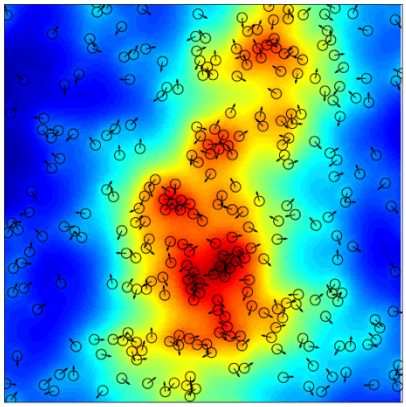
Frontiers in Computational Methods for Active Matter



February 10 - 12, 2020
CECAM-HQ-EPFL, Lausanne, Switzerland

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1 Description

In view of the broad range of active matter systems, various numerical approaches have been developed to model such systems. Some of the major challenges arising in modeling active systems are: (i) Active matter is a multiscale material similar to other complex fluids such as milk or blood, (ii) Active fluids are intrinsically out of equilibrium due to energy consumption on microscopic scale, (iii) The interactions between active particles can be highly nonlinear and are often of multibody character (e.g. hydrodynamic interactions or interactions due to chemical stimuli), (iv) Active particles are mostly not simple geometrical objects, such as hard spheres, but rather of complex shape due to propulsion and other functional units. So far, various system-specific methods with different levels of resolution, ranging from micro- to macroscale, have been developed and employed. For example, active Brownian dynamics and partial differential equations (PDE) (such as generalized Navier Stokes equations), have been used to model active fluids in a very coarse-grained way. However, coarse gaining of active systems in not trivial and modification of microscopic details can strongly alter the macroscopic behaviour. It is unclear e.g. how particle-wall and particle-particle interactions translate into proper boundary conditions and transport coefficients of the corresponding macroscale PDE. On the other hand, mesoscale techniques (e.g. lattice Boltzmann method) try to bridge different length and time scales and to model properly the hydrodynamic interaction between active particles. However, these techniques have to compromise strongly between microscopic accuracy and macroscopic system size. Another point is that the existing techniques need to be further developed to cope with real-world applications. For example, the typical environment for micro-organisms is not a simple fluid but rather a suspension of extracellular polymeric substances (e.g. proteins, lipids and DNA), which can strongly influence the motility and interactions of the moving objects. Another long-term goal for the modeling of biological active matter is to include the adaptive behavior of micro-organisms, i.e. the ability to detect and respond to different stimuli such as material properties of the surrounding (durotaxis) or chemical concentrations (chemotaxis or quorum sensing), which requires a coupling between intracellular and extracellular models.

Similar modeling challenges apply to synthetic active matter. For example, a microscopic modeling and understanding of propulsion based on autophoresis (e.g. thermo or diffusiophoresis) is required to design artificial active materials that are capable of making decisions (based on sensory input) and adapting to environmental changes in a self-organized manner. We will also discuss trendsetting developments of unconventional computing, namely of “materials that compute”. Recent studies indicate that active materials can be used to construct logical units and in long-term to implement autonomous computation schemes.

The goal of this workshop is to bring together the experts in modeling soft condensed matter and biological systems to tie recent advances in computational techniques and the most recent ideas and concepts of active matter theory. This workshop will provide the opportunity to compare state of the art computational active matter approaches and to open the discussion on the existing challenges and problems.

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2 Program

Day 1 - Monday February 10, 2020

- 8:45 to 9:00 - Welcome

Session I: Active Brownian particles, filaments and membranes | Pressure | Surface tension

- 9:00 to 9:45 - Presentation **- Gerhard Gompper**
  Computational approaches to active filaments, membranes, and cells
- 9:45 to 10:30 - Presentation **- Ignacio Pagonabarraga**
  Activity induced phase transitions: from MIPS to chiral self-sorting
- 10:30 to 11:00 - Coffee Break
- 11:00 to 11:45 - Presentation **- Roland G. Winkler**
  Active Brownian particles: local pressure in nonequilibrium systems
- 11:45 to 12:30 - Presentation **- Yariv Kafri**
  Steady-state currents in active matter: origin and implications
- 12:30 to 14:00 - Lunch

Session II: Lattice gas models | Active granular particles | Squirmers | Phoresis

- 14:00 to 14:45 - Presentation **- Joakim Stenhammar**
  Lattice Boltzmann modeling of collective dynamics in microswimmer suspensions
- 14:45 to 15:30 - Presentation **- Thorsten Pöschel**
  Collective behavior and self-organisation of active granular particles
- 15:30 to 16:00 - Coffee Break
- 16:00 to 16:45 - Presentation **- Holger Stark**
  The squirmer as a model microswimmer: collective patterns under gravity and squirmer rods
- 16:45 to 17:30 - Presentation **- Sebastien Michelin**
  Chemical and hydrodynamic coupling in the self-propulsion of phoretic particles and active droplets
- 17:30 to 19:30 - Poster Session & Discussion

Day 2 - Tuesday February 11, 2020

Session III: Continuum models | Active motion in fluids

- 9:00 to 9:45 - Presentation **- Hartmut Löwen**
  Dynamical density functional theory of microswimmers: collective dynamics, circle swimming, and binary mixtures

- 9:45 to 10:30 - Presentation **- Raphael Wittkowski**
  Field-theoretical modeling of active matter

