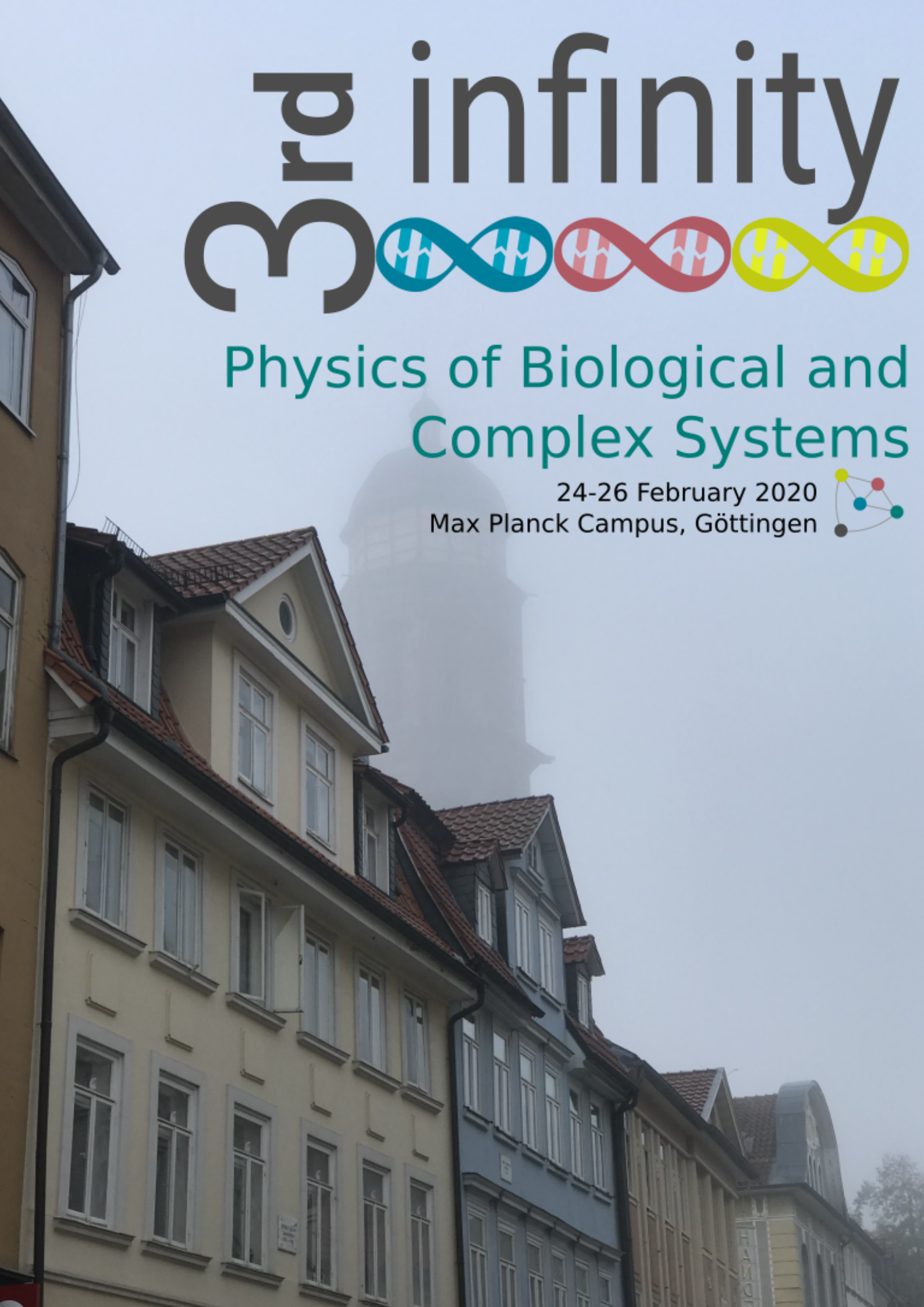

3rd infinity
Physics of Biological and Complex Systems
24-26 February 2020
Max Planck Campus, Göttingen

Third Infinity 2020 Abstract Booklet

February 13, 2020

Third Infinity 2020 Abstract booklet
Göttingen, Germany, February 24 - 26, 2020
Editor: Kristian Blom

Göttingen, 2020

Cover design: Venecia Chavez Medina

Distributed free of charge

Preface

From all of us here in Göttingen at the Physics of Biological and Complex Systems chapter of the International Max Planck Research School, it is our pleasure to welcome you at the fourth edition of the Third Infinity Conference. This conference is jointly organized by PhD students at the MPI for Dynamics and Self-organisation, the MPI for Biophysical Chemistry, and the University of Göttingen.

Third Infinity aims to provide an interdisciplinary platform for motivated researchers across the globe, both young and experienced, to exchange and foster scientific research concerning the Physics of Biological and Complex Systems. The focus is to expose its participants to cutting-edge advancements in their fields through invited talks given by elite speakers and active, person to person interactions. Third Infinity also looks for ardent students to present and report their recent findings and developments through student talks and poster sessions with each session being led by a notable and experienced scientist and world leader in the field. The greatest benefit of any conference is the opportunity for scientists from around the world to meet and share ideas about their work and the work of others. At Third infinity, it is our priority to ensure a fertile social environment to enable new scientific collaborations and friendships to blossom.

The conference will take place over a period of three days and is proud to welcome six invited speakers from five different countries to lead each of the six sessions. In addition, a total of 17 oral contributions and two poster sessions will be held while a Keynote talk by Cristina Marchetti will be given on the morning of the second day. We look forward to three days of cutting-edge science and a chance to unite great minds from all over the world during the 4th edition of the Third Infinity Conference here, in Göttingen, the city of science.

Your Third Infinity 2020 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).

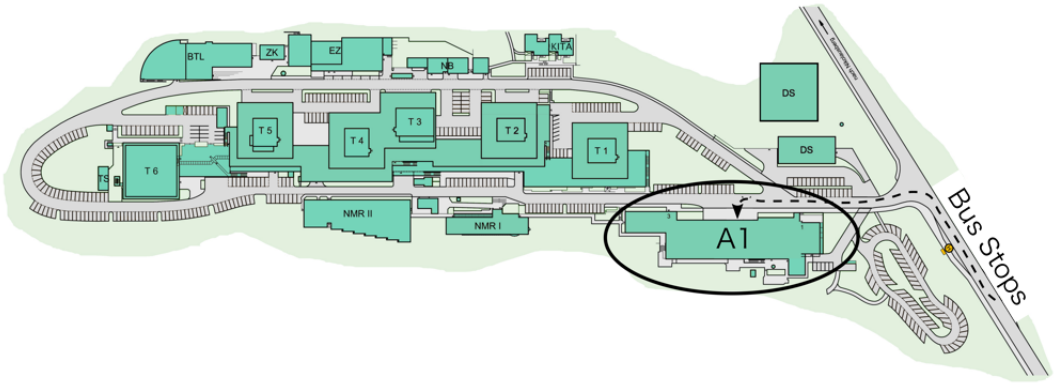
Organization committee

From left to right: Maximilian Vossel, Jimmy the Alpaca, Martin James, Kristian Blom, Aina Gallemí Pérez, Venecia Chavez Medina

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.



Registration

The registration desk is in the foyer, just left of the main entrance. Registration will begin on Monday, February the 24th, 2020 at 09:00 and officially remains open until 09:45. For attendees who are not able to make it 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 assist you, please ask a committee member for help. We will be easily identified by a volunteer badge and shirts bearing the Third Infinity logo.

The registration includes:

- Admission to all oral and poster presentations
- Coffee breaks
- Lunches

Identification badge

A conference identification badge will be included as part of the registration process. Please wear your badge at all times so you can easily be identified by the other conference participants and by the organizing team.

Coffee breaks

Coffee breaks will be held in the foyer between sessions and in the morning before the session starts. Coffee, water, tea, juices and (vegan) snacks will be available for everyone. We kindly, but firmly, ask our guests to respectfully adhere to these times in order to keep the talks on schedule.

Poster sessions

On Monday the 24th and Tuesday the 25th of February there will be a poster session from 17:30 till 18:30. **On Monday all odd-numbered posters are scheduled, and on Tuesday 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.

Internet

For those who are eligible, the Eduroam WiFi network should suffice for those wishing to connect to the Internet during the conference. Otherwise, guest login credentials for the MPI's WiFi network will be included in the registration materials.

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 Vapiano, located close to the city centre of Göttingen. The dinner will take place on Monday evening the 24th of February, 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 the dinner, therefore we kindly ask you to bring your bank card or cash money to pay for the dinner.

The exact location of Vapiano is: Weender Landstraße 1, 37073, Göttingen

Conference picture

A photographer will be present during the conference to take photos during the talks and throughout the events. On Monday, February the 24th, after the Fluid Dynamics session, 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.

Colour code

The following colour code is adapted in this conference booklet to denote the different subjects that will be discussed in each of the sessions:

 Soft Matter

Fluid Dynamics 

 Active Matter

Statistical Physics 

 Complex Networks

Biomedicine 

 Molecular Biophysics

Spectroscopy 

 Nonlinear dynamics

Schedule

Monday 24.02.2020

9:00-9:45	Registration and coffee	
9:45-10:00	Opening remarks	
10:00-10:45	Stefan U. Egelhaaf Soft matter under external driving	Soft Matter
10:45-11:05	Vitali Telezki	Soft Matter
11:05-11:25	Daria Maltseva	Soft Matter
11:25-11:45	Florian Oltsch	Soft Matter
11:45-13:00	Lunch	
13:00-13:45	Björn Hof The onset of turbulence in shear flows - a matter of life and death	Fluid Dynamics
13:45-14:05	Bastian Bäuerlein	Fluid Dynamics
14:05-14:25	Guus Bertens	Fluid Dynamics
14:25-14:45	Christian Küchler	Fluid Dynamics
14:45-15:15	Coffee break and event photo	
15:15-16:15	Arianna Bottinelli Open access and the challenge of open science	
16:15-17:15	FlashTalks	
17:30-18:30	Poster session (odd numbers)	
19:30	Dinner	

Tuesday 25.02.2020

9:00-9:15	Coffee	
9:15-9:30	Remarks by program speaker	
9:30-10:15	Cristina Marchetti KEYNOTE The physics of active matter	Active Matter
10:15-10:35	Henning Reinken	Active Matter
10:35-10:55	Juliane Klamser	Active Matter
10:55-11:15	Yoav Pollack	Active Matter
11:15-11:35	Babak Nasouri	Active Matter
11:35-13:00	Lunch	
13:00-13:45	Udo Seifert Stochastic thermodynamics: concepts and applications	Statistical Physics
13:45-14:05	Sarah Loos	Statistical Physics
14:05-14:25	Deepak Gupta	Statistical Physics
14:25-14:45	Alessio Lapolla	Statistical Physics
14:45-15:05	Carlos Alberto Plata Ramos	Statistical Physics
15:05-15:30	Coffee break	
15:30-17:30	Panel discussion The future of doctoral education in physics Panelists: Dr. Arianna Bottinelli, Dr. Clemens Buss, Prof. Dr. Helmut Grubmüller and Dr. Jana Lasser Moderator: Dr. Katrin Wodzicki	
17:30-18:30	Poster session (even numbers)	

Wednesday 26.02.2020

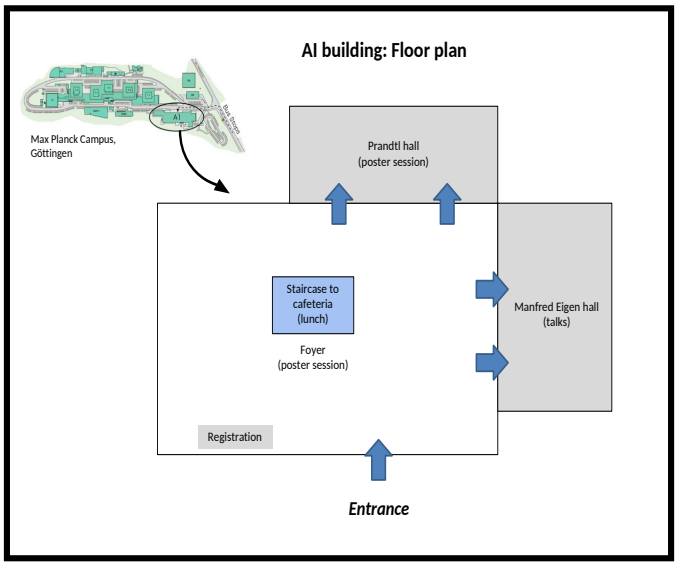
9:50-10:00	Coffee	
10:00-10:45	Elena Agliari Complexity in neural networks: the good with the bad	Complex Networks and Nonlinear Dynamics
10:45-11:05	Ohad Shpielberg	Complex Networks and Nonlinear Dynamics
11:05-11:25	Diego Tapias	Complex Networks and Nonlinear Dynamics
11:25-11:45	Sayedeh Hussaini	Complex Networks and Nonlinear Dynamics
11:45-12:00	Closing remarks	

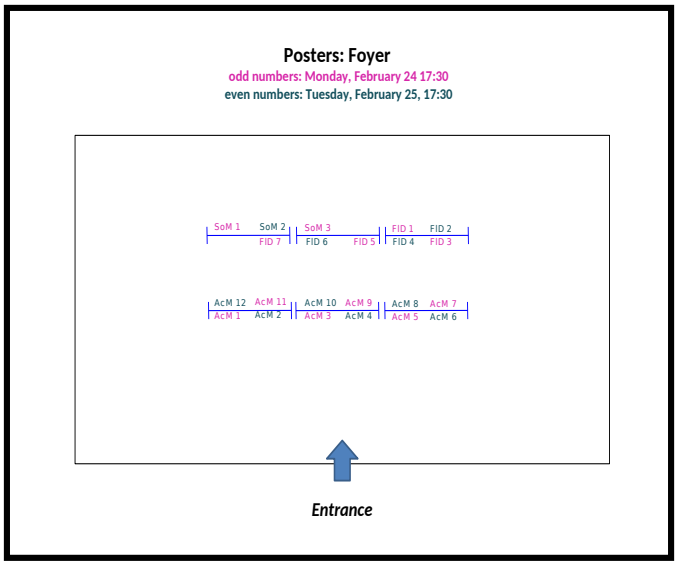
3rd infinity

https://thirdinfinity.mpg.de

Venue: Manfred Eigen hall,
Max Planck Institute for Biophysical Chemistry

Poster plan


AI building: Floor plan
Max Planck Campus, Göttingen
Prandtl hall (poster session)
Staircase to cafeteria (lunch)
Foyer (poster session)
Manfred Eigen hall (talks)
Registration
Entrance


Posters: Foyer
odd numbers: Monday, February 24 17:30
even numbers: Tuesday, February 25, 17:30
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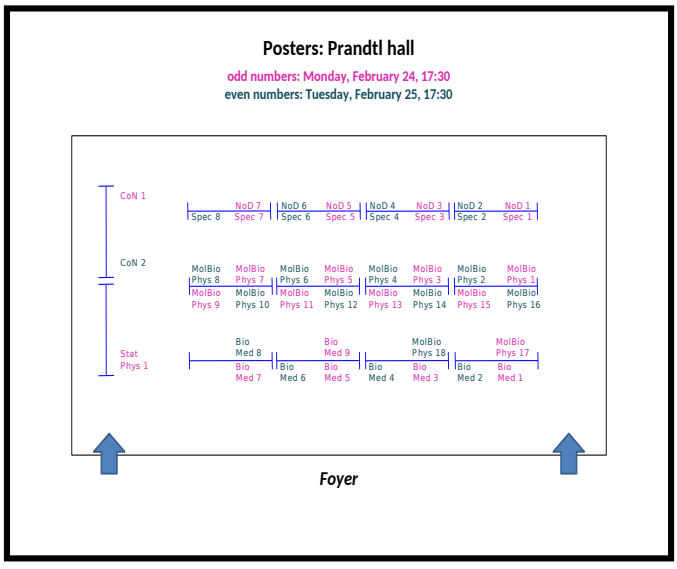
Entrance


Posters: Prandtl hall
odd numbers: Monday, February 24, 17:30
even numbers: Tuesday, February 25, 17:30
CoN 1
CoN 2
Stat Phys 1
NoD 7 Spec 8 Spec 7
NoD 6 Spec 6
NoD 5 Spec 5
NoD 4 Spec 4
NoD 3 Spec 3
NoD 2 Spec 2
NoD 1 Spec 1
MolBio Phys 8 MolBio Phys 9
MolBio Phys 7 MolBio Phys 10
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MolBio Phys 1 MolBio Phys 16
Bio Med 8 Bio Med 7
Bio Med 9 Bio Med 6
Bio Med 5
Bio Med 4
MolBio Phys 18 Bio Med 3
MolBio Phys 17 Bio Med 2 Bio Med 1
Foyer

Panel discussion

The future of doctoral education in physics

This panel discussion will examine whether current doctoral programs in natural science in general and physics in particular, fit to current needs of both finding talents for academia and preparing for the diversification of career paths after the Ph.D. While the existing structured programs have rather been designed to prepare for careers in academia, they might not fully meet the needs of all Ph.D. students given the increasing numbers of Ph.D. students who are striving for very different types of career paths outside of academia. So how well do those programs prepare for different career paths? What is nowadays expected in academia, and how does this differ from expectations in other sectors? Could and should programs be changed to prepare for different career paths as well?

