the access data for the MPI's WiFi network can be provided upon your request.

Contact information

Antje Erdmann
Phone: +49 551 201-2322
Email: 3rdinfinity@gwdg.de
Website: https://thirdinfinity.mpg.de/

Emergency contact

In case of an emergency, please dial 110 (police) or 112 (fire and/or medical emergency). In case of an emergency requiring immediate pharmaceutical attention, an emergency pharmacy is centrally located in Göttingen:

Goethe-Apotheke
Goethe-Allee 17
37073 Göttingen
Tel.: +49 551 56364

Social Program

Conference dinner

The conference dinner will be held at Kartoffelhaus restaurant, located in the city center of Göttingen. The dinner will take place on the evening of Wednesday the 21st of September, starting at 19:30. The dinner is open to all those who opted for the conference dinner during the registration process, but is not mandatory.

Please note that the Third Infinity Organization will not pay for alcoholic drinks during the conference dinner.

The exact location of Kartoffelhaus is: Goethe-Allee 8, 37073 Göttingen (https://www.kartoffelhaus-goettingen.de/)

Conference picture

A photographer will be present all throughout the conference to take photos during the talks and the rest of the events. On Wednesday, September 21st, during the afternoon coffee break from 15:00 to 15:30, we will be taking a group picture to celebrate everyone's presence. We ask all participants to meet outside in front of the conference building. During the coffee break, an announcement will be made to make sure everyone is aware and able to participate.

THIRD INFINITY 2022

Schedule

Wednesday 21.09.2022

8:30-9:30	Registration	
9:30-9:45	Opening remarks	
9:45-10:30	KEYNOTE: Bjorn Stevens	Nonlinear Dynamics & Complex Networks
10:30-10:50	Fabián Álvarez Garrido	
10:50-11:10	Lukas Bentkamp	
11:10-11:30	Diego Tapias	
11:30-12:00	Coffee break	
12:00-13:00	Panel discussion	
13:00-14:00	Lunch	
14:00-15:00	Workshop : Science Communication	
15:00-15:30	Coffee break and **event photo**	
15:30-16:00	Jochen Guck	Biophysics from Experiments to Computation
16:00-16:20	Theresa Bender	
16:20-16:40	Christian F. Pantoja	
16:40-17:00	David Joseph	
17:00-18:30	Poster session	
19:30	Science table	

Thursday 22.09.2022

9:40-10:10	Anne Grapin Botton	Biophysics from Experiments to Computation
10:10-10:30	Sayedeh Hussaini	
10:30-10:50	Aina Gallemi Perez	
10:50-11:20	Coffee break	
11:20-11:50	Thomas Speck	Active Matter & Statistical Physics
11:50-12:10	Yiwei Zhang	
12:10-12:30	Vincent Ouazan--Reboul	
12:30-12:50	Maximilian Kurjahn	
12:50-13:10	Lorenzo Piro	
13:10-14:10	Lunch	
14:10-14:40	Remi Monasson	Alumni Talks
14:40-15:00	Moshir Harsh	
15:00-15:20	Filipe Thewes	
15:20-15:40	Atul Tanaji Mohite	
15:40-16:10	Coffee break	
16:10-16:25	Hinrich Arnoldt	
16:25-16:40	Laura Turco	
16:40-16:55	Mirna Kramar	
16:55-17:10	Questions from students	
17:10-18:10	Poster session	
18.10-20.00	Extended poster session with pizza	

Friday 23.09.2022

9:20-9:30	Announcement alpaca prize	
9:30-10:00	Andela Saric	Biophysics from Experiments to Computation
10:00-10:20	Vedran Miletic	
10:20-10:40	Nicolai Kozlowski	
10:40-11:00	Lukas Hasecke	
11:00-11:30	Coffee break	
11:30-12:00	Marc Timme	Nonlinear Dynamics & Complex Networks
12:00-12:20	Sebastian Contreras	
12:20-12:40	Jonas Dehning	
12.40-13.10	D-fine	
13:10-14:10	Lunch	
14:10-14:25	Marcel Bremerich	Alumni talks + Career fair & Company talks
14:25-14:40	Benjamin von Ardenne	
14:40-14:50	Questions from students	
14:50-15:50	Coffee break and career fair	
15:50-16:10	Life Science Factory	
16:10-16:30	Indiscale	
16:30-17:10	Workshop: Introduction to LinkAhead (from Indiscale)	
17:10-17:40	Marc Timme: closing talk	
17:40-18:00	Final remarks+ lottery and awards	
18:00-21:00	Pizza and networking (+music band)	

All **talks** will be held in the **Manfred Eigen Hall**
Poster sessions and **workshops** will take place in the **Prandtl Hall**
The **career fair** booths will be placed in the **Foyer** on Friday, September 23

Scan the QR code for booklet+info!

Panel discussion

Science communication: our debt to society?

Information crisis. Health crisis. Environmental crisis. In a time of interconnected global challenges, good scientific communication becomes a social responsibility. But who is responsible for this ? Who can benefit from science communication? What should be communicated and how? The panel discussion will cast a light on science communication from the perspectives of a scientist, a journalist, and a science communicator. The participants will be directly involved in the discussion, navigating across and beyond scientific borders together with the panelists.

Dr. Manuel Maidorn, Press officer for the Max Planck Institute for Dynamics and Self-Organization, has kindly agreed to moderate the discussion. The panelists are:

1. Melissa Sollich, International Communications, University of Göttingen and Postdoc Network Coordinator, Göttingen Campus

2. Dr. Johannes Zierenberg, Postdoctoral researcher at the Max Planck Institute for Dynamics and Self-Organization

3. Fred Schwaller, PhD, Science writer, journalist, and communicator

(Wednesday, 21 September, 12:00-13:00, Manfred Eigen lecture hall)

Workshops

Workshop on the topic: "Science Communication - Storytelling"

Telling an exciting and memorable story is one of the key components for efficient science communication. After a quick, get-to-know-you session, you will work together to create a story about a scientific topic and present it to a defined audience. Depending on your target group, you may evolve different communication strategies to get your message across correctly, clearly and in adequate detail. The workshop will be held by Melissa Solich, Science Communicator and Coordinator of the Göttingen PostDoc Net and Dr. Manuel Maidorn, Press Officer at the Max Planck Institute for Dynamics and Self-Organization.
(Wednesday, September 21, 14:00-15:00, in Prandtl lecture hall)

Workshop on the topic: "LinkAhead Introduction"

Data management involves the storing, searching, retrieving and analyzing of data sets and their connections and circumstances. Good data management makes valuable data reusable for yourself and for others. It also makes data findable (Where did I put that USB disk again?) and adds real utility to data, because data can be embedded into context. (Which machine settings did my supervising post-doc use when they acquired that file?)

The open-source toolkit CaosDB can help with all these tasks, and much more: The structure of data can be modified later without losing old information, so scientists have all the flexibility they ever need. And it comes with a powerful Python client, so access is as easy as a few lines of code.

In this hands-on workshop, we will create a data structure and then insert, link and retrieve some data. Attendees who want to follow the workshop on their own machines should install CaosDB's Python library and additional tools with 'pip install caosdb caosadvancedtools' and make sure that they can load the library in Python with 'import caosdb'.
(Friday, September 23, 16:30-17:10, Manfred Eigen lecture hall)

Alumni sessions

Hinrich Arnoldt

Hinrich Arnoldt works as academic sales manager at Comsol Multiphysics GmbH since 2020. He joined the company in 2014 as technical sales engineer. Previously, he studied the physics of complex systems at the Max Planck Institute for Dynamics and Self-Organization. He earned his diploma and PhD studying neural network and evolutionary dynamics.
(Thursday, September 22, 16:10-16:25, Manfred Eigen lecture hall)

Laura Turco

Laura studied Biomedical Engineering at the Politecnico of Milano, Italy and in Uppsala, Sweden and obtained a PhD at the Max Planck Institute for Dynamics and Self-organization in Göttingen. She then did her Postdoc on microfluidic/microfabrication for tissue engineering and synthetic biology. She then established a group on microfluidics and medical applications, while managing the cleanroom facility at the Max Planck Institute for Dynamics and Self-organization in Göttingen. Her latest research focused on bioink development and bioprinting technologies for engineered myocardium. Since 2021, she joined Bayer within the International Future Leadership Program and has been in several department within product supply (Quality, Production, Operational Excellence).
(Thursday, September 22, 16:25-16:40, Manfred Eigen lecture hall)

Mirna Kramar

Mirna studied Chemistry at the University of Zagreb, Croatia and Biophysics at the Technical University of Dresden, Germany. In 2016, she joined the MPI-DS in Göttingen and started her PhD within the GGNB-PBCS, studying the phenomena underlying the behaviour of the unicellular slime mould. Mirna defended her PhD in 2020, after which she moved to Paris for her postdoctoral work at the Institut Curie.
(Thursday, September 22, 16:40-16:55, Manfred Eigen lecture hall)

Marcel Bremerich

Marcel obtained his physics diploma from the Clausthal University of Technology in 2007. In 2012 obtained his Ph.D. from the Biophysics program at GGNB University of Göttingen. After finishing his Ph.D. thesis in the group of Prof. Dr. Christoph Schmidt, he joined the group of Prof. Dr. Daisuke Mizuno at Kyushu University, Japan, as a postdoctoral fellow. Since 2013 he works as a Scientist and Application Specialist for diagnostic membranes in the R&D department at Sartorius Stedim Biotech GmbH. He is dedicated to production and quality control support, customer service, and research on fluid flow dynamics in porous media.
(Friday, September 23, 14:10-14:25, Manfred Eigen lecture hall)

Benjamin von Ardenne

Benjamin obtained his bachelor's and master's (graduated with distinction) degrees at the University of Göttingen. In 2018 he obtained his Ph.D. with summa cum laude at the Max-Planck Institute for Biophysical Chemistry in the International Max Planck Research Schools (IMPRS) "Physics of Biological and Complex Systems". From 2014 to 2019 he became an entrepreneur and software developer for full-platform mobile apps. Then from 2019 to 2020 a software developer at loanboox, CH, Zürich. From 2020 to 2021 a senior data scientist and AI engineer at JUST ADD AI (JAAI) GmbH, Bremen. And since 2022 the CEO at lector.ai GmbH (part of JAAI Group), Bremen.
(Friday, September 23, 14:25-14:40, Manfred Eigen lecture hall)

Talks

Wednesday morning talks

Nonlinear dynamics and complex networks

Wed 21st
9:45–10:30

Keynote

Earth system models — physics and fantasies

Prof. Bjorn Stevens

MPI for Meteorology, Hamburg

bjorn.stevens@mpimet.mpg.de

Earth system models are about as old as the automobile. Since the very beginning, and almost by definition, these models have mixed physics with fantasy to create images of future worlds. In outlining the evolving balance between the two, and the factors that determine it, I will describe the frontiers of present understanding, insights we can still hope to glean, and fantasies we may wish to pursue. I will aim to present my ideas in ways that encourage discussion on more general topics, such as the role of modeling versus simulation, and authority versus reason, in research programs designed to advance understanding of complex systems.

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Towards an effective description of turbulent superstructures in simple shear flows

Wed 21st
10:30–10:50

Fabián Álvarez Garrido[1], Michael, Wilczek[2]

[1]Univesität Bayreuth

[2]Theoretical Physics I, University of Bayreuth, Bayreuth

fabian.alvarez-garrido@uni-bayreuth.de

Turbulent flows driven by large-scale forces such as convection, shear, or rotation may display large-scale coherent flows, namely turbulent superstructures, coexisting with fully developed turbulence on the small scales. A complete description of these flows involves innumerable degrees of freedom, yet turbulent superstructures seem to evolve according to a comparably lower-dimensional set of equations. In addition, despite the ubiquity of turbulent superstructures, their interplay with the smaller scales is not yet fully understood. We study a simple shear-driven flow, the three-dimensional Kolmogorov flow. The large scales in this flow feature the formation of large-scale vortex pairs.Moreover, the system exhibits permanent dynamics between states having a different number of vortex pairs. Employing amplitude equations, we characterize the dynamics of the large scales close to the onset of the vortex pairs. We show that the dynamics close to the onset correspond to the one of a two-dimensional flow. Furthermore, we show that far from the onset, the derived model captures the structure of the large-scale vortices. Based on data from direct numerical simulations, we introduce new stochastic terms to these amplitude equations to model the contribution of the small scales to the dynamics of the large ones. These modified amplitude equations can qualitatively reproduce the dynamics of these large-scale vortex pairs and shed light on the role of small-scale turbulence in the formation of turbulent superstructures.

Temporal large-scale intermittency in turbulent flows

Wed 21st
10:50–11:10

Lukas Bentkamp[1], Michael Wilczek[1]

[1]University of Bayreuth

lukas.bentkamp@uni-bayreuth.de

Turbulent flows are ubiquitous in nature and technology. The temporal structure of their largest scales can be very diverse: For instance, ocean currents may maintain a persistent large-scale shear generating turbulence. By contrast, atmospheric turbulence is driven periodically by diurnal cycles.In three-dimensional turbulence, energy is transported from these large scales to the small scales. Since the smallest scales result from the nonlinear dynamics across the scales, they are often thought of as independent of the large scales. However, as famously remarked by Landau in 1944, sufficiently slow variations of the large scales should nonetheless be expected to impact small-scale statistics. Such variations, termed large-scale intermittency, are often found in experiments and simulations while differing from flow to flow.Here we evaluate the impact of large-scale fluctuations on velocity, velocity gradient, and acceleration statistics. We introduce controlled temporal variations of the energy

injection rate into direct numerical simulations of turbulence. We find that slow variations can strongly impact flow statistics, amplifying the tails of the measured distributions. Moreover, we show that the stronger tails can be mimicked by an ensemble of stationary flows. For this, we superpose ensemble statistics such that the temporal variations of flow measures, such as the energy dissipation rate, are matched. Overall, our work demonstrates that in order to ensure comparability of statistical results in turbulence, one needs to take large-scale intermittency into account.

Wed 21st
11:10–11:30

Subaging in underparametrized Deep Neural Networks

Diego Tapias[1], Carolina Herrera[2], Edison Montoya[3]

[1]Georg-August-Universität Göttingen
[2]Universidad de Antioquia
[3]BCFort

diego.tapias@theorie.physik.uni-goettingen.de

I will introduce a simple classification problem to show that the dynamics of finite–width Deep Neural Networks in the underparametrized regime gives rise to effects similar to those associated with glassy systems, namely a slow evolution of the loss function and aging. Remarkably, the aging is sublinear in the waiting time (subaging) and the power–law exponent characterizing it is robust to different architectures under the constraint of a constant total number of parameters.

Wednesday afternoon talks

Biophysics from experiments to computations

Physical states of cells between life and death

Wed 21st
15:30–16:00

Prof. Jochen Guck

Max Planck Institute for the Science of Light, Erlangen, Germany
jochen.guck@mpl.mpg.de

While most current research in the life sciences focuses on molecular, biochemical aspects of cell processes, we are interested in the emergent physical properties of cells and their importance for biological function. One reason why such properties are not yet generally considered is also a paucity of appropriate tools for their quantification. We are developing novel photonic and microfluidic tools to quantify these physical properties, including real-time deformability cytometry, optical diffraction tomography, and Brillouin microscopy. I will introduce these techniques, which physical properties are being measured, and how those relate to better understanding of cell function, improved disease diagnosis, and novel insights into transitions between life and death.