- 10:30 to 11:00 - Coffee Break

- 11:00 to 11:45 - Presentation **- Jonasz Slomka**
  Generalized Navier-Stokes equations for active fluids in flat and curved geometries

- 11:45 to 12:30 - Presentation **- Amin Doostmohammadi**
  Stabilizing active flows: hydrodynamic screening and topological constraints

- 12:30 to 14:00 - Lunch

Session IV: Phase field models | Active nematics | Self-propelled rods

- 14:00 to 14:45 - Presentation **- Julia Yeomans**
  Modelling collective cell mechanics

- 14:45 to 15:30 - Presentation **- Michael Hagan**
  Particle-based simulations of three-dimensional nematics in and out of confinement

- 15:30 to 16:00 - Coffee Break

- 16:00 to 16:45 - Presentation **- Seth Fraden**
  Boundaries tame flow in active fluids of extensile filaments

- 16:45 to 17:30 - Presentation **- Fernando Peruani**
  Self-propelled rods as a paradigm of active matter: from scalar to vectorial active matter

- 19:00 to 21:30 - Social Dinner

Day 3 - Wednesday February 12, 2020

Session V: Cells and tissues

- 9:00 to 9:45 - Presentation **- Daniel Sussman**
  Active vertex models of epithelial tissue
- 9:45 to 10:30 - Presentation **- Ludger Santen**
  Cytoskeletal dynamics and motor driven transport
- 10:30 to 11:00 - Coffee Break
- 11:00 to 11:45 - Presentation **- Jens Elgeti**
  Active matter driven by growth - a particle-based model
- 11:45 to 12:30 - Presentation **- Falko Ziebert**
  Phase field approach for substrate-based cell motility in complex environments
- 12:30 to 12:45 - Closing Word

3 Abstracts

Computational approaches to active filaments, membranes, and cells

Gerhard Gompper, Thorsten Auth, Jens Elgeti, Roland G. Winkler
Research Center Jülich, Germany

Active matter exhibits a wealth of emerging non-equilibrium behaviors [1]. A paradigmatic example is the interior of cells, where active components, such as the cytoskeleton, are responsible for its structural organization and the dynamics of the various components. Of particular interest are the properties of active polymers and filaments [2]. The intimate coupling of active forces, thermal noise, hydrodynamic interactions, and polymer connectivity implies the emergence of novel structural and dynamical features.

Different propulsion mechanisms capture the physics of a variety of systems, such as chains of active Brownian particles [3], polar filaments propelled along their contours [4,5], or cytoskeletal polar filaments propelled by motor proteins [6,7]. This leads to interesting single-particle behavior, such as a softening of a semiflexible filament of active Brownian particles at intermediate levels of activity [3], or a sperm-like beating motion of a filament pushing a load. At high polymer densities in two dimensions, collective dynamics characterized by active turbulence is observed [5].

Closed polymer rings (in two-dimensions) can be considered as a model of cell membranes. Here, active internal components lead to enhanced fluctuations [8] and an intimate coupling of propulsion forces, membrane deformability, cell shape, and cell sensing and reactivity [9,10].

In all these systems, computational models of active matter play an essential role to elucidate their non-equilibrium behavior [11].

[1] J. Elgeti, R.G. Winkler, and G. Gompper*, Rep. Prog. Phys.* **78***, 056601 (2015)*
[2] R.G. Winkler, J. Elgeti, and G. Gompper, *J. Phys. Soc. Japan* **86***, 101014 (2017)*
[3] T. Eisenstecken, G. Gompper, and R.G. Winkler, *J. Chem. Phys.* **146***, 154903 (2017)*
[4] R.E. Isele-Holder, J. Elgeti, and G. Gompper, *Soft Matter* **11***, 7181 (2015)*
[5] Ö. Duman, R.E. Isele-Holder, J. Elgeti, and G. Gompper*, Soft Matter* **14***, 4483 (2018)*
[6] A. Ravichandran, Ö. Duman, M. Hoore, G. Saggiarato, G.A. Vliegenthart, T. Auth, and G. Gompper*, eLife* **8***, e39694 (2019)*
[7] G. Vliegenthart, A. Ravichandran, M. Ripoll, T. Auth, and G. Gompper*, arXiv:1902.07904 (2019)*
[8] S.M. Mousavi, G. Gompper, and R.G. Winkler, *J. Chem. Phys.* **150***, 064913 (2019)*
[9] C. Abaurrea Velasco, S.D. Ghahnaviyeh, H.N. Pishkenari, T. Auth, and G. Gompper*, Soft Matter* **13***, 5865 (2017).*
[10] C. Abaurrea Velasco, T. Auth, and G. Gompper*, arXiv:1812.09932 (2018)*
[11] M.R. Shaebani, A. Wysocki, R.G. Winkler, G. Gompper, and H. Rieger*, arXiv:1910.02528, Nat. Rev. Phys., to appear (2019)*

Boundaries tame flow in active fluids of extensile filaments

Seth Fraden,
Brandeis University, USA

We study active nematics in two different geometries, disks and annuli, with the goal to explore how boundaries transform the nature of the active flow. The systems are comprised of bundles of microtubules, which are driven to extend symmetrically along the bundle axis by multivalent kinesin motors. When the 2D active nematics are confined to a disk with parallel boundary conditions, the samples are required to have a net topological charge of +1. For large diameters, the behavior of the nematic resembles the unconfined case, exhibiting turbulent flow with pairs of +1/2 and -1/2 defects created and destroyed at a steady state. However, as confinement is increased, the director adopts a “yin and yang” pattern characterized by a pair of co-rotating +1/2 defects, and the 2D nematic transitions from turbulent to coherent circulatory flow.

