Program

Computational Advances in Active Matter

Monday:
Agent-Based Modeling for Cells and Bacteria

09:00 – 10:00  Registration
10:00 – 10:15  Welcome by the Lorentz Center
10:15 – 10:30  Welcome by the Organizers
(de Graaf, Joost)
10:30 – 11:15  Invited Talk:
Collective Motion in Active Matter: From Active Brownian to Cognitive Self-Steering Particles (Gompper, Gerhard)
11:15 – 11:45  Topical:
Crowding-Enhanced Diffusion of Highly Entangled Self-Propelled Stiff Filaments (Kurzthaler, Christina)
11:45 – 12:00  Short Contribution:
How do dense systems of large persistence self-propelled particles relax? (Keta, Yann-Edwin)
12:00 – 12:15  Short Contribution:
Combining agent-based and continuous field simulations for chemically communicating active matter (Ziepke, Alexander)
12:15 – 13:30  Lunch Break
13:30 – 15:00  Demonstration:
Morpho: A computational framework for shapeshifting and shape optimization (Atherton, Tim)
15:00 – 15:30  Topical:
Pulsating active matter (Fodor, Etienne)
15:30 – 16:00  Coffee Break
16:00 – 17:30  Discussion:
Challenges for Agent-Based Modeling (Ilie, Ioana)
17:30 – 19:00  Wine & Cheese Party
**Tuesday:**  
**Vertex and Mesh-Based Modeling for Tissues and Colonies**

09:15 – 10:00  *Invited Talk:*  
Hybrid cellular Potts modeling of cell-extracellular matrix interactions driving cell shape, cell migration and collective cell behavior (Merks, Roeland)

10:00 – 10:30  *Topical:*  
Interacting Active Matter: Beyond two dimensions (Doostmohammadi, Amin)

10:30 – 11:00  *Coffee Break*

11:00 – 12:30  *Demonstration:*  
Tutorial on the Vertex Model for Tissue Mechanics (Sknepnek, Rastko)

12:30 – 14:00  *Lunch Break*

14:00 – 14:45  *Invited Talk:*  
Active Cell Sorting (Yeomans, Julia)

14:45 – 15:15  *Topical:*  
Dynamics of active surfaces (Voigt, Axel)

15:15 – 15:30  *Short Contribution:*  
Active Nematic Vertex Models in a Channel: Generating Flows (Rozman, Jan)

15:30 – 15:45  *Short Contribution:*  
Mechanical feedback as a regulator of tissue dynamics (Perez-Verdugo, Fernanda)

15:45 – 16:15  *Coffee Break*

16:15 – 17:45  *Discussion:*  
Challenges for Vertex and Mesh-Based Modeling (Pollack, Yoav)
Wednesday:
Continuum/Hydrodynamic Methods for Active Systems

09:15 – 10:00  Invited Talk:
Multicellularity and continuum mechanics: Classical concepts and new challenges (Giomi, Luca)

10:00 – 10:30  Topical:
Spatial models of cell-microenvironment interaction (Tsingos, Erika)

10:30 – 11:00  Coffee Break

11:00 – 12:30  Demonstration:
Mesoscale simulations as a tool to study complex systems (Valeriani, Chantal)

12:30 – 14:00  Lunch Break

14:00 – 14:45  Invited Talk:
Hydrodynamics of Active Suspensions (Stark, Holger)

14:45 – 15:15  Topical:
Models and simulations of the dynamics of confined active suspensions (Lushi, Enkeleida)

15:15 – 15:30  Short Contribution:
Chemotaxis of a pair of chiral squirmers (Ruma, Maity)

15:30 – 15:45  Short Contribution:
Billiards with Spatial Memory (Jalaal, Mazi)

15:45 – 16:15  Coffee Break

16:15 – 17:45  Discussion:
Challenges for Continuum Descriptions (Fedosov, Dimitri)

19:00 onward  Workshop Dinner
Thursday:
Field Theoretical Methods for Active Phases

09:15 – 10:00  Invited Talk:
Phase field models in active matter: lyotropic active nematics and topology of multicellular monolayers (Marenduzzo, Davide)

10:00 – 10:30  Topical:
Phase field modeling of crawling cells and cell mechanics (Ziebert, Falko)