The discussion will further have a closer look at the changes within the academic career path. What started off as an independent research project closely supervised by one established scientist resulting in a monograph has morphed into a more structured program in a larger group of Ph.D. students supervised by a Thesis Advisory Committee and resulting in journal publications. How does this development affect the quality of research output and the lives of Ph.D. students? Does supervision by a principal investigator and a Thesis Advisory Committee support their career development better?

The strong focus on publications and discussion on evaluation of individual publication records raises additional questions: How do publications help us in differentiating good science from great science? Alternatively, good scientists from great scientists? Speaking about the selection of great scientists: Despite years of efforts to address the gender gap, it persists. What are the reasons behind this gap? What do we need to change to keep the great female scientists in academia?

Finally, the Ph.D. phase is quite challenging. Long working hours, high expectations, competition and, many different duties demand high engagement. Difficulties to maintain a healthy work-life balance unfortunately has become common among Ph.D. candidates. How to stand up for your rights under these conditions without risking a good relationship with your supervisor and colleagues? And how could Ph.D. programs contribute here?"

Dr. Katrin Wodzicki, the head of the Human Resources and Organization Development Unit of the University of Göttingen, has kindly agreed to moderate the discussion. The panelists are

1. Dr. Arianna Bottinelli
2. Dr. Clemens Buss
3. Prof. Dr. Helmut Grubmüller
4. Dr. Jana Lasser

Talks (23)

Session 01: Soft Matter

24 Feb
10:00-10:45

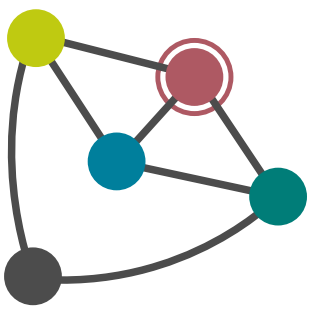
Soft Matter under External Driving

Stefan Egelhaaf

Universität Düsseldorf

stefan.egelhaaf@hhu.de

Soft matter is very susceptible to external stimuli, as 'soft' suggests. Already small forces or modest potentials can significantly affect the behaviour of soft matter. I will start by explaining how this is related to the infinities and how this especially affects the third infinity. Then, this characteristic behaviour will be illustrated with two examples. In both cases, we apply external stimuli and observe the response on all relevant length scales using conventional and confocal microscopy. First, the effects of mechanical deformation (shear) on the structure and dynamics of colloidal hard spheres is investigated. Second, an external potential is imposed on the colloids by exposing them to an extended modulated light field. In particular the effect of the potential on the particle dynamics is quantitatively and systematically studied.



Theoretical Investigation of Structure Formation by Dipolar Swimmers

24 Feb
10:45-11:05

Vitali Telezki, Stefan Klumpp

Institute for the Dynamics of Complex Systems, Georg-August University of Göttingen
vitali.telezki@theorie.physik.uni-goettingen.de

Dipolar swimmers describe a class of artificial and biological active particles with an internal magnetic moment. One example for biological dipolar swimmers are magnetotactic bacteria. Magnetotactic bacteria orient in magnetic fields with the help of a specific cell organelle, the magnetosome chain, a chain of membrane-enclosed magnetic iron-oxide nanocrystals. The resulting orientation allows the bacteria to navigate along magnetic field lines. Because of the interplay between different physical interactions such as steric, hydrodynamic and magnetic interactions, complex collective behaviour is expected to emerge in dense systems of dipolar swimmers. We use Brownian dynamics simulations to investigate the collective behaviour of these dipolar swimmers in confinement. In a first step, we focus on the structure formation of dipolar swimmers in small systems and analyse what structures can emerge and how they depend on the self-propulsion velocity and the magnetic moment of the swimmers. In addition, we investigate how the geometry and the interactions with the confinement affect the emerging structures.

Interaction of the TRPML1 ion channel's N-terminus with biomembranes

24 Feb
11:05-11:25

Daria Maltseva[1], Tina Berger[2], Benedikt Goretzki[2], Kerstin Viet[2], Charlotte Guhl[2], Mischa Bonn[1], Ute Hellmich[2], Grazia Gonella[1]

[1]Max Planck Institute for Polymer Research
[2]Institute for Pharmacy and Biochemistry, Johannes Gutenberg-Universität Mainz
maltsevad@mpip-mainz.mpg.de

The N-terminus of the transient receptor potential mucolipin 1 (TRPML1) ion channel is partly disordered and usually not reported in the available TRPML1 cryo-EM structures [1]. It contains binding sites for PI(4,5)P2 (plasma membrane lipid) and PI(3,5)P2 (lysosomal lipid) [2]. We test the influence of negatively-charged phospholipids on the secondary structure formation of the N-terminus by forming monolayers at the air/buffered aqueous solution interface. The data suggest a predominantly α-helical structure and orientation at the interface which is enhanced in presence of negatively charged lipids. We also obtain information on the effect of the peptide binding on the order in the phospholipid monolayer and observe that the adsorption of the peptides also clearly affects the phospholipid headgroup and only slightly the tails [3].

[1] P. Schmiege, et al. Nature 550, 366 (2017)
[2] X.-P. Dong, et al., Nature Comm. 1, 1 (2010)
[3] T. Berger, et al., In preparation

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24 Feb
11:25-11:45

Phase separation provides a mechanism to reduce noise in cells

Florian Oltsch[1], Adam Klosin[1], Tyler Harmon[1,2], Alf Honigmann[1,3], Frank Jülicher[2,3,4], Anthony Hyman[1,3,4], Christoph Zechner[1,3,4]

[1]Max Planck Institute of Molecular Cell Biology and Genetics
[2]Max Planck Institute for the Physics of Complex Systems
[3]Cluster of Excellence Physics of Life, TU Dresden
[4]Center for Systems Biology Dresden

oltsch@mpi-cbg.de

Noise in gene expression can cause significant variability in protein concentration. How cells deal with variation in protein concentration is an important question in biology. In this talk, I will show that liquid-liquid phase separation provides an effective mechanism to reduce variability in protein concentration. First, I will introduce our theoretical framework that discusses phase separation in the presence of active protein production and turnover. This stochastic non-equilibrium model allows us to study how fluctuations in protein concentration are affected by phase separation. I will then present under which physical conditions noise buffering by phase separation can be effective. Subsequently, I will show experimental data to test our theoretical predictions.

Session 02: Fluid Dynamics

The onset of turbulence in shear flows - a matter of life and death

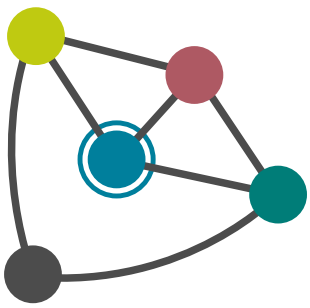
24 Feb
13:00-13:45

Björn Hof

IST Austria

bjoern.hof@ist.ac.at

Past studies of the transition to turbulence in pipes and related shear flows could neither predict the respective critical points for the onset of turbulence nor the nature of this transition. The main difficulty is that in this class of flows turbulence arises despite the linear stability of the laminar flow and that it results from perturbations of finite amplitude. I will show that under such circumstances the transition is driven by a stochastic spreading process: each turbulent spot will eventually die but it may produce offspring beforehand. This setting precisely corresponds to the rules of a stochastic process called 'directed percolation'. By introducing periodic boundary conditions in laboratory experiments we demonstrate for Couette and pipe flow that the transition to turbulence indeed falls into the directed percolation universality class. In particular I will also show that insights into the transition process can be exploited to control turbulence.



Nonlinear resonances of fluid sloshing exhibit Duffing dynamics

24 Feb
13:45-14:05

Bastian Bäuerlein, Kerstin Avila

University of Bremen, Leibniz IWT

baeuerlein@uni-bremen.de

Over a 100 years ago the German engineer Georg Duffing introduced his model for a harmonic oscillator with a nonlinear cubic spring force. Since then the Duffing oscillator established itself as one of the most important mathematical models for describing nonlinear vibrations in many different fields. It has become especially influential in chaos theory, with its transition from a simple ordinary oscillation to fully chaotic motion for increasing driving amplitudes. Although there is plenty of research on the analytical and numerical solutions of the Duffing equation, it is not straightforward to accurately observe these solutions in real physical systems. Up to date most experiments have been specifically tailored to depict the Duffing oscillator, reaching from a cart rolling in a double well potential to nanoscale oscillator devices used for energy harvesting or timing in pacemakers. In our work we experimentally investigate the sloshing motion of water in a partially filled rectangular container under lateral harmonic forcing. With this system we can accurately replicate the transition to advancing complexity for an increasing amplitude in analogy to the Duffing oscillator model. For very low forcing we observe planar standing waves with their resonance frequency matching potential theory predictions. An increase in driving leads to nonlinear effects. We can produce key features of the Duffing oscillator, like a folded asymmetric resonance curve, coexisting states and period-three-motion. The shifted resonance curve leads to a pronounced hysteresis, with transition between states at a phase-lag between driving and sloshing motion of 90°.

Results from the Zugspitze Experiment: an in-situ cloud-droplet particle-tracking experiment

24 Feb
14:05-14:25

Guus Bertens[1], Gholamhossein Bagheri[1], Haitao Xu[2], Eberhard Bodenschatz[1], Jan Moláček[1]

[1]Max Planck Institute for Dynamics and Self-Organization,
[2]Tsinghua University, Beijing

guus.bertens@ds.mpg.de

It is well-known that rain formation has four phases: nucleation, condensation, turbulent coalescence, and gravitational coalescence. Condensation is effective for droplet sizes of up to 20 μm, whereas gravitational coalescence is effective for droplet sizes larger than 100 μm. Turbulence is responsible for bridging the gap between these two, but how exactly it does this, is not known. One of the first to study the effect of turbulence on rain formation were Saffman Turner (1956). While beautiful in its simplicity, their theory has some shortcomings: it doesn't take droplet clustering (e.g. Bec et al. PRL 98, 084502 (2007)) or the sling effect (e.g. Bewley

et al. New J. Phys 15 (2013) 083051) into account. Many studies have tried to resolve these issues. To keep the problem tractable many theoretical studies assume droplets are monodisperse and/or neglect gravity. This makes the results of limited relevance to clouds. Numerical and experimental studies are often limited to low Reynolds numbers, and hence cannot faithfully reproduce cloud conditions. To avoid these issues, one must measure inside clouds. Here we present an in-situ cloud-droplet tracking experiment. The experiment is located on top of the environmental research station Schneefernerhaus, at 2650 m altitude, just below the peak of Mt. Zugspitze in the German Alps. At this location clouds occur close to the ground, which obviates the need for planes or helicopters. At the heart of the experiment are three high speed cameras, capable of recording 1 Mpx at 10 kHz. They are pointed at a small volume, approximately $(2.5\ \mathrm{cm})^3$ in size, illuminated by a 75 W green laser. The cameras are mounted on rails and can be moved by a linear motor, in order compensate for the mean wind. Images are processed with an in-house particle tracking code, that is remniscent of the Shake-The-Box algorithm (Schanz et al. Exp Fluids (2016) 57:70). The code is particularly suitable for processing low light imagery, in which many droplet images are out of focus. We report measurements of the radial distribution function (RDF) for separations of 0.1 to 20 mm. Furthermore we can estimate relative radial velocities (RRV), and condition both quantities on approximate droplet size.

Towards Universal Statistics of Turbulent Flows

24 Feb
14:25-14:45

Christian Küchler[1], Gregory P. Bewley[2], Eberhard Bodenschatz[1]

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

christian.kuechler@ds.mpg.de

Turbulence is characterised by complex fluid motions acting on a wide range of length scales. The largest scales are typically dominated by the flow geometry or the way turbulent kinetic energy is injected into the flow. In the regime of the smallest length scales, the viscous dissipation to heat is the main energy transport mechanism. The Reynolds number of the flow is a measure for the separation of the largest and smallest flow scales. A long-standing paradigm is the existence of an intermediate range of scales, where the influence of viscosity and flow geometry is negligible and the inertial transfer of energy from large to small scales takes a universal form. We present experimental results, where an inertial range can be observed that is independent of Reynolds number suggesting such universality. Our experiments were conducted in a high-pressure wind tunnel filled with pressurised SF6. These conditions allow the existence of very small flow structures. At the same time we can finely control the energy injection with an ultra-flexible active grid. We show that the statistics of velocity fluctuations picked up by ultra-small hot wire sensors (NSTAPs, see e.g. Vallikivi et al. (2014)) are well described by a turbulence model that accounts for the temporal decay of turbulent kinetic energy (Yang et al. (2018)). We further show that we observe a transition to a universal

form of these statistics. Finally, we show that this universal form is not tied to the viscous or forcing range.

Session 03: Open Access

Open Access and the challenge of Open Science

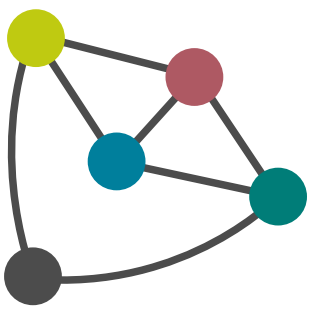
24 Feb
15:15-16:15

Arianna Bottinelli

Springer Nature

arianna.bottinelli@nature.com

Open Access, and more generally Open Science, has been the subject of intensive debates over the past 20 years, providing a new and libre way of publishing, disseminating, and accessing research. In this talk, I will discuss Open Science and Open Access publishing within the physical sciences. I will draw from the Nature Research portfolio of journals, including Communications Physics, and introduce some of the measures supporting Open Science.



Session 04: Active Matter

25 Feb
09:30-10:15

Keynote

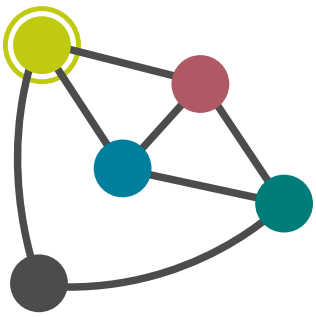
The physics of active matter

Cristina Marchetti

UC Santa Barbara

cmarchetti@ucsb.edu

Assemblies of interacting self-driven entities form soft active materials with intriguing collective behavior and mechanical properties. Examples abound in nature on many scales, from the flocking of birds to cell migration in morphogenesis. They also include synthetic systems, from engineered microswimmers to self-catalytic colloids and autonomously propelled liquid crystals. What unifies these systems is that they are driven out of equilibrium by dissipative processes that act on each individual particle, hence break the time reversal symmetry of the dynamics at the microscale. This results in surprising behavior. For instance, active fluids flow with no externally applied driving forces, active gases do not fill their container, and active particles spontaneously organize when passive ones would not. In this talk I will discuss the physics of active matter with examples from both the living and non-living worlds. I will show that by combining minimal physical models with continuum theory and simulations we are making advances towards capturing quantitatively the laws of spontaneous organization of active systems. This theoretical progress has implication for both formulating design principles for new smart materials and understanding cellular and multicellular organization.



Artificial topological defects organize bacterial motion

25 Feb
10:15-10:35

Henning Reinken*, Sebastian Heidenreich[2], Daiki Nishiguchi[3], Andrey Sokolov[4], Igor Aranson[5], Markus Bär[6], Sabine Klapp*

*Technische Universität Berlin
[2]Physikalisch-Technische Bundesanstalt
[3]University of Tokyo
[4]Argonne National Laboratory
[5]Pennsylvania State University
[6]Physikalisch-Technische Bundesanstalt

henning.reinken@itp.tu-berlin.de

Active systems spontaneously self-organize into complex spatio temporal structures such as flocks, bands, vortices, and turbulence. These collective states are susceptible to weak geometrical confinement, as has been demonstrated in experiments on suspensions of Bacillus subtilis, where turbulent motion is organized into a highly ordered bacterial vortex lattice by arrays of tiny obstacles [1]. Using a continuum-theoretical approach [2], we show how self-induced topological defects imposed by the artificial obstacles guide the flow profile of the active fluid and enable the stabilization of vortex patterns with tunable properties. Beyond the stabilization of square and hexagonal lattices, we also provide a striking example of a chiral, antiferromagnetic lattice induced by arranging the obstacles in a Kagome-like array. In this setup, the interplay of lattice topology, activity and length-scale selection generates a net rotational flow.

[1] D. Nishiguchi et al., Nat. Commun. 9 , 4486 (2018)
[2] H. Reinken et al., Phys. Rev. E 97 , 022613 (2018)

Thermodynamic phases in two-dimensional active matter

25 Feb
10:35-10:55

Juliane Klamser, Sebastian C. Kapfer, Werner Krauth

École supérieure de physique et de chimie industrielles de la ville de Paris

juliane.klamser@espci.fr

For equilibrium systems with short-range interactions, two-dimensional systems are the marginal case between the absence of long-range order in one dimension and the existence of crystalline order in three dimensions. In two dimensions, particle systems are known [1] to form a liquid, a hexatic, or a solid phase at finite temperature, characterized by different degrees of positional and orientational order. I present our recent study [2, 3] about how these two-dimensional equilibrium phases are affected by self-propulsion, driving the system out of equilibrium. Our results are for a two-dimensional interacting many-particle system, without alignment interactions, following a modified Metropolis dynamics, which introduces persistent motion and breaks detailed balance. For purely repulsive pair-wise interactions, we show that the equilibrium phases (liquid, hexatic, and solid) survive far from equilibrium. The persistence (activity) changes the phase boundaries, and its variation

can induce two-step melting at constant density. Motility-induced phase separation, the characteristic non-equilibrium phenomenon of self-propelled particles, appears at sufficiently high activity. I discuss the full phase diagram, numerical characterization of different phases and their defining order. I conclude by comparing phase diagrams for other well-known models of active matter, namely active Brownian and active Ornstein-Uhlenbeck particles. Focuses are differences and their possible microscopic origin, thereby commenting on the universality of two-dimensional active particle phases.