We compute the dynamics in disks with total topological charge of +1, 0 and -1. These boundary conditions in passive nematics lead to three very different director patterns. In contrast, for active nematics, we find for all three cases a similar yin yang pattern of two +1/2 defects in the center of the disk accompanied by a circulating flow independent of the boundary conditions, with the topologically required -1/2 defects relegated to the boundary. This insensitivity to topological constraints distinguishes active from passive liquid crystals.

When the active nematics are confined to annuli we observe 3 states as a function of the width of the annulus and the radius of the inner portion of the annulus. The states are robust circulation of multiple +1/2 defects, "dancing" pairs of +1/2 defects with weak circulation, and a periodic state in which circulation of defects

alternates with the periodic annihilation of defects at the inner boundary and nucleation of defects at the outer boundary.

We compute the dynamics in annuli for total topological charge zero and compare theory and experiment. We hypothesize that the major discrepancies between theory and experiment arise from the neglect of materials lines that occur in the extensile microtubules, but are not accounted for in the continuum hydrodynamic theories.

[1] T. Sanchez, D.T. Chen, S.J. DeCamp, M. Heymann and Z. Dogic*, Nature* **491***, 431 (2012)*
[2] K.T. Wu, J.B. Hishamunda, D.T.N. Chen, S.J. DeCamp, Y.W. Chang, A. Fernandez-Nieves, S. Fraden and Z. Dogic, *Science* **355***, 1284 (2017)*
[3] M. M. Norton, A. Baskaran, A. Opathalage, B. Langeslay, S. Fraden, A. Baskaran and M.F. Hagan, *Phys. Rev. E* **97***, 012702 (2018)*
[4] A. Opathalage, M. M. N., Michael P. N. Juniper, S. A. Aghvami, B. Langeslay, S. Fraden, Z. Dogic, *Proc. Natl. Acad. Sci.* **116***, 4788 - 4797 (2019)*

Active matter driven by growth - A particle-based model

Jens Elgeti,
Forschungszentrum Jülich, Germany

Active matter is matter, driven out of equilibrium by its microscopic constituents. Now imagine cells dividing or a tumor growing -- a growing material is also active matter. However, activity does not enter via the stress, but in material conservation. The material generates itself. Growth implies a change in volume. In physical terms, the conjugate force to a change in volume is a pressure. Thus, in order to grow, cells must exert mechanical pressure on the neighboring tissue. In turn, pressure influences growth. This yields to interesting novel phenomena like infinite compressibility, self contracting materials and steady tread-milling states.

We use particle based simulations to study mechanical properties and effects in growing matter. These simulations have been helpful in understanding, interpreting and designing experiments. I will present an overview of the simulation technique, and several examples of how this model helped to gain insight in mechanical processes underlying tissue growth, ranging from growth of cancer spheroids under pressure, to in silico competition experiments [5-7] and tumor evolution [8].

[1] Basan et al., *HFSP J.* **3***, 265 (2009)*
[2] Montel et al., *Phys. Rev. Lett.* **107***, 188102 (2011)*
[3] Delanrue et al., *Phys. Rev. Lett.* **110***, 138103 (2013)*
[4] Podewitz et al., *EPL* **109***, 58005 (2016)*
[5] Basan et al., *Phys Biol* **8***, 026014 (2011)*
[6] Podewitz et al., *New J Physics* **18***, 083020 (2016)*
[7] Ganai et al., *New J Phys* **21***, 063017 (2019)*
[8] Büscher et al., *arxiv:1910.03263 (2019)*

Stabilizing active flows: hydrodynamic screening and topological constraints

Amin Doostmohammadi,
University of Copenhagen, Denmark

Active flows are often characterized by the emergence of chaotic patterns of swirling flows and jets, known as active turbulence. In this talk I will discuss how hydrodynamic screening of active flows can act as a robust way of controlling and guiding active particles into dynamically ordered coherent structures. I will also explain how combining hydrodynamics with topological constraints can lead to further control of dynamic morphologies of active matter emulsions.

[1] A. Doostmohammadi and J. M. Yeomans, *EPJST* **227***, 2401 (2019)*
[2] L. Metselaar, J. M. Yeomans, and A. Doostmohammadi, *Phys. Rev. Lett.* **123***, 208001 (2019)*

Particle-based simulations of three-dimensional nematics in and out of confinement

Michael Hagan,
Brandeis University, Waltham, USA

Active nematics are liquid crystals whose constituent particles transduce energy into motion. The ordered nematic state is unstable to the proliferation of topological defects, which undergo birth, streaming dynamics, and annihilation to yield a seemingly chaotic dynamical steady-state. Although bulk active nematics in two dimensions have been extensively studied, recent experiments show that active nematics exhibit qualitatively different behaviors when under confinement or in three dimensions. For example, defects tend to form as neutrally charged disclination loops in bulk three-dimensional samples. I will describe using particle-based Brownian dynamics simulations to elucidate the behaviors of dry active nematics in three dimensions, in bulk systems and under confinement. Time permitting, I will also discuss approaches to use such particle-based simulations to inform continuum hydrodynamic models of active nematics.

