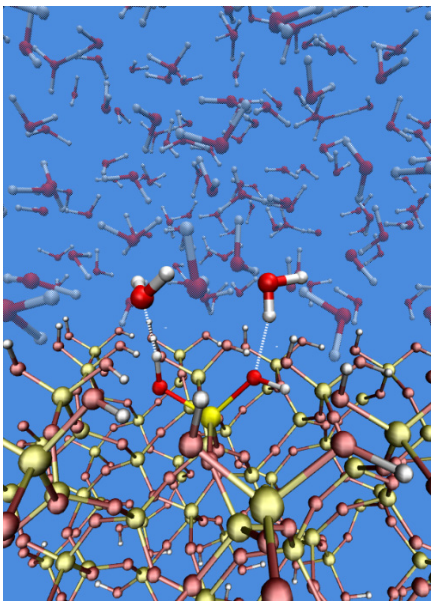
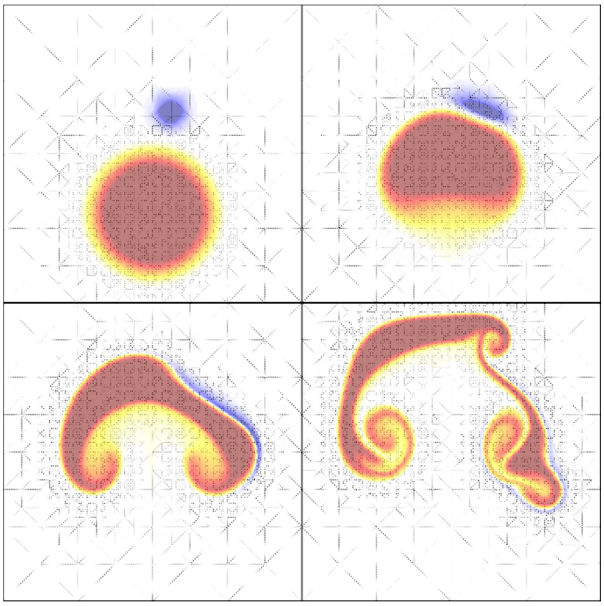
Women in Applied Maths & Soft Matter Physics

Multiscale Simulation Methods for Soft Matter Systems





October 26, 2015 – October 28, 2015

Schloss Waldthausen, Germany

Sara Jabbari Farouji

Maria Lukacova

Friederike Schmid

Johannes Gutenberg University Mainz, Germany

TRR 146

MATERIALS IN MAINZ SCIENCE

Mainz

JG|U

General Information

Organising Committee

Sara Jabbari Farouji (sjabbari@uni-mainz.de)
Institut für Physik
Maria Lukacova (lukacova@mathematik.uni-mainz.de)
Institut für Mathematik
Friederike Schmid (friederike.schmid@uni-mainz.de)
Institut für Physik

Johannes Gutenberg-Universität Mainz
Staudingerweg 9
55128 Mainz
Germany

Conference Coordinator

Markus Haack (mhaack@uni-mainz.de)
Johannes Gutenberg-Universität Mainz
Institut für Physik, Staudingerweg 9
Room 03-523
55128 Mainz
Germany