[1] Sebastian C. Kapfer and Werner Krauth, Phys. Rev. Lett. 114, 035702 (2015)
[2] Juliane U. Klamser, Sebastian C. Kapfer and Werner Krauth, Nat. Commun. 9, 5045 (2018)
[3] Juliane U. Klamser, Sebastian C. Kapfer and Werner Krauth, J. Chem. Phys. 150, 144113 (2019).

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25 Feb
10:55-11:15

Fast *vs.* gradual death in assemblies of immotile growing cells

Yoav Pollack, Philip Bittihn, Ramin Golestanian

Max Planck Institute for Dynamics and Self-Organization

yoav.pollack@ds.mpg.de

Cell life-cycle processes such as growth, division and death, often all happen on a similar timescale, as do the resultant mechanical and dynamical responses of the cell assembly (such as a colony, biofilm or tissue). An archetypal example is *E. Coli* where growth, division and the subsequent relative motion of the daughter cells all happen at roughly the same rate. However there are also examples of another type of system showing abrupt processes, including 'snapping' cell division in Actinobacteria and 'explosive' bacterial lysis. Here we test whether going from the first type of system to the other by introducing a second fast timescale in one of the microscopic processes can affect the macroscopic mechano-dynamics. Specifically we simulate a closed 1D channel of generalized cells that grow and divide to fill up the channel and are removed (via death or extrusion) when pressure builds up. We focus on varying the timescale of the cell removal process, keeping growth and division timescales fixed. We show a clear distinction in the macroscopic system properties between abrupt *vs.* gradual cell removal, such as a significant increase in the homeostatic pressure.

25 Feb
11:15-11:35

Phoretic interactions of two chemically-active particles

Babak Nasouri, Ramin Golestanian

Max Planck Institute for Dynamics and Self-Organization

babak.nasouri@ds.mpg.de

Catalytically-coated active particles in a viscous medium interact with one another by altering the chemical and hydrodynamic fields in their surroundings. Such phoretic interactions may drive particles in motion and are strongly dependent on the physico-chemical properties of the system, namely: the response of the particles to the interaction fields, and geometric factors such as inter-particle distances and particle sizes. In this work, we discuss an analytical approach which can accurately capture the dynamical behavior of two phoretic spherical particles, for any given configuration.

Session 05: Statistical Physics

25 Feb
13:00-13:45

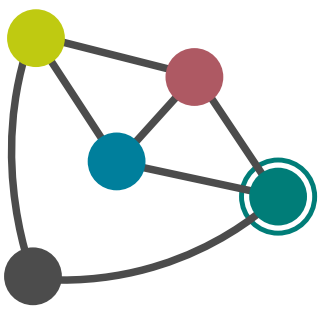
Stochastic thermodynamics: Concepts and applications

Udo Seifert

University of Stuttgart

useifert@theo2.physik.uni-stuttgart.de

For the macroscopic world, classical thermodynamics formulates the laws governing the transformation of various forms of energy into each other. Stochastic thermodynamics extends these concepts to micro- and nano-systems embedded or coupled to a heat bath where fluctuations play a dominant role. Examples are colloidal particles in time-dependent laser traps, single biomolecules manipulated by optical tweezers or AFM tips, and transport through quantum dots. For these systems, exact non-equilibrium relations like the Jarzynski relation, fluctuation theorems and, most recently, a thermodynamic uncertainty relation have been discovered. First, I will introduce the main principles and show a few representative experimental applications. In the second part, I will discuss the universal trade-off between the thermodynamic cost and the precision of any biomolecular, or, more generally, of any stationary non-equilibrium process. By applying this thermodynamic uncertainty relation to molecular motors, I will introduce the emerging field of "thermodynamic inference" where relations from stochastic thermodynamics are used to infer otherwise yet inaccessible properties of nano-scale systems. I will close with recent insights into the minimal requirements for creating coherent oscillations at finite temperature.



Delay in Thermodynamics: The fundamental problem and possible approaches

25 Feb
13:45-14:05

Sarah Loos, Sarah A.M., Sabine Klapp

Technische Universität Berlin

sarahloos@itp.tu-berlin.de

Real-world stochastic systems are often non-Markovian. This might be due to hydrodynamic backcoupling, viscoelastic effects, persistence in active swimmers, or an external feedback control loop acting on the system. Despite the omnipresence of memory, the incorporation of non-Markovian dynamics in the framework of stochastic thermodynamics is yet not fully understood [1, 2]. In fact, fundamental problems remain, which are associated with the acausality of the backward process in the total entropy production functional. We discuss this crucial issue focusing on the case of discrete time delay, and show the implications of different approaches. As a first example, we review the outcome of a direct calculation on the basis of the acausal path integrals, which requires redefining the definition of entropy production, and, in fact, yields a functional which by construction can be calculated for any nonlinear system. Furthermore, we suggest a Markovian embedding approach [3]. While this strategy allows us to employ the standard formulae, and is technically much simpler, it demands the interpretation of entropy production of auxiliary variables. For the case of a feedback controller, we offer an appropriate interpretation.

[1] Munakata, Rosinberg, PRL 112, 180601 (2014)
[2] Loos, Klapp, Sci. Rep. 9, 2491 (2019)
[3] Loos, Hermann, Klapp, preprint: arXiv:1910.08371 (2019)

Work fluctuations and Jarzynski equality in stochastic resetting

25 Feb
14:05-14:25

Deepak Gupta[1], Carlos Plata[1], Arnab Pal[2]

[1] University of Padova,
[2] Tel Aviv University

phydeepak.gupta@gmail.com

We consider the paradigm of an overdamped Brownian particle in a potential well, which is modulated through an external protocol, in the presence of stochastic resetting. Thus, in addition to the short range diffusive motion, the particle also experiences intermittent long jumps which reset the particle back at a preferred location. Due to the modulation of the trap, work is done on the system and we investigate the statistical properties of the work fluctuations. We find that the distribution function of the work typically, in asymptotic times, converges to a universal Gaussian form for any protocol as long as that is also renewed after each resetting event. When observed for a finite time, we show that the system does not generically obey the Jarzynski equality which connects the finite time work fluctuations to the difference in free energy, albeit a restricted set of protocols which we identify herein.

In stark contrast, the Jarzynski equality is always fulfilled when the protocols continue to evolve without being reset. We present a set of exactly solvable models, demonstrate the validation of our theory and carry out numerical simulations to illustrate these findings.

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25 Feb
14:25-14:45

Asymmetric Thermal Relaxation Processes and Non-Markovian Mpemba effect

Alessio Lapolla, Aljaž Godec

Max Planck Institute for Biophysical Chemistry

alessio.lapolla@mpibpc.mpg.de

Thermal relaxation process have been at the heart of non-equilibrium physics for several decades. Pioneered by Newton's law of cooling and later by Onsager's linear irreversible thermodynamics the approach to thermal equilibrium remained a frontier of statistical mechanics. Notwithstanding these efforts the fundamentals of relaxation to equilibrium from far-from-equilibrium initial conditions remains only poorly understood. Here we show on hand of exact solutions of two paradigmatic physical models, that both Markovian as well as non-Markovian physical observables display a puzzling asymmetry in the relaxation dynamics: in absence of inertial effects cooling processes are slower than heating. In addition, we provide evidence for the so-called stochastic Mpemba effect for non-Markovian observables, that is, under certain conditions a non-Markovian physical observable starting further away from thermodynamic equilibrium can relax faster.

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25 Feb
14:45-15:05

Melting curve of a mixture of random DNA oligomers

Carlos Alberto Plata Ramos[1], Samir Suweis[1], Tommaso Bellini[2], Amos Maritan[1]

[1]University of Padova
[2]University of Milano

carlos.plata@unipd.it

A gas of random DNA oligomers in contact with a thermal bath is analyzed. Each DNA oligomer is a strand that can be paired with another one forming a double-stranded DNA. The free energy associated to this pair has an enthalpic and an entropic contribution. Depending on the specific sequences and the shifts in the pairing this bond may be more or less stabilizing. We put forward a classical statistical mechanics approach to the problem of counting the number of paired oligomers in the system. Specifically, we compute, both exactly and in the thermodynamic limit, the partition function of the system, which is the theoretical object containing all its statistical information. Using the partition function, we look into the role of temperature in the expected fraction of paired oligomers obtaining the melting curve that usually is measured in experiments. In the numerical analysis of our theoretical prediction for the melting curve, we start just considering the contribution coming

from perfect pairing, that is, we neglect any possible error in the paring. Then, we study the effect of introducing the possibility of errors. The parallelism between the formation of double-stranded DNA and diatomic molecules is especially useful to test our predictions with the results of the theory of basic chemical reactions. Our approach allow us to clarify some misconceptions ubiquitous in the literature regarding self-complementary sequences.

Session 06: Complex Networks and nonlinear dynamics

26 Feb
10:00-10:45

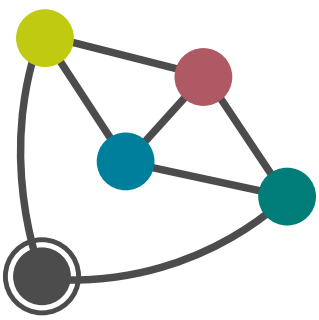
Complexity in neural networks: the good with the bad

Elena Agliari

Sapienza University of Rome

agliari@mat.uniroma1.it

In the first part of the seminar I will describe neural networks from a statistical-mechanics perspective. Focusing on networks trained for retrieval tasks, I will discuss their complexity and show how it is related to network's performance: on the one hand, complexity is a desirable feature as it (potentially) increases the amount of information stored in the network, on the other hand, beyond a critical threshold, it dramatically impairs retrieval. Finally, I will introduce an algorithm for information storage, inspired by neurophysiological mechanisms occurring during mammal's sleep, which yields to an "optimal complexity".



Imitating nonequilibrium steady states using time-varying equilibrium force in many-body diffusive systems

26 Feb
10:45-11:05

Ohad Shpielberg, Takahiro Nemoto

College de France, Pasteur Institute

ohad19@gmail.com

An equivalence between nonequilibrium steady states (NESS) driven by a time-independent force and stochastic pumps (SP) stirred by a time-varying conservative force is studied for general many-body diffusive systems. When the particle density and current of NESS are imitated by SP time-averaged counterparts, we prove that the entropy production rate in the SP is always greater than that of the NESS, provided that the conductivity of the particle current is concave as a function of the particle density. Searching for a SP protocol that saturates the entropy production bound reveals an unexpected connection with traffic waves, where a high density region propagates against the direction of the particle current.

Spectral and time domain properties of the Barrat-Mézard model on a Random Regular Graph

26 Feb
11:05-11:25

Diego Tapias, Peter Sollich

Institute for Theoretical Physics, University of Göttingen

dandroveros@gmail.com

Trap models consider the configuration space dynamics of a glass as that of a point hopping between local energy minima or "traps". In the version introduced by Barrat and Mézard (BM), the transition rates between traps are chosen of Glauber form so that transitions into deeper traps happen at essentially fixed rate while rates for upward transitions take the standard Arrhenius form. In contrast with the Bouchaud trap model, where every transition includes activation to the top of the landscape, the BM trap model dynamics is therefore governed mainly by entropic barriers instead of energetic ones, i.e. by the search for lower-lying traps. This conclusion holds when every trap is accessible from every other, i.e. the network of traps is fully connected. This is clearly an oversimplification, however, as in physical amorphous systems only a small subset of local energy minima will be reachable from any given configuration. In order to capture the effects of configuration space connectivity, we consider the BM trap model dynamics on a sparse network given by a random graph, focusing on the spectral properties of the master operator. We use a general approach based on the cavity method that gives access to the density of states in the limit of large networks. We find remarkably rich behaviour as a function of temperature and network connectivity, including spectra with multiple peaks and qualitative changes with temperature even within the glass regime. We also discuss the differences to the Bouchaud trap model on the same kind of network; these arise from the functional form of the transition rates and the topological properties of the network, which physically result in a unique combination of entropic and activated effects. Finally, we numerically solve the master equation in time using a

Gillespie algorithm and compare the evolution of key dynamical observables (one- and two-time correlation functions) with the information that can be extracted from the spectral analysis.

Control the Dynamics of a Spiral Wave in the Cardiac Tissue Using Optogenetics

26 Feb
11:25-11:45

Sayedeh Hussaini, Rupamanjari Majumder, Valentin Krinski, Ulrich Parlitz, Stefan Luther, Claudia Richter

Max Planck Institute for Dynamics and Self-Organization

sayedeh.hussaini@ds.mpg.de

The emergence of spiral waves in the heart influences its regular function, resulting in lethal cardiac arrhythmias. Undesired side effects of the conventional clinical methods to control this abnormal state of the system have motivated the development of alternative low-energy approaches to restore normality. Cardiac optogenetics shows its potential to be used as a tool for deepening our understanding of the dynamics of these nonlinear waves. Here we present a numerical study to control spiral wave dynamics using optogenetics. The two-dimensional simulation is based on the ionically realistic Bondarenko model of mouse ventricular cardiomyocytes, which is coupled to a model for the light-activated protein Channelrhodopsin-2. We show that constant global sub-threshold illumination increases the resting membrane voltage, which leads to decrease in the action potential amplitude and slows down conduction velocity of the excitation wave in the domain. In the presence of a spiral wave existing in the domain, we applied global periodic illumination, with the same periodicity as the non-illuminated spiral. This led to deviations in the trajectory of the wave tip from circular to epicycloidal and hypocycloidal patterns, based on the phase of the spiral at the time of the illumination. In order to terminate the spiral wave, we tried to guide it towards the boundary. We induced spiral wave drift by applying a constant and pulsed rectangular shaped region of sub-threshold illumination. The spiral wave exhibits drift towards the illuminated area, possibly because of emergent spatio-temporal instabilities in the voltage distribution at the border between the illuminated and non-illuminated zones.

Flashtalks (11)

Analytical solutions for non-Markovian Brownian systems far from thermal equilibrium

24 Feb
16:15-16:18
SoM1

Timo Dörries, Sarah Loos, Sabine H.L. Klapp

Technical University Berlin

timo@dorries.de

Markovian Langevin equations are an established tool to describe stochastic motion. However, in many real-world systems, memory effects play a crucial role and e.g. complex environments can yield to stochastic motion characterized by different timescales. Analytical solutions are in general difficult to obtain here. We propose (linear) toy models where we non-reciprocally couple auxiliary variables to a Brownian particle, each auxiliary variable corresponding to one characteristic timescale. Projecting out the auxiliary variables, we obtain a non-Markovian Langevin equation with memory and colored noise. By deriving closed expressions for up to three auxiliary variables, we can systematically study the connection between the coupling topology and the resulting autocorrelation functions. Further, by studying the connection between topology and thermodynamical properties, we demonstrate that models with non-reciprocal coupling automatically have a net heat production, i.e. describe nonequilibrium systems [1, 2]. Finally, we show that a minimal model with two auxiliary variables yields correlation functions similar to those describing hydrodynamic backflow in an optical trap [3].

[1] S.A.M. Loos et al., arXiv:1910.08372 (submitted)
[2] S.A.M. Loos and H.L. Klapp, Scientific Reports 9, 2491 (2019)
[3] Franosch et al., Nature , 85-88 (2011)

Fluid dynamics

Rotating turbulent Rayleigh-Bénard convection at very large Rayleigh numbers

24 Feb
16:18-16:21
FID01

Marcel Wedi[1], Dennis v. Gils[2], Guenter Ahlers[3], Eberhard Bodenschatz[1], Stephan Weiss[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Twente University
[3]University of California

marcel.wedi@ds.mpg.de

Thermal convection is of major importance in various astro- and geophysical systems, exemplary are buoyancy driven flows in the atmosphere or in the stellar interior. Due to the rotation of the hosting celestial bodies the convection is both, highly turbulent and strongly influenced by Coriolis forces. An idealized model system to study thermal convection is Rayleigh-Bénard convection (RBC), which consists of a horizontal fluid layer heated at the bottom and cooled at the top. Within the Oberbeck-Boussinesq approximation this system is controlled by two parameters only, the thermal driving, expressed dimension-less in the Rayleigh number Ra and the fluid specific Prandtl number Pr. The applied rotation is expressed by the inverse Rossby number 1/Ro. With an experimental RBC realization we aim to study the influence of rotation on the heat transport and the temperature field at very large Ra in the High Pressure Convection Facility (HPCF) in Göttingen. The facility consists of a cylindrical cell of 1.10 m diameter and 2.20 m height that is filled with pressurized sulfur hexafluoride (SF6) at up to 19 bar. The height of the cell and the large density of SF6 enable us to reach Ra as high as $2x10^{15}$ at $0.74 < Pr < 0.96$. The cell is mounted on a rotating table and connected to the non-rotating world via water feed-throughs and slip rings. With these, the signals of more than 100 thermistors close to the sidewalls are collected. With this setup we reach Ek down to 10^{-8}, possibly entering the geostrophic regime. We study the effects of rotation on the heat transport and the temperature distribution inside the cell.