10:30 – 11:00  Coffee Break

11:00 – 12:30  Demonstration:
Active Stokesian Dynamics (Elfring, Gwynn)

12:30 – 14:00  Lunch Break

14:00 – 14:45  Invited Talk:
Non-reciprocal active matter across the scales (Golestanian, Ramin)

14:45 – 15:15  Topical:
Large scale physics of phase separating active systems (Nardini, Cesare)

15:15 – 15:30  Short Contribution:
Symmetry-protected coarsening of non-reciprocal matter (Binysh, Jack)

15:30 – 15:45  Short Contribution:
Defect lines morphologies in three dimensional active nematics (Digregorio, Pasquale)

15:45 – 16:15  Coffee Break

16:15 – 17:45  Discussion:
Challenges for Numerical Field Theories (Krommydas, Dimitrios)
**Friday:**

**Future Directions and Education**

09:15 – 10:00  *Invited Talk:*
Unjamming glasses and removing grain boundaries with active colloids
(Dijkstra, Marjolein)

10:00 – 10:30  *Topical:*
Controlling Collective Motion and Pattern Formation in Magnetic Microswimmers via External Fields (Jabbari, Sara)

10:30 – 11:00  *Coffee Break*

11:30 – 12:00  *Topical:*
Exploring Shape Formation through Active Mechanics in Thin Sheets (Matoz-Fernandez, Daniel)

12:00 – 12:15  *Short Contribution:*
Automatic differentiation of active matter simulations (ADAMS) (Davis, Luke)

12:15 – 12:30  *Short Contribution:*
Flippy: User-friendly and open-source framework for lipid membrane simulations (Dadunashvili, George)

12:30 – 14:00  *Lunch Break*

14:00 – 15:30  *Discussion:*
Developing a Community: Schooling, Training, and Strategic Outlook (the organizers)

15:30 – 16:15  *Invited Talk:*
Challenges and Opportunities in Computational Modelling of Active Systems: Emerging Interactions in Active Suspensions (Pagonabarraga, Ignacio)

16:15 – 16:30  *Closing Statements:*
(Henkes, Silke)
Titles and Abstracts

Monday:

Gerhard Gompper (Forschungszentrum Jülich)
Collective Motion in Active Matter: From Active Brownian to Cognitive Self-Steering Particles

Active Brownian particles and aligning Vicsek particles are the most frequently employed models to describe the dynamics and collective behavior of motile active matter [1]. For living systems, activity and locomotion is combined with sensing of the environment and adaption of motion. Furthermore, geometrical confinement strongly affects individual and collective particle motion. We study such system by considering two paradigmatic cases: (i) Active Brownian Particles (ABPs) in porous media [2], and (ii) active particles with minimal cognition and self-steering [3-7]. The model of cognitive self-steering particles consists of "intelligent" active Brownian particles (iABPs), which are equipped with an orientational response -- with limited maneuverability -- to an instantaneous visual input of the positions of neighbors within a vision cone [3-6]. In addition, dry [3-5] or wet [6] environments, as well as a combination with alignment interactions (like flocks of birds and schools of fish) [7] play an essential role.


Christina Kurzthaler (MPI Physics of Complex Systems)
Crowding-Enhanced Diffusion of Highly Entangled Self-Propelled Stiff Filaments

Active matter systems, such as swimming microorganisms or synthetic self-propelled particles, are intrinsically out of equilibrium and entail a variety of unusual transport phenomena. In this talk, I will discuss the physics of a strongly interacting crowded system of self-propelled stiff filaments. We use event-driven Brownian dynamics simulations and an analytical theory to elucidate the intricate interplay of crowding and self-propulsion. We find a remarkable increase of the effective diffusivity upon increasing the filament number density by more than one order of magnitude. This counterintuitive “crowded is faster” behavior can be rationalized by extending the concept of a confining tube pioneered by Doi and Edwards for highly entangled, crowded, passive to active systems. We predict a scaling theory for the effective diffusivity as a function of the Péclet number and the filament number density. Subsequently, we show that an exact expression derived for a single self-propelled filament with motility parameters as input can predict the nontrivial spatiotemporal dynamics over the entire range of length and timescales. In particular, our theory captures short-time diffusion, directed swimming motion at intermediate times, and the transition to complete orientational relaxation at long times.