Opening the black box: Investigating deep learning models for 12-lead ECG classification

Wed 21st
16:00–16:20

Theresa Bender[1], Jacqueline Beinecke[1], Henning Dathe[1], Anne-Christin Hauschild[1], Dagmar Krefting[1], Nicolai Spicher[1]

[1]Department of Medical Informatics, University Medical Center Göttingen

theresa.bender@med.uni-goettingen.de

Computer-aided diagnosis of electrocardiography (ECG) signals culminated recently in remarkable achievements of methods from the field of deep learning (DL). These networks are trained on large amounts of training data and their high accuracy could eventually pave the way for DL-supported diagnosis in clinical practice. However, the sheer number of trained parameters makes it difficult up to impossible to explain their decisions. As this impedes their potential for clinical application, the field of Explainable AI (XAI) attempts to open these black boxes. In this work, we aim for explaining the decisions of a state-of-the-art deep learning network for classification of 12-lead ECG signals.We analyze data of the China Physiological Signal Challenge 2018 dataset that contains more than 6000 12-lead ECG recordings. We limit our analysis to data from patients showing atrial fibrillation (AF) and left bundle branch block (LBBB) which we expect to lead to different types of features being learned, and healthy controls. We use the pre-trained and freely-available DL-model by Ribeiro et al. accepting 10 seconds of a 12-lead ECG data as input yielding a probability of the record showing AF/LBBB. We use the XAI method "Integrated gradients" (IG) implemented in iNNvestigate which assigns a positive or negative relevance value to each input sample.We analyze the IG output quantitatively by averaging relevances for each signal w.r.t. lead and label. Mean relevances of each lead are significantly higher for AF and LBBB compared to healthy controls. Lead V1, suggested by textbooks on ECG interpretation for AF detection, shows a high median difference between AF and healthy controls. Furthermore, results indicate that the DNN learns clinically-relevant features in individual heartbeats, such as abnormal QRS-complexes in LBBB, or missing P-waves in AF. Additionally, features of healthy heartbeats, such as positive T-waves in lead aVL, are learned.

Quantitative Spatially Resolved NMR to Study Biomolecular Liquid-Liquid Phase Separation

Wed 21st
16:20–16:40

Christian F. Pantoja[1], Alain Ibáñez de Opakua[1], Markus Zweckstetter[2]

[1]Deutsches Zentrum für Neurodegenerative Erkrankungen
[2]Max Planck Institute for Multidisciplinary Sciences

christian.pantoja-rivillas@dzne.de

Liquid-Liquid Phase Separation has emerged as a fundamental process underlying the formation of membrane-less organelles in cells [1]. Intrinsically disordered proteins (IDPs) are key promotors of phase separation and biomolecular condensation, because they can engage in multivalent interactions. Liquid-state NMR spectroscopy is an important method for the study of IDP phase separation, because it provides

high-resolution insights into the dynamic conformational ensembles of IDPs. However, quantitative analysis of the physico-chemical composition of IDP-mediated biomolecular condensates and their phase properties is challenging[2]. Here, we introduce an improved spatially resolved NMR experiment that allows efficient suppression of the water signal in phase-separated systems, which is critical for the accurate quantification of components inside phase-separated IDP condensates. We show that the quantitative spatially resolved NMR enables determination of high accuracy phase diagrams of IDP phase separation in equilibrium and the label-free determination of partition coefficients of small molecules inside condensates. Analysis of the physico-chemical properties and composition of biomolecular condensates using spatially resolved liquid-state NMR methods will be important to unravel the molecular mechanisms of biomolecular condensation and their regulation by small molecules.

Low power optimal control pulses improve the performance of multidimensional Bio-molecular solution NMR experiments at ultrahigh-field 1.2 GHz (28.2 T) spectrometers

Wed 21st
16:40–17:00

David Joseph[1], Christian Griesinger[2]

[1]Max Planck Institute for Multidisciplinary Sciences
[2]Dept. of NMR-based Structural Biology, Max Planck Institute for Multidisciplinary Sciences

dajo@nmr.mpibpc.mpg.de

Bio-molecular NMR studies are usually limited by the sensitivity and resolution, especially for concentration limited samples such as IDPs, in-cell samples and metabolomics studies, etc. Hence it is essential to use a strong magnet such as the recently made available 1.2 GHz (28.2 T) ultrahigh-field magnet to improve the S/N as well as the resolution of the spectra acquired on these samples. To achieve uniform manipulation of the spins dispersed in such a large frequency range broadband pulses are required. This means the commonly used hard pulses would require a strong B1 field and a high power source to generate these pulses. Hence, tolerance to such high power is a stringent criterion that needs to be satisfied by probe designs and is a limiting factor on the dimension of the CryoProbes coils, which are popular in solution bio-NMR studies due to their increased S/N ratio. At present this limitation is visible at the ultrahigh field magnets and for the above reason, the commercial manufacturer of 1.2 GHz spectrometers (Bruker) provides only a 3 mm CryoProbe. This is a serious limitation for studying concentration limited samples where measuring on a 5 mm CryoProbe with a larger sample volume would have provided an additional improvement in the S/N ratio. In this work, we have designed a set of low power optimal control pulses for broadband universal rotation of 1H and 15N nuclei (24 times less power on 1H, 3 times lower power on 15N) using the optimal control module in open source software Spinach. A new approach to designing optimal control based low power band selective pulses is introduced (with power of either 4 / 7 times or 2 / 3.5 times lower power on 13C). These pulses were then utilized to construct low power 2D-OC-[1H,15N]-HSQC experiemnts and

3D-OC-HNCO sequence. In all the OC-pulse sequances constructed we observed a performance improvement and they were highly tolerant to B1 miscalibration and hence are user friendly and can be fully automated at the spectrometer. We are confident that these low power optimal control bio-NMR experiments can enable large volume measurements (or 5 mm CryoProbes) at the 1.2 GHz magnets and at the new generation of ultrahigh-field magnets we expect to see in the future. We are also expanding and developing a library of optimal control bio-NMR experiments to be used at these ultrahigh-field magnets.References1. D. L. Goodwin, I. Kuprov, Journal of Chemical Physics, 2016, 144, 204107.2. Khaneja N. et al. JMR 2005, 172, 296-305.3. Luchinat, E., Barbieri et al. J Biomol NMR; 2021, 75, 97-107.4. F. Schilling et al. Angew. Chem. Int. Ed. 2014 , 53, 4475-4479.5. Coote, P.W. et al. Nat Commun 2018, 9, 3014.

Thursday morning talks

Biophysics from experiments to computations

Self-organization in pancreas organoids: from complex ductal networks to differentiation

Thu 22nd
9:40–10:10

Prof. Anne Grapin Botton

Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany
botton@mpi-cbg.de

To understand pancreas development, as a complement to in vivo investigations, we designed simplified in vitro systems that can be monitored and manipulated more extensively than the whole embryo. We established three-dimensional culture conditions that enable the efficient expansion, differentiation and morphogenesis of pancreatic progenitors isolated from mouse embryos, human fetuses or produced from human pluripotent stem cells (hPSCs). The mouse system is architecturally the most elaborate, encompassing all epithelial pancreatic cell types spatially arranged similarly to the developing organ in vivo. Notably, acinar cells, the cells that produce digestive enzymes, are found at the tip of emerging branches and a network or ducts connects them, though lacking the outlet found in vivo. Endocrine cells form a small percentage interspersed between ducts. We investigated the mechanisms leading to organoid self-organization, notably lumen formation, branching, differentiation and collective movements. Starting from the onset of organoid formation we observe a first step of epithelial cell aggregation and compaction which is necessary to enable growth. Under some conditions, collective movements, which are not observed in single cells, emerge from the collective. The talk will largely focus on the analysis of these collective movements and on the conditions that enable their emergence. We will further discuss how a network of ducts with narrow elongated lumen forms rather than single spherical lumen found in many organoids and their links to branching morphogenesis.This is work with Byung Ho Lee, Irene Seijo Barandiaran, Tzer Han Tan, and Heike Petzold.

Thu 22nd
10:10–10:30

Resonant Feedback Control of Cardiac Arrhythmia Using Optogenetics

Sayedeh Hussaini[1], S. L. Laedke [1], J. S. Schetelig [1],A. M. Kyzy [1], L. N. Diaz-Maue1 [1], V. Biktashev [3], R. Majumder [1], V. Krinski [2], S. Luther [1]

[1]Max Planck Institute for Dynamics and Self-Organisation
[2]INPHYNI, CNRS, SOPHIA Antipolis, France
[3]Exeter University, Exeter, England

sayedeh.hussaini@ds.mpg.de

Introduction: Rotating spiral waves in the heart are associated with life-threatening cardiac arrhythmias. Today, strong, globally resetting electrical shocks are used to terminate cardiac fibrillation. Significant side effects have motivated the development of alternative low-energy approaches, (S.Luther, *Nature* (2011)). For this purpose a detailed understanding of the dynamics of spiral waves is required. Cardiac optogenetics opens novel paths to study the mechanisms underlying the onset, perpetuation, and control of cardiac arrhythmias. The termination of ventricular arrhythmias has been demonstrated in optogenetic Langendorff-perfused mouse hearts using global and structured illumination (R. Uribe, *Front Physiol* (2018), S. Hussaini, *eLife* (2021)). In this study, we use optogenetics as a tool to numerically and experimentally investigate the control method of resonant feedback pacing, in which global periodic illumination is applied to cardiac tissue.
Methods: We use a two-dimensional computational model to describe the spatiotemporal evolution of membrane voltage across an optogenetically modified murine cardiac monolayer . Additionally, we report the results of our ex vivo studies using 5 Langendorff-perfused hearts from αMHC-ChR2 transgenic mice.
Results: Our study shows a significant increase in termination efficiency of resonant feedback stimulation using periodic global illumination, compared to a single global optical pulse corresponding to conventional defibrillation. The dose-response curve demonstrates termination rates of more than 50% and 100% at the lowest and highest light intensity of 3.1 and 100 µW/mm2 for the resonant feedback case. In contrast, it shows a decrease in termination rate to 0 % and ≈45 % for the single optical pulse. Our simulations suggests that resonant drift is the underlying mechanism for termination of arrhythmia in mouse heart at very low LIs. Further experimental validation of these results is ongoing.
Conclusion: Resonant feedback pacing demonstrates effective low-energy defibrillation in numerical simulations and experimentally in intact mouse hearts (S. Hussaini, Ph.D. thesis, *eDiss* (2021)).

Actomyosin cortex dynamics in the wound healing of cardiac fibroblasts

Thu 22nd
10:30–10:50

Aina Gallemi Perez[1], Marco Tarantola[1]

[1]Max Planck Institute for Dynamics and Self-Organization

aina.gallemi-perez@ds.mpg.de

In synthetic biology, one of the main challenges is to identify which properties should the synthetic constructs present so that they match and properly interact with our biological systems of interest. In this regard, the actomyosin cortex, which is highly engaged during cellular spreading and migration, and therefore, during wound healing, should be highlighted. This is especially relevant in cardiac research, where fibroblasts undergo the so-called fibroblast to myofibroblast transition (FMT) -which can lead to fibrosis and cancer development- in order to acquire increased mobility. We believe that by better understanding the cortical and wound healing dynamics of cardiac fibroblasts, we may be able to provide synthetic biology with clear targets on which to develop biomedical strategies to enhance the natural cardiac healing response. Accordingly, we employ atomic force microscopy (AFM) to analyse how the rheological properties of the actomyosin cortex change throughout the adhesion process. In addition, we study the impedance-based wound healing dynamics of fibroblasts on gaps of different sizes, and the corresponding cellular micromotions. Finally, we use immunostained samples to optically identify the closure mechanisms that cells undertake while healing. The combination of techniques here employed provides a comprehensive description of the adaptability of the actomyosin cortex and its impact on recovery dynamics and mechanism throughout wound size.

Thursday midday talks

Active Matter and Statistical Physics

Thu 22nd
11:20–11:50

Active particles: insights into living matter

Prof. Thomas Speck

Johannes Gutenberg University, Mainz

thomas.speck@uni-mainz.de

The notion of motile active matter has been useful to describe and understand the dynamic collective states in systems ranging from birds to bacteria. It is delineated from other non-equilibrium systems through autonomous motion (i.e. no external guiding field) and the local conversion of environmental or residual free energy into directed motion. These traits are shared with the molecular building blocks of living matter. To gain theoretical insights, minimal models have been pivotal in statistical physics. In this talk, I will present a few examples how modifications to one such minimal model, active Brownian particles, can be used to gain fundamental insights into the emergence of synchronization and collective behavior in the absence of detailed regulation: quorum sensing, motility interfaces, and crawling cells.

Binary mixtures of deforming particles: The role of metastability

Thu 22nd
11:50–12:10

Yiwei Zhang[1], Alessandro Manacorda[1], Etienne Fodor[1]

[1]University of Luxembourg

yiwei.zhang@uni.lu

Phase separation occurs in miscible liquids where components have distinct properties. In reactors, components undergo stochastic change in their properties which affect the liquid composition. While phase separation and reaction-diffusion have already been studied extensively as separate ingredients, how they combine in non-ideal reactors remains poorly understood. To bridge this gap, we consider repulsive particles with fluctuating size subject to one-body landscape and nonequilibrium synchronisation. The landscape features minima which, regarding size as reaction coordinate, distinguish three states: Particles with finite size, either A- or B-type, and point particles. In this context, synchronisation penalizes A particles in B-rich phases, and vice versa, so that the system eventually accommodates a uniform state. We report the phase diagram depending on the stability of each state and the corresponding particle sizes. Combining hydrodynamic and phenomenological arguments, we recapitulate how metastability regulates the interplay between synchronisation and repulsion. Our results reveal the role of nonequilibrium kinetic factors at play in non-ideal reaction-diffusion systems.

Non-equilibrium phase separation in mixtures of catalytically active particles: size dispersity and screening effects

Thu 22nd
12:10–12:30

Vincent Ouazan-Reboul[1], Jaime Agudo-Canalejo[1], Ramin Golestanian[2]

[1]Max Planck Institute for Dynamics and Self-Organization

[2]Max Planck Institute for Dynamics and Self-Organization and Rudolf Peierls Centre for Theoretical Physics, University of Oxford

vincent.ouazan-reboul@ds.mpg.de

Biomolecular condensates in cells are often rich in catalytically active enzymes. This is particularly true in the case of the large enzymatic complexes known as metabolons, which contain different enzymes that participate in the same catalytic pathway. One possible explanation for this self-organization is the combination of the catalytic activity of the enzymes and a chemotactic response to gradients of their substrate, which leads to a substrate-mediated effective interaction between enzymes. These interactions constitute a purely non-equilibrium effect and show exotic features such as non-reciprocity. Here, we analytically study a model describing the phase separation of a mixture of such catalytically active particles. We show that a Michaelis–Menten-like dependence of the particles' activities manifests itself as a screening of the interactions, and that a mixture of two differently sized active species can exhibit phase separation with transient oscillations. We also derive a rich stability phase diagram for a mixture of two species with both concentration-dependent activity and size dispersity.

