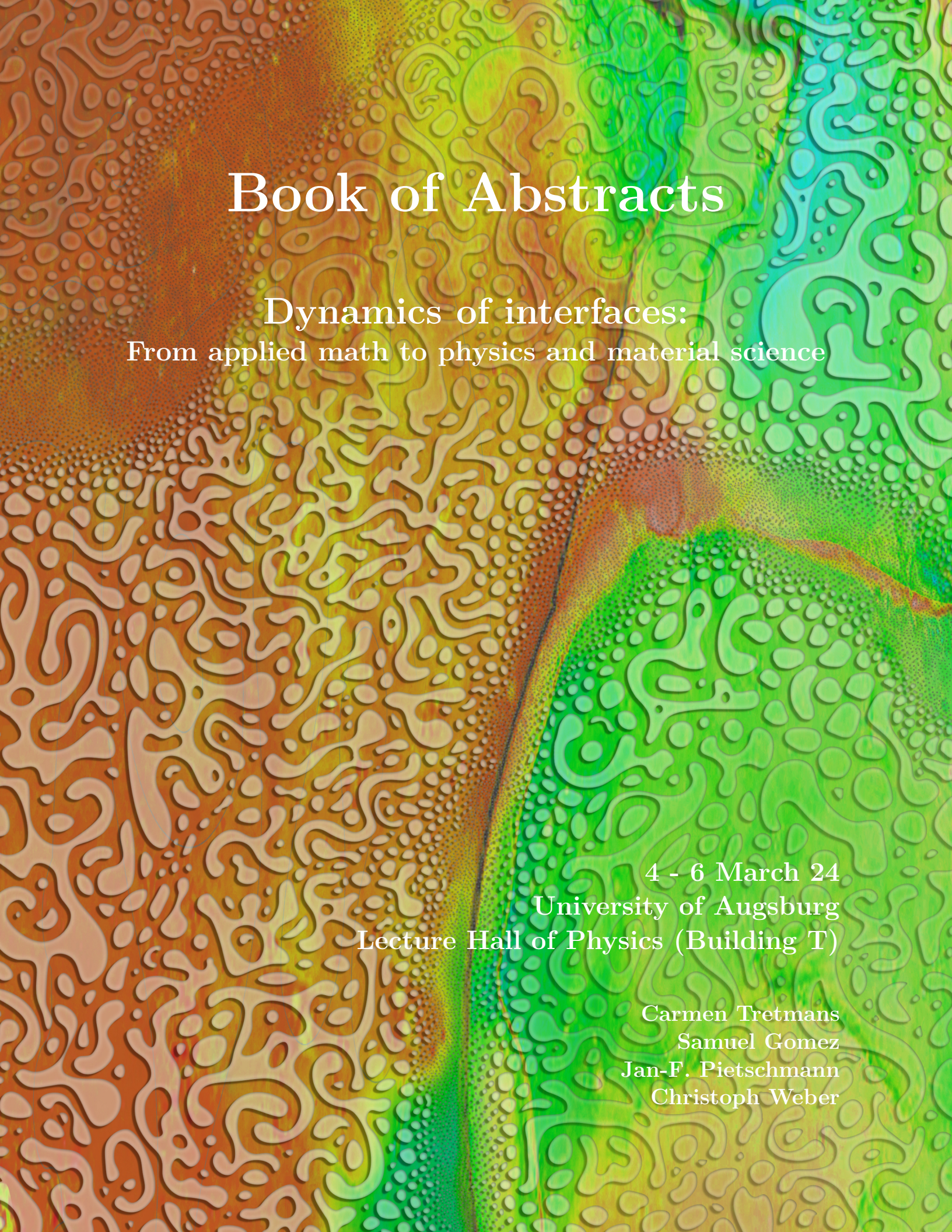


Book of Abstracts

Dynamics of interfaces:
From applied math to physics and material science

4 - 6 March 24
University of Augsburg
Lecture Hall of Physics (Building T)

Carmen Tretmans
Samuel Gomez
Jan-F. Pietschmann
Christoph Weber

Numerical simulation of active cell surfaces - from pattern formation to cell division

Sebastian Aland (Hochschule für Technik und Wirtschaft Dresden)

Shape changes of single cells are governed by the actomyosin cortex, a thin layer of active material underneath the cell surface. Aside from controlling rigidity, the cortical surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules. The complex interplay of molecule transport and surface hydrodynamics gives rise to pattern formation and self-organized shape dynamics. Despite the biological importance of these phenomena, the system is far from being understood.

To improve this understanding, we present numerical simulations of such an active surface immersed in viscous fluids. The cortex is modelled as a viscoelastic surface material, described by a freely evolving Finite-Element grid. The dynamics are coupled to a surface concentration equation of force-generating molecules (e.g. actomyosin). We analyze the emerging mechanochemical patterns and shape changes and show that the activity of the surface can lead to cell division or cell migration.

Spatiotemporal bacteria-phage competition regulates order in growing bacterial colonies

Igor Aronson (Pennsylvania State University)

Bacteriophages are viral predators of bacteria. Understanding the bacteria-phage competition is crucial for horizontal gene transfer and treatment of antibiotic-resistant bacterial infections. While bacteria and phages live and evolve in colonies and biofilms growing on solid surfaces, most studies of bacteria-phage interactions are conducted in well-agitated liquid cultures, ignoring spatial heterogeneity. We use computational modeling to examine bacteria-bacteriophage population dynamics in physically structured environments such as hard agar. We have demonstrated that spatial heterogeneity in phage distribution determines the resulting plaque shapes.