Yann-Edwin Keta (Leiden University)

How do dense systems of large persistence self-propelled particles relax?

We employ activity-driven dynamics (ADD) to study the relaxation of dense systems of large persistence self-propelled particles on time scales large compared to the persistence time. On the time scale of the persistence time, the dynamics is intermittent: elastic branches in which the system moves collectively in response to changes in the self-propulsion forces are interrupted by instantaneous plastic events during which a subset of the system changes its local structure. On average, this dynamics is diffusive. However, we show that dynamical heterogeneities play a crucial role which indicates that there are correlations between rearrangements.


Alexander Ziepke (Ludwig-Maximilians-Universität München)

Combining agent-based and continuous field simulations for chemically communicating active matter

Self-organization in active matter plays a vital role in various biological and artificial systems. In numerous cases, communication is a key mechanism for forming and localizing critical structures, such as the fruiting body in Dictyostelium discoideum or aggregation clusters in quorum-sensing bacteria. In a recent study, we suggest a model for chemically communicating active matter that endows self-propelled polar agents with information processing and signal-relaying capabilities [1]. As the length scales of the dynamics of the self-propelled active agents and the chemical signaling molecules are distinct, we employ a combination of discrete simulations of the active agents and a continuum field theory for the reacting and diffusing chemicals. These simulations reveal that self-sustained nonlinear signaling contributes significantly to the formation of complex self-organized aggregates through a hierarchy of intermediate collective dynamic states.


Tim Atherton (Tufts)

Morpho: A computational framework for shapeshifting and shape optimization

TBA
We reveal that the mechanical pulsation of locally synchronized particles is a generic route to propagate deformation waves. We consider a model of dense repulsive particles whose activity drives periodic change in size of each individual [1]. The dynamics is inspired by biological tissues where cells consume fuel to sustain active deformation [2, 3]. We show that the competition between repulsion and synchronization triggers an instability which promotes a wealth of dynamical patterns, ranging from spiral waves to defect turbulence. We identify the mechanisms underlying the emergence of patterns, and characterize the corresponding transitions. By coarse-graining the dynamics, we propose a hydrodynamic description of an assembly of pulsating particles, and discuss an analogy with reaction-diffusion systems.

Tuesday:

Roeland Merks (Universiteit Leiden)

Hybrid cellular Potts modeling of cell-extracellular matrix interactions driving cell shape, cell migration and collective cell behavior

To form the patterns and behaviors that we observe in multicellular development, cells must carefully coordinate their behavior through biophysical and biochemical cues. Numerical modeling and theory are essential for analyzing the mechanism of such coordinated, collective cell behavior. To do so, single-cell models must be sufficiently detailed so they correctly capture essential aspects of individual cells and do not oversimplify. At the same time, the models must be sufficiently simple and computationally efficient so general principles can be understood and the models can be upscaled to multicellular systems. My team analyzes single cell behavior and multicellular development using a combination of mathematical, computational and experimental approaches. Our central tool is the cellular Potts model (CPM), a widely-used, lattice-based framework for modeling cell behavior. We typically couple the CPM with simulation models of the cellular microenvironment and relevant intracellular dynamics, a technique known as hybrid CPMs. I will present a series of our recent hybrid CPMs for modeling individual cell behavior, and show how these can be used to study the coordinated cell behavior that is seen in biological development. I will first discuss a series of models used to analyze observations such as anomalous cell migration patterns of immune cells, the effect of extracellular matrix stiffness on cell shape, cellular force transduction in fibrous ECMs, and models of anisotropic force generation.

I will then discuss how insights from single cell models translate to understanding of multicellular development. In our ongoing work, we are developing strategies for experimental falsification and iterative correction of multicellular models of angiogenesis. Recent versions of our cell-ECM interaction models focus on how our descriptions of focal adhesions, the mechanosensitive ‘feet’ of cells by which they hold on the extracellular matrix, must be improved to analyze mechanical cell-ECM interactions. Also we invest in computational improvements to advance towards more detailed multicellular models. Altogether, I will present the use of cell-based modeling in analyzing how local cell-microenvironment interactions coordinate cell behavior during multicellular patterning.