Self-buckling of filamentous cyanobacteria reveals gliding forces

Thu 22nd
12:30–12:50

Maximilian Kurjahn[1], Antaran Deka[1], Antoine Girot[2], Leila Abbaspour[3], Stefan Klumpp[3], Maike Lorenz[4], Oliver Bäumchen[5], Stefan Karpitschka[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Max Planck Institute for Dynamics and Self-Organization. Experimental Physics V, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany
[3]Max Planck School Matter to Life, Georg-August-Universität Göttingen. Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen
[4]Department of Experimental Phycology and SAG Culture Collection of Algae, Albrecht-von-Haller Institute for Plant Science, Georg-August-Universität Göttingen
[5]Experimental Physics V, University of Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

maximilian.kurjahn@ds.mpg.de

Filamentous cyanobacteria are one of the oldest and today still most abundant lifeforms on earth, with manifold implications in ecology and economics. These phototrophic organisms form long and flexible filaments that do not actively swim in bulk liquid but exhibit gliding motility in contact with solid surfaces. The underlying force generating mechanism of their gliding apparatus is not yet understood. We measure their bending modulus with micropipette force sensors, and investigate how filaments buckle after gliding onto an obstacle. Comparing Kirchhoff theory to the experiments, we derive the active forces and the friction coefficients associated with gliding from the observed critical filament length for buckling. Remarkably, we find that these two quantities are strongly coupled, while dependencies on other observables are largely absent. The critical length also aligns with the peak of their natural length distribution, indicating the importance of buckling for their collective.

Optimal navigation for microswimmers in complex and noisy environments

Thu 22nd
12:50–13:10

Lorenzo Piro[1], Benoit Mahault[1], Ramin Golestanian[1]

[1]Max Planck Institute for Dynamics and Self-Organization

lorenzo.piro@ds.mpg.de

Finding the fastest path to a desired destination is a vitally important task for microorganisms moving in a fluid flow. We address this problem by designing new navigation strategies that allow for travel time optimization of microscopic self-propelled particles in complex and noisy environments. Inspired by the control maps provided by the stochastic optimal control framework, here we design new simple strategies that allow microscopic self-propelled particles to adapt their motility in response to external stimuli such as light gradients, mimicking the tactic behaviours observed in a number of natural and artificial microswimmers. This is in contrast to strategies relying on the results of optimal control theory or machine learning algorithms and

which require control over the microswimmer motion via external feedback loops. Remarkably, even though the strategies we propose rely on simple principles, they show arrival time statistics strikingly similar to those obtained from stochastic optimal control theory, as well as performances that are robust to environmental changes and strong fluctuations. These features, as well as their applicability to more general optimization problems such as navigation on curved manifolds, make these strategies promising candidates for the realization of optimized semi-autonomous navigation.

Thu 22nd
14:10–14:40

Designing biomolecules from artificial and natural evolutionary data

Prof. Remi Monasson

École Normale Supérieure, Paris, France

monasson@lpt.ens.fr

The massive availability of sequence information now makes possible to learn models of homologous proteins or RNA sequences, thought to share a common structure and function. In turn these models can be sampled to generate new sequences, never sampled by Evolution, and yet functional. I will show several applications to design new DNA aptamers, proteins and enzymatic RNAs. I will also discuss how these models can be made simple enough to be interpretable, and what they can tell us about the sequence-to-phenotype mapping underlying the structural and functional features of these biomolecules.

Accurate dynamics from memory in chemical reactions with small copy numbers

Thu 22nd
14:40–15:00

Moshir Harsh[1], Sollich Peter [1]

[1]Institut für Theoretische Physik, Georg-August-Universität Göttingen

moshir.harsh@theorie.physik.uni-goettingen.de

Chemical reactions in the regime of small copy numbers of species such as gene regulation or protein interaction networks show large fluctuations, making mean field solutions as given by mass action kinetics unreliable. Accurate calculations of the one and two-time quantities of these stochastic processes remain a challenging problem; numerical solutions to the master equation or stochastic simulations can be deployed, but these are computationally intensive and do not allow likelihood inference from dynamical trajectories.Here, we present a method that captures the fluctuations beyond mean field using self-consistently determined memory: by integrating information from the past we can systematically improve our ap- proximation for the dynamics of chemical reactions. This memory is not added ad-hoc, but can be shown to arise naturally by considering the effective action of the Doi-Peliti field theory of chemical reactions. The effective action is treated perturbatively but we can self-consistently resum a very large class of diagrams resulting in a stable expansion.We can treat any general network of chemical reactions by deriving an analytical expression for the corrections to the mean-field free energy inspired from the diagrammatic perturbation theory calculations. We demonstrate this method and its accuracy on single and multi-species binary reactions across a range of parameter values. We show how this approach also opens a route to making inferences from experimentally measured dynamics.

Composition Dependent Instabilities in Mixtures With Many Components

Thu 22nd
15:00–15:20

Filipe Thewes[1], Matthias Krüger[2], Peter Sollich[3]

[1]ITP - Göttingen
[2]Institut für Theoretische Physik, Georg-August-Universität Göttingen
[3]King's College London

filipe.cunhathewes@uni-goettingen.de

Understanding the phase behavior of mixtures with many components is a key step toward a physics-based description of intracellular compartmentalization. Here, we study the instabilities of a mixture model where the second virial coefficients are taken as random Gaussian variables. Using tools from free probability theory we obtain the spinodal curve and the nature of instabilities for a mixture with an arbitrary composition, thus lifting the assumption of uniform mixture component densities pervading previous studies. We illustrate our results with examples and show that, by controlling the volume fraction of only a few components, one can systematically change the nature of the spinodal instability and achieve demixing for realistic scenarios. This type of instability is an interplay between entropic effects

due to non-uniform composition and variability of interactions. Our approach allows for the inclusion of any finite number of structured interactions which leads to the competition between different forms of demixing as density is increased.

Thu 22nd
15:20–15:40

Optimising Energetics of Field Theories: Pareto Front and Phase Transitions

Atul Tanaji Mohite[1], Etienne Fodor[1]

[1]University of Luxembourg

atul.mohite@uni.lu

Understanding finite time optimal processes is a frontier of non-equilibrium statistical physics. Phase transitions are ubiquitous in Physics with many applications. Field theories have been extremely successful in characterizing the universal properties of various phase transitions, and in delineating a few canonical models which capture the essential Physics at play in a large class of systems [1-3]. Interestingly, a generic framework for optimizing the energetic cost associated with the finite-time driving of such systems is still largely missing. What is the optimal process for a change of phase in finite time? Here, building on recent advances in stochastic thermodynamics and optimal transport theory [4-7], we show how to analytically derive the optimal driving protocols that minimize work for a finite driving time, which we apply to cases with either conserved or non-conserved scalar order parameter in the weak noise regime. We compute exact closed-form analytical expressions for the optimal driving protocols and the optimum energy cost associated with them. Moreover, we formulate a numerical multi-optimization problem to simultaneously optimize the mean and variance of work, leading to revealing a first-order phase transition inthe corresponding Pareto front, which features the coexistence of multiple optimal protocols. Overall, our results elucidate how to drive field theories to minimize the average and fluctuations of energy cost, with the potential to be deployed to a broad class of systems.

Friday morning talks

Biophysics from experiments to computations

One becomes two: non-equilibrium assemblies that split cells across evolution

Fri 23rd
9:30–10:00

Prof. Andela Šarić

IST Austria

andela.saric@ist.ac.at

The molecular machinery of life is largely created via self-organisation of individual molecules into functional larger-scaled assemblies. Such processes are multi-scale in nature and constantly driven far from thermodynamic equilibrium. Our group develops minimal coarse-grained models to investigate how driven macromolecular assemblies result in living machines, and how such processes can fail, leading to diseases.
Today I will present our research on computational modeling of active filaments that dynamically reshape and cut cells. I will present the comparison of our simulation results to live cell data on reshaping processes across evolution — from cellular trafficking to cell division in archaea and bacteria. Beyond their biological context, our models can help guide the design of artificial structures that are able to mimic life at the nanoscale.

Extending Non-Equilibrium Pulling Method in GROMACS with Arbitrary User-Defined Atom Weight Factor Expressions

Fri 23rd
10:00–10:20

Vedran Miletić[1], Matea Turalija[1]

[1]Group for Applications and Services on Exascale Research Infrastructure, Faculty of Informatics and Digital Technologies, University of Rijeka

vmiletic@inf.uniri.hr

Numerous non-equilibrium methods are used in modern molecular dynamics simulations. Specifically, non-equilibrium pulling can be used to simulate protein unfolding, ligand unbinding, and uniform flow as well as perform umbrella sampling. Recently, GRoningen MAchine for Chemical Simulations (GROMACS), a popular molecular dynamics simulation software package, introduced a transformation pull coordinate that allows arbitrary mathematical transformations of pull coordinates. This enables changing the pull direction, rate, and force during the simulation in a user-defined way. While these are generally useful, performing uniform flow simulation requires changing the force applied to the atoms of the pull group during the simulation. The extension of GROMACS we developed offers the ability to specify an arbitrary user-defined atom weight factor expression. This approach allows hard-coded smooth or non-smooth weighting of the pull group as a special case. This approach additionally allows the positions in y and z coordinates as well as the velocities in all three coordinates to affect weighting. The implementation is publicly available on GitLab and will be submitted for inclusion in a future version of GROMACS.

Uncertainty in Markov State Models for Protein Dynamics

Fri 23rd
10:20–10:40

Nicolai Kozlowski[1], Malte Schäffner[1], Andreas Volkhardt[1], Helmut Grubmüller[1]

[1]Theoretical and Computational Biophysics Department, Max Planck Institute fur Multidisciplinary Sciences

nkozlow@mpinat.mpg.de

Markov State Models (MSMs) are a tool to describe and analyze protein dynamics. They are useful in particular to determine characteristic timescales of protein motion. For larger biomolecules such as proteins it is challenging to obtain sufficient sampling for the timescales to converge, which is thus a frequent concern. There are, however, also several other sources of uncertainty, such as choice of lag time and the number of dimensions in the dimension reduction preprocessing step (e.g. time-lagged independent component analysis tICA), the number of Markov states, or choice of the MSM lag time as well as random number generation and the width of the Bayesian transition probability distribution. To quantify and rank the uncertainties in MSM timescales induced by these choices, we constructed MSMs for four small macromolecules using several parameter combinations and amounts of sampling. We found that the largest uncertainty is due to insufficient sampling, somewhat smaller uncertainties arise from changing the number of Markov states,

whereas uncertainties caused by changing the number of dimensions after tICA, the MSM lag time or tICA lag time and the Bayesian transition probability distribution width are often similar to the uncertainty due to random number generation, and hence likely to be not of concern.

Nuclear quantum effects matter

Fri 23rd
10:40–11:00

Lukas Hasecke[1], Ricardo A. Mata[1]

[1]Georg-August-Universität Göttingen

lhaseck@gwdg.de

Nowadays we are facing a new dawn in the comprehension of protein function, based on the rapid advancements in both experimental and theoretical methods over the last decades. Especially through the recent improvements of cryo-electron microscopy and X-ray crystallography protein structures can be resolved with high resolution. Those accurately determined structures are an ideal base for quantum chemistry calculations which can elucidate the mechanisms behind the efficient work of enzymes. [1]Particularly important for the enzyme activity are the contributions from hydrogen bonds. One especially interesting type of those bonds are low-barrier hydrogen bonds which play a central role in enzymatic proton wires. Moreover, the formation of those bonds has also been associated with a substantial stabilisation of the intermediates and transition states occurring during enzymatic reactions. [2]Regarding the computational side, most available electron structure methods solely treat the electrons quantum mechanically and omit the quantum character of other particles. However, nuclear quantum effects should not be ignored in enzymes. One major contribution of these effects is given by the delocalisation of protons in hydrogen-bond networks. [3] Additionally, several other observations demonstrate the impact of nuclear quantum effects like delocalisation, zero-point vibration and hydrogen tunneling on the reactivity of enzymes. Therefore, large errors are expected by using conventional quantum chemical methods for the simulation of systems where the quantum nature of the protons becomes increasingly relevant. With the aim to address this problem an adaptive nuclear-electronic orbital approach is developed to efficiently analyse the impact of nuclear quantum effects in enzymatic systems, particularly in hydrogen bond networks.[1] Dai, S. et al. Nature 573, 609–613 (2019).[2] Rindfleisch, S., Krull, M., Uranga, J. et al. Nat Catal 5, 332–341 (2022).[3] Wang, L. et al. PNAS 111 (52), 18454-18459 (2014).

Thursday midday talks

Nonlinear dynamics and complex networks

Fri 23rd
11:30–12:00

Tipping Points and Inference in Complex Systems

Prof. Marc Timme

Strategic Professor Chair for Network Dynamics
Institute of Theoretical Physics Center for Advancing Electronics Dresden (cfaed)
TU Dresden, Germany

marc.timme@tu-dresden.de

The dynamics of networks enables the function of a variety of systems we rely on every day, from gene regulation and metabolism in the cell to the distribution of electric power and communication of information. Understanding, steering and predicting the function of interacting nonlinear dynamical systems, in particular if they are externally driven out of equilibrium, relies on obtaining and evaluating suitable models, posing at least two major challenges. First, how can we extract key structural system features of networks if only time series data provide information about the dynamics of (some) units? Second, how can we characterize nonlinear responses of nonlinear multi-dimensional systems externally driven by fluctuations, and consequently, predict tipping points at which normal operational states may be lost? Here we report recent progress on nonlinear response theory extended to predict tipping points and on model-free inference of network structural features from observed dynamics.This is work with Jose Casadiego, Mor Nitzan, Hauke Haehne, Georg Boerner, Moritz Thuemler and others.

- Topical Review: Marc Timme Jose Casadiego, J. Phys. A 47:343001 (2014).
- Casadiego et al., Nature Comm. 8:2192 (2017).
- Nitzan et al., Science Adv.:e1600396 (2017).
- Haehne et al., Phys. Rev. Lett. 122:158301 (2019).[5] Moritz Thuemler et al., accepted (2022).