Steady-state currents in active matter: origin and implications

Yariv Kafri,
Technion - Israel Institute of Technology, Israel

It is well known that under rather generic circumstances active systems can generate currents due to, say, an external potential. In the talk, I will discuss several implications of this fact on the physics of different systems. Specifically, I will focus on interactions between objects immersed in an active fluid, the effects of disorder on active particles, escape problems, and surface tension between an active fluid and a solid surface.

Dynamical density functional theory of microswimmers: collective dynamics, circle swimming, and binary mixtures

Hartmut Löwen, A. M. Menzel, and C. Hoell
Heinrich Heine University Düsseldorf, Germany

When active microswimmers self-propel, they set the surrounding fluid into motion. These induced fluid flows affect the configuration of other microswimmers in the suspension. As a consequence of such kinds of hydrodynamic coupling, different types of dynamic collective behavior can emerge. We study this situation in (semi-)dilute suspensions of active microswimmers using a particle-scale statistical approach. Based on a discrete minimal microswimmer model, we develop corresponding dynamical density functional theories [1,2,3,4]. Mainly, we concentrate on two different scenarios of spontaneous symmetry breaking arising from the hydrodynamic interactions. First, under spherical confinement, the swimmers may concentrate in high-density spots blocked by the confinement barrier [1,2]. Second, without the spherical confinement, the hydrodynamic interactions may induce the onset of polar orientational order and thus collective motion [3,4,5]. Variations include the possibility of circle swimming [2], externally imposed flow fields [3], and the behavior of binary mixtures of active microswimmers composed, for instance, of pushers and pullers [4,5]. In the latter case, we observe the majority species to impose its behavior onto the minority species.

[1] A. M. Menzel, A. Saha, C. Hoell, and H. Löwen, *J. Chem. Phys.* **144***, 024115 (2016)*
[2] C. Hoell, H. Löwen, and A. M. Menzel, *New J. Phys.* **19***, 125004 (2017)*
[3] C. Hoell, H. Löwen, and A. M. Menzel*, J. Chem. Phys.* **149***, 144902 (2018)*
[4] C. Hoell, H. Löwen, and A. M. Menzel, *J. Chem. Phys.* **151***, 064902 (2019)*
[5] G. Pessot, H. Löwen, and A. M. Menzel*, Mol. Phys.* **116***, 3401 (2018)*

Chemical and hydrodynamic coupling in the self-propulsion of phoretic particles and active droplets

Sebastien Michelin,
Ecole Polytechnique, France

Chemically-active particles and droplets have recently emerged as canonical systems to study the behavior of synthetic active matter. To gain motility, they exploit two chemical properties of their interface with the surrounding fluid: (i) a chemical activity, namely the exchange of chemical solutes with their environment (e.g. catalytic reactions) and (ii) a phoretic mobility, that converts non-uniform solute concentration into fluid slip or mechanical stress. This not only provides them with the ability to self-propel without any external macroscopic control but also introduces new interactions routes between them as each particle/droplet now drifts in the chemical and hydrodynamic footprints of its neighbors, which critically conditions their interactions and collective dynamics. In this presentation, I will present some recent developments on the modeling and simulations of the individual and collective behavior of such synthetic micro swimmers.

Activity induced phase transitions: from MIPS to chiral self-sorting

Ignacio Pagonabarraga,
EPFL, Switzerland

I will consider simple statistical models to address fundamental aspects of active systems and will analyze the implications that different features of self-propulsion and particle shape has in the emergence of structures in suspensions of model self-propelled particles. I will discuss the potential of schematic models to address fundamental questions that still remain open, such as the connection of the effective phase diagram and pressure with effective equilibrium concepts. These approaches allow to understand the transformations that characterize these systems as effective phase transitions out of equilibrium.

Self-propelled rods as a paradigm of active matter: from scalar to vectorial active matter

Fernando Peruani,
Université Nice Sophia Antipolis, France

The physics of self-propelled discs (SPDs) and self-propelled rods (SPRs) is fundamentally different. SPDs undergo phase separation, while SPRs can also exhibit collective motion. By varying the aspect ratio of SPR, it is possible to connect two classes of active matter — scalar and vectorial active matter — and understand how motility-induced phase separation gets destabilized and orientational order emerges in active systems. We will see that a representation of active particles by smoothed continuum fields represents a powerful computational and analytical tool that allows unifying seemingly disconnected realms of active matter.

[1] F. Peruani, A. Deutsch, and M. Bär, *Phys. Rev. E* **74***, 030904 (2006)*
[2] S. Weitz, A. Deutsch, F. Peruani, *Phys. Rev. E* **92***, 012322 (2015)*
[3] R. Grossmann, I.S. Aranson, F. Peruani*, arXiv:1906.00277 (2019)*
[4] M. Bär et al., *arXiv:1907.00360 (2019)*

Collective behavior and self-organisation of active granular particles

Thorsten Pöschel, Michael Engel, Christian Scholz, Harol Torres
Universität Erlangen-Nuernberg, Germany

Biological organisms and artificial active particles self-organize into swarms and patterns. Open questions concern the design of emergent phenomena by choosing appropriate forms of activity and particle interactions. A particularly simple and versatile system are 3D-printed robots on a vibrating table that can perform self-propelled and self-spinning motion. Here we study a mixture of minimalistic clockwise and counter-clockwise rotating robots, called rotors. Our experiments show that rotors move collectively and exhibit super-diffusive interfacial motion and phase separate via spinodal decomposition. On long time scales, confinement favors symmetric demixing patterns. By mapping rotor motion on a Langevin equation with a constant driving torque and by comparison with computer simulations, we demonstrate that our macroscopic system is a form of active soft matter.