Amin Doostmohammadi (University of Copenhagen)

Interacting Active Matter: Beyond two dimensions

I will discuss mechanics of how cells use finger-like protrusions known to interact with their surrounding medium. First, I will present experimental and theoretical results of active mirror-symmetry breaking in subcellular skeleton of filopodia that allows for rotation, helicity, and buckling of these cellular fingers in a wide variety of cells ranging from epithelial, mesenchymal, cancerous and stem cells. I will then describe in-vivo experiments together with theoretical modeling showing how during frog embryo development specialized active cells interact with an active epithelium. In particular, I will discuss how specialized cells probe and modify an epithelial layer, and how they insert themselves and integrate within the epithelium. Finally, I will describe new computational results on the fluid-to-glass transition in 3D cell layers.
Rastko Sknepnek (University of Dundee)
Tutorial on the Vertex Model for Tissue Mechanics

Epithelial tissue is a thin layer of compactly packed cells that line the outer surfaces of organs and blood vessels throughout the body, as well as the inner surfaces of cavities in many internal organs. To maintain proper function, cells in epithelia are not static but constantly die and are being replaced. In addition, during processes such as embryonic development, wound healing, and cancer invasion, epithelial cells can also collectively migrate. These features make epithelia a dense active system and understanding collective cell behaviours in epithelial tissue in focus on intensive research. Vertex model has been one of the central tools for modelling physical properties of epithelial tissues. Implementing the vertex model in a simulation is, however, not trivial. In this tutorial, we will discuss basic physics of epithelial tissues and how translate it into the vertex model. We will then discuss how to implement the vertex model using a combination of C++ backend and Python interface. We'll also discuss good and bad coding practices and how to design a maintainable scientific software. The tutorial will be accompanied by an example code at https://github.com/sknepneklab/VMTutorial (the repository will be available ~24 hours before the tutorial).

Julia Yeomans (University of Oxford)
Active Cell Sorting

The spontaneous sorting of cells according to properties such as size, cell fate or deformability is an important process in development and, possibly, cancer progression. Phase ordering is ubiquitous and well understood in passive systems which can be described in terms of a free energy. Extensions to active models have demonstrated a range of features absent in equilibrium. We will describe sorting in model cell layers, driven by activity differences between cells. We contrast results from continuum, phase field and vertex models.

Axel Voigt (TU Dresden)
Dynamics of active surfaces

TBA

Jan Rozman (University of Oxford)
Active Nematic Vertex Models in a Channel: Generating Flows

The importance of nematic order to mechanical properties of epithelia is becoming increasingly evident. Several approaches have, therefore, been developed to adapt vertex models, a commonly used cell-level method for modelling epithelial mechanics, to also include nematic activity. Analogously to continuum active nematic models that exhibit a sequence of activity-dependent flow profiles when confined to a channel, we analyse an active nematic vertex model in a channel. We find that the usual substrate-friction based vertex model dynamics do not produce channel-wide flows. However, the recently proposed vertex-vertex friction model, a proxy for viscosity, leads to the formation of unidirectional flows. Moreover, we show that vertex-
vertex friction allows for long-range velocity correlations, reminiscent of cells flows in morphogenesis, whereas substrate friction dynamics only allow for short-range correlations. This work, therefore, underlies the importance of internal dissipation for collective behaviours in epithelia.

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**Fernanda Pérez-Verdugo** (Carnegie Mellon University)

**Mechanical feedback as a regulator of tissue dynamics**

Epithelial tissue dynamics involve a complex interplay between mechanical forces and biochemical activity. However, the integration of mechanics with signaling has remained challenging in computational models. Here, I will present two feedback mechanisms that govern tissue shape, topology, and spatial dynamics. First, I will show the negative feedback between tension and strain, which generates higher-order topological structures that cannot be achieved in conventional vertex models and leads to a robust control of tissue fluidity. Secondly, I will discuss how positive feedback between strain and contractility, manifested as a stretch-induced contraction model, elucidates the emergence of spontaneous waves and excitable patterns in tissues. Taken together, these studies provide examples of how mechano-chemical coupling can result in adaptive mechanical responses.
Wednesday:

**Luca Giomi** (Leiden University)

**Multicellularity and continuum mechanics: classic concepts and new challenges**

I will review various continuum theories of multicellular systems, such as tissues, bacterial colonies and cell layers. In particular, I will illustrate how different layers of complexity can be progressively painted over the essential canvas of continuum mechanics to achieve the desired degree of realism and accuracy. I will highlight the advantages as well as the shortcomings of this approach and attempt to identify a few conceptual and technical challenges for the years to come.