Understanding (and fighting) the COVID-19 pandemic with models

Fri 23rd
12:00–12:20

Sebastian Contreras[1], Jonas Dehning[1], Emil Iftekhar[1], Paul Spitzner[1], Philipp Dönges[1], Sebastian Mohr[1], Joel Wagner[1], Simon Bauer[1], Alvaro Olivera-Nappa[2], Johannes Zierenberg[1], Viola Priesemann[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Universidad de Chile

sebastian.contreras@ds.mpg.de

Mathematical models for the spread of infectious diseases have been crucial to designing and assessing interventions in the COVID-19 pandemic. Using compartmental susceptible-infectious-removed (SIR-like) models, we demonstrate the existence of different tipping points that separate regimes where outbreaks are likely to propagate (linearly or exponentially) or die out. These regimes can be enabled by non-pharmaceutical interventions, such as testing and contact tracing, and modulated by their stringency. In addition, factors such as the self-regulation of contacts following increased risk perceptions and vaccination also play a significant role, especially in the long-term and transition to endemicity. In my talk, I will discuss some of the critical ingredients that models need to incorporate to shed light on the influence of these concepts on the controllability of an outbreak and the long-term dynamics of an infectious disease.

The impact of the UEFA European Football Championship on the spread of COVID-19

Fri 23rd
12:20–12:40

Jonas Dehning[1], Sebastian B. Mohr[1], Sebastian Contreras[1], Philipp Dönges[1], Emil Iftekhar[1], Oliver Schulz[2], Philip Bechtle[3], Viola Priesemann[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Max Planck Institute for Physics, Munich
[3]University Bonn

jonas.dehning@ds.mpg.de

Large-scale international events like the UEFA Euro 2020 football championship offer a unique opportunity to quantify the impact of match-related social gatherings on COVID-19, as the number of matches played by participating countries resembles a randomized trial. Moreover, soccer-related activities have a marked gender-imbalance that we can exploit for inference. In our work, we build a differentiable Bayesian SEIR-like model. Its parameters are inferred with Hamiltonian Monte-Carlo using the PyMC3 package. Our model simulates COVID-19 spread in each country using a discrete renewal process and gender-resolved case numbers. On average, 3.2

Closing talk

Fri 23rd
17:10–17:40

Towards Systainability?
– Self-Organized Nonlinear Dynamics of Energy Systems

Prof. Marc Timme

Chair for Network Dynamics, TU Dresden

marc.timme@tu-dresden.de

In 2015, the United Nations set sustainable development goals to be reached by 2030 for planet earth and its inhabitants, including humans. Many of the goals, such as climate action, sustainable cities and clean energy rely on novel technologies, used under societal and economic boundary conditions. Here we argue that, in addition, a systemic understanding of how to suitably design and operate such technologies is required to make them truly sustainable. We provide several examples: for instance, energy transmission grids, in which adding new transmission lines may cause system outages due to Braess paradox; moreover, climate change cannot be achieved in the current mode of economic action because direct heating, resulting from the first law of thermodynamics, would bring oceans to boiling temperature by 2500. Finally, the planetary constraints themselves may limit us to increase energy consumption for one or a few generations only. Thus, considering considering full-scale, collectively self-organized dynamics of entire complex systems rather than only of their components, is key to achieve their systemic sustainability - and thus systainability of our only planet.

Posters

Nonlinear dynamics and complex networks

Protein Dynamics in the Complex Physical Environment of the Synapse

Poster 1
Wed 21st
17:00–18:30

Simon Dannenberg[1], Sarah Mohammadinejad[1], Stefan Klumpp[1]

[1]Institut für Dynamik komplexer Systeme, Georg-August-Universität Göttingen
simon.dannenberg@uni-goettingen.de

The synapse is a complex environment that is densely packed withproteins and has an internal geometry structured by membranes. Thisaffects the mobility of proteins involved in signal transmission andhence, their availability at corresponding reaction sides.In our work we use dynamic Monte Carlo simulations to investigatethe individual influences of different physical features of the synapseon protein mobility. The simulations are parameterized by mobilitymeasurements via FRAP experiments. By simulating protein mobil-ity in synapses with different geometric features such as synapse vol-ume and vesicle number, we study the influence of these features onconcentration profiles in the synapse and other key aspects of signaltransmission.

Interplay Between Risk Perception, Behavior, and COVID-19 Spread

Poster 2
Thu 22nd
17:10–18:10

Emil Iftekhar[1], Philipp Dönges[1], Joel Wagner[1], Sebastian Contreras[1], Emil Iftekhar[1], Simon Bauer[1], Sebastian Mohr[1], Jonas Dehning[1], André Calero Valdez[2], Mirjam Kretzschmar[3], Michael Mäs[4], Kai Nagel[5], Viola Priesemann[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]University of Lübeck, Lübeck, Germany
[3]University Medical Center Utrecht, Utrecht University, Utrecht, Netherlands
[4]Department of Sociology, Karlsruhe Institute of Technology, Karlsruhe, Germany
[5]Chair of Transport Systems Planning and Transport Telematics, Technische Universität Berlin, Berlin, Germany
emil.iftekhar@ds.mpg.de

Pharmaceutical and non-pharmaceutical interventions (NPIs) have been crucial for controlling COVID-19. They are complemented by voluntary health-protective behavior, building a complex interplay between risk perception, behavior, and disease spread. We studied how voluntary health-protective behavior and vaccination willingness impact the long-term dynamics. We analyzed how different levels of mandatory NPIs determine how individuals use their leeway for voluntary actions. If mandatory NPIs are too weak, COVID-19 incidence will surge, implying high morbidity and mortality before individuals react; if they are too strong, one expects a rebound wave once restrictions are lifted, challenging the transition to endemicity. Conversely, moderate mandatory NPIs give individuals time and room to adapt their level of caution, mitigating disease spread effectively. When complemented with high vaccination rates, this also offers a robust way to limit the impacts of the Omicron variant of concern. Altogether, our work highlights the importance of appropriate mandatory NPIs to maximise the impact of individual voluntary actions in pandemic control.

Poster 3
Wed 21st
17:00–18:30

Distinguishing noise from high-dimensional chaos

Inga Kottlarz[1], Ulrich Parlitz[1,2]

[1]Max-Planck-Institute for Dynamics and Self-Organization
[2]Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen

inga.kottlarz@ds.mpg.de

The ordinal pattern-based Complexity-Entropy Plane is a popular tool in nonlinear dynamics for distinguishing noise from chaos. While successful attempts to do so have been documented for low-dimensional maps and continuous-time systems, high-dimensional systems have been somewhat neglected so far. To address the question in which way time series from highdimensional chaotic attractors can be characterized by their location in the Complexity-Entropy Plane we analyze data from the high-dimensional continuous-time Lorenz-96 system, the discrete generalized Hénon map and the Mackey-Glass equation as a delay system and discuss the crucial role of the lag and the pattern length or the ordinal pattern, and the length of the available time series.

Align data organisation along the stages of scientific work

Poster 4
Thu 22nd
17:10–18:10

Baltasar Ruechardt[1]

[1]Max Planck Institute for Dynamics and Self-Organization

baltasar.ruechardt@ds.mpg.de

Data management is crucial to reuse scientific data; knowledge cannot be created if the path that led to it was not properly documented, observations cannot be understood without the setup that allowed them being properly documented. I suggest a concept to structure data and data creation processes building up on the file system layout suggested in Spreckelsen et al. [1] along the stages of scientific work that I previously defined. Applying this concept allows to keep an overview over data and data creation processes, to share them easily, complying with the FAIR principles [2] and to contextualise daily scientific work into the bigger picture. [1] Spreckelsen, Florian, Baltasar Rüchardt, Jan Lebert, Stefan Luther, Ulrich Parlitz, and Alexander Schlemmer. "Guidelines for a Standardized Filesystem Layout for Scientific Data." Data 5, no. 2 (June 2020): 43. https://doi.org/10.3390/data5020043. [2] Wilkinson, Mark D., Michel Dumontier, IJsbrand Jan Aalbersberg, Gabrielle Appleton, Myles Axton, Arie Baak, Niklas Blomberg, et al. "The FAIR Guiding Principles for Scientific Data Management and Stewardship." Scientific Data 3, no. 1 (March 15, 2016): 160018. https://doi.org/10.1038/sdata.2016.18.

Energy Dissipation Rate Estimates from Airborne Atmospheric Measurements with the Max Planck CloudKites

Poster 5
Wed 21st
17:00–18:30

Marcel Schröder[1], Freja Nordsiek[1], Oliver Schlenczek[1], Antonio Ibañez Landeta[1], Johannes Güttler[1], Eberhard Bodenschatz[1], Gholamhossein Bagheri[1]

[1]Max-Planck-Institute for Dynamics and Self-Organization

marcel.schroeder@ds.mpg.de

The energy dissipation rate is one of the most important characteristics of a turbulent flow across the entire range of scales, and of particle-turbulence interaction. To investigate cloud microphysics and turbulence in clouds and in the atmospheric boundary layer, we infer coarse-grained time series of the energy dissipation rate from one-dimensional wind velocity time records by specially developed airborne platforms, the Max-Planck-CloudKite + (MPCK+) and the mini-Max-Planck-CloudKites (mini-MPCK). During the EUREC4A-ATOMIC field campaign in the Caribbean January-February 2020, both instruments are deployed aboard balloon-kite hybrids launched from RV Maria S. Merian and RV Meteor conducting in situ measurements of the wind velocity and meteorological as well as cloud microphysical properties with high spatial and temporal resolution. We present estimates of the energy dissipation rate from in situ velocity time records by the MPCKs during the EUREC4A-ATOMIC field campaign and preliminary assessment of turbulence features.

Modular architecture facilitates noise-driven control of synchrony in neuronal networks

Poster 6
Thu 22nd
17:10–18:10

F. Paul Spitzner[1], Hideaki Yamamoto[2], F. Paul Spitzner[1], Taiki Takemuro[2], Victor Buendía[3], Carla Morante[4], Tomohiro Konno[5], Shigeo Sato[2], Ayumi Hirano-Iwata[2], Viola Priesemann[1], Miguel A. Muñoz[6], Johannes Zierenberg[1], Jordi Soriano[4]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Research Institute of Electrical Communication, Tohoku University, Sendai, Japan
[3]Max Planck Institute for Biological Cybernetics, Tübingen, Germany
[4]Department de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain
[5]Graduate School of Pharmaceutical Sciences, Tohoku University, Sendai, Japan
[6]Departamento de Electromagnetismo y Física de la Materia, Universidad de Granada, Granada, Spain

paul.spitzner@ds.mpg.de

Brain functions require both segregated processing of information in specialized circuits, as well as integration across circuits to perform high- level information processing. One possible way to implement these seemingly opposing demands is by flexibly switching between synchronous and less synchronous states. Understanding how complex synchronization patterns are controlled by the interaction of network architecture and external perturbations is thus a central challenge in neuroscience, but the mechanisms behind such interactions remain elusive. Here, we utilise precision neuroengineering to manipulate cultured neuronal networks and show that a modular architecture facilitates desynchronization upon asynchronous stimulation, making external noise a control parameter of synchrony. Using spiking neuron models, we then demonstrate that external noise can reduce the level of available synaptic resources, which make intermodular interactions more stochastic and thereby facilitates the breakdown of synchrony. Finally, the phenomenology of stochastic intermodular interactions is formulated into a mesoscopic model that incorporates a state-dependent gating mechanism for signal propagation. Taken together, our results demonstrate a network mechanism by which asynchronous inputs tune the inherent dynamical state in structured networks of excitable units.

Large scale fow structure formation in trubulent Rayleigh Bénard Convection

Poster 7
Wed 21st
17:00–18:30

Hiufai Yik[1], Eberhard Bodenschatz[1], Olga Shishkina[1], Stephan Weiss[2]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Institute of Aerodynamics and Flow-Technology, German Aerospace Center

hyik@ds.mpg.de

Thermal convection is a topic of great interest in astrophysics, geophysics, and industry. While weakly driven flows are generally well understood, knowledge of flows under strong thermal forcing, where turbulence dominates, is limited. In recent years, researchers have focused on predicting global quantities such as global heat

transport and velocity, which are easier to study in smaller setups. Only in recent years, with advances in numerical and experimental techniques, is the study of large-scale flow structures coming into focus. We investigate how different boundary conditions affect flow structures experimentally and numerically. The experiment is performed at the High Pressure Convection Facility (HPCF) in Göttingen. The convection cell has dimensions of 3.5m(L) x 0.35m(W) x 0.7m(H). The boundaries at the top and bottom are divided lengthwise into 4 sections to create the desired boundary pattern. The spatial heat flux and temperature along the center of the convection cell are measured to determine the flow pattern at extremely high Rayleigh numbers up to 1x10$\hat{1}$3. The experiment is complemented by direct numerical simulations conducted with the state-of-the-art code GOLDFISH at lower Rayleigh numbers so that we can better understand how and why the flow patterns develop.

Autocorrelations from emergent bistability in homeostatic spiking neural networks on neuromorphic hardware

Poster 8
Wed 21nd
17:00–18:30

Johannes Zierenberg[1], Benjamin Cramer[2], Markus Kreft[2], Sebastian Billaudelle[2], Vitali Karasenko[2], Aron Leibfried[2], Eric Müller[2], Philipp Spilger[2], Johannes Weis[2], Johannes Schemmel[2], Miguel A. Muñoz[3], Viola Priesemann[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Heidelberg University
[3]Universidad de Granada

johannes.zierenberg@ds.mpg.de

A unique feature of neuromorphic computing is that memory is an implicit part of processing through traces of past information in the system's collective dynamics. The extent of memory about past inputs is commonly quantified by the autocorrelation time of collective dynamics. Based on past experimental evidence, a potential explanation for the underlying autocorrelations are close- to-critical fluctuations. Here, we show for self-organized networks of excitatory and inhibitory leaky integrate-and-fire neurons that autocorrelations can originate from emergent bistability upon reducing external input strength. We identify the bistability as a fluctuation-induced stochastic switching between metastable active and quiescent states in the vicinity of a non-equilibrium phase transition. This bistability occurs for networks with fixed heterogeneous weights as a consequence of homeostatic self-organization during development. Specifically, in our experiments on neuromorphic hardware and in computer simulations, the emergent bistability gives rise to autocorrelation times exceeding 500 ms despite single-neuron timescales of only 20 ms. Our results provide the first verification of biologically compatible autocorrelation times in networks of leaky integrate-and-fire neurons, which here are not generated by close-to-critical fluctuations but by emergent bistability in homeostatically regulated networks. Our results thereby constitute a new, complementary mechanism for emergent autocorrelations in networks of spiking neurons, with implications for biological and artificial networks, and introduces the general paradigm of fluctuation-induced bistability for driven systems with absorbing states.

Session: Active Matter and Statistical Physics

Poster 9
Wed 21st
17:00–18:30

Dynamics of multicomponent mixtures

Maryam Akaberian[1]

[1]Georg-August-Universität Göttingen

maryam.akaberian@uni-goettingen.de

Using a Model description for the time evolution of a multicomponent liquid mixture we obtain an explicitexpression for the mobility matrix in equilibrium. By introducing the hypothesis that this mobility should notdepend heavily on the thermodynamics, we are able to evaluate our expressions in terms of quantities that canbe easily obtained from experiments or numerical simulations. We describe multicomponent mixtures dynamics by considering a simple model which is called painted particle model and later extrapolate it mixture with distinguishable particles.