Our predictions about the T-phage family agree with experimental observations.

We have shown that phage infection results in large-scale reorganization and phage transport through the growing colony beyond the local motion of phages. As the phage plaque grows, the surviving cells align to the radial direction, maximizing the cells' probability of encountering phages. Increasing the radial order decreases the local number of topological defects since the defects close to the hole in the colony center are "flushed" by the bacterial flow.

Beyond controlling the shapes and sizes of phage plaques with the initial placement of cells and phage, we hint at how to shrink or eliminate a microcolony.

A critical transition regulates coarsening, scaling, and shape instabilities in active emulsions

Giacomo Bartolucci (University of Barcelona)

Active droplets are ubiquitous in liquid mixtures such as the cell cytoplasm or pools of short polymers that mimic the primordial soup. In such emulsions, chemical reactions are driven out of equilibrium by continuous turnover of chemical fuel. Despite the importance of active emulsions, their coarsening, scaling behaviour, and shape instabilities remain poorly understood. To shed light on these phenomena, we introduce a minimal model that allows us to characterize the steady state of single, chemically active droplets. We find a novel critical transition whose control parameter is the quantity conserved by the reaction. Below this transition, single droplets remain finite in infinite systems while, above it, they grow until a shape instability occurs. Crucially, this transition determines if shape instabilities lead to droplet division or elongation. In emulsions of many droplets, on the other hand, the same transition reveals how phases scale when a finite number of droplets are initialized in the nucleation and growth regime and what happens when such systems get quenched into the spinodal. We conclude by focusing on the formation of an intriguing stationary state composed of spherical shells and describing its experimental realization in coacervate systems.

Active Droplets: Droplets Regulated by Chemical Reaction Cycles

Job Boekhoven (Technische Universität München)

Active droplets are droplets regulated by chemical reaction cycles. Such droplets are common in our cells as membrane-less organelles, i.e., organelles that rely on the phase separation of RNA and proteins from the cytosol. Due to their non-equilibrium nature, these droplets are endowed with properties we do not observe for in-equilibrium self-assembly.

Excited by these unique properties, we developed a chemical reaction cycle that continuously activates and deactivates molecules for phase separation at the expense of chemical fuel. The interplay of activation and deactivation results in fascinating behavior. In this lecture, I will present the highlights of our findings, offer design rules for active droplets, and give an outlook of their role in the synthesis of life.

Shaping early molecular live by physical selection pressures

Dieter Braun (Ludwig-Maximilians-Universität München)

We will only fully understand the origin of life when we can recreate it in the laboratory. I report on our latest progress in building an autonomous evolution machine. A first step towards molecular evolution is the assembly of RNA from single nucleotides. We found that a moderate temperature difference at an air-water interface is an ideal micro-reactor for this process. The fluctuating interface continuously forms new dry spots by evaporation, driving the ring-opening polymerization of 2',3'-cyclic nucleotides toward RNA strands [2] and their length selective accumulation [4], including sequence-dependent phase transitions [1] and showing fast evolution for DNA model systems [3]. The reaction only required a moderate alkaline pH and operated in a wide range of temperatures (4-80°C). The propagation of information is critical. Under the same pH conditions as above, we found templated ligation of RNA strands with 2',3'-cyclic ends. We see that both the formation and ligation is enhanced by amino acids. Surprisingly, the interface setting also shows signatures of modern cell biology: RNA is encapsulated into vesicles when lipids are added [4]. Even the components of modern cells assemble at the interface: a highly diluted PURE system accumulated at the air-water interface, triggering the expression of proteins such as GFP. Thus, interfaces control a remarkable variety of key steps in the evolution of life, making us optimistic that a prebiotic evolutionary machine can be created in the laboratory sooner rather than later.

[1] G. Bartolucci, A. C. Serrão, P. Schwintek, A. Kühnlein, Y. Rana, P. Janto, D. Hofer, C. B. Mast, D. Braun, and C. A. Weber. Sequence self-selection by cyclic phase separation. *Proceedings of the National Academy of Sciences*, 120(43):e2218876120, 2023.

[2] A. V. Dass, S. Wunnava, J. Langlais, B. von der Esch, M. Krusche, L. Ufer, N. Chrisam, R. C. A. Dubini, F. Gartner, S. Angerpointner, C. F. Dirscherl, P. Rovó, C. B. Mast, J. E. Šponer, C. Ochsenfeld, E. Frey, and D. Braun. Rna oligomerisation without added catalyst from 2,3-cyclic nucleotides by drying at air-water interfaces. *ChemSystemsChem*, 5(1):e202200026, 2023.

[3] A. Ianeselli, M. Atienza, P. W. Kudella, U. Gerland, C. B. Mast, and D. Braun. Water cycles in a Hadean CO2 atmosphere drive the evolution of long DNA. *Nature Physics*, 18(5):579–585, May 2022.

[4] M. Morasch, J. Liu, C. F. Dirscherl, A. Ianeselli, A. Kühnlein, K. Le Vay, P. Schwintek, S. Islam, M. K. Corpinot, B. Scheu, D. B. Dingwell, P. Schwille, H. Mutschler, M. W. Powner, C. B. Mast, and D. Braun. Heated gas bubbles enrich, crystallize, dry, phosphorylate and encapsulate prebiotic molecules. *Nature Chemistry*, 11(9):779–788, Sept. 2019.