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**Erika Tsingos** (Utrecht University)

**Spatial models of cell-microenvironment interaction**

In animal development, cells maneuver through a complex environment consisting of both other cells and extracellular matrix proteins. How do physical cues and chemical signals contribute to regulate cell behavior and cell fate decisions? I will present two examples where I address this question using agent based modelling approaches. First, a cell center-based model of the vertebrate thymus, the organ where immature progenitors mature into T cells ready to mount an immune response. In this organ, progenitors move through a maze-like network of thymic cells guided by extracellular gradients of cytokines, which ultimately decide the balance between two T cell subtypes [1].

Second, I will present recent work on combining a cellular Potts simulation with a mechanical bead-spring chain model that recapitulates long-ranged interactions between cells and extracellular matrix fibers [2]. I will end by giving a perspective on how the model can be used to study how ECM mechanics impact on cancer metastasis.


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**Chantal Valeriani** (Complutense University of Madrid)

**Mesoscale simulations as a tool to study complex systems**

Dissipative Particle Dynamics (DPD) is one of the most efficient mesoscale coarse-grained approach for modelling not only soft but also active matter systems, such as suspensions of microswimmers and bacterial biofilms. On the one side, since DPD dynamics obeys Navier-Stokes equations and preserve hydrodynamics, we have implemented swimmer models (such as the squirmer model) within the DPD framework and studied suspensions of squirmers under different conditions, ranging from confinement to an externally applied force. On the other side, we have recently applied DPD to capture the essentials of topological and compositional features of the components of a bacterial biofilm, a viscoelastic medium consisting of micron-sized bacteria
cross-linked to a self-produced network of extracellular polymeric substances (EPSs) embedded in water.

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**Holger Stark** (Technische Universität Berlin)

**Hydrodynamics of Active Suspensions**

Hydrodynamic flow fields generated by microswimmers influence decisively their collective dynamics and their motion in complex environments. I will illustrate this along two lines. First, using hydrodynamic multipoles one can demonstrate that active particles in a parabolic potential form a cluster that acts as a fluid pump. Furthermore, hydrodynamic multipoles can also be used to understand the swimming and rheology of active particles in complex fluid environments with an elastic or inertial contribution. Second, we perform explicit simulations with the method of multi-particle collision dynamics of the squirmer model microswimmer. Under gravity they exhibit a variety of fascinating emergent collective dynamics, including plumes, convective rolls, and spawning clusters. Finally, the state diagram of squirmer rods depends on their pusher/puller type. In particular, pusher rods exhibit active turbulence as a compromise between disordering hydrodynamic interactions and steric alignment.

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**Enkeleida Lushi** (New Jersey Institute of Technology)

**Models and simulations of the dynamics of confined active suspensions**

Mathematical modelling and computations of the dynamics of active suspensions is a rich area of research that spans many approaches. I will describe some of the work our group and the broader community has been doing in this front, especially focusing on the models and numerical simulations of fluid-immersed active particles in a variety of non-trivial confinements. Comparisons with relevant experiments will be shown, and we will outline possible directions for future work.

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**Maity Ruma** (Aalto University)