Poster 10
Thu 22nd
17:10–18:10

Bounding Uncertainty of Empirical First Passage Times of Reversible Markov Processes

Rick Bebon[1], Aljaz Godec[1]

[1]Max Planck Institute for Multidisciplinary Sciences

rick.bebon@mpinat.mpg.de

The first-passage time denotes the time at which a stochastic process first reaches a predefined threshold for the first time. First-passage concepts are deeply ingrained in the theory of multiple fields to study e.g. chemical reactions, cell signaling, gene regulation, the foraging behavior of bacteria and animals, and the dynamics of stock options. Moreover, first-passage time problems are central to characterize the kinetics of barrier crossings in energy landscapes, the persistence of non-equilibrium systems, and the statistics of entropy production, and are intimately connected to the statistical properties of extreme values. We derive universal concentration inequalities for first-passage times of ergodic reversible Markov processes on discrete and continuous-state spaces. For a sample of $N \geq 1$ independent realizations of the first-passage process, we prove a bound on the probability that a sample mean deviates from the true mean first-passage time by more than any given amount. Complementary, we derive an upper bound on the corresponding expected maximal positive and negative deviations. Our results provide a novel and rigorous quantification of the uncertainty of first-passage times inferred from experiments and computer simulations as a result of limited sampling and furthermore lay grounds for a more systematic model-free inference of kinetic rates.

Synchronisation and enhanced catalysis of mechanically coupled enzymes

Poster 11
Wed 21st
17:00–18:30

Mike Chatzittofi[1], Jaime Agudo-Canalejo[1], Tunrayo Adeleke-Larodo, Pierre Illien, Ramin Golestanian[1]

[1]Max-Planck-Institute for Dynamics and Self-Organization

mike.chatzittofi@ds.mpg.de

Enzymes are the catalysts of the chemical processes that take place in livingorganisms. These processes, during which chemical energy is converted to me-chanical energy and heat, occur stochastically as a result of a noise-activatedbarrier-crossing event. Despite this stochasticity, it has been shown recentlythat two mechanically coupled enzymes can synchronize their catalytic reaction[1]. Even more interestingly, the coupling enhances the catalysis of the twoenzymes. This effect can be understood as arising from a bifurcation in thedeterministic dynamics of the system. In this work, we use a similar approachto describe the dynamics of an enzyme by assuming that the enzyme is attachedto a passive molecule. The goal is to design the properties of the enzyme so thatits motion favours a "chemical reaction", for example dissociation or a shapeswitch of the molecule. A bifurcation in the deterministic dynamics can cause achange in the molecules state after one enzymatic reaction. The stochastic sim-ulations, also show that the enzyme's activity affects the state of the molecule.The Kramers' rate for this two-dimensional problem is also calculated.

J. Agudo-Canalejo, T. Adeleke-Larodo, P. Illien, and R. Golestanian, Phys.Rev. Lett. 127, 208103 (2021).

From Micromechanics to Collective Dynamics of Filamentous Cyanobacteria

Poster 12
Thu 22nd
17:10–18:10

Antaran Kumar Deka[1], Maximilian Kurjahn[1], Leila Abbaspour[2], Antoine Girot[1,3], Oliver Baumchen[1,3], Stefan Karpitschka[1]

[1]Max Planck Institute for Dynamics and Self-Orgnization
[2]Max Planck School Matter to Life, Georg-August-Universität Göttingen and Institute for Dynamics of Complex Systems, Georg-August-Universität Göttingen
[3]Experimental Physics V, University of Bayreuth

antaran.deka@ds.mpg.de

Filamentous Cyanobacteria belong to the oldest known phototrophic forms of life on the planet. Responsible for the "Great Oxidation Event" millions of years ago, they enabled the development and sustenance of animal and human life. Today they are abundant in many eco-systems, forming benthic mats or suspended aggregates which can grow to gigantic blooms, sometimes posing serious economical and ecological threats. In their aggregates, the long, flexible, and actively gliding filaments entangle into complex structural patterns which are dynamic and adaptive to environmental conditions, presumably enhancing the capability of acclimatization. Neither the micro-mechanics of the individual filaments, nor their gliding motility,

nor the pattern formation mechanism in their aggregates are understood.Here, we measure the bending stiffness of individual, living filaments from three species, using Micropipette Force Sensors. The results are subsequently used to analyze the self-buckling behavior of filaments that glide onto obstacles, which in turn reveals their gliding forces and friction coefficients. This enables us to calibrate the essential parameters of an agent based active polymer model for filamentous cyanobacteria. The patterns and dynamics generated by the calibrated two-dimensional model are remarkably similar to experimental observations of filamentous cyanobacteria in quasi-two-dimensional confinement. The agreement indicates that the self-organization of the colonies of filamentous cyanobacteria might indeed be captured by the statistical physics of simple active polymers.

Poster 13
Wed 21st
17:00–18:30

Necessity for Coarse Graining Empirical Densities and Currents in Continuous Space

Cai Dieball[1], Aljaz Godec[1]

[1]Max Planck Institute for Multidisciplinary Sciences

cai.dieball@mpinat.mpg.de

We present general results on fluctuations and spatial correlations of the coarse-grained empirical density and current of diffusion in equilibrium or non-equilibrium steady states on all time scales. Although the underlying dynamics is assumed to be Markovian, the time averaging and coarse graining hardwired in the definition of the functionals under consideration give rise to a non-Markovian time evolution and non-trivial statistics. We unravel a deep connection between current fluctuations and generalized time-reversal symmetry. We highlight the essential role of coarse graining in space from athematical, thermodynamical, and experimental points of view. Spatial coarse graining is required to uncover salient features of currents that break detailed balance, and a thermodynamically "optimal" coarse graining ensures the most precise inference of dissipation. Defined without coarse graining, the fluctuations of empirical density and current are proven to diverge on all time scales in dimensions higher than one, which has far-reaching consequences for large-deviation limits in continuous space and for continuum limits of Markov-jump processes. We apply the results to examples of irreversible diffusion. Our findings provide new intuition about time-averaged observables and allow for a more efficient analysis of single-molecule experiments.

Ciliary chemosensitivity is enhanced by cilium geometry and motility

Poster 14
Thu 22nd
17:10–18:10

David Hickey[1], Andrej Vilfan[1], Ramin Golestanian[1]

[1]Max Planck Institute for Dynamics and Self-Organization

david.hickey@ds.mpg.de

Cilia are hairlike organelles with roles in motility and sensing. We investigate whether locating chemoreceptors on cilia provides sensitivity advantages and whether motile sensory cilia have further advantages. Using a simple advection-diffusion model, we compute capture rates of diffusive molecules to a cilium. We find that due to its geometry, a non-motile cilium in a quiescent fluid has a capture rate equal to that of a circular absorbing region with quadruple the surface area, and when the same cilium is exposed to an external shear flow, the equivalent surface area is sextuple that of the quiescent case. Alternatively, if the cilium beats in a non-reciprocal manner in an otherwise quiescent fluid, its capture rate increases with the beating frequency to the power of 1/3, and this motility advantage is seen to apply even in simulated cilium bundles. Altogether, our results show that the geometry of cilia provide one reason why many receptors are found on cilia and point to the advantage of combining motility with chemoreception, for a singular cilium as well as groups of cilia.

Collective dynamics in systems of growing rods

Poster 15
Wed 21st
17:00–18:30

Lukas Hupe[1], Jonas Isensee[2], Philipp Bittihn[2], Ramin Golestanian[3]

[1]Max Planck Institute for Dynamics and Self-Organization

[2]Max-Planck-Institute for Dynamics and Self-Organization. Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany.

[3]Max-Planck-Institute for Dynamics and Self-Organization. Institute for the Dynamics of Complex Systems, Georg-August-Universität Göttingen, Germany. Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom.

lukas.hupe@ds.mpg.de

Recent research shows that in confined populations of growing and dividing rods, such as microcolonies of bacteria, a complex interplay between growth activity, fluctuating inter-particle forces and boundary effects can lead to emergent collective dynamics, including global flow of cellular matter and alignment due to the nematic symmetry of local mechanical interactions. Here, we use a new versatile framework for agent-based simulations to explore these effects in systems with different geometries containing two-dimensional spherocylinders. We observe the emergence of orientational order in rectangular channels and analyse its dependence on both microscopic parameters of the rods and the geometry of the confinement. Further observations of complex orientation patterns in open polygonal domains hint at a link between shear rate anisotropy and orientation.

Poster 16
Thu 22nd
17:10–18:10

Stress anisotropy in confined populations of growing rods

Jonas Isensee[1], Lukas Hupe[1], Ramin Golestanian[1,2], Philip Bittihn[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom
jonas.isensee@ds.mpg.de

Growing colonies of rod-shaped bacteria commonly feature order and alignment of the constituent particles. This is generally thought to be the result of the active stresses generated by growth, mechanical volume exclusion interactions between cells, and shear-flow-induced effects due to confinement. However, how these contributing factors interact to give rise to the observed global alignment patterns remains elusive.We study, in-silico, colonies of growing rod-shaped particles of different aspect ratios confined in channel-like geometries. A spatially resolved analysis of the stress tensor reveals a strong relationship between near-perfect alignment and an inversion of stress anisotropy for particles with large length-to-width ratios. We show that, in quantitative agreement with an asymptotic theory, strong alignment can lead to a decoupling of active and passive stresses parallel and perpendicular to the direction of growth, respectively. Our results illustrate the complexity arising from the inherent coupling between nematic order and active stresses in growing active matter which is influenced by geometric and configurational constraints due to confinement.

Poster 17
Wed 21st
17:00–18:30

Competition drivers in confined cellular aggregates: Does dead matter matter?

Yoav G. Pollack[1], Philip Bittihn[1], Ramin Golestanian[1,2]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, OX1 3PU, UK
yoav.pollack@ds.mpg.de

Competition of different species or cell types for limited space is relevant in a variety of biological processes such as biofilm development, tissue morphogenesis and tumor growth. Predicting the outcome for non-adversarial 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 in confinement. We show that passive by-products of the processes maintaining homeostasis can significantly alter fitness, enabling cell types with lower homeostatic pressure to outcompete those with higher homeostatic pressure. We reveal that growing matter with a higher homeostatic proportion of active cells can better exploit local growth opportunities that continuously arise at interfaces. We elucidate this effect in theoretical arguments and simulations that include finite-time mechanical persistence of dead cells. Our results suggest that self-organization of cellular aggregates into active and passive matter can be decisive for competition outcomes and that optimizing the proportion of growing (active) cells can be as important to survival as sensitivity to mechanical cues.

The orientation field generated by a moving defect: multivalued solutions of the diffusion equation

Poster 18
Thu 22nd
17:10–18:10

Jacopo Romano[1]

[1]Max Planck Institute for Dynamics and Self-Organziation

jacopo.romano@ds.mpg.de

We provide the exact solution of the diffusion equation for multivalued fields, which can be regarded as the simplest model for nonequilibrium dynamics of the angular field generated by topological defects. We show that the solution can be given in a closed form in terms of the past trajectory of the defects and discuss its more relevant expansions. By doing so, we are able to shed light on the new features which characterize the dynamics of defects out of equilibrium and which distinguish these systems qualitatively and quantitatively from their equilibrium counterpart.

Quantification and optimization of mixing efficiency in active microfluidic systems

Poster 19
Wed 21st
17:00–18:30

Yihong Shi[1], Andrej Vilfan[1], Ramin Golestanian[1]

[1]Max Planck Institute for Dynamics and Self-Organization

yihong.shi@ds.mpg.de

Fluids at microscales are typically characterized by very low Reynolds numbers, where viscous forces dominate, and inertia is negligible. Because all the flows are time-reversible, fluid mixing requires an interplay between flow and diffusion. The process of mixing is equally relevant in the biological microfluidic environment, where cilia (hair-like cellular protrusions that beat periodically) are involved in the transport and mixing of fluids, as well as in a few sensory functions.We applied the concept of mutual information to quantify the degree of mixing efficiency in a closed microfluidic compartment. As a simple model system we investigated the mixing in the fluid between two rotating concentric cylinders. We solved the advection-diffusion equation for particles in the fluid with a spectral method. The limits of short and long times can be reproduced analytically. Interestingly, the overall mixing efficiency, quantified as a reduction of mutual information, is maximized by certain velocity sequences that vary according to some rules. These results demonstrate that mutual information can be used as a universal measure to measure the mixing efficiency in biological and other microfluidic environments.

Poster 20
Thu 22nd
17:10–18:10

Nucleation of chemically active droplets

Noah Ziethen[1], David Zwicker[1]

[1]Max Planck Institute for Dynamics and Self-Organization

nziethe@ds.mpg.de

Liquid-liquid phase separation emerged as a crucial organizing principle inside biological cells giving rise to a plethora of intracellular compartments. These biomolecular condensates are involved in many cellular processes on all scales. Unique to the cellular context, these condensates can consist of only a few hundred molecules and are affected by non-equilibrium processes. In particular, active chemical conversion between condensate material and proteins in the surrounding cytoplasm can control their size. Moreover, the significant concentration fluctuations due to the small molecule numbers imply that spontaneous nucleation and dissolution are likely. Yet, it is unclear how the driven reactions affect these stochastic processes. Here, we investigate the influence of chemical reactions on the nucleation behavior of active droplets using a stochastic field theory. We find a decrease in the nucleation rate with the increased strength of the chemical reactions. Using classical nucleation theory, we can reduce the full dynamics to an analytical expression for the free energy, which only depends on the droplet radius and the strength of the chemical reactions. The chemical reactions increase the energy barrier, which the system needs to overcome, to form a droplet. Additionally, the region of metastability in the phase diagram is shifted by the chemical reactions. The binodal and the spinodal line are moved towards the center of the phase diagram. Cells might use these effects to control the nucleation behavior of intracellular droplets or even suppress their formation completely.

Neutrophil mechanotransduction during durotaxis

Poster 21
Wed 21st
17:00–18:30

Fatemeh Abbasi[1], Matthias Brandt[2], Timo Betz[1]

[1]Georg-August-Universität Göttingen
[2]Institute of Cell Biology, ZMBE, University of Münster
fatemeh.abbasi@phys.uni-goettingen.de

In Vivo, cells experience complex tissue environments with various chemical and physical features. 3D confinement is one of the major physical obstacles for cells in their natural environment. Neutrophils are among the most abundant immune cells in our body, which have to cope with various physical constrictions on their way from production to the infection site. In addition to confinement, the stiffness of themicroenvironment is another mechanical feature these rapidly moving cells are exposed to. Neutrophils experience various tissue stiffness, from 1 kPa (bone marrow) to 20 MPa (bone). Previous studies have demonstrated that these cells are responsive to their microenvironment stiffness by adjusting their adhesion and spreading. Based on this knowledge we decided to combine confinement and stiffness change and investigate the impact of 3D stiffness gradient on cell behaviour and migration, a fact called durotaxis. We hypothesized that stiffness gradient might be a triggering factor of neutrophil migration toward the infection site. We confine neutrophils in between 2 layers of polyacrylamide hydrogels with 2 different stiffness and keep this distance stable for the desired period of time to investigate cell mechanotransduction during durotaxis from different points of view. Our preliminary results regarding the neutrophil durotaxis show a surprising and transient force peak on the soft substrate during cell shifting.