Mechanics of cellular granules: from stiff gas vesicles to soft hollow condensates

Françoise Brochard-Wyart (Institut Curie)

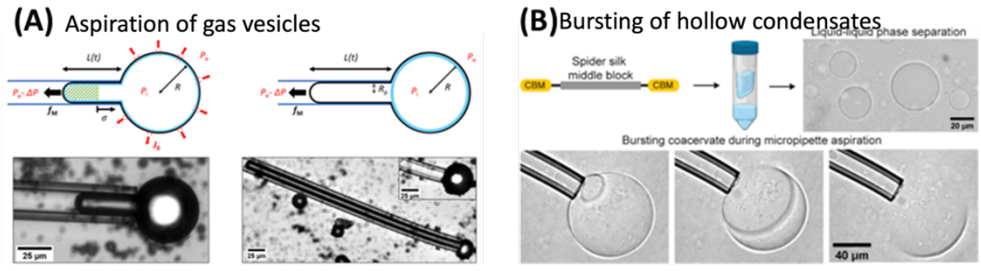
Joint work with G.Beaune, I.Tunn, JH.Al-Terke.Timonem and R.H. Ras, M.B.Linder.

In cells, proteins self-organize into fascinating structures, forming hydrophobic cages or protein condensates that perform specialized functions within the cell. We show that pipette

aspiration is a technique of choice to investigate the mechanical properties from the study of two cases:

A) Gas Vesicles. Produced in bacteria as a means of achieving cellular buoyancy. these air-filled protein nanostructures have been genetically encoded in cells to act as contrast agents for ultrasound imaging and as cell-killing agents through inertia-induced cavitation. To study their mechanical properties, they need to be formed on a larger scale. Here we report the formation and properties of giant gas vesicles, microbubbles encapsulating perfluoro-n-butane and coated with surface-active proteins adsorbed on their surface. We develop a model to analyze the suction of these compressible coated bubbles and compare it with incompressible liquid-filled capsules. The sucked bubble does not reach a steady state and the length of the tongue increases at constant speed. This is interpreted as a leakage of gas through the porous membrane. In the case of a porous capsule, we discuss the validity of the classical picture of E. Evans based on the Laplace law relating the membrane tension to ΔP and define a "sealing" parameter Q as the ratio of τ_M,the relaxation time of the viscous membrane flow, and τ_L,the relaxation time of the leakage flow. When Q is large, the membrane stress is given by the Laplace relation, but when Q is small, the classical picture no longer holds. We discuss future applications of these fascinating vesicles in tissue engineering and regenerative medicine. Gas vesicles can be targeted to specific tissues, enabling non-invasive imaging and diagnostics, and could be used for drug delivery and oxygen transport.

B) Hollow condensates. Biomolecular condensates, also known as coacervates are formed by the physical process of liquid-liquid phase separation (LLPS). Coacervates have crucial functions as membraneless organelles in cells to store the proteinaceous building blocks that form high performing biomaterials. Numerous biomolecular hollow or core-shell coacervates have been reported in cells and bioengineered *in vitro*. The relationship between the molecular structure of these coacervates and their rheological and interfacial properties remains largely unexplored. To fill this gap, we use micropipette aspiration to characterize hollow coacervates prepared from bioengineered spider silk proteins. We observed that coacervates can burst like vesicles upon aspiration. The bursting shows that the protein concentration is not homogeneous inside the condensate but forms a dense layer (shell) on the surface. We develop a model to analyse the aspiration and the bursting of these hollow coacervates, which leads to the measurement of the surface and bulk viscosity as well as an estimate of the shell thickness and viscosity. Understanding and controlling the formation and bursting of hollow coacervates will open new avenues for their use as material building blocks of chemical reaction compartments, or drug delivery systems.



Predictive contact line dynamics through phase field modelling

Andreas Carlson (University of Oslo)

Moving contact lines i.e., the point where three immiscible phases meet, appear in a myriad of applications as well as in biological systems. I will present how using phase field modelling allows us to capture the dynamics of the contact line by coupling its motion to the fluid flow. In particular, I will discuss how we use experiments in combination with phase field simulations to probe physical effects of the flow in rapid dynamic wetting of droplets on solid surfaces and the contact line motion of liquid free surfaces.

Elastocapillary Worthington jet & droplets produced by bursting bubbles

Ayush Dixit (University of Twente)

Joint work with Alexandros Oratis, Konstantinos Zinelis, Detlef Lohse1 and Vatsal Sanjay.

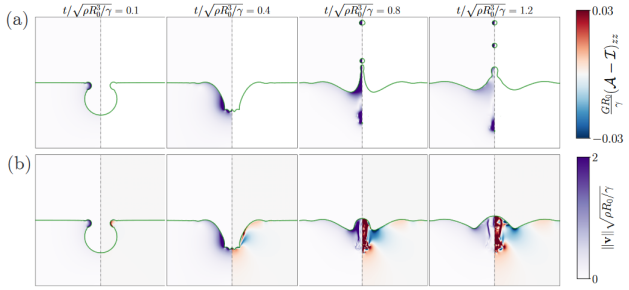


Figure 1: Collapse of bubble cavity in (a) Newtonian and (b) polymeric medium. The panels correspond to dimensionless time $t/\sqrt{\rho R_0^3/\gamma}$ at 0.1, 0.4, 0.8 and 1.2, respectively, illustrating dimensionless velocity and the additional dimensional polymeric stress (zz component). Both cases have the same fluid properties, except for G, which is 0 for the Newtonian case (a) and is $0.01\gamma/R_0$ for the polymeric case (b). The added polymers are observed to suppress the formation of aerosol. Here, ρ, γ and R_0 are the density of the liquid, surface tension and initial bubble radius, respectively.