**Chemotaxis of a pair of chiral squirmers**

In this work, we study the chemotactic navigation of a pair of hydrodynamically interacting low Reynolds number swimmers propelling in helical paths [1]. We observe that the hydrodynamic interaction between the swimmers helps them to reach the chemical target quicker than a single swimmer [1, 2]. We have used the chiral squirmer model [2, 4] to understand the chemotactic behaviour and mechanical properties of the swimmers. The former model swimmer possesses a translational V and an angular velocity Ω, see fig. 1(a), (b). Chiral squirmers exhibit synchronized bounded motion apart from the regular monotonic attraction and repulsion depending on its nature, i.e., puller or pusher type. In bounded motion, they synchronize, approach each other, and separate from each other periodically [2, 4]. Here, we have considered only the linear chemical gradient, see fig. 1(c). We observe that in a chemical landscape the former synchronized swimming mechanism helps them to reach the chemical target faster. This study is helpful in understanding the collective dynamics of swimmers in a complex environment.
It has been proposed that spatial memory can lead to more efficient navigation and collective behaviour in biological and synthetic active systems. This raises important questions about the fundamental properties of dynamical systems with spatial memory. We present a framework based on mathematical billiards in which particles remember their past trajectories and react to them. Despite the simplicity of its fundamental deterministic rules, such a system is strongly non-ergodic and exhibits highly intermittent statistics, manifesting in complex pattern formation. We show how these self-memory-induced complexities emerge from the temporal change of topology and the consequent chaos in the system. We study the fundamental properties of these billiards and particularly the long-time behaviour when the particles are self-trapped in an arrested state. We exploit numerical simulations of several millions of particles to explore pattern formation and the corresponding statistics in polygonal billiards of different geometries. Our work illustrates how the dynamics of a single-body system can dramatically change when particles feature spatial memory and provide a scheme to further explore systems with complex memory kernels.
Thursday:

Davide Marenduzzo (University of Edinburgh)
Phase field models in active matter:
lyotropic active nematics and topology of multicellular monolayers

I will discuss some recent simulations of active matter system by phase field methods. First, we will consider the phase behaviour and dynamics of a lyotropic active nematic fluid, and show that the coupling between concentration and order can lead to microphase separation. The latter regime is notable in view of the absence of an explicit demixing term in the underlying free energy. Second, we shall use a multiphase field model to study a monolayer of deformable cells with intercellular and substrate friction. Here, our computer simulations show that nematic order emerges close to the solid-to-liquid transition in the monolayer, and that the topology of hexatic and nematic defects are intimately related.

Falko Ziebert (Heidelberg University)
Phase field modeling of crawling cells and cell mechanics

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 framework for motile cells in complex environments and cells under external stresses. Effects that can be treated by the framework include cell guidance on substrates with modulated adhesion or stiffness; collective cell migration; motion in 3D confinement and on curved or topographically structured substrates; mechanics of cells in complex environments and under external loads/stresses.

Gwynn Elfring (University of British Columbia)
Active Stokesian Dynamics

TBA

Ramin Golestanian (MPI-DS & Oxford)
Non-reciprocal active matter across the scales

Broken action-reaction symmetry has been recently explored in active matter in the context of nonequilibrium phoretic interactions between catalytically active colloids and enzymes [1], and shown to lead formation of self-propelled active molecules that break time-reversal symmetry [2], oscillating active complexes that break time-translation symmetry [3], chiral bound-states [4], and active phase separation with specified stoichiometry [5, 6]. Non-reciprocal interactions have been found to lead to rich physical phenomena involving various forms of spontaneous symmetry-breaking in other related nonequilibrium contexts [7, 8]. Recent applications of non-reciprocal
active matter have revealed exotic behaviour such as the appearance of effervescent travelling patterns [9] and shape-shifting multifarious self-organization [10], spontaneous escape of kinetic barriers [11], dynamical pattern formation in quorum-sensing active matter [12], as well as implications of the physics of non-reciprocal interactions on the origin of life [13,14,15].


Cesare Nardini (CEA & University of Paris-Saclay)
Large scale physics of phase separating active systems

Phase separating active systems display surprising phenomenology that is absent in passive fluid-fluid or liquid-vapor phase separation. One of the reasons for this is that the Ostwald process – the main mechanism leading to the completion of phase separation in equilibrium fluids – can go into reverse in active fluids. When this happens, the active system self-organizes, depending on the global density, in a micro-phase separated state or in a bubbly phase separated state, which corresponds to a coexistence between the micro-phase separated state and the homogeneous phase. In this talk I will describe the large scale properties of micro and bubbly phase separation. This was studied by performing large-scale numerical simulations of particle models, of an active field theory and of a minimal model in which the micro-separated domains are regarded as the degrees of freedom. If time allows I will also discuss recent insights into active turbulent flows that we obtained from numerical simulations of a continuum theory describing micro-swimmer suspensions. With full control in terms of microscopic parameters, we will discuss the spectra of turbulent flows as well as the properties of the transition between the homogeneous/isotropic state and the active turbulent one.