Binding study of Mammea A/AA with plasma protein (HSA and BSA): spectroscopy UV-vis and MD simulations.

Poster 22
Thu 22nd
17:10–18:10

Baruch Ateba Amana[1]

[1]University of Douala
bateba@fs-univ-douala.cm

Mammea A/AA (MA), an active compound of Mammea African stem bark extract, exhibit biological properties as antimicrobial, anticancer and antioxidant. To further prospect its usage as drug, the unusual ratiometric absorbance of MA was exploited to monitor its binding to plasma proteins (HSA and BSA). To further understand the difference of the binding parameters in HSA and BSA, 60ns of MD simulations were undertaken and to explain the different solvatochromism observed for the two proteins. Our study demonstrate that MA can be applied as molecular probe to follow biomolecules interactions.Keywords: Mammea A/AA; plasma proteins; fluorescence quenching; molecular modeling.

Influence of vimentin intermediate filaments on microtubules in cells

Poster 23
Wed 21st
17:00–18:30

Anna Blob[1], Roman David Ventzke[2], Thomas Giacomo Nies[3], Laura Schaedel[4], Axel Munk[3], Sarah Köster[1]

[1]Institute for X-Ray Physics, Georg-August-Universität Göttingen
[2]Institute for X-Ray Physics, Georg-August-Universität Göttingen, Institute for Mathematical Stochastics, Georg-August-Universität Göttingen
[3]Institute for Mathematical Stochastics, Georg-August-Universität Göttingen
[4]Center for Biophysics, Saarland University

anna.blob@uni-goettingen.de

The cytoskeleton in eucaryotic cells is an intricate network of three different filamentous proteins: microtubules, actin filaments and intermediate filaments. Together, they are essential for the mechanical properties as well as important functions of the cell, such as intracellular transport and division. Each filament type has its own unique features, and, in particular, microtubules, can withstand large compressive forces and show characteristic buckling and bending behavior that is still not fully understood. In addition to the special properties of each cytoskeletal filament type, there is also evidence for important interactions between them: It has been shown that vimentin intermediate filaments stabilize microtubules in vitro and can template the microtubule network in migrating cells. Following up on this idea, we are interested in the influence of vimentin networks on microtubule mechanics. Investigating how the bending of microtubules depends on both the microtubule network itself and the vimentin network will improve our understanding of the mechanical consequences of the interaction within and between these filament systems. We compare microtubule networks in vimentin-knockout and wildtype mouse fibroblasts on micropatterns. Microscopy images are processed and analyzed with respect to the curvature of microtubules. We find that the local curvature of microtubules depends on the cellular region and on both microtubule density and vimentin density.

Effects of Cryo-EM Cooling on Structural Ensembles

Poster 24
Thu 22nd
17:10–18:10

Lars Bock[1], Helmut Grubmüller[1]

[1]Max Planck Institute for Multidisciplinary Sciences

lars.bock@mpinat.mpg.de

The recent revolution in cryo electron microscopy (cryo-EM) allows the determination of structures of macromolecular complexes at atomic resolution. Cryo-EM also provides information on structural heterogeneity and ensembles of macromolecules. To obtain cryo-EM images of macromolecules, the samples are first rapidly cooled down to liquid nitrogen temperatures. The rapid cooling preserves some information of the room temperature ensemble. However, to what extent the structural ensemble is perturbed by the cooling is currently unknown. To quantify the effects of cooling, we first estimated the temperature drop rate by solving the heat equation

which suggests that cooling takes place within microseconds. Then, we started all-atom explicit-solvent molecular dynamics (MD) simulations of the ribosome from 41 snapshots taken from a room temperature ensemble with linearly decreasing temperature at 11 different cooling rates each with simulation lengths ranging from 0.1 ns to 128 ns. In the simulations, we observed that cooling leads to a marked decrease in the structural heterogeneity of the cooled ensemble. To test if and how this effect depends on the cooling rate, we used Bayesian statistics to test three thermodynamic and kinetic models of the cooling process. The observation that a kinetic two-state model improves the prediction of the decrease in heterogeneity compared to the cooling-rate independent thermodynamic model suggests that kinetic effects do contribute markedly. The combination of the estimated temperature drop rate with the kinetic model suggests that small barriers between the states (<10 kJ/mol) are overcome during cooling and do not contribute to the heterogeneity of the structural ensemble obtained by cryo-EM. In contrast, conformational states separated by barriers above 10 kJ/mol are expected to be trapped during plunge-freezing. The obtained parameters for the kinetic model will allow one to quantify the heterogeneity of biologically relevant room-temperature ensembles from cryo-EM structures.

Study and analysis of plant growth and development results using biophysics tools and informational simulation

Poster 25
Wed 21st
17:00–18:30

Maamar Boukabcha[1]

[1]Hassiba BEN BOUALI University of Chlef, Faculty of natural sciences and life, Chlef, Algeria

boukamaa@gmail.com

Plant growth and development is a very important natural phenomenon among the complex systems of living complexes. To study this phenomenon during plant growth and development, we use many methods and means including biophysics and informatics tools. Informatics simulation of plant growth has a long history, where simulation of plant growth and development results data by computer programs plays an important role in extracting different results. The study and analysis of data on the results of different growth and development of plants across the world remains continuous through different ages and places under different experimental and natural conditions.Key words: plant growth, biophysical tools, simulation, modeling.

λ-dynamics in GROMACS with the Fast Multipole Method: Constant pH MD and beyond

Poster 26
Thu 22nd
17:10–18:10

Eliane Briand[1]

[1]Max Planck Institute for Multidisciplinary Sciences
eliane.briand@mpinat.mpg.de

The residue protonation state of biomolecules is usually treated as fixed in molecular dynamics (MD) simulations: this is equivalent to a time-varying pH. Numerous approaches are found in the literature to obtain a more realistic constant pH by dynamically altering protonation, however these tend to be too slow or too complicated for routine use. Building upon the established λ-dynamics method with Hamiltonian interpolation, we aim to make constant pH MD (CPH-MD) accessible to the non-expert by an intuitive interface, a user-oriented documentation, and a performance high enough for use beyond small proteins through FMM electrostatics.

Imaging Single Cells with an Optical Stretcher and X-ray Phase-Contrast Tomography

Poster 27
Wed 21st
17:00–18:30

Jan-Philipp Burchert[1], Madleen Busse[2], Roland Stange[3], Tim Salditt[1], Sarah Köster[1]

[1]Institute for X-Ray Physics, Georg-August-Universität Göttingen
[2]Department of Physics and Munich School of Biomedical Engineering, Technical University of Munich
[3]RS Zelltechnik GmbH, Schöllnach

jan-philipp.burchert@uni-goettingen.de

X-rays penetrate deep into matter and allow us to image structures with high spatial resolution, which makes them attractive for investigating individual biological cells. Here, we combine x-ray phase contrast tomography with an x-ray compatible optical stretcher to image single cells in solution, thus in their physiological environment, and avoid the need for freezing, drying or embedding of the samples. The cells are trapped in a contactless manner in a fixed position by the optical stretcher and probed by the x-ray beam. The flow from the microfluidic device sets the cells in slow rotational motion, which enables tomographic imaging. We apply this combination of techniques to unfixed and fixed NIH3T3 fibroblasts, which are partially stained with an x-ray contrast agent. The experimental data show that we can acquire images of these cells with our setup. Moreover, the comparison of the different preparations and two beam energies will improve the image quality in future experiments.

Selectivity Filter Occupancy and Gating Transitions in the MthK Potassium Channel

Poster 28
Thu 22nd
17:10–18:10

Reinier de Vries[1], Wojciech Kopec, Bert L. De Groot

[1]Max Planck Institute for Multidisciplinary Sciences
reinier.devries@mpinat.mpg.de

Potassium Channels are one of the most ubiquitous classes of proteins and are found across all forms of life. Potassium permeation is controlled in several different ways in most potassium channels. The selectivity filter plays a crucial role here. MthK is a bacterial calcium gated potassium channel and used as a model for calcium-gated potassium channels. Recently several structures of closed and inactivated MthK have been published. We use atomistic molecular dynamics simulations to study the different states of this channel and explore the possibility of using these to elucidate the mechanism by which the channel changes between different gating configurations. To study the effect of this different conformations on the selectivity filter configuration we measure the occupancy of the different binding sites in the selectivity filter. Ammonium ions are often used as a substitute for potassium in NMR experiments due to their similar properties and have been shown to have similar occupancy patterns in molecular dynamics simulations of other potassium channels. We therefore also perform simulations using ammonium ions and compare the selectivity filter occupancy to simulations with potassium ions. This allows for later comparison of selectivity configuration data with ssNMR experiments.

Selected references:
Direct Detection of Bound Ammonium Ions in the Selectivity Filter of Ion Channels by Solid-State NMRCarl Öster, Kumar Tekwani Movellan, Benjamin Goold, Kitty Hendriks, Sascha Lange, Stefan Becker, Bert L. de Groot, Wojciech Kopec, Loren B. Andreas, and Adam LangeJournal of the American Chemical Society 2022 144 (9), 4147-4157 DOI: 10.1021/jacs.1c13247Ball-and-chain inactivation in a calcium-gated potassium channelChen Fan1, Nattakan Sukomon, Emelie Flood , Jan Rheinberger, Toby W. Allen and Crina M. NimigeanNature 580, 288–293 (2020). DOI: /10.1038/s41586-020-2116-0
Molecular mechanism of a potassium channel gating through activation gate-selectivity filter coupling. Wojciech Kopec1 , Brad S. Rothberg and Bert L. de GrootNat Commun 10, 5366 (2019). DOI: 10.1038/s41467-019-13227-w

Poster 29
Wed 21st
17:00–18:30

Introducing a peptide mimicking neuroligin 2 for collybistin 2 activation

Lara Dohmen[1], Claudia Steinem[2], Olaf Jahn[3], Lars van Werven[3]

[1]Institute for organic and biomolecular chemistry
[2]Institute for Organic and Biomolecular Chemistry, Georg-August-Universität Göttingen
[3]Max-Planck-Institute for Multidisciplinary Sciences

lara.dohmen@uni-goettingen.de

The assembly of the GABAergic post-synapse is a key step in synaptogenesis and crucial for the regulation of neuronal communication. Its formation depends a plethora of different proteins. The scaffolding protein gephyrin is one critical component for assembly, since it is essential for clustering of the inhibitory GABAA-receptor. Thereby, collybistin 2 (CB2) is necessary to recruit gephyrin to the postsynaptic membrane. Due to its self-associated conformation, CB2 requires activation by neuroligin 2 (NL2) in order to change to an active state.[1] Owing to its complexity, the formation of the GABAergic inhibitory post synapse is extremely prone to disfunctions causing a spectrum of neuronal diseases.[2,3,4] Thus, it is crucial to understand the mechanism underlying the process of synapse organization.For a better comprehension, it is essential to investigate single protein interactions in detail without the influence of unknown components. Therefore, we use an in vitro system, which allows us to examine interaction properties in a bottom-up approach in a highly controlled manner. Solid supported hybrid monolayers (SHMs) serve as a membrane model system. We aim at investigating the interaction between collybistin 2 and neuroligin 2, which is able to activate CB2 for binding to phosphoinositides in the membrane. As neuroligin 2 is an intermembrane protein, its insertion into solid supported membranes is not feasible. Therefore, we established another approach to introduce the protein to the in vitro system. Via ATR-IR spectroscopy we were able to show the successful attachment of a NL2-mimicking peptide, harboring the cytosolic CB2 binding site, to the membrane via a reaction between a cysteine and a maleimide-lipid. This opens up a new way of investigating the interactions between CB2 and NL2. We plan to use reflectometric interference spectroscopy to quantify the binding behavior of different CB2-forms to SHMs in dependence of the NL2-mimicking peptide.

Coarsening of biomolecular condensates regulate crossover placement in Meiosis I

Poster 30
Thu 22nd
17:10–18:10

Marcel Ernst[1], David Zwicker[1]

[1]Max Planck Institute for Dynamics and Self-Organization

marcel.ernst@ds.mpg.de

During meiosis, genetic information from female and male chromo- somes is exchanged in a process called crossover. The dynamics that determine the positioning of these crossovers is largely not understood. Experimental observations consistently reveal two key findings: First, the number of crossovers per chromosome is at least one and is usu- ally small, between one and three. Second, there is crossover interfer- ence, which prevents nearby crossovers on a single chromosome. We hypothesize that crossovers are determined by biomolecular conden- sates, which coarsen by exchanging material along chromosomes. We present theoretical and numerical results suggesting scaling laws anal- ogous to Lifshitz-Slyozov-Wagner theory that predict the final number of crossovers, and their spatial structure as a function of coarsening time, chromosome length, and the initial amount of material. These results are consistent with current experimental findings in Arabidopsis thaliana and suggest how cells use a fundamental coarsening process to regulate spatial patterns.

Reconstituting ATP synthase and monitoring its activity in photoacid-containing vesicles

Poster 31
Wed 21st
17:00–18:30

Hendrik Flegel[1], Amelie Jane Meyer[2], Julia Bock[2], Tobias Weege[2], Heuer Alexa[2], Claudia Steinem[2]

[1]Institute of Organic and Biomolecular Chemistry
[2]Georg-August-University, Institute of Organic and Biomolecular Chemistry Göttingen, Germany

hendrik.flegel@uni-goettingen.de

The ATP synthase is one of the most important protein complexes and responsible for synthesizing the energy currency ATP from ADP and phosphate. This transmembrane protein is a molecular motor driven by an electrochemical gradient called proton motive force pmf. Since the pmf is composed of the pH difference ΔpH and the electric potential $\Delta\varphi$ across the respective membrane, ATP synthesis can be induced by a proton gradient.While the proton pathway within the protein during ATP synthesis is rather understood, the question of how the protons reach the protein entrance is still elusive. A new experimental approach enables the control of proton release in time and location. We use photoacid molecules exhibiting different pKa values in the ground and in the first excited state. Hence, upon light excitation the photoacid becomes highly acidic and a proton release follows. Placing these proton sources either on the membrane surface or in bulk solution should allow differentiation between the transfer of interfacial and bulk protons towards

the ATP synthase. Therefore, the reconstitution of FOF1 ATP synthase from thermophilic Bacillus in large unilamellar photoacid-containing vesicles with the right protein orientation is required. Here, we employ the photoacid 8-hydroxy-1,3,6-pyrenetrisulfonate (HPTS). While water soluble HPTS is entrapped in the vesicle lumen, the amphiphilic derivative C12-HPTS can be incorporated within the vesicle membrane. It remains to be elucidated whether it is necessary to prepare vesicles with an asymmetric distribution of photoacid molecules in order to ensure a proton gradient across the membrane. To verify whether the developed reconstitution protocols and the presence of the photoacid itself have any influence on the protein activity, the highly sensitive luciferin-luciferase assay is used. The successful reconstitution of the key structures described above will be the first step towards examination of the influence of proton localization on protein activity.