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[2] C. Scholz, M. Engel, T. Pöschel, *Nature Comm.* **9***, 931 (2018)*
[3] C. Scholz, S. D'Silva, T. Pöschel*, New J. Phys.* **18***, 123001 (2016)*
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Cytoskeletal dynamics and motor driven transport

Ludger Santen,
Saarland University, Germany

The cytoskeleton is an inhomogeneous network of semi-flexible filaments, which are involved in a wide variety of active biological processes, as for example motor-driven intracellular transport and active filament dynamics [1-5]. In this contribution we will discuss different lattice gas approaches to bidirectional intracellular transport. The key factors of efficient bidirectional transport will be discussed [2] as well as an approach to self-organized lane-formation [3].

The cytoskeletal filaments are very dynamic objects [4] which are embedded in a dense and cross-linked network. It has been shown that, in cells, they typically exhibit significant bending on all length scales. We will introduce model of a semi-flexible filament deformed by different types of cross-linkers, for which one can compute and investigate the bending spectrum. We will discuss different implementations of model. Our simulation results show that the spatially localized forcing and the non-thermal dynamics both introduce deviations from the thermal-like q(-2) spectrum [5].

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[2] R. Jose, L. Santen*, JSTAT (accepted) (2020)*
[3] R. Jose, L. Santen*, Self-organized lane formation in bidirectional transport of molecular motors (submitted)*
[4] M. Ebbinghaus, L. Santen, *Biophys. J.* **100***, 832 (2011)*
[5] I. Weber, C. Appert-Rolland, G. Schehr, L. Santen*, EPL* **120***, 38006 (2017)*

Generalized Navier-Stokes equations for active fluids in flat and curved geometries

Jonasz Slomka,
ETHZ, Switzerland

Recent experiments show that active fluids stirred by swimming bacteria or ATP-powered microtubule networks can exhibit complex flow dynamics and emergent pattern scale selection. Here, I will investigate a simplified phenomenological approach to ‘active turbulence’, a chaotic non-equilibrium steady-state in which the solvent flow develops a dominant vortex size. This approach generalizes the incompressible Navier-Stokes equations by accounting for active stresses through a linear instability mechanism, in contrast to externally driven classical turbulence. This minimal model can reproduce experimentally observed velocity statistics and is analytically tractable in planar and curved geometry. Exact stationary bulk solutions include Abrikosovtype vortex lattices in 2D and chiral Beltrami fields in 3D. The model readily generalizes to curved geometries. On a two-sphere, we present exact stationary solutions and predict a new type of upward energy transfer mechanism realized through the formation of vortex chains, rather than the merging of vortices, as expected from classical 2D turbulence. In 3D simulations on periodic domains, we observe spontaneous mirror-symmetry breaking realized through Beltrami-like flows, which give rise to upward energy transfer, in contrast to the classical direct Richardson cascade. Our analysis of triadic interactions supports this numerical prediction by establishing an analogy with forced rigid body dynamics and reveals a previously unknown triad invariant for classical turbulence.

The squirmer as a model microswimmer: collective patterns under gravity and squirmer rods

Holger Stark,
TU Berlin, Germany

We use squirmers and hydrodynamic simulations based on the method of multi-particle collision dynamics to explore the collective dynamics of microswimmers under gravity and of elongated microswimmers.

Under the influence of gravity, we find a variety of different phenomena depending on the ratio of swimming to bulk sedimentation velocity. Single squirmers can float or slide above the bottom wall. A collection of squirmers exhibits a very dynamic sedimentation profile with dense layering at the bottom and exponential decay towards the top, where large-scale convective flow arises. When the squirmers become bottom-heavy, they exhibit inverted sedimentation, plumes and convective rolls, and spawning clusters. Finally, a single layer of squirmers under gravity shows different collective dynamics including “hydrodynamic Wigner fluids” and swarming.

We also form squirmer rods and explore their collective dynamics when they are trapped in a plane similar to the active biofilaments in the experiments of Dogic et al. We explore the phase behavior of rigid rods and comment on the role of flexibility and on the behavior of pusher and puller rods.

Lattice Boltzmann modeling of collective dynamics in microswimmer suspensions

Joakim Stenhammar,
Lund University, Sweden

Due to their non-equilibrium character, the collective dynamics of active matter systems is often dominated by hydrodynamic interactions. One example is the collective motion of swimming bacteria, which interact through their long-ranged stresslet flow-fields to create a state of so-called “active turbulence”. However, due to the computational difficulties of accurately treating hydrodynamically interacting particles, the computational modeling of such collective motion has so far been challenging. In this talk, I will present a point-force implementation of stresslet microswimmers, where the hydrodynamic flow fields are treated using an efficient lattice Boltzmann (LB) algorithm, to model such systems. The use of a point-force model, where each swimmer is modeled only through its long-ranged hydrodynamic flow field, enables the simulation of several million particles, enough to study the emergence and properties of active turbulence as well as the dynamics of tracer transport in microswimmer suspensions.