Bubbles are often generated in liquids due to agitations at the free surface. Such bubbles rise to the surface and burst, producing droplets that can transport pathogens from the contaminated surrounding medium. After the film cap bursts, capillary waves travel over the interface and focus on the base, often generating Worthington jets that may eject fast droplets. Overall dynamics produced by bubble bursting depend crucially on the viscosity and cavity geometry which have been exhaustively studied. Yet, the surrounding rheology

can also significantly influence the dynamics. Introducing non-Newtonian properties, such as adding polymers, changes the flow behaviour, resulting in properties intermediate between simple liquids and elastic solids that can consequently suppress aerosol generation [2, 3]. However, the dynamics produced by bubble-bursting in a viscoelastic medium are yet to be fully understood. Here, we use direct numerical simulations using the volume of fluid method [1] to describe the bubble cavity collapse in a viscoelastic medium (figure 1). The study focuses on demystifying the underlying mechanisms of aerosol suppression and fine spray formation in polymeric liquids by analyzing the role of elastic modulus G and relaxation time λ on the dynamics [4]. We show that at low polymer concentrations, the dynamics are similar to that in Newtonian medium whereas at high polymer concentrations, the resulting elasticity resists the elongation of the Worthington jet and, consequently, suppresses the formation of the aerosols. Interestingly, near the polymer concentration threshold, the generated droplets are smaller than in Newtonian fluids, potentially enhancing aerosol dispersal.

[1] S. Popinet and collaborators. Basilisk c. `http://basilisk.fr`, 2013–2024. (Last accessed: January 2024).

[2] V. Sanjay, D. Lohse, and M. Jalaal. Bursting bubble in a viscoplastic medium. *Journal of Fluid Mechanics*, 922:A2, 2021.

[3] U. Sen, C. Datt, T. Segers, H. Wijshoff, J. H. Snoeijer, M. Versluis, and D. Lohse. The retraction of jetted slender viscoelastic liquid filaments. *Journal of Fluid Mechanics*, 929:A25, 2021.

[4] J. H. Snoeijer, A. Pandey, M. A. Herrada, and J. Eggers. The relationship between viscoelasticity and elasticity. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 476(2243):20200419, 2020.

Two-Phase biomembranes: Modeling, analysis and numerical computations

Harald Garcke (Universität Regensburg)

Biomembranes and vesicles consisting of multiple phases can attain a multitude of shapes, undergoing complex shape transitions. We study a Cahn–Hilliard model on an evolving hypersurface coupled to Navier–Stokes equations on the surface and in the surrounding medium to model these phenomena. The evolution is driven by a curvature energy, modelling the elasticity of the membrane, and by a Cahn–Hilliard type energy, modelling line energy effects.

A stable semidiscrete finite element approximation is introduced and, with the help of a fully discrete method, several phenomena occurring for two-phase membranes are computed. Finally, we will discuss new analytical and numerical results for situations where the coupling to the bulk is neglected.

Capillary interactions between soft capsules, hard particles and droplets at thin fluid films

Jens Harting (Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich)

Joint work with Maarten Wouters, Othmane Aouane, Qingguang Xie, Lei Yang and Marcello Sega.

The ordering of particles in the drying process of a colloidal suspension is crucial in determining the properties of the resulting film. For example, microscopic inhomogeneities can lead to the formation of cracks and defects that can deteriorate the quality of the film considerably. We study this multiscale problem, using our recently developed lattice Boltzmann method which allows for the simulation of soft deformable particles, hard colloids or even droplets (liquid lenses) attached to liquid interfaces. Although capillary interactions between rigid particles are well studied, much is still to be understood about the behaviour of soft particles or liquid lenses and the role of their softness during the final stages of film drying. Our measured menisci deformations and lateral capillary forces show that the deformations become smaller with increasing particles softness resulting in weaker lateral interaction forces. At large interparticle distances, the force approaches that of rigid particles.

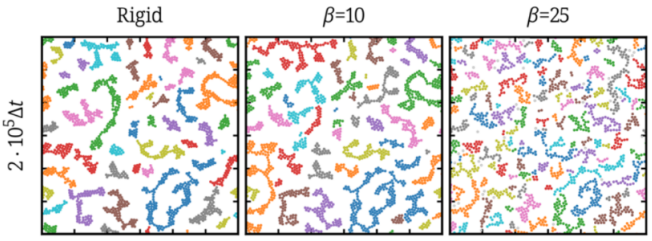


Figure 2: particle softness and capillary interactions in a drying film

[1] F. Pelusi, F. Guglietta, M. Sega, O. Aouane, and J. Harting. A sharp interface approach for wetting dynamics of coated droplets and soft particles. *Physics of Fluids*, 35(8):082126, Aug. 2023. _eprint: https://pubs.aip.org/aip/pof/article-pdf/doi/10.1063/5.0160096/18103259/082126_1_5.0160096.pdf.