Conformational dynamics of Elongation Factor G: an in silico study

Poster 32
Thu 22nd
17:10–18:10

Sara Gabrielli[1], Helmut Grubmueller[1], Lars Bock[1]

[1]Max Planck Institute for Multidisciplinary Sciences

sara.gabrielli@mpinat.mpg.de

Elongation Factor G (EF-G) is a GTPase that is involved in protein synthesis in bacterial cells. After peptide bond formation, EF-G binds to the ribosome and accelerates tRNA translocation. Although recent cryo-EM data of early translocation steps have shown a large overall reorientation of EF-G in the ribosome following Pi release, little is known about intermediate conformations explored during this rearrangement. The high flexibility of domain IV observed inCryo-EM studies and its proximity to the A-site tRNA suggest that the dynamics of domain IV might play a fundamental role during translocation. In order to investigate the conformational dynamics and energetics of EF-G, we use extensive all-atom Molecular Dynamics simulations. Simulations of E. Coli EF-G in solution have indeed revealed that the most pronounced inter-domain motion is the rotation of domains IV-V relative to domains I-III. The results have also provided an insight on the conformations that are intrinsically favoured in the protein, i.e. independently from the interactions with the ribosomal environment. Starting from the observations here reported, we plan to soon integrate and compare the results with simulations of EF-G in the ribosome.

Interactions between Cytoskeletal Filaments

Poster 33
Wed 21st
17:00–18:30

Magdalena Haaf[1], Anna Schepers[1], Sarah Köster[1]

[1]Institute for X-Ray Physics

magdalena.haaf@uni-goettingen.de

The cytoskeletal filaments –actin, microtubules, and intermediate filaments (IFs)– constitute an interpenetrating network which performs essential cellular functions. Next to the mechanical properties of the single filaments, the interactions between the filamentous proteins play an important role in cytoskeletal network mechanics. To gain a deeper understanding of the composite network it is useful to quantify suchinteractions in a controlled setting. Cell experiments have revealed a functional and structural interplay between F-actin and vimentin IFs. However, in reconstituted systemsstudies of mixed networks come to conflicting conclusions. To clearly solve this conflict, it is crucial to simplify the system even further to the single filament level. We use a quadruple optical trap in combination with microfluidics and fluorescence microscopy to directly quantify interaction strength and dynamics between F-actin and vimentin IFs. Our approach allows us to characterize the interactions independent of network morphology. This setup further enables us to probe the influence of electrostatic and hydrophobic effects on the interactions between single filaments.

DFT simulation of Ion Permeation in Potassium Channels

Poster 34
Thu 22nd
17:10–18:10

Chenggon Hui[1], Wojciech Kopec[1], Bert de Groot[1]

[1]Max Planck Institute for Multidisciplinary Sciences

chenggong.hui@mpinat.mpg.de

Potassium channels are the most widely distributed ion channels. It permeates potassium ions at a high rate. (150mA or an ion per 10 ns). The MD simulated conductance is much lower than the experiment result and the ion force field is typically blamed. We used ab initio MD at the DFT level to specifically investigate the process of ion permeation through the narrowest part of the channel (selectivity filter).

Metabolic tumor imaging with rapidly signal-enhanced 1-13C-pyruvate-d3

Poster 35
Wed 21st
17:00–18:30

Theresa Hune[1], Salvatore Mamone[1], Henning Schroeder[1], Anil Jagtap[1], Sonja Sternkopf[1], Gabriele Stevanato[1], Sergey Korchak[1], Claudia Fokken[1], Christoph Müller[2], Andreas Schmidt[2], Dorothea Becker[1], Stefan Glöggler[1]

[1]Max Planck Institute for Multidisciplinary Sciences
[2]DKTK, Freiburg

thhu@mpinat.mpg.de

Using para-hydrogen to enhance NMR signals is a convenient way to overcome the inherently low sensitivity of NMR spectroscopy. Via hydrogenation of a side arm that can be chemically removed later on, this technique is now applicable to a wide range of molecules. High signal intensities enable diagnostically valuable tools like Magnetic Resonance Spectroscopic Imaging (MRSI). MRSI is a non-invasive method for the characterization of metabolism in vivo that combines the features of an NMR spectrum with an anatomical MRI image. Changes in metabolism are often the first signs for pathological changes in tissues and have therefore a high diagnostic value.In this work, hyperpolarized 1-13C-pyruvate was used to investigate cancer metabolism in vivo. Crucial steps are the hydrogenation of vinyl pyruvate using para-enriched hydrogen as well as the polarization transfer from the protons to the carbon of interest via irradiation with radiofrequency pulses. Bond cleavage and purification procedures, including catalyst filtering, lead to an aqueous solution with a concentration of 50 mM of the hyperpolarized metabolite which was then used for in vivo experiments. As a model, subcutaneous human melanoma xenografts in Balb/c nu/nu mice were chosen.The hyperpolarized pyruvate was injected into the tail vein of the mice and metabolic images and spectroscopic data were acquired. In order to quantify the conversion of pyruvate to lactate, a series of NMR spectra was acquired after the injection. They show that pyruvate is rapidly converted into lactate and alanine. The concentration profiles were fitted using a model-free approach based on the area under the curves. The rate constants of the conversion were determined. For the images, an EPSI sequence (Echo Planar Spectroscopic Imaging) was used. The images show pyruvate as well as lactate at the site of the tumor, demonstrating the feasibility of this method for tumor diagnostics.

Resonant Feedback Control of Cardiac Arrhythmia Using Optogenetics

Poster 36
Thu 22nd
17:10–18:10

Sayedeh Hussaini[1], S. L. Laedke [1], J. S. Schetelig [1],A. M. Kyzy [1], L. N. Diaz-Maue1 [1], V. Biktashev [3], R. Majumder [1], V. Krinski [2], S. Luther [1]

[1]Max Planck Institute for Dynamics and Self-Organisation
[2]INPHYNI, CNRS, SOPHIA Antipolis, France
[3]Exeter University, Exeter, England

sayedeh.hussaini@ds.mpg.de

Introduction: Rotating spiral waves in the heart are associated with life-threatening cardiac arrhythmias. Today, strong, globally resetting electrical shocks are used to terminate cardiac fibrillation. Significant side effects have motivated the development of alternative low-energy approaches, (S.Luther, *Nature* (2011)). For this purpose a detailed understanding of the dynamics of spiral waves is required. Cardiac optogenetics opens novel paths to study the mechanisms underlying the onset, perpetuation, and control of cardiac arrhythmias. The termination of ventricular arrhythmias has been demonstrated in optogenetic Langendorff-perfused mouse hearts using global and structured illumination (R. Uribe, *Front Physiol* (2018), S. Hussaini, *eLife* (2021)). In this study, we use optogenetics as a tool to numerically and experimentally investigate the control method of resonant feedback pacing, in which global periodic illumination is applied to cardiac tissue.
Methods: We use a two-dimensional computational model to describe the spatiotemporal evolution of membrane voltage across an optogenetically modified murine cardiac monolayer . Additionally, we report the results of our ex vivo studies using 5 Langendorff-perfused hearts from αMHC-ChR2 transgenic mice.
Results: Our study shows a significant increase in termination efficiency of resonant feedback stimulation using periodic global illumination, compared to a single global optical pulse corresponding to conventional defibrillation. The dose-response curve demonstrates termination rates of more than 50% and 100% at the lowest and highest light intensity of 3.1 and 100 µW/mm2 for the resonant feedback case. In contrast, it shows a decrease in termination rate to 0 % and ≈45 % for the single optical pulse. Our simulations suggests that resonant drift is the underlying mechanism for termination of arrhythmia in mouse heart at very low LIs. Further experimental validation of these results is ongoing.
Conclusion: Resonant feedback pacing demonstrates effective low-energy defibrillation in numerical simulations and experimentally in intact mouse hearts (S. Hussaini, Ph.D. thesis, *eDiss* (2021)).

Time-Domain Simulations of Pulsed ENDOR Sequences

Poster 37
Wed 21st
17:00–18:30

Annemarie Kehl[1], Robert Zeier[2], Steffen Glaser[3], Marina Bennati[1]

[1]Max Planck Institute for Multidisciplinary Sciences
[2]Forschungszentrum Jülich
[3]TU München

akehl@gwdg.de

A well-established tool to detect the interaction between an electron spin and a nucleus is ENDOR spectroscopy. To derive structural parameters from the experiment usually simulations of the spectra are performed.Generally, these are frequency domain simulations, i.e. the resonance frequencies are calculated from the spin Hamilton operator and simulated as a 'stick' spectrum. Then, the 'stick' spectrum is convoluted with a line-shape function containing a line broadening and a line shape function according to the pulse sequence. This approach is relatively fast and easily accessible to extract structural information from the experiment. However, the effect of the pulse sequence on the experiment is only simulated in a pre-defined

way. A tool to directly simulate the effects of pulse sequences are time domain simulations, i.e. calculating the effect of the pulses on the spin density matrix over the whole time period of the experiment.[1] Here we will demonstrate the use of time domain simulations to evaluate and understand the spin-dynamics in advanced pulse ENDOR sequences such as cross-polarization (CP) ENDOR, spin lock ENDOR and NOVEL-based ENDOR.[2] In the simulation different physical aspects should be considered, e.g. the anisotropic term (so-called B term) of the hyperfine coupling, the g-anisotropy and effects of powder patterns This allows not only for an assignment of the effects detected in experimental spectra, i.e. the asymmetries in single-crystal ENDOR spectra due to the detection of the B-term. It also provides a theoretical tool to identify the potential strengths and weaknesses of pulse sequences, as well as the parameters that might be optimized.

Literature:

I. Bejenke, et.al., Molecular Physics 2020,118:18

R. Rizzato, et.al., Molecular Physics, 2013, 111, 2809

Poster 38
Thu 22nd
17:10–18:10

Ion Conduction Mechanisms in Potassium Channels Revealed by Permeation Cycles

Chun Kei Lam[1], Bert de Groot[1]

[1]Max Planck Institute for Multidisciplinary Sciences

chun-kei.lam@mpinat.mpg.de

Potassium channels are responsible for the selective yet efficient permeation of potassium ions across cell membranes. Despite a vast amount of available high-resolution structures of potassium channels, those conformations inform mostly only static information on ion permeation processes. Here we employed molecular dynamics simulations and Markov state models to obtain dynamical details of ion permeation. The full permeation routes expressed in terms of selectivity filter occupancy are illustrated. We show that the water-free permeation represents the dominant permeation mode over a wide range of potassium concentration, temperature, and membrane voltage for the pore of MthK, demonstrating the robustness of the direct knock-on mechanism. Our results shed light on the underlying permeation details that happen in the selectivity filter which are valuable in studying conduction mechanisms in potassium channels.

Structure Determination from Fluctuation X-ray Scattering

Poster 39
Wed 21st
17:00–18:30

Michael Maihöfer[1], Helmut Grubmüller[1]

[1]Max Planck Institute for Multidisciplinary Sciences

michael.maihoefer@mpinat.mpg.de

Fluctuation x-ray scattering is an exciting new method for determining biomolecular structures in solution. It promises to give structural information under native, biological conditions of the molecule. However, only few photons are scattered per image, and the orientation of each scattering molecule is unknown. For these reasons, the reconstruction from the scattering images remains a challenging task. To address this problem, we develop a bayesian framework, that finds the most probable structure that gives rise to the scattering images. It explicitly accounts for the unknown molecular orientations by marginalizing out all possible orientations. To reduce the computational cost, this is done by summing over many randomly chosen orientations.We show that with our method it is possible to recover structures to near-atomic resolution.

Cytoskeletal Networks in Cells Under Strain

Poster 40
Thu 22nd
17:10–18:10

Ruth Meyer[1], Anna V. Schepers[2], Peter Luley[2], Sarah Köster[2]

[1]Institute for X-Ray Physics

[2]Institute for X-Ray Physics, Georg-August-Universität Göttingen

ruth.meyer@uni-goettingen.de

The cytoskeleton of eukaryotic cells mainly consists of three types of filamentous proteins: F-actin, microtubules and intermediate filaments (IFs). In contrast to microtubules and actin filaments, IFs are expressed in a cell-type specific manner, and keratins are found in epithelial cells. In certain cell types, the IF keratin forms a layer close to the membrane, referred to as an "IF-cortex". It has been observed that this IF-cortex arranges in a "rim-and-spokes" structure in epithelia. Based on this hypothesis, IFs and actin filaments might add complementary mechanical properties to the cellular cortex. When stretching single IFs, it was previously shown that IFs remain undamaged even at high forces. 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. The experiment is conducted by seeding cells on an elastic substrate and then stretching the substrate uniaxially or equibiaxially to high strains. In combination with fluorescence and atomic force microscopy, this setup allows us to study the structure and the mechanical properties of actin and IF networks close to the cell membrane.

Study of permeation and gating mechanisms in K+ channels using molecular dynamics simulations

Poster 41
Wed 21st
17:00–18:30

Andrei Mironenko[1], Bert L. de Groot[1], Wojciech Kopec[1]

[1]Max Planck Institute for Multidisciplinary Sciences

amirone@mpibpc.mpg.de

K+ channels feature high conductance rates combined with high selectivity for K+ ions. One of the central questions regarding K+ channels has been the permeation mechanism: the exact order, in which K+ ions and water molecules traverse the narrowest, highly conserved part of the channel - the selectivity filter (SF) - that would explain the highly efficient permeation. Another important feature of K+ channels is that they are often gated by ligands and voltage, which involves complex allosteric interactions between multiple domains of the channel. Clarifying the mechanistic and energetic underpinnings of this process is a challenging task.In this work, we employ molecular dynamics simulations to study two such questions. First, we investigate the ion permeation mechanism in two SF mutants of the KcsA channel - G77A and T75A. We show that these mutants disrupt the water-free permeation seen in the WT KcsA, and lead to a low-conductance, low-selectivity potassium permeation - in line with our previous observations that co-permeation of water decreases the K+ permeation efficiency. Then, we shift our focus onto the Slo1 channel: it is gated synergistically by Ca2+ and voltage, and in the Ca2+-free state it presumably undergoes pore dehydration that hinders ion permeation. Our MD simulations with applied voltage reveal that the Ca2+-bound structure is indeed potassium conductive, while the Ca2+-free is functionally closed. We further observe that spontaneous unbinding of Ca2+ from the cytosolic gating ring of the conductive Slo1 causes pore dehydration and lipid entry, coupled with a conformational transition to the closed state - thus suggesting a closing mechanism for the channel.