Shearing an Active Glass

24 Feb
16:21-16:24
FID02

Rituparno Mandal, Peter Sollich

Institute for Theoretical Physics, Georg August Universität Göttingen

rituparno.mandal@uni-goettingen.de

Recent experiments and simulations have revealed glassy features of cytoplasm, tissues and dense assemblies of self propelled colloids. This prompts the fundamental question of whether non-equilibrium (active) amorphous materials are essentially equivalent to their passive counterparts, or whether they can present qualitatively different behaviour. To tackle this challenge we investigate the yielding and mechanical behaviour of a model active glass former, a Kob-Andersen glass in two

dimensions where each particle is driven by a constant propulsion force whose direction varies diffusively over time. Using extensive Molecular Dynamics simulations, we focus in particular on the effects of the intermittent dynamics in the regime of highly persistent activity and reveal a novel type of shear induced orientational ordering in the system.

Self-Organization in Chemically Active Systems

24 Feb
16:24-16:27
AcM01

Vincent Ouazan-Reboul, Jaime Agudo-Canalejo, Ramin Golestanian

Max Planck Institute for Dynamics and Self-Organization

vincent.ouazan-reboul@ds.mpg.de

Individual enzymes show a variety of physically interesting behaviors in the presence of their substrate, in particular, they have been reported to undergo directed motion (chemotaxis) and to display an increase in their diffusion coefficient [1]. The ability of an enzyme to chemotax as a response to the chemical activity of some other enzyme leads to chemical field-mediated interactions, which have the property of being non-reciprocal. In [2] a minimal model for self-organizing behavior of chemically active particles was developed, with some simplifying assumptions: all particles shared the same diffusion coefficient, had constant chemical activities, and communicated through a single chemical species. This minimal model can exhibit phase separation of the particles starting from an homogeneous state. Here, we extend this model to particles with different diffusion coefficients and concentration-dependent activities interacting through an arbitrary number of chemical species. We have been able to establish instability conditions for the case of two species interacting through a single chemical, and to calculate the initial stoichiometry of the phase-separated state. We find that, in contrast to the minimal model, the system can now exhibit oscillatory behavior. Future work will be focused on applying our model to more biologically realistic enzymatic cycles. Indeed, it has been reported that enzymes that participate in common catalytic pathways tend to co-localize in clusters known as metabolons [3].

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[3] Sweetlove, L. J., Fernie, A. R. (2018, December 1). The role of dynamic enzyme assemblies and substrate channelling in metabolic regulation. Nature Communications, Vol. 9.

24 Feb
16:27-16:30
StatPhys01

Negative differential response in chemical reactions

Emanuele Penocchio[1], Riccardo Rao[2], Massimiliano Esposito[1], Gianmaria Falasco[1], Tommaso Cossetto[1]

[1]University of Luxembourg
[2]Institute for Advanced Study
emanuele.penocchio@uni.lu

Reaction currents in chemical networks can decrease when increasing their driving affinities. Such negative differential response (NDR), a hallmark of nonequilibrium physics, is found in reaction schemes of major biological relevance, namely, substrate inhibition and autocatalysis. We display it by deriving the full counting statistics of two minimal representative models by large deviation methods. We explore the consequences of NDR for biochemical networks in terms of precision-dissipation tradeoff and stability against external perturbations. Furthermore, we go beyond the realm of biochemistry and examine the relevance of NDR in artificial applications, showing how it limits the performance of dissipative self-assembly.

Biomedicine

Synchronization-based Reconstruction of Electromechanical Wave Dynamics in Elastic Excitable Media

24 Feb
16:30-16:33
BioMed01

Jan Lebert, Jan Christoph

University Medical Center Göttingen

jan.lebert@med.uni-goettingen.de

In elastic excitable media, such as the heart, mechanical contraction is triggered by nonlinear waves of electrical excitation, which propagate rapidly through the tissue due to intercellular electrochemical coupling. However, in the heart, the excitation waves are not completely observable in experiments, as it lacks adequate imaging technology that could penetrate the tissue and provide panoramic, three-dimensional visualizations of the highly dynamic excitation wave phenomena from within the depths of the cardiac muscle. As a result, the electrophysiological mechanisms that are associated with the onset and progression of severe heart rhythm disorders such as atrial or ventricular fibrillation remain insufficiently understood. In recent work, it was demonstrated that cardiac fibrillation can be characterized by three-dimensional mechanical vortex dynamics, which appear to be fingerprints of electrical scroll vortex waves. Here, we present a novel synchronization-based data assimilation approach with which it is possible to reconstruct excitation wave dynamics within the volume of elastic excitable media by observing spatiotemporal deformation patterns, which occur in response to excitation. The mechanical data are assimilated in a numerical replication of the measured elastic excitable system, and within this replication, the data drive the intrinsic excitable dynamics, which then coevolve and correspond to a reconstruction of the original dynamics. We provide a numerical proof-of-principle and demonstrate the performance of the approach by recovering even complicated three-dimensional scroll wave patterns, including vortex filaments of electrical excitation from within a deformable bulk tissue with fiber anisotropy. In the future, the reconstruction approach could be combined with high-speed imaging of the heart's mechanical contractions to estimate its electrophysiological activity for diagnostic purposes.

24 Feb
16:33-16:36
BioMed02

Nano^2 - Nanotube-nanobody conjugates for near-infrared immunolabeling and sensing

Florian Mann[1], Z. Lv[2], J. Großhans[2], F. Opazo[3], S. Kruss[1]

[1]Institute for Physical Chemistry, University of Göttingen
[2]Institut Für Entwicklungsbiochemie UMG/Georg-August Universität Göttingen
[3]Center for Biostructural Imaging of Neurodegeneration

florian.mann@med.uni-goettingen.de

Single-walled carbon nanotubes (SWCNT) are a highly interesting material for biomedical applications as they show a strong, non-bleaching fluorescence in the near-infrared (nIR, 900-1700 nm) leading to enhanced tissue penetration [1]. Until now, these striking optical features were utilized e.g. in the creation of (bio)sensors for the detection of analytes ranging from small neurotransmitters [2] to large proteins [3]. In addition to sensing, SWCNTs have also been exploited in many studies as transport agents for drugs or even macromolecular cargo into cells or even cancer tissue [4]. Here, we present a strategy that combines these outstanding properties of SWCNTs with the highly specific molecular recognition of nanobodies. Nanobodies are the smallest recombinant antibody fragments that are still functional and are only about 20% of the size of an original antibody [5]. In this work, we make use of a hybrid functionalization strategy for the oriented attachment of green fluorescent protein (GFP)-binding nanobodies to the nanotube's surrounding organic phase. The use of GFP-targeting nanobodies opens up a large space of possible applications. First, we demonstrate that it is possible to label single GFP-tagged kinesin motors in living drosophila embryos and track their directional movement during embryogenesis. In addition, we target cell surface receptors and use the SWCNT's fluorescence for sensing of small molecules. In summary, we show that nanobody conjugated SWCNTs show great potential for targeted nIR imaging, sensing and labeling.

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Molecular biophysics

Direct measurement of interactions between single intermediate filaments

24 Feb
16:36-16:39
MolBioPhys01

Anna Schepers[1], Charlotta Lorenz[1], Stefan Klumpp[2], Sarah Köster[1]

[1]Institute for X-Ray Physics, Georg August University Göttingen
[2]Institute for Dynamics of Complex Systems, Georg August University Göttingen
aschepe@uni-goettingen.de

The cytoskeleton consists of F-actin, microtublues and intermediate filaments (IFs), which form a complex composite network. F-actin and microtubule networks have been studied extensively and a large variety of cross-linkers are known. By contrast, the interactions in reconstituted IF networks are less well understood. It has, however, been shown that multivalent ions cause bundling and network stiffening. Whereas rheological experiments give insight into the network properties, it is challenging to distinguish the contributions of filament stiffening and of increased attraction. Combining optical trapping and fluorescence microscopy enables us to bring two single vimentin IFs in contact and directly study the interactions between the filaments. By amplifying electrostatic attraction or diminishing the hydrophobic interactions we are able to study the nature of the interactions between IFs. These results, in combination with studies of the mechanical properties of single IFs, allow us to model the interactions with Monte-Carlo simulations, thereby gaining a deeper understanding of cytoskeletal structures.

Influence of Phosphorylation on Vimentin Mechanics

24 Feb
16:39-16:42
MolBioPhys02

Julia Kraxner[1], Julia Menzel[2], Ivan Silbern[3], Henning Urlaub[3], Blanche Schwappach[2], Sarah Köster[1]

[1]Institute for X-ray Physics, University of Göttingen
[2]Universitätsmedizin Göttingen, Department of Molecular Biology
[3]Bioanalytical Mass Spectrometry, Max Planck Institute for Biophysical Chemistry
julia.kraxner@physik.uni-goettingen.de

The mechanical properties of biological cells are determined by the cytoskeleton. This composite biopolymer network consists of microtubules and microfilaments, which are conserved throughout all cell types, and different types of intermediate filaments (IFs), which are expressed in a cell-type specific manner. The adaption to specific mechanical requirements may be further achieved by post-translational modifications of the proteins. In this context, phosphorylation which adds negative charges to the modified site, plays an important role. Regarding IFs, phosphorylation heavily affects disassembly of the filaments and provides binding sites for proteins like 14-3-3 which is a regulator for signaling proteins. Here, we study partially phosphorylated single vimentin IFs by analyzing stress-strain curves recorded with an optical tweezer setup which combines microfluidics and fluorescence microscopy.

Furthermore, we investigate the influence of bound 14-3-3 on the mechanics and the contribution of single phosphorylation sites by phosphomimetics. Our results show that additional charges within the filament soften the vimentin filaments and the binding of 14-3-3 weakens the filaments even more.

Graphene-Based Metal-Induced Energy Transfer for Sub-Nanometer Optical Localization

24 Feb
16:42-16:45
MolBioPhys03

Arindam Ghosh, Akshita Sharma, Alexey I. Chizhik, Sebastian Isbaner, Daja Ruhlandt, Roman Tsukanov, Ingo Gregor, Narain Karedla, Jörg Enderlein

Third Institute of Physics, Georg-August-University Göttingen

arindam.ghosh@phys.uni-goettingen.de

Super-resolution microscopy methods which are based on single-molecule localization (SMLM) such as PALM [1] , STORM [2] , fPALM [3] , dSTORM [4] or PAINT [5] have found manifold applications from fundamental physics to life sciences. These methods achieve lateral localization accuracies of a few nanometers, but encounter big challenges when it comes to the localization along the optical axis (third dimension). Recently, Metal-Induced Energy Transfer or MIET [6, 7] was introduced as a technique for axial localization of fluorescent emitters with nanometer accuracy [8, 9]. It exploits the energy transfer from an excited fluorophore to surface plasmons in a thin metal film. Here, we show that using graphene as the "metal" layer , one can increase the localization accuracy of MIET by nearly an order of magnitude We demonstrate this potential of graphene-based MIET (gMIET) by axially localizing single emitters, and by estimating supported lipid bilayer (SLB) thickness values with Ångström accuracy. We also present preliminary results concerning the structure and dynamics of mitochondrial membranes.

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Magnetically Induced Alignment of Natural Products for Stereo-chemical Structure Determination via NMR

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Spec01

Niels Karschin[1], Christian Griesinger[1], Klaus Wolkenstein[2]

[1]Max Planck Institute for Biophysical Chemistry
[2]Department of Geobiology, University of Göttingen

nkarsch@gwdg.de

In the field of natural products the determination of molecular structure is one of the fundamental steps in characterizing the isolated compounds. Unfortunately, due to the structural complexity and conformational heterogeneity of many natural products, they cannot be crystallized. For the solution of these problems, NMR in anisotropic phases has gained increasing popularity since it leads to partial alignment of the molecules and thus provides unique and global structural constraints such as residual dipolar couplings (RDC) and residual chemical shift anisotropies (RCSA). However, it suffers from the necessity to dissolve the analyte in special media such as liquid crystals or polymer gels. Generally, small degrees of alignment are also caused by an interaction of the magnetic field with aromatic moieties. A key feature of this mechanism is that the alignment can be predicted via DFT. We have shown that both RDC and RCSA can be acquired from natural products without special sample preparation using magnetically induced alignment. On the two examples of a novel natural product with a large aromatic system and the alkaloid Strychnine featuring a single aromatic ring these data, together with the predicted alignment, yield the correct stereochemical configuration with high certainty.

Posters (56)

Soft matter

Effective simulation of many interacting droplets

SoM2

Ajinkya Kulkarni, David Zwicker

Max Planck Institute for Dynamics and Self-Organization

ajinkya.kulkarni@ds.mpg.de

Liquid-liquid phase separation plays an important role in organizing material inside biological cells by forming liquid droplets. So far it is unclear how a large number of droplets behave in the heterogeneous environment of the cell. Numerically, such systems are studied using Monte-Carlo simulations, Molecular Dynamics simulations, or by solving the Cahn-Hilliard equation. All these methods are computationally expensive since they have to resolve spatial structures on the scale of individual particles. This severely limits the system sizes that can be studied. We propose a novel simulation method to tackle this limitation. Our method describes droplets explicitly by a position and a radius, while the dilute phase is represented by a concentration field. We assume that droplets are far enough away from each other and only interact by exchanging material via the dilute phase. Since it is sufficient to describe the dilute phase by a coarse discretization of the diffusion equation, our method is orders of magnitude faster than the traditional ones. As a result, we can simulate the dynamics of many droplets on length- and timescales relevant to biological cells.

Effective simulation of many interacting droplets

SoM3

Karlo Komorowski[1], Jannis Schaeper[1], Michael Sztucki[2], Lewis Sharpnack[2], Gerrit Brehm[1], Sarah Köster[1], Tim Salditt[1]

[1]Institute for X-Ray Physics, University of Göttingen
[2]European Synchrotron Radiation Facility

karlo.komorowski@stud.uni-goettingen.de

We have used small-angle x-ray scattering (SAXS) to study the adhesion of lipid vesicles in the strong coupling regime induced by divalent ions. The bilayer structure and the interbilayer distance between adhered vesicles was studied for different DOPC:DOPS mixtures varying the surface charge density of the membrane, as well as for different divalent ions. The results are in good agreement with the strong coupling theory and the corresponding like-charge attraction based on ion-correlations, which falls beyond the classical Poisson–Boltzmann theory of electrostatics. Using time-resolved SAXS combined with the stopped-flow rapid mixing technique, we find that in highly charged bilayers the adhesion state is only of transient nature, and that the adhering vesicles subsequently transform to a phase of multilamellar vesicles. Aside from the stopped-flow SAXS instrumentations used primarily for these results, we also evaluate microfluidic sample environments for vesicle SAXS.

Fluid dynamics

FID03 Resolved energy budget of superstructures in Rayleigh-Bénard convection

Gerrit Green[1], Dimitar G. Vlaykov[2], Juan Pedro Mellado[3], Michael Wilczek[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]University of Exeter
[3]Universitat Politècnica de Catalunya

gerrit.green@ds.mpg.de

Coherent large-scale flow patterns in the presence of turbulent small-scale fluctuations are a ubiquitous phenomenon in natural flows. Currently, the interaction of these so-called turbulent superstructures with small-scale fluctuations is not understood in detail. In order to clarify this interaction, we study superstructures by means of direct numerical simulations in Rayleigh-Bénard convection. This idealized model system shows a complex coexistence of turbulent fluctuations and superstructures. Here, we employ a filtering approach to separate the superstructures from the small-scale fluctuations. We study the resolved energy budget at the scale of the superstructures and characterize the different contributions to the budget, such as the energy input by buoyancy, the direct dissipation, and the energy transfer between scales. We find that the energy transfer primarily acts as an energy sink but exhibits a complex structure in the boundary layer. Our detailed analysis of the energy budget sheds light on the interaction between superstructures and small-scale fluctuations and may help to guide the development of reduced-order models.

FID04 Experimental investigation of a sheared thermally unstable boundary layer

Giuseppe Gabriele Nunnari, Stephan Weiss

Max Planck Institute for Dynamics and Self-Organization

ga.nunnari@gmail.com

In many natural and industrial systems, heat is transported by mixed convection. There, the flow is driven not only by buoyancy due to temperature differences but also by an externally applied pressure gradient. Prominent examples are atmospheric boundary layers in nature or active cooling devices in numerous engineering applications. We investigate experimentally the turbulent boundary layer that develops on top of a heated horizontal plate that is subject to a colder mean wind. In the experiment, we use a three-meter long (streamwise) and one meter wide (spanwise) plate that consists of a 1m long adiabatic section, followed by a 2m long heated section. The heat transported away by the flow is quantified by measuring the temperature drop across the Lexan plate at 21 different lateral positions. The plate is placed inside an open wind tunnel 1.2 meter wide and 1.5 meter high with a 9

meter long test section. We use constant temperature anemometry (CTA) and thermistors to measure velocity and temperature profiles. We try to determine scaling relations for the heat flux as functions of the Grasshof and Richardson numbers. In particular, we study the transition from fully forced to dominantly free convection. Furthermore, we hope to gain a better understanding of the difference between a shear-turbulent boundary layer and a laminar boundary layer which is perturbed by thermal plumes.