[2] T. Scheel, Q. Xie, M. Sega, and J. Harting. Viscous to inertial coalescence of liquid lenses: A lattice boltzmann investigation. *Phys. Rev. Fluids*, 8:074201, Jul 2023.

[3] M. Wouters, O. Aouane, M. Sega, and J. Harting. Capillary interactions between soft capsules protruding through thin fluid films. *Soft Matter*, 16:10910–10920, 2020.

[4] M. Wouters, O. Aouane, M. Sega, and J. Harting. Lattice boltzmann simulations of drying suspensions of soft particles. *Philosophical Transactions of the Royal Society of London, Series A: Mathematical, Physical and Engineering Sciences*, 379(2208), Oct. 2021.

[5] L. Yang, M. Sega, and J. Harting. Capillary-bridge forces between solid particles: Insights from lattice boltzmann simulations. *AIChE Journal*, 67(9):e17350, 2021.

Patterns in active fluids on surface

Sabine Klapp (Institute of Theoretical Physics, TU Berlin)

In this talk we will discuss recent results on the collective behavior and pattern formation of active systems exhibiting vortices and clustering on surfaces. The first example concerns suspensions of microswimmers exhibiting mesoscale turbulence. We employ a continuum-theoretical approach which can be derived microscopically [4] and allows for a quantitative modelling of experiments [5]. Considering systems in periodic arrays of obstacles, we explore the transition from a vortex state to mesoscale turbulence. We find an intriguing similarity with a second-order phase transition characterized by critical exponents in the 2D Ising universality class and an effective temperature that can be related to a particle-dependent quantity, that is, the motility [3]. We also present a state diagram indicating the route to turbulence in the absence of obstacles [2].
The second example concerns systems of repulsive active particles with non-reciprocal alignment coupling. The resulting collective dynamics involves, beyond flocking and motility-induced phase separation, also frustrated states induced by non-reciprocity. We investigate the large-scale behavior of these systems using a mean-field-like continuum theory and linear stability analysis [1]. In addition, we present particle-based simulations of the underlying Langevin equations. The latter allow us to characterize the complex dynamics microscopically, and to assess the role of correlations.

[1] K. L. Kreienkamp and S. H. L. Klapp. Clustering and flocking of repulsive chiral active particles with non-reciprocal couplings. *New Journal of Physics*, 24(12):123009, dec 2022.

[2] H. Reinken, S. Heidenreich, M. Bär, and S. H. L. Klapp. *in preparation.*

[3] H. Reinken, S. Heidenreich, M. Bär, and S. H. L. Klapp. Ising-like critical behavior of vortex lattices in an active fluid. *Phys. Rev. Lett.*, 128:048004, Jan 2022.

[4] H. Reinken, S. H. L. Klapp, M. Bär, and S. Heidenreich. Derivation of a hydrodynamic theory for mesoscale dynamics in microswimmer suspensions. *Phys. Rev. E*, 97:022613, Feb 2018.

[5] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson. Organizing bacterial vortex lattices by periodic obstacle arrays. *Communications Physics*, 3(1):76, May 2020.

Chemically Active Wetting

Susanne Liese (Universität Augsburg)

Joint work with Xueping Zhao, Christoph Weber and Frank Jülicher.

Wetting of liquid droplets on passive surfaces is ubiquitous in our daily lives, and the governing physical laws are well-understood. However, the comprehension of wetting laws becomes challenging when surfaces exhibit activity. We propose chemically active wetting as a new class of active systems where the surface is active due to a binding process that is maintained away from equilibrium. The derived non-equilibrium thermodynamic theory reveals that active binding fundamentally alters wetting behavior, resulting in stable, non-equilibrium states with droplet shapes resembling pancakes or mushrooms. The peculiar shapes can be explained by an analogy to electrostatics, where binding sinks and sources

form pairs analogous to electrostatic dipoles along the triple line. This analogy extends to a broader concept, where localized chemical activity generates a multipole field of the chemical potential. The underlying physics holds significance in biological contexts such as cells, where proteins forming droplets can bind to membranes with the simultaneous turnover of biological fuels.

Modern simulation methods for complex multi-physics problems in computational cell biology

André Jürgen Massing (Norwegian University of Science and Technology)

Many continuum mechanics based models in computational cell biology require the numerical solution of highly non-trivial partial differential equations (PDEs) on complicated or moving surfaces. For instance, phase-separation in multi-component lipid-based membranes, diffusion-driven protein-crowding, and cell motion driven by cytoskeleton reorganization are all processes which can be modeled by complex partial differential equations posed on the cell membrane surface. Another example is the Extracellular-Membran-Intracellular (EMI) model which is mixed-dimensional problem which couples an elliptic partial differential equation on the extra/intracellular domains with a system of nonlinear ordinary differential equations (ODEs) over the cell membranes to model of electrical activity of explicitly resolved brain cells.

In this talk, we give an introduction to a novel and general discretization framework which allows for an easy discretization of surface-bounded differential equations and their seamless coupling to additional, e.g. bulk-related PDEs. The framework is first explained by considering some simple prototype PDEs posed on either bulk or surface domains. Then, we demonstrate how the discretization technology can be used to simulate EMI model on resolved neural cell geometries and diffusion-type problems on moving domains. One major goal of this talk is to stimulate discussions on how sophisticated numerical methods could help approach challenging problems in computational cell biology/biophysics.