Active vertex models of epithelial tissue

Daniel Sussman,
Emory University, USA

Simple models of confluent epithelial cells have provided powerful and, at times, predictive organizing principles for understanding the unusual dynamical and mechanical properties of dense tissue and cellular aggregates. In this talk I will focus on a geometrically inspired class of models, focusing on our work related to two stylized facts. Firstly, these models seem to possess anomalous properties in the disordered bulk phase and also unusual interfacial surface tension between coexisting populations of cells. Secondly, however, the way these models combine an active, molecular-dynamics-like basis with a topological or graph-based network of interactions poses challenges to the sorts of efficient, large-scale numerical studies that are required to validate these unusual properties and compare them with experimental systems.

Active Brownian particles: local pressure in nonequilibrium systems

Roland G. Winkler, Shibananda Das, and Gerhard Gompper
Forschungszentrum Jülich, Germany

Motile active systems develop an intrinsic swim stress through their locomotion, which influences their dynamics and collective behavior [1,2,3]. Such stresses are particularly interesting, since there is no equilibrium counterpart and, thus, no thermodynamic description exists. The stress of a fluid on a confining wall is given by its mechanical wall forces, independent of the passive or active nature of the fluid [3]. In systems at thermal equilibrium, an equation of state exists and local stress can be defined via Clausius’ virial theorem or thermodynamically by the Helmholtz free energy. However, for nonequilibrium active systems, a comparable local description is missing, which has hampered the characterization of inhomogeneous active systems.

We derive an expression for the active stress of spherical active Brownian particles (ABPs) in a local volume inside of a confined, wall-bound system [4]. On the one hand, we find a new virial expression for the local active stress, and, on the other hand, we identify an original active-momentum contribution due to particle flux across a virtual plane. The local stress is quantified in computer simulations of non-interacting ABPs and ABPs interacting by a short-ranged repulsive Lennard-Jones potential. We demonstrate that the stress on the wall and the local bulk stress are identical, which confirms the existence of a pressure equation of state for spherical ABP systems. Most importantly, our calculations demonstrate that active pressure is not a boundary effect, but is caused by momentum transport due to activity. Moreover, it opens up the possibility to calculate stresses locally, even in inhomogeneous systems, which we confirm by calculating the local stress in a phase separated system of ABPs.

[1] J. Elgeti, R. G. Winkler, and G. Gompper, *Rep. Prog. Phys.* **78***, 056601 (2015)*
[2] S. C. Takatori, W. Yan, and J. F. Brady, *Phys. Rev. Lett.* **113***, 028103 (2014)*
[3] R. G. Winkler, A. Wysocki, and G. Gompper*, Soft Matter* **11***, 6680 (2015)*
[4] S. Das, G. Gompper, and R. G. Winkler, *Sci. Rep.* **9***, 6608 (2019)*

Field-theoretical modeling of active matter

Raphael Wittkowski,
Universität Münster, Germany

Besides experiments and computer simulations, field-theoretical models constitute an important approach for studying the properties of active matter. Several field theories for active matter have already been derived and successfully applied in recent years. Among the most popular models are Active Model B, Active Model B+, and Active Model H. This talk gives an introduction to the field-theoretical modeling of active matter. It presents some of the most popular models as well as powerful methods that allow to derive such field theories.

Modelling collective cell mechanics

Julia Yeomans,
Oxford University, United Kingdom

The collective dynamics of epithelial cell layers shows many features seen in active systems. Examples include velocity correlations over several cell lengths, motile topological defects and collective rotation and oscillations in confinement. I shall discuss the extent to which models of active materials, and in particular phase field models, can reproduce the experiments and explain why initially isotropic cells can act as extensile active nematics.

[1] R. Mueller, J. M. Yeomans and A. Doostmohammadi*Phys. Rev. Lett.* **122***, 048004 (2019)*

Phase field approach for substrate-based cell motility in complex environments

Falko Ziebert,
Ruprecht-Karls-Universität Heidelberg, Germany

Cells crawling on substrates or in more complex environments, either individually or collectively, are an important representative class of active matter systems.

I will give a brief introduction to substrate-based crawling motility of eukaryotic cells and survey our recent advances in its modeling. After another brief introduction into the phase field method, capable of numerically efficiently tracking deformable and moving boundaries and interfaces, I present a modular modeling approach for motile cells in complex environments. This approach [1] allows us to describe, e.g., cell guidance on substrates with modulated adhesion or stiffness [2], collective cell migration [3], as well as motion in 3D confinement and on curved or topographically structured substrates [4]. I will also briefly discuss the example of cellular shape waves [5], where the computational approach allows for additional insight via semi-analytic methods (employing asymptotic reduction and multiple scales).

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4 Posters

The role of dimensionality in the collective dynamics of microswimmers

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Long-ranged hydrodynamic interactions often dominate the collective behaviour in suspensions of microswimmers. Suspensions of rear-actuated (pusher) bacteria at sufficient densities exhibit large-scale, chaotic flows, so-called bacterial turbulence. It is well established that the transition to bacterial turbulence is due to a hydrodynamic instability resulting from the reorientation of the swimmers caused by the pusher stresslet flow fields [1], while front-actuated (puller) suspensions do not show any such collective behaviour. To study the collective phenomena of microswimmers, we use large-scale (up to N=5·10^6) particle-resolved lattice Boltzmann simulations [2,3]. We model the microswimmers as two point forces, representing the drag force on the body and the propulsive force from the flagella, yielding an extended stresslet acting on the fluid, while ignoring near-field effects and excluded volume interactions.