Jack Binysh (University of Bath)
Symmetry-protected coarsening of non-reciprocal matter

Non-reciprocal interactions in active elastic media cause work cycles and wave propagation forbidden in equilibrium. These linear phenomena yield motifs for programming mechanical
actuation, but also hint at a new class of non-linear emergent phenomena in active solids. Here, we develop a continuum model of nonlinear odd elasticity, benchmarked against microscopic simulation and table-top experiments. Combining non-reciprocity and non-linearity in momentum-conserving materials yields long-wavelength instabilities and travelling nonlinear patterns that coarsen over time. We explore how coarsening responds to environmental stimuli, giving a toolkit of distinct patterns for designing locomotion and actuation in active solids. Our results position odd elastic solids as an illustrative example of nonlinear physics in the absence of reciprocity, and point towards applications of these animate materials towards shape change, crawling, and swimming.

Pasquale Digregorio (Università degli Studi di Bari and INFN Sezione di Bari)
Defect lines morphologies in three dimensional active nematics.

Within a living cell, motor proteins like kinesin are responsible of the transport of intracellular components. The functioning of this active transport is well known and it has been employed to build synthetic assemblies of microtubules, which are stirred at the level of the single components and evolve out of thermal equilibrium. Such system is a paradigmatic example of an active material and its realisation has originated lasting efforts aimed to understand its crucial properties. In particular, the presence of activity drives chaotic flow at the large scale and the proliferation of topological defects, which retain some unique properties compared with passive liquid crystals. We analyse in detail the morphology and dynamics of these topological defects and how they depend on the local active stress.
Friday:

Marjolein Dijkstra (Utrecht University)

Unjamming glasses and removing grain boundaries with active colloids

The relaxation dynamics of a colloidal glass can be sped up by orders of magnitude by introducing activity [1]. As a consequence, the glass transition shifts to higher packing fractions upon increasing the activity, allowing the study of sphere packings with fluid-like dynamics close to random close packing. We apply these findings to devitrify glassy systems consisting of mixtures of active and passive hard spheres [2]. We show that the crystallization of hard-sphere glasses can be dramatically promoted by doping the system with small amounts of active particles. Our results suggest a novel way of fabricating crystalline materials from (colloidal) glasses. This is particularly important for materials that get easily kinetically trapped in glassy states, and the crystal nucleation hardly occurs. In addition, we show that grain boundaries can be removed in a polycrystalline material by the addition of active particles [3,4].


Sara Jabbari (University of Amsterdam)

Controlling Collective Motion and Pattern Formation in Magnetic Microswimmers via External Fields

The ability to control and regulate the collective motion of microswimmers via external fields holds great promise for various high-tech applications, including micro-scale cargo transport, targeted drug delivery, and microfluidic devices. To understand how interplay between an external alignment field and fluid-mediated interactions affects collective behaviour and transport of microswimmers, we develop a mesoscopic continuum kinetic theory. Our model is based on a Smoluchowski equation for a particle probability density function in an alignment field coupled to a mean-field description of the flow arising from the activity of dipolar swimmers and the alignment torque. This framework allows us to study the hydrodynamic stability and transport of microswimmers with weak magnetic dipole moments such as magnetotactic bacteria and active magnetic colloids in an external field. Combining linear stability analysis and non-linear 3D continuum simulations, we show that for sufficiently high activity and moderate magnetic field strengths, a homogeneous polar steady state is unstable and distinct types of splay and bend-twist instabilities for puller and pusher swimmers emerge. The instabilities arise from the amplification of anisotropic hydrodynamic interactions due to the external alignment and lead to a partial depolarisation and a reduction of the average transport speed of the swimmers in the field direction. Interestingly, at higher field strengths the homogeneous polar state becomes stable and a transport efficiency identical to that of active particles without hydrodynamic interactions is restored. We will discuss potential computational developments which allow us to explore the competition between hydrodynamic and dipole-dipole interactions on shaping the collective dynamics of magnetic swimmers in an external field.