Analysis of cortical tension on lumen formation of epithelial spheroids

Poster 42
Thu 22nd
17:10–18:10

Amaury Perez Tirado[1,2], Andreas Janshoff[2]

[1]Institut für Physikalische Chemie
[2]Institute of Physical Chemistry University

amaury.pereztirado@uni-goettingen.de

Coordinated epithelial cells aggregates and forms spheroids in the presence of three-dimensional extracellular matrix conditions. In the process of morphogenesis, they form a shell layer with an encapsulated lumen that grows until reaching a stable phase. Recent studies have showed the formation and adaptation of the cells during the cystogenesis, using techniques of optical microscopy. The study of epithelial cell as barriers and monolayers has been explored but the mechanical properties of these cyst structures and the variations of the lumen pressure during the process of formation are not completely understood. We are proposing the use of force spectroscopy

on epithelial cyst on different stages of the growth to analyze the cortical tension of the cellular surface though the fitting of a model based on the pre-stress of the surface, the areastrain and the viscoelastic properties. The preliminary results showed a hydrostatic pressure between 200 and 400 kPa on cyst with diameters between 50 and 70 μm. This study revealed the importance of mechanical properties of the cell membrane to keep the homeostasis in the formation of epithelial spheroids

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Fluorescence Lifetime Image Scanning Microscopy

Poster 43
Wed 21st
17:00–18:30

Niels Radmacher[1]

[1]Faculty of Physics, University of Göttingen

niels.radmacher@phys.uni-goettingen.de

The spatial arrangement and relative composition of proteins in cells can be an essential clue for the health of an organism. Thus capturing high-resolution images of living cells in native environment is a vital tool for diagnostics in medicine and biology.Image Scanning Microscopy (ISM) provides twice the resolution of a confocal microscope by replacing the single-point detector with a CCD chip.Another excellent tool for bio-imaging is Fluorescence Lifetime Imaging Microscopy (FLIM), which allows for distinguishing different markers by their specific lifetime.Combining these two techniques into a Fluorescence Lifetime Image Scanning Microscope (FL-ISM) enables superresolution microscopy with fluorescence lifetime multiplexing for live cell and tissue imaging. This requires an array of single-photon detectors such as SPADs (Single Photon Avalanche Diodes) or MPMTs (Multianod Photomultiplier Tube).Our results show simultaneous fluorescence lifetime multiplexing for up to three different structures in two spectral regions. At the same time, we are keeping acquisition times comparable to other Fluorescence Lifetime Imaging techniques.

Characterizing proton transport in giant unilamellar vesicles using a microfluidic approach

Poster 44
Thu 22nd
17:10–18:10

Dominik Ruppelt[1], Elena Ackermann[1], Claudia Steinem[1]

[1]Georg-August-Universität Göttingen

dominik.ruppelt@uni-goettingen.de

Proton-transfer across lipid membranes belongs to the most prevalent reactions in living cells and, thus, understanding the mechanism of action of proton-translocating peptides and proteins is of great importance. In vivo, vesicle bulk assays are traditionally used involving large unilamellar vesicles and some kind of pH-sensitive fluorescent dye. However, this approach is accompanied by certain drawbacks since it does not provide any information about the behavior of single vesicles. Furthermore, since the establishment of a pH-gradient after the addition of a peptide is difficult, most assays rely on the insertion of the peptide after establishing a pH-gradient making the resulting data a convolution of insertion, peptide assembly and

proton transport kinetics. Therefore, innovative approaches allowing the observation of proton transport on a single-vesicle level are favorable.Here, we adopted a setup based on the microfluidic trapping of giant unilamellar vesicles for the analysis of transmembrane proton translocation. The fluorescent dye pyranine was entrapped in GUVs before these were immobilized in micro-structured features based on PDMS and the compound of interest was pre-inserted. The setup allows for a rapid buffer exchange and with this the fast formation of a pH-gradient across the membrane yielding the proton transport without the limitations present in bulk assays. To provide a proof of principle of our system, we monitored differences in the proton transport mediated by the channel gramicidin and the carrier molecule CCCP. Based on our findings, we were able to differentiate between a channel and carrier solely on their proton translocation rates.

Poster 45
Wed 21st
17:00–18:30

Measuring photophysical transition rates with fluorescence correlation spectroscopy and antibunching

Damir Sakhapov[1], Ingo Gregor[2], Narain Karedla[3], Joerg Enderlein[2]

[1]Third Institute of Physics, Biophysics
[2]Third Institute of Physics
[3]The Rosalind Franklin Institute

damir.sakhapov@phys.uni-goettingen.de

Fluorescence correlation spectroscopy (FCS) is outstanding when measuring diffusion properties of molecules. Studies of photophysical rate constants, however, are hindered by their strong dependence on excitation intensity dependence, a quantity notoriously difficult to determine in an FCS framework. Here, we perform fluorescence antibunching measurements to determine absolute values of excitation intensity in the confocal volume. The core idea is to measure antibunching times at different excitation intensities, which can then be used to extract absolute numbers for the excitation rate of the studied molecules. These numbers can then be used to determine absolute values for the intersystem crossing and phosphorescent rates of the studied dye.

Insights into the operation mode of ABCE1 via Markov Models

Poster 46
Thu 22nd
17:10–18:10

Malte Schäffner[1], Helmut Grubmüller[1]

[1]Theoretical and Computational Biophysics, Max Planck Institute for Multidisciplinary Sciences

malte.schaeffner@mpinat.mpg.de

ABCE1 is a remarkable structural exception of the ubiquitous ATP Binding Cassette(ABC) superfamily. Unlike almost all other members, ABCE1 lacks transmembranedomains and comprises only the 'core engine' of all ABC proteins, and therefore is anideal prototype for studying the mechanism of ABC proteins in general. Each of itstwo homologous nucleotide binding domains (NBD) contains one nucleotide bindingsite, which can be in an open and a closed state. Despite this near symmetry, andquite unexpectedly, the kinetics has been found quite asymmetric: Whereas a E238Qpoint mutant that impairs ATP hydrolysis in one of the two binding sites reduced theoverall turnover rate of the enzyme by a factor of two–as one might expect–a E485Qpoint mutant that impairs the other site, staggeringly, shows a so far unexplained ten-fold increase.To address this issue, we used Markov models to study how such asymmetry canarise. Specifically we asked if previously proposed long range couplings or allostericinteractions between the two binding sites are really required to explain thisobservation. Indeed, using a Bayesian approach, we found Markov models thatquantitatively match the measured kinetics as well as additional occupation data, andnevertheless did not require any coupling or allostery beyond the structure-inducedproperty that opening and closing always involves both NBSs. The unexpected fastkinetics of the second mutant is explained in terms of dominant reaction pathways,which change drastically for the second mutant allowing circumvention of the rate-limiting step present in wild-type and first mutant. We expect that this Bayes/Markovapproach can help, quite generally, to gain a systematic and quantitativeunderstanding of enzymatic kinetics governed by coupled chemical andconformational dynamics as a basis for rational enzyme optimization.

Bayesian Structure Determination from Single Molecule X-Ray Diffraction

Poster 47
Wed 21st
17:00–18:30

Steffen Schultze[1], Helmut Grubmüller[1]

[1]Max-Planck-Institute for Multidisciplinary Sciences

steffen.schultze@mpinat.mpg.de

Single molecule X-Ray diffraction experiments are a promising new method for the structure determination of biomolecules. The reconstruction of the structure from these experiments is quite challenging: The scattering images are sparse, each containing only 15 photons on average, and the signal to noise ratio is very low. In addition, the orientations of the molecules at the time of scattering are unknown. Available analysis methods require at least 100 photons per image, or a very large number (e.g. 10^9) of images. We present a novel Bayesian approach that requires

fewer photons per image and, at the same time, relatively few images. It is flexible in that many different representations of the electron density can be used, both in Fourier space and directly in real space. Using synthetic data, we demonstrate the method is able to recover the structure of the protein crambin at 6-7Å resolution using only 10^6 images, and at 3.8Å resolution using 10^8 images.

Poster 48
Thu 22nd
17:10–18:10

Analyzing EEG networks throughout the lifespan

Nicolai Spicher[1], Theresa Bender[2], Ennio H. Idrobo-Ávila[2], Niels K. Focke[3], Dagmar Krefting[2]

[1]University Medical Center Göttingen
[2]Department of Medical Informatics, University Medical Center Göttingen
[3]Clinic of Neurology, University Medical Center Göttingen

nicolai.spicher@med.uni-goettingen.de

Aging is a complex process with a multitude of effects on physiology and psychology with impact on behavior and social-emotional skills. Over the course of life, the brain undergoes measurable structural and functional changes but it is unclear what defines (un)healthy aging. With neurodegenerative diseases (e.g. dementia) on the rise, understanding the network interactions involved in aging is essential. In this work, we use time delay stability (TDS, Bashan et al. 2021) as a method to analyze changes in aging in sleeping subjects. We use electroencephalography (EEG) data of the SIESTA study containing polysomnography data acquired in European sleep centers with N=488 subjects (391 healthy controls, 97 sleep apnea patients) in the range [20,95] years. Next to healthy controls, we analyze sleep apnea patients to get an idea of the influence of non-ageing-related issues The EEG electrode placement was frontal/central/occipital left/right with a sampling rate of 200Hz. Sleep data was manually annotated by experts in sleep medicine, following the Rechtschaffen and Kales (1968) guidelines, resulting in four different stages: deep sleep (DS) / light sleep (LS), REM sleep, wake state (W). We split EEG signals into five frequency bands of the same width (δ=0-4Hz / ϑ=4-8Hz / α=8-12Hz / σ=12-16Hz / β=16-20Hz) and used a MATLAB implementation of TDS. It allows to compute the degree interaction between the 16 different EEG electrode pair combination, that we averaged in a single value. Our results show that in healthy patients network strengths declines w.r.t age. In sleep apnea patients we observe parabola-shaped curves reaching maxima in middle age (45-55 years). In principle network strength is stronger in more awake states. In future work, we aim for working towards disentangling health- and aging-related issues.

Formation and maintenance of Calcium channel clusters: A bottom-up approach

Poster 49
Wed 21st
17:00–18:30

Nikolas Teiwes[1], Niko Schwenzer[2], Celine Pohl[1], Ingo Mey[1], Stephan Lehnart[2], Claudia Steinem[1,3]

[1]Institute of Organic and Biomolecular Chemistry
[2]Research Unit for Cellular Biophysics and Translational Cardiology
[3]Max Planck Institute for Dynamics and Self-Organization

nikolas.teiwes@uni-goettingen.de

The native plasma membrane is tremendously overwhelming. Lipid Rafts, Protein Clusters and other emergent membrane properties are due to cellular and cytosolic complexity poorly understood. To investigate the function and dynamics of membrane components and simultaneously adjust the surrounding environment, a new in vitro system is needed. To empower further membrane analysis Giant Plasma Membrane Vesicles (GPMVs) derived from cells are spread on solid supported & porous silicon dioxide (SiO2) substrate, creating solid-supported plasma membrane bilayers (SPMB) & pore-spanning plasma membranes (PSPM).Amongst other investigations, GPMVs, SPMBs and PSPMs allow for the characterization of phase behavior, diffusion and viscosity of abstracted cellular membrane. Subsequently, we present besides a proof of principle of these promising bottom-up systems, insights to fundamental properties.

Actin and Spine shape dynamics as Synaptic tag

Poster 50
Thu 22nd
17:10–18:10

Mitha Thomas[1], Michael Fauth[2]

[1]Third Institute of Physics - Biophysics, Georg-August-Universität Göttingen
[2]Third Institute of Physics, Georg-August-Universität Göttingen

mitha.thomas@phys.uni-goettingen.de

Long-term potentiation of synapses is an important form of synaptic plasticity. It occurs in two phases: an early phase which constitutes a transient increase in synaptic strength, and a late phase which sustains this increase for a longer duration. The synaptic tagging and capture hypothesis states that the late phase is possible if the stimulus leads to a transient 'synaptic tag' in concurrence with the synthesis of plasticity-related proteins, which reorganise the post synaptic density. What acts as a 'tag' remains largely unknown. We follow the hypothesis that actin dynamics in interaction with spine geometry acts as a synaptic tag and test this using computational modelling. We build on an existing model for non-LTP conditions that links spine geometry and actin dynamics. Actin dynamics is assumed to occur in discrete foci and involve mechanisms for filament branching, capping, severing and uncapping. To investigate LTP, we first study a single actin focus and introduce time-dependence for the above mechanisms. We observe that an increase in branching rate entails an increase in the lifetime of the focus and in actin activity. Likewise, increasing the capping rate bring down actin activity and leads to a shorter-lived

focus. Varying the rates of multiple processes, we observe that severing and uncapping simultaneously bring about significant effects on actin activity. Next, we simulate multiple foci introducing nucleation rate. While nucleation is increased, an increased number of foci and, hence, actin activity is observed. In summary, we show that the concerted modulation of multiple processes facilitates actin activity but the modulation of actin dynamics by itself only leads to short-lived changes. Thus, coupling to spine geometry is necessary. To verify this, we introduce a simplified spine area dynamics based on the number of foci and indeed observe alterations on time-scales that are suggestive of synaptic tag.

Poster 51
Wed 21st
17:00–18:30

An integrated NNBD-based platform for molecular phenotypic analysis in DCM patient-specific iPSC-cardiomyocytes and CRISPR-Cas9-engineered controls

Hang Xu[1]

[1]Georg-August-Universität Göttingen

hang.xu@med.uni-goettingen.de

Human induced pluripotent stem cell-derived cardiomyocytes (iPSC-CMs) emerged as an alternative tool in precision and systems medicine. New analysis strategies in combination with systems medicine approaches will help to realize the full potential of molecular disease phenotypic data derived from patient-specific iPSC-CMs for evolving additional treatment directions in cardiovascular disease and heart failure. Dilated cardiomyopathy is a major cause of heart failure and we could previously recapitulate molecular DCM phenotypes using patient-specific iPSC-CMs carrying inherited DCM-causing mutations. Here, we employed CRISPR/Cas gene editing to introduce a dilated cardiomyopathy (DCM)-causing mutation in the sarcomeric protein troponin T, TnT-R141W, into WT control iPSCs (MUT). In parallel to performing RNAseq and proteomic analysis for assessment of molecular signaling in WT control and Cas9-mutation-introduced, isogenic iPSC-CMs (MUT), we developed a new approach for data analysis at the molecular level. We implemented a non-negative blind deconvolution (NNBD) method to quantify molecular disease phenotypes such as calcium handling, beating force, and contractility in iPSC-CMs at the single cell level. The NNDB-based method enabled data parametrization, fitting, and analysis in WT controls versus isogenic MUT iPSC-CMs. Of note, Cas9-edited TnT-R141W iPSC-CMs revealed significantly reduced beating force and prolonged contractile event duration. The NNBD-based platform provides an alternative framework for improved quantification of molecular disease phenotypic data and may contribute to development of novel diagnostic tools.

Conservation genomic of Endangered Langur

Liye Zhang[1], Lutz Walter, Christian, Roos Liye Zhang

[1]German primate center

lzhang@dpz.eu

Poster 52
Thu 22nd
17:10–18:10

Many mammal species are threatened with extinction or have declining populations, but the consequences of large-scale population size reductions on the genomic make-up of species are yet not much explored. We here investigated the population history and genetic load of the Cat Ba langur , a primate species endemic to Vietnam's famous Halong Bay and with approximately 70 individuals one of the most threatened primates of the world

Author Index

Nonlinear Dynamics and Complex Networks

Biophysics from Experiment to Computation

Active Matter and Statistical Physics