Numerical simulation of droplets on biomembranes

Marcel Mokbel (TU Bergakademie Freiberg)

Biological cells utilize membranes and liquid-like droplets, known as biomolecular condensates, to structure their interior. The interaction of droplets and membranes, despite being involved in several key biological processes, is so far little understood.
In this talk, we present a first numerical method to simulate the continuum dynamics of droplets interacting with deformable membranes via wetting. The method combines the advantages of the phase-field method for multi-phase flow simulation and the arbitrary

Lagrangian-Eulerian (ALE) method for an explicit description of the elastic surface. The model is thermodynamically consistent, coupling bulk hydrodynamics with capillary forces, as well as bending, tension, and stretching of a thin membrane.

Dynamics of Longitudinal Pulses within Lipid Interfaces: Physical, Computational, and Biological Aspects

Matan Mussel (University of Haifa)

In this talk, we will describe a numerical investigation of the nonintuitive properties of longitudinal pulses that propagate within lipid interfaces close to the order–disorder phase transition. These properties include saturation of pulse amplitude, annihilation upon collision, electrical and chemical changes that co-propagate with the disturbance, and a transient change in permeability that may create oscillatory and excitability responses. Pointing out striking similarities to action potentials observed in excitable cells, we suggest that longitudinal pulses may be harnessed for material-based computation, mimicking biological or artificial neural algorithms. We illustrate the system's strong performance across various inputs by implementing regression and classification tasks. Additionally, we demonstrate that longitudinal pulses propagate more information than is typically considered by conventional models of neural computation. We conclude by discussing the possibility that acoustics in lipid interfaces might play a functional role in cellular communication. This suggests that non-electric information encoded within the biological pulse may be overlooked if one focuses solely on electrical measurements.

Numerical approximation of solid-state dewetting with anisotropic surface energies

Robert Nürnberg (University of Trento)

Joint work with Harald Garcke, Patrick Knopf and Quan Zhao.

We present a diffuse-interface model for the solid-state dewetting problem with anisotropic surface energies. The introduced model consists of the anisotropic Cahn–Hilliard equation, with either a smooth or a double-obstacle potential, together with a degenerate mobility function and appropriate boundary conditions on the wall.
Upon regularizing the introduced diffuse-interface model, and with the help of suitable asymptotic expansions, we recover as the sharp-interface limit the anisotropic surface diffusion flow for the interface together with an anisotropic Young's law and a zero-flux condition at the contact line of the interface with a fixed external boundary. Numerical results based on an appropriate finite element approximation are presented to demonstrate the excellent agreement between the proposed diffuse-interface model and its sharp-interface limit.

Long-range interactions and disorder facilitate pattern formation in spatial complex systems

Fabrizio Olmeda (IST Austria)

Complex systems with global interactions tend to be stable if interactions between components are sufficiently homogeneous. In biological systems, which often have small copy numbers and interactions mediated by diffusing agents, noise and non-locality may affect stability. Here, we derive stability criteria for spatial complex systems with local and non-local interactions from a coarse-grained field theory with multiplicative noise. We show that long-range interactions give rise to a transition between regimes exhibiting giant density fluctuations and pattern formation. This instability is suppressed by non-reciprocity in interactions. Our work provides a theoretical framework to quantify the effect of disorder and long-range interactions in a wide-range of spatially extended complex systems, with application ranging from ecosystems to phase separation.

A multiscale approximation of a Cahn–Larché system with phase separation on the microscale

Malte A. Peter (Universität Augsburg)

We consider the process of phase separation of a binary system under the influence of mechanical deformation and we derive a mathematical multiscale model, which describes the evolving microstructure taking into account the elastic properties of the involved materials. Motivated by phase-separation processes observed in lipid monolayers in film-balance experiments, the starting point of the model is the Cahn–Hilliard equation coupled with the equations of linear elasticity, the so-called Cahn–Larché system. Owing to the fact that the mechanical deformation takes place on a macroscopic scale whereas the phase separation happens on a microscopic level, a multiscale approach is imperative. We assume the pattern of the evolving microstructure to have an intrinsic length scale associated with it, which, after nondimensionalisation, leads to a scaled model involving a small parameter $\varepsilon > 0$, which is suitable for periodic-homogenisation techniques. For the full nonlinear problem, the so-called homogenised problem is then obtained by letting $\varepsilon \to 0$ using the method of asymptotic expansion. Furthermore, we present a linearised Cahn–Larché system and use the mathematically rigorous method of two-scale convergence to obtain the associated limit problem, which turns out to have the same structure as in the nonlinear case, in a mathematically rigorous way. Properties of the limit nonlinear distributed-microstructure model are discussed and numerical simulations based on a finite-element approach are used to illustrate the model behaviour.

This is joint work with L. Reischmann (DLR-Institute of Test and Simulation for Gas Turbines).

Phase-field simulations of absorber layer formation for printed photovoltaics

Olivier Ronsin (Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich)

Joint work with M. Majewski, M. Siber, Y. Ameslon and J. Harting.