Collisional droplet growth in a turbulent environment FID05

Tobias Bätge, Michael Wilczek

Max Planck Institute for Dynamics and Self-Organization

tobias.baetge@ds.mpg.de

Studying the growth of droplets is crucial for a better understanding of cloud physics and especially rain formation. Up to now it is uncertain what mechanisms drive droplet growth. Here we focus on the role of droplet collisions and coalescence, which we are investigating in a combined theoretical and computational approach. In particular, we are focusing on statistical evolution equations which capture the growth of an individual droplet in a statistically stationary turbulent suspension. This theoretical approach is complemented by computational investigations, which will allow us to gain insights into the role of the small-scale structure of turbulence on collisional growth.

Encoding memory in biological network hierarchy FID06

Mirna Kramar, Karen Alim

Max Planck Institute for Dynamics and Self-Organization

mirna.kramar@ds.mpg.de

Remembering sources of food and threat is essential for survival. While higher animals rely on their nervous system, even very simple organisms are able to encode sensory information that aids them in tackling complex environments. The true slime mould *Physarum polycephalum* is a giant unicellular eukaryote whose body consists of a protoplasm-filled network of tubes which undergoes constant reorganization. The mechanism behind the reorganization of *P. polycephalum*'s body upon food encounter has not been explained previously. Here, we identify the imprint the food stimulus leaves on network morphology as memory and show that the network relies on tube growth and flows to encode stimulus information. We hypothesise an encoding mechanism introducing a local release of a chemical agent that affects the mechanical properties of the tubes and spreading through the network by protoplasmic flows. Using a theoretical model, we test our hypothesis and find the model yields a correct prediction of flow-dependent stimulus response. Finally, we investigate the role of network hierarchy in memory encoding and show that both

hierarchy and the orientation of tubes are relevant in stimulus encoding. Our findings demonstrate *P. polycephalum*'s ability to encode memory and likely open doors to the use of the organism in bioinspired design.

FID07

Memory capacity of flow network morphology

Komal Bhattacharyya, David Zwicker, Karen Alim

Max Planck Institute for Dynamics and Self-Organization

komal@ds.mpg.de

The slime mould *Physarum polycephalum* is a very simple unicellular but seemingly intelligent organism with a network-like body. Its complex behaviour requires the ability to propagate, store and process information. Recently, it has been shown that *Physarum* propagates information about stimuli with the fluid flows throughout its network. Most inspiringly, *Physarum* was observed to adapt its networks tube radii globally in response to stimuli, reaching a steady-state as a long term response that keeps a memory of the stimuli in its network morphology. Inspired by this observation we here investigate the capacity to store information about previous stimuli in the morphology of an adaptive flow network. We model the organism as a flow network whose radii can change when optimising the network to have the least energy dissipation. We observe how the system reacts to localised changes and the timescale of its responses to applied stimuli by numerical simulation. Through theoretical understanding, we aim to pinpoint the information storing and processing capabilities of adaptive flow networks in general and *Physarum* networks specifically.

Active matter

Nonuniversality in scalar active matter with diffusivity edge under periodic confinement

AcM02

Benoît Mahault, Ramin Golestanian

Max Planck Institute for Dynamics and Self-Organization

benoit.mahault@ds.mpg.de

Scalar active matter is often described at the mean field level by nonlinear Fokker-Planck equations with density-dependent diffusion coefficients integrating fast degrees of freedom, as well as various equilibrium and/or nonequilibrium processes. A generic class, characterized by a diffusivity vanishing above some threshold density, was recently introduced [*Golestanian*, Phys. Rev. E 100, *010601(R)*]. In presence of harmonic confinement, such 'diffusivity edge' was shown to lead to condensation in the ground state, with the associated transition exhibiting formal similarities with Bose-Einstein condensation (BEC). Many active systems, such as self-propelled Janus particles, can however self-assemble into finite-size coexisting clusters. To account for such feature in the diffusivity edge framework, a periodic egg-crate confinement, that provides multiple sites for condensation, is considered in arbitrary dimensions. While for high barriers separating two minima the system essentially behaves as in the single harmonic trap case, for shallow potentials the transition is qualitatively different as the exponent associated to the scaling of the condensate fraction with an effective temperature is found to be nonuniversal. We nevertheless show from a generalized thermodynamic description that the overall phenomenology of BEC, such as the divergence of the isothermal compressibility at the transition, holds in both cases.

Size control of Active Droplets

AcM03

Jan Kirschbaum, David Zwicker

Max Planck Institute for Dynamics and Self-Organization

jan.kirschbaum@ds.mpg.de

Droplets have emerged as an important organization principle inside cells. To control the size and distribution of droplets, the cell has to overcome the uncontrolled growth due to surface tension, called Ostwald ripening. We show that droplet size can be controlled by enzymatic, ATP-driven chemical reactions, which switch a protein between a phase separating and a soluble form. In this case, the system constantly consumes chemical energy to prevent Ostwald ripening. By using the framework of linear non-equilibrium thermodynamics, we get more insight into the non-equilibrium process, which was not possible in earlier descriptions based on mass action kinetics. Our results suggest that only the combination of external driving and heterogeneous distribution of enzymes leads to a stable droplet size. We further analyze the non-equilibrium steady state in terms of thermodynamic fluxes and

entropy production. This allows us to link the stable droplet size to the chemical energy consumption. Taken together, our work reveals the conditions under which droplet size can be controlled in non-equilibrium environments like cells.

AcM04

Filament Sensor – A tool for near real-time analysis of stress fiber formation in stem cells

Lara Hauke[1], Benjamin Eltzner[2], Carina Wollnik[1], Stephan Huckemann[2], Florian Rehfeldt[1,3]

[1]Third Institute of Physics - Biophysics, University of Göttingen,
[2]Institute for Mathematical Stochastics, University of Göttingen,
[3]Experimental Physics 1, University of Bayreuth

lara.hauke@phys.uni-goettingen.de

Mechanically induced differentiation of human mesenchymal stem cells (hMSC) drives these cells towards different lineages with respect to Young's elastic modulus E of the microenvironment. While differentiation is commonly investigated by changes in lineage-specific protein expression, which occur over a period of days to weeks, the pattern formation of the cytoskeleton shows significant differences within the first 24 hours after seeding. Therefore, the stress fiber structure of hMSCs, quantified by an order parameter S, can be used as an early morphological marker for mechano-induced differentiation. We use a massively parallel live-cell imaging set-up to record cells under physiological conditions (37 °C, 5 % CO_2) over a period of 24-48 hours. This way we obtain a large, statistically sufficient data set. To minimize the impact of the fluorescent marker, we use an optimized lifeact-TagRFP transfection of hMSCs to visualize the structure and formation of actin-myosin stress fibers. We aim for a full representation of filament processes over time and space, allowing for statistical analysis. The current understanding and classification of stress fibers (dorsal, ventral, arcs) are based on their location in the cell and function during migration. In contrast, we concentrate on an unbiased classification due to their temporal and spatial persistence that should also correlate with function. This is represented by significantly different persistence in space and time and crosstalk with other cytoskeletal components. For this task we developed the 'FilamentSensor', a freely available tool for near real-time analysis of stress fibers. We present experimental data where we can distinguish the cytoskeletal structures of hMSCs on 1 kPa, 10 kPa and 30 kPa elastic substrates with 99 % confidence. We are working on single filament tracking, a sophisticated analysis of the structure in terms of orientation fields, 3D filament tracing, and tracking, and correlation of focal adhesions and stress fibers.

Minimal actomyosin cortices

AcM05

Nils Liebe[1], Ingo Mey[1], Andreas Janshoff[2], Claudia Steinem[1]

[1]Institute of Organic and Biomolecular Chemistry, University of Göttingen
[2]Institute of Physical Chemistry, University of Göttingen

nils.liebe@uni-goettingen.de

The cell cortex is a highly regulated network, which is attached to the plasma membrane. This network consists of filamentous actin (F-actin), which forms a thin actin sheet on the inner face of the cell membrane composed of single and bundled filaments. In this cortex, the F-actin is regulated by a vast array of different actin binding proteins (ABPs) like cross-linkers. The actin cortex is bound via linker-proteins like ezrin, radixin and moesin (ERM-family) to the membrane receptor-lipid phosphatidylinositol-4,5-bisphosphate (PtdIns(4,5)-P2). The direct connection between the cortex and the membrane is necessary to convert forces among both structures. The motor protein myosin II is able to reorganize the actin cortex and hereby to apply mechanical forces via the actin-membrane connection to the cell membrane. This work addresses the organization and reorganization of a membrane bound minimal actin cortex (MAC), using physiological binding conditions. Several model systems for MACs have been used to study the active behavior of membrane bound actin-networks in two- (2D) and three-dimensional (3D) systems. In this work, a 2D *in vitro* bottom up approach is used, due to the higher efficacy for small scale effects like on single filaments. The MAC is physiologically bound to supported lipid membranes via the receptor-lipid PtdIns(4,5)-P2 and the linker-protein ezrin. The myosin induced dynamics are analyzed by means of high-resolution confocal laser microscopy (CLSM). Besides the overall network reorganization by myosin, the underlying binding behavior between actin and myosin is investigated for a more detailed insight of the reorganization mechanism.

Modelling the Dynamics of Actomyosin Networks

AcM06

Ilyas Kuhlemann, Andreas Janshoff, Burkhard Geil

Institute of Physical Chemistry, Georg-August-Universität Göttingen

ikuhlem@gwdg.de

To complement our experiments on actomyosin networks, we develop a versatile brownian dynamics simulation framework to study the active dynamics of 3D biopolymer networks. Filaments are simulated as a highly coarse-grained linear bead-spring model where all beads experience harmonic potentials for stretching and bending modes while all other bead/bead interactions are reduced to hard-sphere potentials. Crosslinking proteins and myosin motors are not simulated as explicit entities - they rather are special "states" of beads, allowing these beads to form bonds with nearby beads of other filaments. While the whole spatial dynamics of the network is simulated via Langevin equations of motion, the kinetics of crosslinking and the myosin motor motions are handled via Gillespie algorithms modeling the temporal state changes in form of a reaction system. In this way the filaments can nucleate,

assemble and disassemble, crosslinks can be formed and can be broken, myosin motors can translate along the filaments and thus extort and distribute forces in the network. The extreme coarse-grained structure of our model will allow us to study the active filament dynamics and the network relaxation as a response to external distortions covering many orders of magnitude in time scales.

AcM07

Cell mechanics and kinematics during collective cell migration

Mark Skamrahl[1], Hongtao Pang[1], Jannis Gottwald[1], Tabea Oswald[1], Alexey Chizhik[2], Andreas Janshoff[1]

[1]Institute of Physical Chemistry, University of Göttingen
[2]Third Institute of Physics, University of Göttingen

mskamra@uni-goettingen.de]

Collective cell migration is not only essential during vital processes such as embryonic development but also crucial to close wounds in a cell layer. Epithelial wound healing has been investigated by our group before, showing that even single-cell defects cause long-range mechanical responses, highlighting the mechanical cooperativity of cells. Yet, the mechanisms responsible for this mechanical cooperativity and acting during collective migration remain unclear. Hence, we now aim to elucidate cell-cell as well as cell-substrate interactions during collective cell migration across entire cell layers applying a variety of different methodologies. To quantify the kinematics of the apparent cell motion we use optical migration assays in combination with velocimetry-based correlation analyses. In addition, direct mechanical insights into collective cell migration are obtained by employing atomic force microscopy. To gain knowledge about the molecular origins of this physical process we use confocal fluorescence microscopy. Employing these techniques, we aim to elucidate the role of cell-cell interactions and intercellular junctions in cell migration. To gain a comprehensive picture of epithelial migration, we apply the recently established MIET (metal induced energy transfer) microscopy technology to investigate cell-substrate interactions during migration with nm-precision. Combining these novel approaches targeting intercellular as well as cell-substrate dynamics will provide new insights into the process of collective cell migration.

The Influence of Strain on Epithelial Cell Monolayers

AcM08

Jonathan Bodenschatz, Ajmail Karim, Andreas Janshoff
University of Göttingen
jonathan.bodenschatz@uni-goettingen.de

The epithelium is ubiquitous and essential in mammalian biology. Epithelial cells cover internal and external body surfaces. They perform critical roles in the body. Even though these cells must withstand large strains without failure, not much is known about how static and dynamical mechanical strain influence epithelial tissues and how the strains influence the mechanical properties of the cells and cell-cell contacts. To answer this question, we have established a polydimethylsiloxane (PDMS) based device and use this novel method to stretch confluent cell monolayers. The mechanical properties of the strained cells are directly measured via indentation with an atomic force microscope (AFM). While changes in cell-cell and cell-substrate contacts, as well as cytoskeletal reorganization are investigated with immunofluorescence and confocal microscopy. This combination of cell stretcher and AFM will provide new insights into the response epithelial cells under strain.

Collective olfactory search in a turbulent environment

AcM09

Lorenzo Piro[1], Mihir Durve[2], Massimo Cencini[3], Luca Biferale[4], Antonio Celani[2]
[1]Max Planck Institute for Dynamics and Self-Organization
[2]Quantitative Life Sciences, The Abdus Salam International Centre for Theoretical Physics - ICTP
[3]Istituto dei Sistemi Complessi, CNR
[4]Department of Physics and INFN, University of Rome Tor Vergata
lorenzo.piro@ds.mpg.de

Finding the distant source of an odor dispersed by a turbulent flow is a vital task for many organisms, either for foraging or for mating purposes. At the level of individual search, animals like moths have developed effective strategies to solve this very difficult navigation problem based on the noisy detection of odor concentration and wind velocity alone. When many individuals concurrently perform the same olfactory search task, without any centralized control, sharing information about the decisions made by the members of the group can potentially increase the performance. But how much of this information is actually valuable and exploitable for the collective task? Here we show that, in a model of a swarm of agents inspired by moth behavior, there is an optimal way to blend the private information about odor and wind detections with the publicly available information about other agents' heading direction. At optimality, the time required for the first agent to reach the source is essentially the shortest flight time from the departure point to the target. Conversely, agents who discard public information are several fold slower and groups that do not put enough weight on private information perform even worse. Our results then suggest an efficient multi-agent olfactory search algorithm that could prove useful in robotics, for instance in the identification of sources of harmful volatile compounds.

AcM10

Hydrodynamics in Ciliary Systems

David Hickey

Max Planck Institute for Dynamics and Self-Organization

david.hickey@ds.mpg.de

Cilia are small hairlike organelles which are involved in many biological processes. Both motile and immotile variants exist. The immotile cilia are hypothesised to act as force sensors, and are able to sense chemicals in the surrounding medium. Motile cilia are often used to generate fluid flow or for propulsion. However, they too can be chemosensitive. Despite the ubiquity of cilium-particle interactions, there has been surprisingly little research into how cilia interact with diffusive ligands in fluids. An intriguing hypothesis is that motile cilia could increase their chemical uptake significantly by stirring or pumping the fluid. My work has focused on numerically modelling particle capture by an individual cilium. By considering a simplified model cilium in a low Reynolds number fluid, I have found adsorption rate constants for a single cilium near a non-slip boundary. Both motile and immotile cilia have been considered, as have fluids with and without bulk flow. Future work will consider a more realistic model cilium and simulating multiple cilia on a two-dimensional array, and will look closely into how cilia might optimally behave in order to maximise their chemical uptake.

AcM11

Phenotypic differences in reversible attachment behavior reveal distinct *P. aeruginosa* surface colonization strategies

Jeremy Vachier[1], Calvin Lee[2], Jaime de Anda[2], Kun Zhao[3], Amy Baker[4], Rachel Bennet[5], Catherine Armbruster[6,7], Kimberley Lewis[4], Rebecca Tarnopol[8], Charles Lomba[2], Deborah Hogan[4], Matthew Parsek[6], George OToole[4], Ramin Golestanian[1,9], Gerard Wong[2]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Department of Bioengineering, Department of Chemistry and Biochemistry, and California NanoSystems Institute, University of California Los Angeles
[3]Key Laboratory of Systems Bioengineering (Ministry of Education), School of Chemical Engineering and Technology,Collaborative Innovation Center of Chemical Science and Engineering, Tianjin University
[4]Department of Microbiology and Immunology, Geisel School of Medicine at Dartmouth
[5]School of Mathematics, University of Bristol
[6]Department of Microbiology, University of Washington
[7]Department of Microbiology and Molecular Genetics, University of Pittsburgh School of Medicine
[8]Department of Plant and Microbial Biology, University of California Berkeley
[9]Rudolf Peierls Centre for Theoretical Physics, University of Oxford

jeremy.vachier@ds.mpg.de

Despite possessing the machinery to sense, adhere to, and proliferate on surfaces, it is commonly observed that bacteria initially have a difficult time attaching to a

surface. Before forming a bacterial biofilm, planktonic bacteria exhibit a random period of transient surface attachment known as 'reversible attachment' which is poorly understood. Using community tracking methods at single-cell resolution, we examine how reversible attachment progresses during initial stages of surface sensing. *Pseudomonas aeruginosa* strains PAO1 and PA14, which exhibit similar exponential trends of surface cell population increase, show unanticipated differences when the behavior of each cell was considered at the full lineage level and interpreted using the unifying quantitative framework of an exactly solvable stochastic model. Reversible attachment comprises two regimes of behavior, processive and nonprocessive, corresponding to whether cells of the lineage stay on the surface long enough to divide, or not, before detaching. Stark differences between PAO1 and PA14 in the processive regime of reversible attachment suggest the existence of two complementary surface colonization strategies, which are roughly analogous to 'immediate'-*vs* 'deferred-gratification' in a prototypical cognitive-affective processing system. PAO1 lineages commit relatively quickly to a surface compared to PA14 lineages. PA14 lineages allow detaching cells to retain memory of the surface so that they are primed for improved subsequent surface attachment. In fact, it is possible to identify motility suppression events in PA14 lineages in the process of surface commitment. We hypothesize that these contrasting strategies are rooted in downstream differences between Wsp-based and Pil-Chp-based surface sensing systems.