We recently showed that the collective behaviour in 3-dimensional pusher suspensions is characterized by long-ranged flow fields, with typical ranges of >30 bacterial body lengths, in accordance with theoretical predictions [1,4]. Bacterial turbulence in 2-dimensional geometries, such as thin films, is, however, much less understood in spite of being of experimental relevance. In this work, we study both pusher and puller suspensions in a quasi-2-dimensional geometry, where the fluid flow is effectively 3-dimensional, but where the swimmers are confined to a thin film by no-slip walls. Our results show that confinement changes the nature of the collective motion in pusher suspensions, from long-ranged to short-ranged, as compared to pusher suspensions in the 3-dimensional case. For confined puller suspensions, we instead observe swimmers clustering at intermediate concentrations. Our results thus indicate a strong effect of dimensionality on the underlying hydrodynamic instabilities of microswimmer suspensions.

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Dynamics of propagating modes and characterisation of ordering in coupled non-equilibrium systems

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We study a coupled non-equilibrium system consisting of two species of particles, one lighter (L) and the other heavier (H), that move stochastically on an energy landscape, which also fluctuates in time. The particles tend to minimize their energy by moving along the local potential gradient and also by modifying the landscape around their position in such a way that the energy is further lowered. By tuning the coupling parameters that govern the action of the H and L particles on the landscape, we obtain a phase diagram that shows two new kinds of ordered phases in both particle species and also the landscape, along with two earlier found phases, and a disordered phase. The newly found ordered phases show algebraically fast coarsening to steady state and rich dynamics. The phase diagram remains qualitatively valid for all densities in one and two dimensions. The disordered phase is characterised using a recently developed formalism of non-linear fluctuating hydrodynamics (NLFH) along with mode-coupling theory that predicts diffusive, KPZ, 3/2-Lévy, 5/3-Lévy, and gold-Lévy universality classes for our system. However, we argue that in verifying the predictions through numerical simulations, the conclusions can be masked by finite size effects.

Density distributions and depth in flocks

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Swarming is the collective behaviour of animal aggregations and can be observed throughout the animal kingdom, from the flocking of birds and shoaling of fish to the motion of human crowds. In these groups global orientational order can emerge from the social behaviour of its constituents. This collective behaviour is not thought to arise from centralised coordination but rather the system is believed to exhibit self-organisation due to the local rules of the interacting elements: coherent motion with local rules manifesting global order.

A large number of theoretical models have been developed in which local interaction rules give rise to global ordering in animal systems however empirical studies have been more rare. Recent field studies have reconstructed the internal dynamics of large flocks of Starlings and experimental evidence suggests that interactions in flocks of birds do not involve a characteristic length scale [1, 2]. Bird flocks have also been revealed to have an inhomogeneous density distribution, with the density of birds near the border greater than near the centre [3]. This observation is counter to what has been observed in some models of collective behaviour. It is also counter-intuitive in relation to some biological theories of animal behaviour, such as the selfish herd hypothesis (in which the centre of the group would be the safest location and all individuals might therefore be expected to seek to occupy it). Developing models with a metric-free characteristic is technically challenging as they typically support a zero density steady-state as the group diffusively expands indefinitely [4].

We introduce a fully topological (metric-free) 3-dimensional model for collective behaviour that incorporates a distributed motional bias, providing control of the density distribution. This model was fitted to empirical data of Starling murmurations using stochastic optimisation to determine a suitable form of bounding function. Simulation data from this model is shown to match published data for the density variation across flocks of Starlings. We find that this requires individuals on the edge of the flock to have an inward motional bias but that birds in the interior of the flock instead must have an outward bias. We then compare this fitted model to a benchmark topological model with no motional bias on the bulk of the flock (only on the surface), which allows us to understand the role of the specific form of distributed motional bias that we have identified. We also discuss the ability of individuals to determine their depth within a flock and show how this might be achieved by relatively simple analysis of their visual environment.

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Integrating inference form data in understandable form with deduction in order to multiscale modeling active molecules

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Traditional modeling exhibit problems when increasing dimensionality, both computational and of deterring whose local minima are really worth representing salient matter states. Integration with data mining is paramount, feasible only when inference is provided in deductive logical form [1], immediately allowing to a posteriori integrating priors by simply correcting, adding or deleting inferred rules, also in order to save computational cost and avoid overfitting while keeping attention to individual behavior within a statistic population. Even mutant are then keen to be forecasted [2] before discovery when multiscale modeling a biologically active important protein with attention to coarse domain interaction allowing Galerkin simulation of the Markovian processing of its statistical behavior when exposed to pathophysiological range of concentrations of its biological mate.

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Flocking and reorientation transition in the 4-state active potts model

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We study the 4-state active Potts model in two dimensions, which is an active lattice gas model on the square lattice with particles performing nearest-neighbor hopping biased according to one of four possible motility states and ferromagnetic on-site alignment. A collective motion emerges at low temperatures from a spontaneous breaking of the discrete symmetry in the form of bands aligned with one of the four directions. This flocking transition is a first-order liquid-gas phase transition with an infinite critical density, as found in previously studied models [1-2]. We compute the velocity-density and the temperature-density phase diagrams and we find a novel reorientation transition of the phase-separated profiles from transversal to longitudinal band motion, which is absent in the Vicsek model [1] and the active Ising model [2]. The longitudinal motion occurs at high velocities due to a strongly biased diffusion. We present a hydrodynamic theory which reproduces very well the results of computer simulations of the microscopic model.