The processing conditions strongly impact the morphology and hence the efficiency of the photoactive layers in organic (OSC) and perovskite (PSC) solar cells. However, the process-structure relationship still remains poorly understood, and a theoretical model for this problem is missing.
We propose a new coupled phase field - fluid mechanics framework gathering the main physical phenomena that drive the morphology formation of the photoactive layer for printed photovoltaics [3, 2]. Solvent evaporation, crystal nucleation, growth and coarsening in polycrystalline materials, liquid-liquid phase separation are taken into account. The kinetic evolution of the investigated mixture is given by the coupled Cahn-Hilliard-Cook, stochastic Allen-Cahn, mass conservation and momentum conservation equations. Furthermore, the dramatic evolution of the kinetic properties during wet film drying are considered. This new approach can help identifying new design rules for ink formulation and processing conditions of drying crystalline mixtures.
For OSC, the possible crystallization pathways and associated morphologies will be discussed [4]. Very convincing comparisons with previously reported in-situ characterization of the film structure will be shown in the case of film drying and thermal annealing: the morphology formation pathways, crystallization kinetics, and final morphology are in line with experimental results [1]. For PSC, simulations showing the impact of the evaporation rate on the final crystalline structure will be shown. The results regarding substrate coverage, film roughness, crystals sizes are in excellent agreement with experimental results, and the process design rules for obtaining high-quality films will be discussed. Overall, this contribution illustrate how advanced Phase-Field simulations can help accelerating the development of 3rd generation photovoltaics and thus contribute to the energy transition.

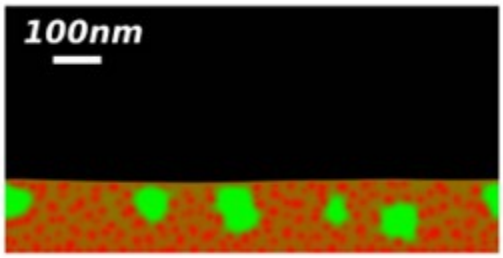


Figure 3: Nanomorphology of a polymer (red) - small molecule (green) bulk-heterojunction at the end of film drying

[1] O. J. J. Ronsin and J. Harting. Formation of crystalline bulk heterojunctions in organic solar cells: Insights from phase-field simulations. *ACS Applied Materials & Interfaces*, 14(44):49785–49800, 2022.

PMID: 36282868.

[2] O. J. J. Ronsin and J. Harting. Phase-field simulations of the morphology formation in evaporating crystalline multicomponent films. *Advanced Theory and Simulations*, 5(10):2200286, 2022.

[3] O. J. J. Ronsin, D. Jang, H.-J. Egelhaaf, C. J. Brabec, and J. Harting. Phase-Field Simulation of Liquid–Vapor Equilibrium and Evaporation of Fluid Mixtures. *ACS Applied Materials & Interfaces*, 13(47):55988–56003, Dec. 2021. American Chemical Society.

[4] M. Siber, O. J. J. Ronsin, and J. Harting. Crystalline morphology formation in phase-field simulations of binary mixtures. *J. Mater. Chem. C*, 11:15979–15999, 2023.

Deformable soft matter

Vatsal Sanjay (University of Twente)

This talk explores the fascinating world of deformable soft matter, focusing on drops and bubbles—ubiquitous in nature and technology. Using exhaustive experimental, numerical, and theoretical approaches, we delve into the intricate dynamics of drop impacts on both rigid and compliant surfaces and the captivating phenomena of retraction and bursting of bubbles. Central to our discussion is unveiling novel insights into hydrodynamic singularities inherent in these systems.

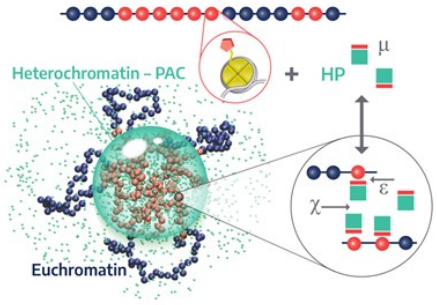
Exploring RNA-Protein Dynamics through Phase Segregation

Andrea Signori (Politecnico di Milano)

Phase separation has emerged as a fundamental concept in Cell Biology. This study delves into a phase-field model elucidating the intricate dynamics of protein-RNA complexes subjected to phase segregation. The system involves a singular protein, two distinct RNA species, and two resultant complexes. The interactions are governed by coupled reaction-diffusion equations intricately intertwined with the formation and evolution of the complexes. Addressing technical challenges, particularly the initialization of the complexes from a pure phase, proves to be a significant challenge in managing the Cahn–Hilliard equation with singular potentials like the Flory–Huggins. Notably, the study establishes the existence of weak solutions in both two and three dimensions. Our discoveries have further implications, reaching into the domain of the standard Cahn–Hilliard equation with a source term, including the Oono type, where such outcomes were previously unexplored.

How polymers control and localize liquid-liquid phase separation

Jens-Uwe Sommer (Leibniz Institute of Polymer Research, TU Dresden)



Liquid-liquid phase separation of proteins is increasingly recognized as a fundamental concept to understand biological functions. Biomolecular condensates are formed at specific places in the cell, but what controls their size and life-time, and by which mechanisms different condensates interact or exchange material (and possibly information) with each other as well as with the environment is still largely unexplored. Biomolecular condensates comprise multiple components, with large biopolymers like RNA and DNA playing a crucial role in their formation. Adopting a perspective rooted in polymer physics, I examine long, flexible polymers within a solution of mixed components, such as proteins in water. Two scenarios are presented in detail: Bridging-induced interactions and polymer-assisted condensation (PAC) which can explain the formation of localized and size-controlled condensates using concepts from polymer physics and phase separation theory. As an example, I explore the case of heterochromatin. Here, the features of PAC offer a rational basis for explaining the preservation of epigenetic information during the cell cycle. Furthermore, the effect of external forces on PAC-condensates and polymerization in mixed solvents are discussed.