Tissue-wide integration of mechanical cues promotes efficiency of auxin patterning

AcM12

João Ramos[1], Alexis Maizel[2], Karen Alim[3]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]COS Heidelberg
[3]Technische Universität München Garching

joao.ramos@ds.mpg.de

New plants organs form by local accumulation of auxin, which is transported by PIN proteins that localize following mechanical stresses. As auxin itself modifies tissue mechanics, a feedback loop between tissue mechanics and auxin patterning unfolds – yet the impact of tissue-wide mechanical coupling on auxin pattern emergence remains unclear. Here, we use a hybrid model composed of a vertex model for plant tissue mechanics, and a compartment model for auxin transport to explore the collective mechanical response of the tissue to auxin patterns and how it feeds back onto auxin transport. We compare a model accounting for a tissue-wide mechanical integration to a model where mechanical stresses are averaged out across the tissue. We show that only tissue-wide mechanical coupling leads to focused auxin spots, which we show to result from the formation of a circumferential stress field around these spots, self-reinforcing PIN polarity and auxin accumulation.

Complex Networks

Synaptic consolidation stabilizes memory representations and improves recall in a network model

CoN01

Jannik Luboeinski, Christian Tetzlaff

Third Institute of Physics, Georg-August-University Göttingen

jannik.luboeinski@phys.uni-goettingen.de

Memory representations in neural systems exhibit a variety of dynamics such as their formation, recall, or consolidation. However, most of the synaptic and neuronal processes underlying these dynamics remain elusive. In this study, we show that a spiking network model combined with calcium-based synaptic plasticity and synaptic consolidation naturally implements the formation, consolidation, and cue-triggered recall of a memory representation. We find that these functionally relevant memory dynamics occur in a regime in which inhibition and excitation are weakly balanced. Within this regime, we investigate how the memory strength depends on parameters such as inhibition or the number of neurons encoding the memory representation. To quantify the memory strength, we employ two different measures of recall quality: the mutual information between the activity distributions during learning and recall, and a coefficient describing the degree of pattern completion. In addition, we investigate the long-term effect of synaptic consolidation on a memory representation and its recall. As expected, synaptic consolidation significantly prolongs the lifetime of the memory representation. Remarkably, we also find that the process of synaptic consolidation improves the recall performance significantly without requiring external stimulation. Further analyses indicate that this passive memory improvement is governed by the interaction between the recall cue and the distribution of early- and late-phase synaptic weights, which is altered by synaptic consolidation. Presenting a recall cue when early-phase changes have already been transferred to the late phase, re-strengthening of early-phase weights occurs, which improves recall. Moreover, we find that an additional, intermediate recall stimulus further amplifies the effect of memory improvement. In summary, by developing and investigating a theoretical network model, we show that the interplay of calcium-based synaptic plasticity and synaptic consolidation accounts for the formation, consolidation, and recall of memory representations and we predict that this interplay enables the passive improvement of memories.

Learning trajectories in an anisotropic spiking neural network on Loihi

CoN02

Carlo Michaelis, Andrew Lehr, Christian Tetzlaff

Georg-August-University Göttingen

carlo.michaelis@phys.uni-goettingen.de

Sequences of neural activity are found across the brain and support complex behavior. In particular animals can learn and perform movement sequences robustly, adaptively and efficiently. However, in spiking neural networks obtaining stable and robust sequential representations is a difficult problem. We used a recently developed anisotropic spiking neural network to represent reliable patterns of neural activity. Using these stable patterns we learned a readout using a regularized regression algorithm. The network was simulated on neuromorphic hardware using the Loihi chip from Intel and applied to a motor task performed by a robotic arm.

Biomedicine

BioMed03

Generation of a mouse ovary cell atlas

Chloe Charalambous, Sara Haag, Debojit Saha, Sarah Mae Penir, Eike Urs Moennich, Melina Schuh

Max Planck Institute for Biophysical Chemistry

chloe.charalambous@mpibpc.mpg.de

Oocytes are egg precursor cells that can mature into fertilizable eggs. A finite pool of oocytes is established in ovaries during embryonic development. These oocytes will progress through a long maturation stage, finally developing into fertilizable eggs in the adult ovary. Oocyte development in both embryonic and adult stages is supported by numerous ovarian cells. It is considered that ovarian cells also mature during embryonic and adult stages to support the different requirements of developing oocytes. How oocytes and ovarian cells mature at synonymous stages of ovarian development is unclear. Moreover, our understanding of the gene regulatory networks that support ovarian development is limited. To further characterize this crucial developmental process we have conducted single-cell sequencing of embryonic and adult ovaries. We anticipate this study will provide a more detailed understanding of how ovarian development occurs.

BioMed04

A nIR Fluorescent nanosensor to visualize serotonin release from human platelets

Meshkat Dinarvand

Institute of Physical Chemistry, University of Göttingen

dinarvandmesh@gmail.com

Serotonin, a neurotransmitter that regulates the tone of activity in the brain, is also involved in regulating immune related responses. Quantifying concentration changes of serotonin in real time with high temporal, spatial and chemical resolution is of great interest but challenging with conventional fluorescent probes/sensors. Our approach is to create nanoscale fluorescent sensors that report about their local chemical environment. Single nanosensors are used to study chemical processes on the single-molecule level while imaging of many sensors provides spatial information. In our work we design sensors with a focus on near infrared (nIR) fluorescent materials because this spectral region lays in the biological transparency window. Here, we used semiconducting single-walled carbon nanotubes (SWCNTs) as non-bleaching nIR fluorescent building blocks. The SWCNTs are functionalized with DNA aptamers to create a sensor with specific molecular recognition. Photophysical changes of these sensors in response to target molecules and other interfering molecules were analyzed by nIR fluorescence spectroscopy and microscopy. Most notably, we gained a deeper understanding of how fast and how strong single molecules

such as serotonin interact with the organic phase and the nanomaterial. As an application, these sensors were used for spatiotemporal nIR imaging of the release of serotonin from serotonin releasing blood platelets. In summary, we introduce the first nIR fluorescent sensor for the important signaling molecule serotonin and use it to image serotonin release by cells.

Towards tailored near infrared fluorescent nano sensors for detecting bacterial interactions

BioMed05

Robert Nißler, Sebastian Kruss

University Göttingen

robert.nissler@chemie.uni-goettingen.de

Single-walled carbon nanotubes (SWCNTs) are an emerging building block for nanoscale sensors and labels because of their unique photophysical properties. Semiconducting SWCNTs fluoresce in the tissue transparency near infrared (nIR) window (840 – 1650 nm) and do not bleach.[1] Due to their 1D nature small perturbations in their environment strongly affect their fluorescence. The major challenges in using SWCNTS for sensing is on the one side their purification [2] and on the other side a tailored surface chemistry for molecular recognition and photophysical signal transduction. Cellular metabolites such as first messengers are important biomolecules used by cells to exchange both energy and information but up to day there are many such molecules for which no sensors exist. DNA is a versatile macromolecule to functionalize and solubilize SWCNTs. Furthermore, DNA acts as a conformational quantum yield switch, which makes it a good candidate to impart signal transduction. However, different sensing strategies are known, but general recognition capabilities need to be further explored. Here, we present three different approaches with DNA to tailor SWCNT surface chemistry and detect biologically important metabolites.

Optogenetic Arrhythmia Termination Using Global Illumination

BioMed06

Raul Alejandro Quinonez Uribe, Stefan Luther, Claudia Richter

Max Planck Institute for Dynamics and Self-Organization

raul.quinonez@ds.mpg.de

Cardiac arrhythmias or in other words, abnormal electrical activity of the heart are characterized by chaotic excitation waves that lead to an unsynchronized contraction and therefore insufficient blood pumping from the heart's chambers into the circulation. To date, both understanding of the electrical cardiac dynamics generating and sustaining arrhythmias as well as arrhythmia treatments lack optimization. Current treatments include electrical shocks and drugs that can lead to pain and side-effects. In this research we implement a biological tool called optogenetics, that photo-sensitizes the heart via light-sensitive ion channels, such as

Channelrhodopsin-2 (ChR-2), allowing us to study cardiac arrhythmia termination using light pulses. We performed experiments on ChR-2 transgenic mice hearts ex-vivo using a Langendorff-perfusion system in order to understand the effect of light intensity and pulse width on optogenetic arrhythmia termination using global stimulation. By tuning the light intensity termination of >90% arrhythmias was achieved using light pulses from 10 to 1000 ms. Moreover the time-lapse from stimulation to termination was characterized and results show that 53% of all arrhythmias (n-403), independent of the light stimulus were terminated in the range between 36-75 ms. These results improve the understanding of cardiac optogenetics as a tool to control arrhythmias shortening the gap between research and applications. A crucial next step is to test this method on bigger animal models.

BioMed07

Endothelialized microchannels as in vitro model for blood vessels and pearmation analysis

Kumari Priti Sinha[1], Lionel Bureau[1], Misbah Chauki[1], Maddalena Wu[2]

[1]University of Grenoble, [2]Sacco Hospital, Milan

pritisinha.026@gmail.com

Microfluidic technology highly developed in physics is now widely used to create tools for cell biology. A variety of bioassays and investigations can be carried on in microfluidic systems where living cells can be cultured: cell migration and interaction, cancer cell invasion, drug delivery assays, wound healing, angiogenesis, thrombosis, studies of blood flow and shear stress etc. The vascular endothelium is considered as a complex organ, which is responsible for the dynamic control of vessel functions. The endothelium is continuously exposed both to shear stress and changes in pressure, including rhythmic fluctuations due to heart beating and to the signals from surrounding tissues. In order to test endothelial cells' behavior in a three dimensional dynamic model reproducing the influence of physiological flow and shear stress as an important part of "everyday life" of the endothelium, we developed and tested a "microvasculature-on-a-chip" microfluidic device and performed several tests to verify its possible biomedical applications. We confirmed possibility to implement our chip to study changes in endothelium permeability in order to study capillary leak syndrome.

Mechanisms of chromosome segregation errors in mammalian oocytes

BioMed08

Eirini Bellou

Max Planck Institute for Biophysical Chemistry

eirini.bellou@mpibpc.mpg.de

Chromosome segregation during female meiosis is remarkably error-prone, especially in humans. Cytogenetic and bioinformatic studies in human eggs indicate exceptional differences in the predisposition of individual chromosomes to missegregation: smaller and acrocentric chromosomes (with kinetochores positioned close to telomeres), are more vulnerable to errors. It is still unclear why this is the case, due to the lack of a suitable model system. Mouse chromosomes are telocentric, and differ structurally from the meta- and acrocentric chromosomes in humans. Pigs have a more human-like karyotype and should be better suited to investigate aneuploidy rates between different types of chromosomes. Thus, the aim of my project is to investigate the mechanistic basis of what predisposes certain chromosomes to missegregation by studying pig oocytes. I will differentially label the distinct chromosome subclasses in live pig oocytes and follow both meiotic divisions using live cell microscopy and kinetochore tracking. I will characterize the behavior of chromosome subclasses by investigating the dynamics of their alignment, kinetics of movement and efficiency in error correction. This study will develop a new model and comprehensive understanding of the relationship between chromosome morphology and aneuploidy

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3d velocity quantification using magnetic resonance imaging in real time

BioMed09

Jost Kollmeier

Max Planck Institute for Biophysical Chemistry

jost.kollmeier@mpibpc.mpg.de

Magnetic resonance imaging (MRI) is intrinsically slow. Due to repetitive line-by-line scanning in Fourier space the acuqisition of a single 2D image normally takes several seconds. Using a real-time MRI approach with a non-linear iterative image reconstruction, it becomes possible to reconstruct images from highly undersampled data sets. This way, a significant speed-up is achieved and MRI movies with up to 50 frames per second are realized. The real-time approach is extended to allow for phase-contrast imaging - a method that quantifies blood flow velocities by exploiting the phase of the complex MRI signal. This work illustrates the image reconstruction technique for multi-directional flow and demonstrates results of real-time 3d flow at the human aortic arch.

MolBioPhys04

A Model of AMPAR-trafficking during E-LTP

Moritz Becker[1], Christian Tetzlaff[1,2]

[1]Third Institute of Physics, Georg-August-University Göttingen, [2]Bernstein Center for Computational Neuroscience

moritz.becker@phys.uni-goettingen.de

AMPA Receptors (AMPARs) are the most abundant mediators of fast excitatory signals at synapses in the brain. It is therefore believed that their trafficking plays an important role in synaptic plasticity, especially in Long-Term Potentiation (LTP). However, the details of how AMPAR-trafficking contributes to the Early-Phase of LTP (E-LTP) are still not fully understood. We therefore constructed a theoretical model that is able to account for different influences on AMPAR-trafficking such as volume changes of the spine head, clustering of receptors due to cooperative binding and changes in exocytosis and binding rates upon LTP induction. We fitted the parameters of this model to experiments and compared the outcomes of the model simulations to LTP experiments under different conditions. We find that in a model that does not account for spine growth and cooperative binding, exocytosis of AMPARs needs to be much higher than experimentally predicted in order to explain the slow decay of E-LTP, which lasts for 2-8h. Therefore, we propose a model in which receptor accumulation at the PSD is increased due to the interplay of cooperative binding of receptors and spine morphological changes. In this model, cooperativity leads to a continuous phase transition between low and almost full occupation of the PSD with immobilized AMPARs. This transition depends on the number of available mobile receptors, which is controlled by the spine size. However, initial spine and PSD size tightly control the effect of cooperativity and spine morphological changes on AMPAR accumulation. Moreover, an exocytic binding factor may be needed under some conditions in order to stabilize AMPARs at synapses after LTP induction, which our model can also account for. In summary, we have developed a compact theoretical model that enables to shed new light on the relationship between E-LTP and the underlying AMPAR-dynamics.

Structure and dynamics of Plasmodium falciparum adhesin VAR2CSA: homology modelling and molecular dynamics simulations

MolBioPhys05

Iván Pulido[1], Camilo Aponte-Santamaría[1,2]

[1]Max Planck Tandem Group in Computational Biophysics, University of Los Andes,
[2]Interdisciplinary Center for Scientific Computing, Heidelberg University

ij.pulido@uniandes.edu.co

VAR2CSA is a protein expressed by the Plasmodium falciparum parasite that mediates the adhesion of infected erythrocytes to placenta. This protein is found at the membrane of infected erythrocytes and its extracellular Duffy-binding-like (DBL) domains interact with the chondroiting-4-sulfate (CSA) glycosaminoglycan matrix of the placenta. The interaction of VAR2CSA with CSA is enhanced by shear stress and DBL domains bind cooperatively to CSA [Rieger et al. Blood 125:383-391, 2015]. Here, we analyzed the structure and dynamics of the extracellular portion of VAR2CSA, via homology modelling and molecular dynamics simulations, as a first step to uncover the, so far unknown, molecular mechanism leading to the shear-enhanced binding cooperativity.

Out of plane bending components in Chlamydomonas flagella observed with multi-plane phase contrast imaging

MolBioPhys06

Soheil Mojiri

Third Institute of Physics, University of Göttingen

soheil.mojiri@phys.uni-goettingen.de

Cilia and flagella are whip-like cellular appendages found in micro-organisms and animals. Motile ciliary structures are mainly responsible for cell locomotion and generation of fluid flow across surfaces of cells and tissues. Investigation of the rapid 3D dynamics of flagella demands a volumetric in vivo imaging technique which is fast, non-invasive and provides high spatial resolution at the same time. However, existing methods do not offer a simple solution meeting these experimental criteria due to technical demands, image analysis complexity or a great deal of uncertainty. We propose the combination of a conventional phase contrast microscope with a customized multi-channel beam-splitter that enables simultaneous acquisition of a stack of eight planes. This method does not require any post-processing. Using this approach, we image beating Chlamydomonas axonemes within a volume of of $40 \times 40 \times 4\,[\mu\mathrm{m}^3]$ with a rate of 250 volumes per second. Our results demonstrate a prevailing correlation between the curvature and the out of plane component (local chirality) of the flagella waveform. The maximum of the correlation amplitude is located at about one third of the axonemal arc length off the basal tip.