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Stochastic modeling of the tug-of-war between kinesin-1 and mammalian dynein motor proteins in intracellular transport

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Microtubule-based intracellular transport is a bidirectional, biased stochastic motion carried out by teams of kinesin and dynein motor proteins. Inside cells dynein and kinesin motors walk processively in opposite directions along microtubules (polar intracellular filaments) in order to transport cargo. It is known that both kind of motors are simultaneously bound to the cargo. Therefore, a tug-of-war between the opposite-directed motor teams is likely to occur. In order to achieve targeted active transport the cell must spatiotemporally regulate the tug-of-war.

As regulation mechanism it is proposed either coordinating the activity of attached motors or regulating the tug-of-war by the motor properties. Recent studies propose that beside coordinating the motor activity by adaptor proteins, dynein can be mechanically activated depending on the number of attached dynein motors in unidirectional gliding assays [1]. Here, we study how the self-regulated dynein activation depends on the number of kinesin and dynein motors in a bidirectional transport system and how it influences the tug-of-war competition. In order to systematically vary the number of kinesin and dynein motors involved in the tug-of-war we use microtubule gliding assays.

Beside the self-regulation by the motor number we test the regulation by the motor properties. Here, we show that the tug-of-war remains unchanged upon a varying ATP concentration and that roadblocks cannot tune the tug-of-war competition.

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Anisotropic diffusion of ellipsoidal tracers in microswimmer suspensions

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To microorganisms immersed in a fluid, passive particles such as dead cells can act as hazards or sources of nutrients, impacting swimming behaviour. It is known that passive tracers exhibit enhanced diffusion in bacterial suspensions due to hydrodynamic interactions[1][2], and that several aspects of the diffusion dynamics are non-trivial. Especially anisotropic tracers are of interest, as their behaviour is poorly understood, and as ellipsoids are potentially better approximations of for example real dead cells than spheres could be.

In this study, we investigate the potential coupling between passive ellipsoidal tracers' translational and rotational motion, using large-scale lattice Boltzmann simulations of dilute and semidilute microswimmer suspensions. Under thermal Brownian motion, an ellipsoid is expected to diffuse quicker along its major axis than along its minor axes. However, experimental data indicate that under enhanced diffusion the opposite is true[2] – translational mean-square displacement and diffusion coefficients are larger along the minor axes.

We consider whether this anisotropic diffusion is due to far-field hydrodynamic interactions, as would be captured by the used lattice Boltzmann method. Factors that are under investigation include swimmer

concentration and tracer size, and we aim to quantify whether the diffusive behaviour is similar in 2D and 3D. Interestingly, the results of our simulations do not align with experiments: In 3D, diffusion remains largely isotropic at low swimmer concentrations, before transitioning into being greater along the tracers' major axis, i.e., the same symmetry as for thermal Brownian motion. This indicates that the balance between hydrodynamic and non-hydrodynamic interactions, such as collisions, can lead to very different behaviours, and that both types of interactions have to be taken into account when interpreting experimental data.

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Dynamics and correlations in active processes with two motility states

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The stochastic dynamics of active particles with distinct motility states is studied analytically. A theoretical framework is developed to describe a generic class of stochastic processes consisting of two states characterized by their activity coefficients and velocity distributions. The generalized activity of each state may range from being antipersistent (slower than diffusion) to persistent motion. The mean square displacement and velocity autocorrelations are obtained analytically for exponentially distributed sojourn times in each state. Various timescales for orientational correlations are characterized and the asymptotic diffusion constant is derived. It is shown how extra memory effects introduced by age-dependent switching probabilities between the states enhance the orientational correlations in non-Markovian processes with power-law sojourn time distributions.

Velocity alignment promotes motility-induced phase separation

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We study the phase behavior of polar Active Brownian Particles moving in two-spatial dimensions and interacting through volume exclusion and velocity alignment. We combine particle-based simulations of the microscopic model with a simple mean-field kinetic model [1] to understand the impact of velocity alignment on the motility-induced phase separation of self-propelled disks. We show that, as the alignment strength is increased, approaching the onset of collective motion from below, orientational correlations grow, rendering the diffusive reorientation dynamics slower. As a consequence, the tendency of particles to aggregate into isotropic clusters is enhanced, favoring the complete de-mixing of the system into a low and high-density phase [2]. In the light of these results, we derive a mean-field model based on [3] to shed some light into the underlying mechanisms controlling the system's phase separation.

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Optimizing correlated active random searches

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Optimal search strategies often minimize the mean first-passage time with respect to a parameter of the stochastic motion (such as particle activity, ratio between the durations of diffusive and directed motion in intermittent walks, etc.) or with respect to a structural property of the environment in which the particle moves. However, the influential factors governing the search ability are correlated in general. For example, a universal coupling between the speed and directional persistence of migrating cells has been reported recently. We introduce a new class of optimal search strategies based on tuning the strength of correlations between the key parameters. We show that speed-persistence correlation does not necessarily improve the efficiency of active random searches in confinement.

Capillary action in scalar active matter

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We study the capacity of active matter to rise in thin tubes against gravity and other related phenomena, like, wetting of vertical plates and spontaneous imbibition, where a wetting liquid is drawn into a porous medium. This capillary action is well known in classical fluids and originates from attractive interactions between the liquid molecules and the container walls, and from the attraction of the liquid molecules among each other. We observe capillarity in a minimal model for scalar active matter with purely repulsive interactions, where an effective attraction emerges due to slowdown during collisions between active particles and between active particles and walls.

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