According to the PAC-model heterochromatin is formed due to condensation of specific proteins (HP) in the presence of the polymer. Methylated sequences of chromatin (red) are trapped and confined in the protein condensate. The resulting droplet serves as reaction chamber for client molecules such as methyltransferase to reestablish the full epigenetic information after cell division, and rejects transcription factors silencing gens in specialized cells.

[1] J.-U. Sommer, H. Merlitz, and H. Schiessel. Polymer-assisted condensation: A mechanism for heterochromatin formation and epigenetic memory. *Macromolecules*, 55(11):4841–4851, 2022.

Phase-Field Models for Organic Solar Cell Production

Carmen Tretmans (Universität Augsburg)

In this talk we discuss a model for the formation of acceptor and donor regions during the production of organic solar cells. The process is based on a spinodal decomposition of two species in a solvent, where the solvent is allowed to evaporate. This yields a coupling of the respective phase field equations via a degenerate mobility. We provide some insight on the modelling and the application as well as several numerical examples based on finite element simulations.

Machine learning with and for phase-field modeling

Olga Wodo (University of Buffalo)

Machine learning and artificial intelligence emerge as new tools to supplement theory and computations in our endeavor to understand materials better and, ultimately, to use these tools for materials design with target properties. In this talk, I will highlight how phase field modeling and machine learning can complement each other to accelerate materials design and discovery. I will focus on the robust microstructure representations needed to reduce high-dimensional phase field data and represent materials' microstructure in machine-friendly formats that include (i) statistical descriptors (e.g., 2-point correlations), (ii) vector of physically meaningful descriptors, and (iii) latent space learned using autoencoder. Using these representations, I will present case studies using phase field data to train machine learning models, extract salient features from large datasets, use phase diagrams to inform material selection and orchestrate inverse microstructure design. The challenges and methods behind these case studies are generic for establishing and inverting materials-process-structure-property relationships of most materials systems. Still, in this talk, organic photovoltaics applications will serve as a platform where complex multi-physics phenomena governing the material behavior and device properties demand effective knowledge extraction, materials selection, and design through computational or machine learning modeling. I will close this talk with the call for FAIR data generation and how good data stewardship can help the community.

Controllable Capillary Assembly of Magnetic Janus Particles at Fluid-Fluid Interfaces

Qingguang Xie (Helmholtz Institute Erlangen-Nürnberg for Renewable Energy)

Self-assembly of particles at fluid-fluid interfaces is a promising route to fabricate functional materials from the bottom-up. However, directing and controlling particles into highly

tunable and predictable structures, while essential, is a challenge. Here, we apply a hybrid approach combining the lattice Boltzmann, and the discrete element methods to investigate the behaviour of magnetic Janus particles adsorbed at a fluid-fluid interface interacting with an external magnetic field. Depending on their tilt angle and shape (e.g. sphere, ellipsoid), the anisotropic particles deform the interface and generate capillary dipoles or hexapoles. Driven by capillary interactions, multiple particles thus arrange into reconfigurable chain-, hexagonal-lattice-, and ring-like structures, which can be actively controlled by varying the external magnetic field. We develop interface energy models to reveal the underlying mechanism and find good qualitative agreement with simulation results. Our results have implications for the fabrication of varied microstructures for use in microdevices, organic electronics, or advanced display applications.

[1] Q. Xie, G. B. Davies, F. Günther, and J. Harting. Tunable dipolar capillary deformations for magnetic janus particles at fluid–fluid interfaces. *Soft Matter*, 11:3581–3588, 2015.

[2] Q. Xie, G. B. Davies, and J. Harting. Controlled capillary assembly of magnetic janus particles at fluid–fluid interfaces. *Soft Matter*, 12:6566–6574, 2016.

[3] Q. Xie, G. B. Davies, and J. Harting. Direct assembly of magnetic janus particles at a droplet interface. *ACS Nano*, 11(11):11232–11239, 2017. PMID: 29035521.

[4] Q. Xie and J. Harting. Controllable capillary assembly of magnetic ellipsoidal janus particles into tunable rings, chains and hexagonal lattices. *Advanced Materials*, 33(8):2006390, 2021.

Wetting Dynamics of Droplet with Surface Binding

Xueping Zhao (University of Nottingham Ningbo China)

Biomolecules, such as proteins and RNAs, can phase separate in the cytoplasm of cells to form biological condensates. Such condensates are liquid-like droplets that can wet biological surfaces such as membranes. Many molecules that can participate in phase separation can also reversibly bind to membrane surfaces. When a droplet wets such a surface, these molecules can diffuse both inside the droplet or in the bound state on the surface. How the interplay between surface binding and surface diffusion affects the wetting kinetics is not well understood. Here, we derive the governing equations using non-equilibrium thermodynamics by relating the diffusive fluxes and forces at the surface coupled to the bulk. We use our theory to study the spreading kinetics in the presence of surface binding and find that binding speeds up wetting by nucleating a droplet inside the surface. Our results are relevant both to artificial systems and to condensates in cells. They suggest that the wetting of droplets in living cells could be regulated by two-dimensional droplets in the surface-bound layer changing the binding affinity to biological surfaces.