MolBioPhys07

Towards Mimicking Cellular Communication: Characterization of Cell-free synthesized Connexin 43 hemichannels

Yeimar Portillo[1], Claudia Steinem[1,2]

[1]Institute of Organic and Biomolecular Chemistry, Georg-August-Universität Göttingen
[2]Max Planck Institute for Dynamics and Self-Organization

yeimar.portillo-castellano@uni-goettingen.de

Gap-junctions support multicellular life providing a unique direct cell-to-cell communication system that allows the transport of molecules to neighboring cells. Assemblies of hexameric connexins, also referred to as connexons or hemichannels, dock with connexons of adjacent cells to form a direct pathway to connect the cytosol of both cells. Connexin-43 (Cx43) is the most ubiquitous isoform and by far the best-characterized connexin. In multicellular systems, cell-cell interactions are highly complex with numerous proteins playing vital roles in cell signaling or cell contacts. Therefore, we are employing a bottom-up approach to mimic cell-to-cell communication in synthetic cell models. The aim of this study is to reconstitute Cx43 into Giant Unilamellar Vesicles (GUVs) as Minimal Cell Compartments (MCCs) to build artificial cells capable of forming multicellular aggregates and mimic intercellular communication by the formation of gap-junctions. For this purpose, Cx43 has been produced and directly inserted into liposomes by using a cell-free expression approach. During the study, the optimization of cell-free conditions for the production of Cx43-proteoliposomes has been carried out. The functional characterization of connexin-43 will be performed with the Black Lipid Membrane technique (BLM) by the fusion of proteoliposomes with pure lipid bilayers to gather insight on the connexon's properties at the single-channel level. Finally, the formation of gap junction channels will be investigated by coupling Cx43-doped GUVs to Cx43-doped pore spanning membranes in a dye transfer assay for functional characterization of cell-cell communication in artificial cell models.

MolBioPhys08

Integrational modelling for sarcomere analysis in DCM patient-specific and CRISPR/Cas9-edited iPSC-cardiomyocytes

Hang Xu, Asset Amenov, Yuanyuan Dai, Nadezda Ignatyeva, Antje Ebert

Universitätsmedizin Göttingen, department of cardiology

hang.xu@med.uni-goettingen.de

Cardiomyocyte contraction is mediated by excitation-contraction coupling, a process which is initiated by Ca2+ -binding to troponin. Mutations in sarcomere regulatory proteins cause dilated cardiomyopathy (DCM) that associated with sudden cardiac death and heart failure. Several models have been developed to simulate contraction at the sarcomere level. These models consist of a series of sarcomere components, and then using differential equations to describe reactions within and between these components, such as in the Markov model and in the cooperative

activation- and crossbridge cycling approximate models. To analyse patient-specific differences of Ca2+ handing and contractility parameters in cardiomyocytes, we are integrating Ca2+ handling and contractility data from induced pluripotent stem cell-derived cardiomyocytes (iPSC-CMs) generated from patients with cardiomyopathy mutations, as well as CRISPR/Cas9-engineered, genome-edited controls. Firstly, we assess parameters that specifically characterize properties of Ca2+ handling and contractility. We then construct relationships of filtered parameters within Ca2+ transient and contractility data. Preliminary results show a linear correlation between contraction duration and beating rate in healthy control iPSC-CMs, but no correlation in DCM iPSC-CMs. Next, to clarify the relationship between Ca2+ handling and contraction, we are going to investigate relationships of complimentary parameters in both types of datasets. Finally, we plan to develop a model would integrate contractility and Ca2+ transient data in healthy control, DCM and CRISPR/Cas9-engineered iPSC-CMs. This model in combination with iPSC technology may provide a platform for prediction modelling of patient-specific parameters in patients with cardiomyopathy.

Leaflet-dependent diffusion in lipid bilayers using Metal-Induced Energy Transfer and Fluorescence Lifetime Correlation Spectroscopy (MIET-FLCS)

MolBioPhys09

Akshita Sharma[1], Narain Karedla[2], Sebastian Isbaner[1], Arindam Ghosh[1], Ingo Gregor[1], Jörg Enderlein[1]

[1]Third Institute of Physics - Biophysics, Georg August University
[2]Physical and Theoretical Chemistry, University of Oxford

akshita.sharma@phys.uni-goettingen.de

Understanding membrane diffusion provides a deeper insight into transport mechanisms and the functioning of proteins in several cellular processes. In this work, we determine the diffusion of labeled lipids in lipid bilayers in a leaflet-dependent manner. We use the recently established single-molecule Metal Induced Energy Transfer (smMIET) [1, 2] technique together with Line-Scan Fluorescence Lifetime Correlation Spectroscopy (LS-FLCS) [3]. In smMIET, the excited-state lifetime of a fluorescent molecule varies monotonically with its distance from a metal surface. This is due to the strong distance-dependent energy transfer from the dye to the surface plasmons of the metal. Due to the steep variation of the fluorescence lifetime with distance from the substrate, we observe a bi-exponential decay of fluorescence from the labeled lipids diffusing in the excitation focus. Using LS-FLCS, we get the temporal- and spatial- autocorrelation functions of the lipids diffusing in the two leaflets. The results show the heterogeneities in the diffusion of lipids in mono-component SLB mainly arising due to the interaction of proximal leaflet with the substrate. Moreover, in the distal leaflet more than one diffusing component was observed, which reflects upon the interaction of the distal leaflet with the proximal leaflet or due to the bilayer defects. This method will have huge potential in understanding the complex dynamics of lipids and proteins in asymmetric membranes.

MolBioPhys10

Positioning of cholesterol around AQP0 studied with molecular dynamics simulations

Juan David Orjuela[1], Po-Lin Chiu[2], Thomas Walz[3], Bert L. de Groot[4], Camilo Aponte-Santamaria[1]

[1]Max Planck Tandem group in Computational Biophysics, University of Los Andes
[2]Arizona State University
[3]The Rockefeller University
[4]Max Planck Institute for Biophysical Chemistry

jd.orjuelam@uniandes.edu.co

Studying lipid–protein interactions is fundamental to understand the complex behaviour of biological membranes. In these systems, membrane proteins affect the organization of lipid bilayers and thus its mechanical properties, and vice-versa the local lipid environment alters membrane-protein function. The most abundant membrane protein in the eye lens is aquaporin-0 (AQP0), with reported roles in water conduction, cell-cell adhesion and cell organization. Electron crystallography and molecular dynamics (MD) simulations have contributed to our understanding of lipid–protein interactions, by providing high-resolution three-dimensional structural and dynamical data, in a systematic manner for diverse lipidic environments. Here, we performed MD simulations to monitor the positioning of cholesterol around AQP0 in a sphingolipid membrane and examined the effect cholesterol concentration has on the localization of this sterol molecule. We thereby expand our previous studies focused on phospholipids, by considering this time cholesterol, which potentially plays a key role in the higher-order organization of AQP0 tetramers in the lens membrane.

MolBioPhys11

Molecular Regnition Imaging of Syntaxin 1

Anna Riedl, Andreas Janshoff

Institute of Physical Chemistry, George-August University Göttingen

annaluisa.riedl@uni-goettingen.de

Molecular recognition imaging offers an opportunity for label-free imaging at a resolution below the diffraction limit of light. Instead of electromagnetic waves the atomic force microscope (AFM) uses the strength of interactions between sample and the AFM probe, the cantilever. For specific detection as well as interaction the tip of the cantilever can be functionalized for example with antibodies. By scanning the sample area, the cantilever is deflected by binding events between the molecules coupled to the tip with the sample surface and each pixel detected in this way can be reconstructed to a map of the considered region. The protein clusters can be detected by a local density-based analysis as regions with a large number of spots with high binding strength. So, investigation of protein clusters is possible without artifacts of preparation or clustering caused by fluorophores. In this project, clustering of Syntaxin 1 will be investigated by anti-Syntaxin antibodies

coupled to the cantilever. Syntaxin 1 is a member of the Q-SNARE protein family and plays an important role in vesicle fusion and hence transmitter release in neuroendocrine cells as well as in neurons. It seems that Syntaxin 1 forms clusters at the membrane of neuroendocrine PC 12 cells and these clusters might influence neurotransmitter release, but these results were achieved by manipulating Syntaxin 1 with fluorophores. A confirmation without altering the protein would answer the question whether Syntaxin 1 clusters are a native state or bias and elucidate the function of protein clusters in endocrine signaling and neurotransmitter releases.

Brownian Dynamics of Disordered Proteins

MolBioPhys12

Steffen Mühle[1], Man Zhou[2], Arindam Ghosh[1], Jörg Enderlein[1]

[1]George-August University Göttingen
[2]University of Oxford

steffen.muehle@phys.uni-goettingen.de

The conformational flexibility and dynamics of unfolded peptide chains is of major interest in the context of protein folding and protein functioning. The rate with which amino acids at different positions along the peptide chain meet sets an upper speed limit for protein folding. By using single-molecule photo-induced energy transfer spectroscopy, we have systematically measured end-to-end and end-to-internal site contact formation rates for several intrinsically disordered protein fragments (IDPs) (11 to 41 amino acids) and have also determined their hydrodynamic radius using dual-focus fluorescence correlation spectroscopy. For interpreting the measured values, we have developed a Brownian dynamics model (based on bead-rod chain dynamics in a thermal bath including hydrodynamic interactions) which quantitatively reproduces all measured data surprisingly well while requiring only two fit parameters. The model provides a complete picture of the peptides' dynamics and allows us to translate the experimental rates and radii into molecular properties of the peptides: We find a persistence length of lP=5.21.9Å, a hydrodynamic radius of a=3.50.7Å per amino acid, and that excluded volume effects play an important role in the dynamics of IDPs.

MolBioPhys13

Reconstitution of ATP synthases in giant unilamellar vesicles by lipid based microfluidics as a first step towards the formation of artificial cells

Kristina Kramer[1], Merve Sari[1], Hannes Witt[1,2], Claudia Steinem[1,2]

[1]Institute of Organic and Biomolecular Chemistry, University of Göttingen
[2]Max Planck Institute for Dynamics and Self-Organization

kristina.kramer@uni-goettingen.de

Understanding the evolution of multicellularity is one of the most important and challenging targets in modern research. Within this project we try to investigate communication and translocation in multicellular organisms built from unicellular compartments by means of synthetic biology. To study such complex processes in living systems, the formation of an interconnected system of minimal cell compartments (MCCs) in a bottom-up fashion is a promising strategy. This should be realized by implementing essential biological components in giant unilamellar vesicles (GUVs) via droplet-based microfluidics. Hereby we seek to build up artificial cells and reach a collective behavior to produce a synthetic tissue. The creation of these so called living foams has some challenges like establishing a reliable way to produce GUVs with a defined size and the physiological reconstitution of different proteins allowing for adhesion, connectivity and communication as well as stabilization by cytoskeletal filaments and energy production. To tackle these challenges modular engineering approaches, relying on a microfluidic system to generate monodisperse GUVs in copolymer stabilized water-in-oil droplets, are appropriate. These copolymer-stabilized GUVs can be equipped by microfluidic setups with different proteins in a gentle manner and released afterwards in a physiological environment. Here we present a way to reconstitute a FOF1 ATP synthase from thermophilic Bacillus in GUVs by using the above-mentioned microfluidic methods. The insertion of ATP synthases within the GUVs is one of the most important requirements towards obtaining artificial tissues since they can act as a renewable energy source ensuring the production of chemical energy in the form of ATP by a conversion of electrochemical gradients. To monitor and study the activity of the ATP synthases in vesicles the highly sensitive Luciferin-Luciferase assay is used. The successful integration of the ATP synthase in GUVs will be the first step towards a living foam.

Studying DNA in Cell Nuclei by Combined X-ray Scanning Nanodiffraction and Holography

MolBioPhys14

Andrew Wittmeier[1], Chiara Cassini[1], Mareike Topperwien, Manuela Denz[1], Johannes Hagemann[2], Markus Osterhoff[1], Tim Salditt[1], Sarah Koester[1]

[1]Institute for X-ray physics, Georg-August-University Göttingen
[2] Deutsches Elektronen-Synchrotron DESY, Hamburg

andrew.wittmeier@phys.uni-goettingen.de

Imaging nanostructures within a cell presents several challenges. Although traditional optical imaging techniques, such as phase contrast or diffraction-limited fluorescence microscopy, are widely used, they cannot access the necessary length scales of subcellular structures such as nuclear DNA. Techniques such as electron microscopy can image the necessary length scales but at the invasive expense of slicing and staining the cell. X-rays overcome these challenges: with their short wavelengths and therefore high penetration depths, they are capable of imaging nanostructures within whole cells, yielding quantitative structural information. Here, we perform both x-ray scanning nanodiffraction and x-ray holography measurements on lyophilized 3T3 fibroblasts. The presented analysis yields structural information regarding the morphology, aggregation state, projected mass density and projected electron density.

Form Cell to Substrate - Formation of a GPMV-based Bottom-up System

MolBioPhys15

Nikolas Teiwes[1], Phila Baumannm[1], Kita Schmidt[1], Lena Strieker[1], Claudia Steinem[1,2]

[1]Institute for Biomolecular Chemistry, University of Göttingen
[2]Max Plank 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. Therefore, it is suitable to spread Giant Plasma Membrane Vesicles (GPMVs) derived from cells inside out on top of a Silicon dioxide (SiO2) Surface, enabling for further membrane analysis. Depending on the method of Vesiculation, a high variety of different GPMVs can be produced. Subsequently, to develop a reliable system, this GPMV Heterogeneity requires fundamental, biophysically characterization. Here, we present besides a Proof of Principle for this promising Bottom-up system, matching insights into biophysical GPMV heterogeneity.

MolBioPhys16

Influence of PI(4,5)P2 and synaptotagmin-1 on the SNARE mediated fusion

Jörn Dietz[1], Andreas Janshoff[1], Raphael Hubrich[1], Claudia Steinem[1], Francisco Angel Perez Lara[2], Reinhard Jahn[2]

[1]University of Göttingen
[2]Max Planck Institute for Biophysical Chemistry
joern.dietz@uni-goettingen.de

We use Tethered particle motion (TPM), the motion of a microparticle tethered to a substrate by a macromolecule, to investigate the binding affinity of membrane reconstituted full length synaptotagmin (syt-1) towards solid supported membranes varying in their lipid compositions, by tracking the position of membrane coated silica beads in x-, y, and z-direction through analysis of their diffraction patterns. We use a commercially available unit (Stand-alone G2 System) for Acoustic Force Spectroscopy (AFSTM) from LUMICKS designed for single-molecule and single-cell manipulation for precise experimentaion with high throughput to assure positions are recorded in real time with nanometer accuracy. Two opposing supports silica bead and glassy surface were separately coated via vesicle spreading, respectively. Membrane coated beads were gently added through the flow chamber. Against buoyancy and thermal fluctuation the membrane coated beads sediment and establish close contact and binding when syt-1 is present. We use POPC:Bodipy (99:1) with reconstituted syt-1 on our microparticle against four different target membranes on glass support to distinguish between free bead movement without any interaction DOPC:DOPS:PIP(4,5)2:TR (99:0:0:1), Phosphatidylserin interaction DOPC:DOPS:PIP(4,5)2:TR (88:11:0:1), syt-1 Phosphatidylinositol interaction DOPC:DOPS:PIP(4,5)2:TR (87:11:1:1), and we compare this to a native lipid composition DOPC:DOPS:DOPE:CHOL:PIP2:TR (46:20:20:11:1:2) under constant buffer condition. Through analysing the particles motion we observe different confinments in their diffusive behaviour by comparing the ensemble average of their mean square displacements.

MolBioPhys17

Confocal single molecule localisation microscopy for superresolved fluorescence lifetime imaging

Jan Christoph Thiele, Eugenia Butkevich, Oleksii Nevskyi, Jörg Enderlein

Third Institute of Physics - Biophysics, University of Göttingen
jan.christoph.thiele@phys.uni-goettingen.de

Localisation based super-resolution microscopy techniques like dSTORM, PALM and PAINT usually rely on wide field or TIRF illumination and wide field detection. This allows for simultaneous acquisition of the whole field of view but comes with the limitations of a camera based detection. Instead, we use a confocal setup with a pulsed excitation, single photon detection and a fast laser scanner. We evaluate different dyes and conditions to achieve slow blinking kinetics and a high number

of photons per switching event. Individual switching events could be localised utilising our confocal scanning approach and the corresponding super-resolved image could be reconstructed. The huge advantage of a single photon detection is that each localisation contains information about the fluorescence lifetime. This enables us to combine dSTORM with metal induced energy transfer (MIET), a distance dependant modulation of the lifetime of a fluorophore by a thin metal film. MIET enables axial localising single fluorophores with a precision below 5 nm. Our goal is to achieve a high, isotropic 3D-localisation accuracy by combining the high lateral precision of dSTORM with the high axial precision of MIET.

A Novel Class of Structure Tensors for Dispersed Fibers in Soft Materials

MolBioPhys18

Moritz Kalhöfer-Köchling, Yong Wang, Eberhard Bodenschatz

Max Planck Institute for Dynamics and Self-Organization

moritz.kalhofer-koechling@ds.mpg.de

Most biological tissues, like muscle, brain, tendon, display a fibrous structure, leading to an anisotropic mechanical behavior. Computational models often times are based on the assumption that fibers form unidirectional families, hugely facilitating simulations since you treatment of individual fibers can be omitted. Recent research, however, shows that even for considerably well aligned tissue, such as myocardium, the dispersed nature of fiber orientation plays an important role for its mechanical response. Angular integration (AI) accumulates contributions of individual fibers in a mathematical concise manner but leads to costly simulations. Based on Taylor series expansions of the AI, we propose a novel class of generalized structure tensors (GST), which are easier to implement, faster to compute, and show better convergence to the AI compared with previous GST models of similar order.