Daniel Matoz-Fernandez (Complutense University of Madrid)
Exploring Shape Formation through Active Mechanics in Thin Sheets

The study of pattern and structure formation in plants and animals remains an active interdisciplinary research topic. D'Arcy Thompson's pioneering work, integrating physical science methods into biology, highlighted mathematical explanations for the diversity of shapes in the living world. Morphogenesis, the developmental shaping of organisms, is controlled by a complex interplay of chemical and mechanical signals, reshaping cells and their environment. Recent discoveries have underscored the role of physics and mechanics alongside biochemistry in this process.

In this talk, we will present our research on the dynamics of active structural remodelling, such as rapid growth in viscoelastic thin sheets, and its role in generating diverse shapes. This phenomenon is a result of the interplay between viscous relaxation and active processes, particularly significant when the rate of active processes surpasses that of viscoelastic relaxation. This concept is vital in understanding morphogenesis, where embryos must undergo precise shape transformations. Our research indicates that keeping a system out of equilibrium, by manipulating chemical and mechanical parameters, can significantly broaden the array of possible morphologies. These findings provide novel insights into the principles of morphogenesis and the development of shape in biological systems.


Luke Davis (University College London)
Automatic differentiation of active matter simulations (ADAMS)

Active matter systems exhibit rich collective behaviours such as motility-induced phase separation, flocking, and active turbulence. The optimal design and control of these striking collective – active – effects opens the door to potential active technologies, such as materials and actuators, that are able to perform a wide-range of functions that are elusive to passive technology. Despite this potential, the optimal design and control of many-body active systems is currently in its infancy, with the main challenges arising from the highly non-equilibrium, stochastic, and many-body degrees of freedom inherent in many active systems. In this short talk, I will briefly summarize our recent progress on the theoretical underpinnings of active control [1]
and present a roadmap for the computational exploration of control and design of rich active matter systems through automatic differentiation techniques.

Fig. 1. Realising optimization of rich and many-body active matter model systems through the coupling of arbitrarily complex simulation code with an automatic differentiation layer.


George Dadunashvili (Ludwig-Maximilians-Universitaet Muenchen)
flippy: User-friendly and open-source framework for lipid membrane simulations

Cell membranes' shapes influence the function of cells and their compartments. Thus, to better understand biological processes on the cellular level, we must understand the physics of membrane reshaping. Since membranes are two-dimensional fluids with complex elastic behavior, it is mostly impossible to predict their shapes analytically. Thus, we need simulations to study membrane reshaping. One popular method for representing membranes in simulations is dynamic triangulation. To update the configuration of the membrane, the nodes of the mesh can move, and the edges can be rewired to make the mesh fluid. In this talk, I will present flippy [1,2], an open-source C++ package for evolving dynamic triangulations. flippy can simulate lipid membrane shapes, their interaction with proteins or external particles, and the effect of external forces. I will discuss the goals around which flippy was designed and present its capabilities by presenting a project on membrane microtubule interactions.


Ignacio Pagonabarraga (University of Barcelona)
Challenges and opportunities in computational modelling of active systems:
Emerging interactions in active suspensions

Flocks of birds, schools of fishes, or bacterial colonies constitute examples of living systems that coordinate their motion. In all these systems their constituent elements generate motion due to energy consumption and can exchange information or react sensitively to chemical cues to move together or to react collectively to external signals. Artificial systems, such as nanorobots, exploit the heterogeneous compositions of their surface to displace because of the heterogeneous chemical processes that take place in the presence of appropriate chemical substances. All these systems, example of active matter, are intrinsically out of equilibrium, and are characterized by long range correlations and large susceptibilities to external perturbations. These features have deep implications in the emergent properties of active systems and pose challenges to the appropriate computational
strategies. I will discuss the implications that these features have in the effective interactions between passive inclusions in an active suspension, where passive particles couple to the active suspension and quickly react to the active particles rearrangements. Hence, their relative dynamics plays an important role in the features that characterize the emergent interactions among the inclusions. Moreover, for systems where active particles develop long range polar order, the presence of passive obstacles triggers spontaneous macroscopic structures that give rise to non-reciprocal interactions. I will also discuss the susceptibility of polar active systems to small inclusions and the implications this has on the nature of their ordered phases.