Scattering fingerprints of hydrodynamic interactions and internal friction in elastic network models of macromolecules

MolBioPhys19

Cai Dieball, Aljaž Godec

Max Planck Institute for Biophysical Chemistry

cai.dieball@mpibpc.mpg.de

Neutron and X-ray scattering are essential techniques for probing structural dynamics of macromolecules in bulk systems. Conversely, single-molecule spectroscopy provides complementary insight on the level of individual molecules. Intriguingly, the aforementioned bulk and single-molecule methods give highly diverging results. In our work we analyze simple polymer and elastic network models of macromolecules to shed light into the divergent views with special emphasis on the importance of hydrodynamic interaction and internal friction. We obtain analytical results for the static and dynamic structure factor and the intermediate scattering function and asses systematically the role of hydrodynamic interaction and internal friction.

Nonlinear dynamics

NoD01 Fast Quantitiative MRI using a Generalized Bloch Model-based Reconstruction

Nick Scholand, Xiaoqing Wang, Sebastian Rosenzweig, Martin Uecker

Department of Interventional and Diagnostic Radiology, University Medical Center Göttingen. German Centre for Cardiovascular Research (DZHK), Partner site Göttingen.

nick.scholand@med.uni-goettingen.de

Magnetic Resonance Imaging (MRI) is a popular non-invasive technique for medical imaging. It provides an excellent soft-tissue contrast and requires no ionizing radiation. In conventional MRI, image contrast qualitatively depends on various physical and chemical properties of the tissue. In contrast, in quantitative MRI these underlying properties are measured directly. Examples for properties which can measured using MRI are flow velocities, temperature, diffusion constants, electric current densities, magnetic field inhomogeneities, and relaxation constants. Here, we propose a method that uses the full Bloch equations in a calibrationless multi-channel model-based reconstruction. The reconstruction technique allows to model arbitrary spin dynamics and therefore becomes independent from specific MR sequences with analytical signal models. Multiple relaxation parameters can be estimated simultaneously, depending on the type of the applied sequences. We validated the proposed technique using simulations and experiments using the inversion-recovery (IR) FLASH and IR bSSFP sequences.

NoD02 Robust Cardiac and Respiratory Self-Gating MRI Using Time-Delayed Embedding (SSA-FARY)

Sebastian Rosenzweig, Nick Scholand, H Christian M Holme, Martin Uecker,

Universitätsmedizin Göttingen, Deutsches Zentrum für Herzkreislaufforschung DZHK

sebastian.rosenzweig@med.uni-goettingen.de

Magnetic Resonance Imaging (MRI) is a valuable tool for the detection and assessment of myocardial disease. Compared to other imaging modalities like Computed Tomography (CT), MRI does not involve the use of damaging radiation and possesses a superior soft tissue contrast. However, MRI has a major limitation: It is slow. This is particularly problematic for cardiac MRI, where both cardiac and respiratory motion is present. One way to overcome this limitation is to monitor cardiac and respiratory motion using external hardware such as an electrocardiogram (ECG) or a respiratory belts. Using this information, data from multiple heart-beats can be combined to generate a single, high-quality synthetic heart-beat. However, the placement of external devices is cumbersome and time-consuming. Alternatively, chunks of the acquired k-space data itself, which make up a so-called auto-calibration (AC) region, can be analyzed to detect cardiac and respiratory motion. This is known as self-gating. Conventionally, a combination of band-pass filters

and peak-detection algorithms is used. However, these techniques lack robustness. Here, we propose the application of dynamical system theory to extract cardiac and respiratory motion. In particular, we utilize the method of delays to embed the AC region in a higher dimensional space, which we then process using Principle Component Analysis (PCA). We validate this method, dubbed SSA-FARY, on numerical simulations and on volumetric self-gated cardiac MRI measurements.

Petrubation of pattern formation in D. Discoideum: Effects of obstacles and flow

NoD03

Torsten Eckstein, Estefania Vidal, Azam Gholami

Max Planck Institute for Dynamics and Self-Organization

torsten.eckstein@ds.mpg.de

The social amoeba Dictyostelium discoideum (D.d.) shows large scale pattern formation under starvation conditions. The cells produce waves of the signalling chemical cyclic adenosine monophosphate (cAMP). We study perturbations of this pattern formation process. Inspired by the natural habitat of the cells (the soil) we study the influence of nonexcitable obstacles. For prestarved cells incubated with caffeine we find initial bulk oscillations followed by target centre formation. These waves are centred on the obstacles, inducing a regular grid of waves and thus streaming territories. Comparing our experiments to simulations leads to similar results, if we include the effect of caffeine and assume a mechanism to break symmetry at the obstacles. Similarly, we take rain induced fluid flows in the soil as a reason to study the influence of an advective flow on the patterns. We find that while the wave period is constant for different flow velocities, both wave speed and thickness scale with it. Additionally, the wave shape is strongly influenced by the flow. We compare this to simulations and find good good agreement, although one simplification does not hold for high speed flows. Finally, we study the mutant cell line pdsA- in a flow setup. Here, we find that the normally not aggregating cell line can be rescued by a fresh buffer flow of adequate magnitude. The cells show damped waves, which decay along the channel. The cell development is crucial in these experiments, as there are two different regimes of pattern formation which start only after an initial 3 hours of flow. Additionally, the cells start spontaneous pattern formation if supplied with a strong enough flow for a certain amount of time. Again, we compare to simulations and find a wave instability induced by the zero boundary condition.

Optimal non-equilibrium decision making to store immune memory

NoD04

Oskar Schnaack[1], Armita Nourmohammad[1,2]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]University of Washington

oskar.schnaack@ds.mpg.de

Our adaptive immune system consists of highly diverse immune receptors to mount specific responses against a multitude of pathogens. During an infection, a fraction of these receptors forms a memory for later encounters. Here, we address a key question: which of the immune receptors should be kept as memory so that they can mount a response against evolved forms of the original pathogen in future infections? To do so, we have developed a theoretical framework, where memory storage is a non-equilibrium decision-making process between an adaptive exploration to mount a specific response and exploitation of existing yet suboptimal memory that can be utilized immediately to suppress an infection. To achieve a long-term benefit for the host, we show that memory generation should involve feedback from receptors' affinity and should favor cross-reactive receptors with a moderate affinity over high-affinity receptors against the infecting pathogen. The recipe for memory generation should be tuned over the host's evolutionary timescale based on the pathogenic evolutionary rates. Our results are consistent with recent experiments that suggest cell fate decisions during memory generation are highly regulated to balance the affinity and cross-reactivity of immune receptors.

Synchronization based reconstruction of the electrical state of the heart

NoD05

Baltasar Rüchardt[1], Jochen Bröcker[2], Stefan Luther[1], Ulrich Parlitz[1]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]University of Reading

baltasar.ruechardt@ds.mpg.de

The electrocardiogram (ECG) is the standard diagnostic tool to assess electrophysiological function of the heart. The relation between the electrical excitation of the heart and the electrical potential on the surface of the body is well understood ('forward problem'). However the reconstruction of the source distribution on the heart from given ECG measurements is challenging, because information is lost when the electrical signal travels through the body in a diffusion-like process ('inverse problem'). The standard methods to handle this loss are regularization methods which impose predefined assumptions on the problem until a solution can be found. This can exclude the true solution and, in general, does not rely on information of the underlying dynamical processes. In contrast, we try to reconstruct the electrical state of the heart from sensor signals with reduced spatial information by means of synchronization, based on a model of the spatial-temporal electrical dynamics.

Convolutional autoencoder and conditional random fields hybrid for predicting spatial-temporal chaos

NoD06

Sebastian Herzog[1], Florentin Wörgötter[2]

[1]Max Planck Institute for Dynamics and Self-Organization
[2]Third Institute of Physics and Bernstein Center for Computational Neuroscience

We present an approach for data driven prediction of high-dimensional chaotic time series generated by spatially extended systems. The algorithm employs a convolutional autoencoder for dimension reduction and feature extraction combined with a probabilistic prediction scheme operating in feature space which consists of a conditional random field. The future evolution of the spatially-extended system is predicted using a feedback loop and iterated predictions. The excellent performance of this method is illustrated and evaluated using Lorenz-96 systems and Kuramoto-Sivashinsky equations of different size generating time series of different dimensionality and complexity.

Multi-scale x-ray phase-contrast tomography of murine hearts

NoD07

Marius Reichardt

The spatial organization of heart muscle exhibits a complex structure on multiple length scales, from the sarcomeric unit to the whole organ. Here we demonstrate a multi-scale three-dimensional imaging approach with three levels of magnification, based on synchrotron x-ray phase contrast tomography. Whole mouse hearts are scanned in an undulator beam, which is first focused and then broadened by divergence. Regions-of-interest are scanned in parallel beam as well as by magnified cone beam geometry using a x-ray waveguide optic. Data is analyzed in terms of orientation, anisotropy and the sarcomeric periodicity via a local Fourier transformation.

Tuning the Rotational Diffusion of Polarizing Agents for Higher DNP Efficiency

Spec02

Marcel Levien, Markus Hiller, Igor Tkach, Marina Bennati, Tomas Orlando

Max Planck Institute for Biophysical Chemistry

mlevien@gwdg.de

Within the last 15 years dynamic nuclear polarization (DNP) has emerged as an efficient tool to boost the sensitivity of various magnetic resonance techniques [1]. Dissolution DNP has proven its applicability in magnetic resonance imaging (MRI) as well as solid-state DNP in nuclear magnetic resonance (NMR) [1]. However, liquid state NMR DNP is still in its infancy. Even though the general possibility of large signal enhancements at large magnetic fields has been demonstrated, many significant features of the polarization transfer mechanism are still to be investigated [2, 3]. As the polarization transfer in liquids is exclusively driven by relaxation (Overhauser Effect), the interplay of different molecular motions and their impact on relaxation is decisive for the DNP efficiency [3]. Here, we show experimentally how translational diffusion and rotation individually influence the coupling factor. The manipulation of either molecular motion was achieved by changing the temperature or the size of the polarizing agent. 1H-DNP measurements at 0.34 T were performed in toluene and chloroform doped with nitroxide derivatives. They reveal the impact of motions with significantly different timescales on the DNP efficiency. Furthermore, systems where scalar relaxation is dominating the polarization transfer were investigated with the same approach by performing 13C-DNP at 1.2 T. Upon the increase of the polarizing agent size, these systems display an increase of the absolute coupling factor. This peculiar behavior may be connected to an additional contact contribution which is modulated on a timescale suitable for high DNP efficiency at low magnetic field. In the future, DNP efficiency may be boosted even further through rational polarizer design.

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17O Hyperfine Spectroscopy to study Water Binding to Protein Radicals

Spec03

Fabian Hecker[1], Mario Chiesa[2], JoAnne Stubbe[3], Marina Bennati[1]

[1]Max Planck Institute for Biophysical Chemistry
[2]Universita di Torino
[3]Massachusetts Institute of Technology

fhecker@gwdg.de

Hyperfine spectroscopy is a powerful tool to probe the ligand sphere of paramagnetic species in a wide variety of observable systems. The 17O nucleus is a valuable probe for the presence of water but its low gyromagnetic ratio, large nuclear spin of I=5/2 and large quadrupole couplings make spectroscopy challenging. It was already extensively employed to investigate the binding of water to transition metal complexes but reports on water binding to protein radicals have been scarse. Amino acid radicals play an important role in biological electron transfer processes in proteins. Four distinct tyrosyl radicals have been identified as intermediates during the 35 Å proton-coupled electron transfer (PCET) in E.coli ribonucleotide reductase, which has been intensively studied as a paradigm for long range protein PCET. Y356 has been of particular interest in the last few years, as it is supposed to reside at the subunit interface of the protein active complex and water molecules are expected to facilitate the radical transfer across the interface. A hydrogen bonding network has been detected using 1H ENDOR, strongly suggesting the binding of waters to Y356. However, conclusive evidence for water involvement in the PCET is missing so far. Here we present 94 GHz ENDOR, and EDNMR as well as 34 GHz HYSCORE on a model system for 17O hyperfine spectroscopy and on Y356 in the active RNR enzyme. The results show that 17O ENDOR and HYSCORE spectroscopy can be used effectively to study water binding to organic nitroxide radicals. The ENDOR experiments on RNR show remarkably sharp coupling features, suggesting close binding of at least one water molecules to Y356 in accordance with our previous experiments. The comparison of both system clearly shows that the most appropriate hyperfine method is determined by the size of the hyperfine and quadrupole coupling.

NMR spectroscopy of human Hsp90

Spec04

Antonia Lott[1], Markus Zweckstetter[2]

[1]Deutsches Zentrum für Neurodegenerative Erkrankungen (DZNE Göttingen),
[2]Max-Planck-Institute for Biophysical Chemistry

antonia.lott@mpibpc.mpg.de

Hsp70 and Hsp90, two central chaperones of the heat shock protein (Hsp) family, play an important role in maintaining protein homeostasis [1]. In addition to their discrete chaperone function, they can build up the Hsp70/Hsp90 chaperone machinery where Hsp70 is linked to Hsp90 via the Hsp-organizing protein (Hop) [2, 3, 4]. It is well known that Hop can bind simultaneously to both chaperones and thereby

enables the orchestrated interplay between Hsp70 and Hsp90 [5], however, structural data at high resolution is not available. This project aims to gain detailed insights into the Hsp70/Hsp90 chaperone machinery by NMR targeting in particular the conformational rearrangements within Hsp90 upon its interaction with Hop and during the association of the Hsp90:Hop complex with Hsp70. A major bottleneck to the structural analysis of the Hsp70/Hsp90 chaperone machinery is its highly dynamic nature. To overcome these intrinsic challenges and gain structural information at single-residue resolution, we use a side-specific isotope labeling strategy combined with 1H-13C methyl-TROSY experiments optimized for high-molecular weight proteins [6]. By that we want to provide fundamental knowledge about the mode of protein (mis-)folding regulated by the Hsp70/Hsp90 chaperone machinery.

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Spec05 Breaking the 1.5Å barrier in single particle cryoEM using an aberration-corrected and monochromated TEM

Ka Man Yip

Max Planck Institute of Biophysical Chemistry

kyip@mpibpc.mpg.de

Despite advances in detector development and software algorithms, it is still difficult to surpass the 1.5Å barrier in single particle cryoEM. Other than challenges in sample preparation, the resolution of single particle cryoEM is also limited by the optical performance of the microscope. Here we introduce a microscope system equipped with coma corrector and monochromator that can break through the 1.5Å barrier with its improved optical performance.

Spec06 Measuring rotational diffusion of fluorophores using Fluorescence Correlation Spectroscopy (FCS) with polarization detection, dark field microscopy and fluorescence anisotropy

Aditya Katti[1], Antoine Delon[2], Jörg Enderlein[1]

[1]Third Institute of Physics, University of Göttingen
[2]Laboratoire Interdisciplinaire de Physique, Grenoble

aditya.katti@phys.uni-goettingen.de

FCS is a technique used to measure diffusion coefficients of fluorescently labeled molecules in nanomolar and picomolar concentrations. Fluorescence fluctuations as and when fluorophores move in and out of the observation volume are recorded and correlated to find the translational diffusion coefficients. However, in scattering and aberrating media like polyacrylamide (PAA) and agarose, the observation volume is distorted which gives inaccurate values. A more robust method to measure diffusion coefficients would be to measure rotational diffusion coefficients. FCS with polarized detection is advantageous in this case as the measurements are dependent on the polarization of the emitted photons and not the shape of the observation volume. Flat gels of PAA with different monomer and cross-linker concentrations were prepared with enhanced green fluorescent protein (EGFP) in the solution. The trapped EGFP rotates slower than in aqueous solution. Dark-field microscopy are helpful as they circumvent all issues associated with fluorescence measurements as scattered light is used as the information. Using gold nanorods of suitable sizes, dark field illuminated defocused images can be used to analyze rotation of these nanorods using a high-speed camera and hence rotational diffusion time can be measured. All these techniques provide an insight into measurement of pressure indirectly using rotational diffusion time as a measure. Fluorescence anisotropy is a method used when the rotational diffusion time and fluorescence emission lifetime of the fluorophore are comparable. Using beads filled with Europium (Eu3+) chelate ions, which have a long lifetime in a bead of suitable size, anisotropy measurements are performed determining the rotational diffusion time of the beads.

An approach to the Liquid-Liquid Phase Separation (LLPS) phenomenon from the NMR point of view

Spec07

Christian Pantoja Rivillas, Markus Zweckstetter

Max Planck Institute for Biophysical Chemistry

Christian.Pantoja-Rivillas@dzne.de

Recently the phenomenon of Liquid-Liquid Phase Separation (LLPS) has gained great interest among the scientific community given its participation in the formation of membraneless organelles that play crucial roles in the cellular environment 1. Great efforts are currently devoted to its structural and functional characterization. However, obtaining structural information at the molecular level of this phenomenon remains elusive given the challenges presented by the dynamics of the system. One of the most powerful analytical techniques in obtaining information at the atomic level is Nuclear Magnetic Resonance (NMR). Given its versatility and the wide variety of experiments available, this technique is presented as a key element in the understanding and characterization of this phenomenon in deep detail. In the present work we show a broad study of the different physical parameters accessible from NMR (T1, T2, Chemical Exchange) for the characterization of the phenomenon of LLPS. The strengths and challenges of current NMR methodologies are evaluated on a model system composed of triethylamine/water. Direct detection in 13C is shown as a plausible alternative in the study of this process given the favorable relaxation properties of this nucleus.

Author Index

Soft matter

Fluid dynamics

Active matter

Complex networks and nonlinear dynamics

Statistical physics