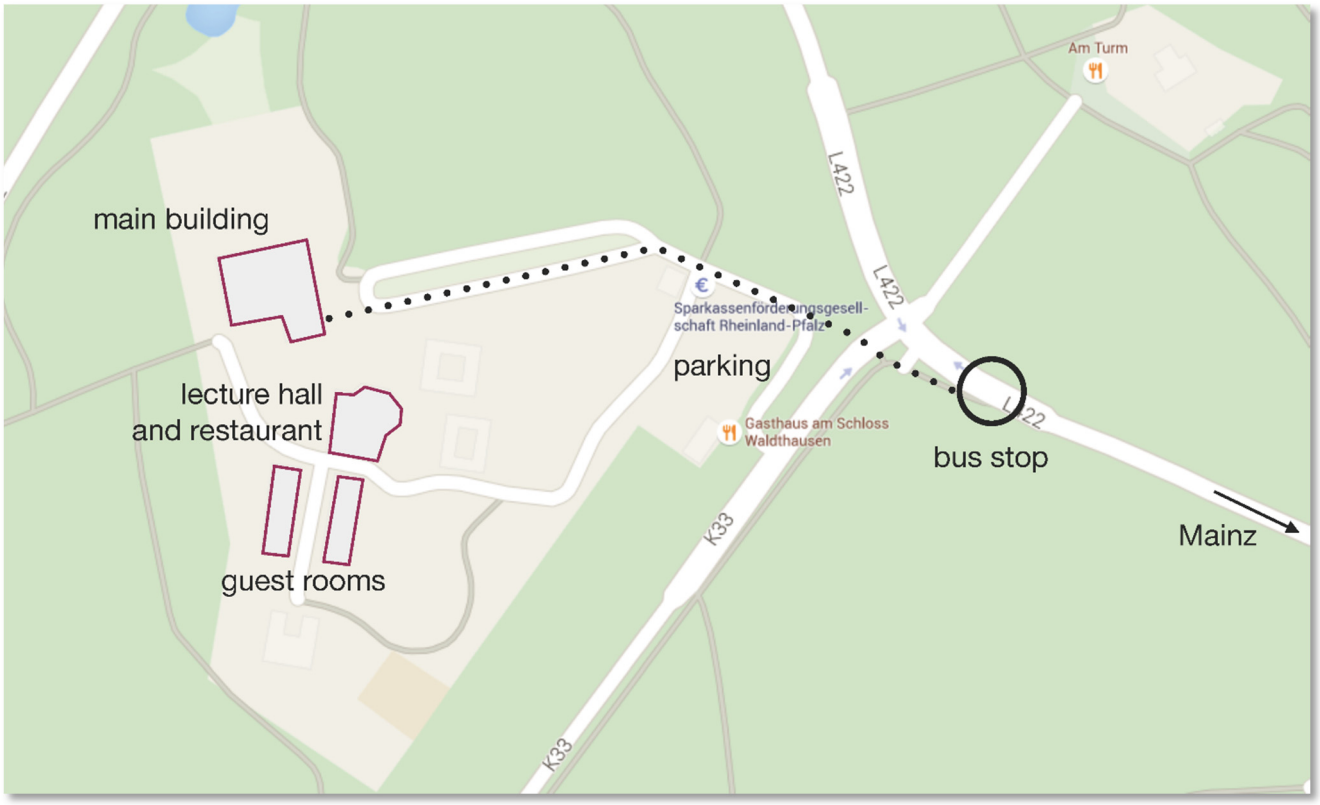
Tel.: +49 (6131) 39 – 20490
Fax.: +49 (6131) 39 – 20496

The Images on the cover page have been provided by Maria Lukacova and Marialore Sulpizi.

Venue

Phone: +49 (6131) – 145199 or +49 (6131) – 145225

Address: Im Wald 1, 55257 Budenheim, Germany



To get there from Mainz by bus:
take line 64 from main station (Hauptbahnhof F) in direction Budenheim.

Opening hours:

- **„Weinstube“** (bar located in the basement of the main building)
  open from 7:30 pm to 12:00 midnight

- **Restaurant:**
  Breakfast from 7:00 am to 9:00 am
  Lunch from 12:00 to 1:45 pm
  Dinner from 6:00 pm to 7:30 pm (during the workshop longer)

Program

Monday, October 26, 2015	
8:00 am - 8:50 am	Registration
8:50 am - 9:05 am	Opening
Session 1: Soft matter – Sara Jabbari	
9:05 am - 10:00 am	**Julia Yeomans** (Oxford University, UK) Modelling active nematics -
10:00 am - 10:15 am	**Francisca Guzman-Lastra** (Univers. Düsseldorf, Germany) Fission and fusion scenarios for magnetic microswimmer clusters -
10:15 am - 10:30 am	**Oksana Manyuhina** (Syracuse University, USA) Disclinations and defect patterns in n-atic liquid crystals
10:30 am - 10:50 am	Coffee break
Session 2: Applied mathematics – Maria Lukacova	
10:50 am - 11:45 am	**Alina Chertock** (North Carolina State University, USA) Asymptotic preserving simulations of kinetic systems for chemotaxis
11:55 am - 12:00 pm	**Nehzat Emamy** (University of Mainz, Germany) A macro-scale flow solver for 3D heterogeneous multi-scale simulations using discontinuous Galerkin FEM
12:00 pm - 12:15 pm	**Anju Saini** (Indian Institute of Technology Roorkee, India) Mathematical Model of Pulsatile Flow of a Dusty Fluid through a symmetrical constricted tube
12:15 pm - 1:45 pm	Lunch break / poster installation

Session 3: Soft matter – Friederike Schmid	
1:45 pm - 2:40 pm	**M. Cristina Marchetti** (Syracuse University, USA) Collective Mechanics of Epithelial Cell Layers
2:40 pm - 2:55 pm	**Swetlana Jungblut** (University of Vienna, Austria) Caveats of mean first-passage time methods applied to the crystallization transition
2:55 pm - 3:20 pm	**Posters flash** 2 min sound bite for each poster presentation
3:20 pm - 5:00 pm	**Poster session** Discussion accompanied by coffee & cake
5:00 pm - 5:10 pm	Refreshment
Session 4: Applied mathematics – Alina Chertock	
5:10 pm - 6:05 pm	**Anja Schlömerkemper** (University of Würzburg, Germany) Mathematical Modeling and Analysis of Magnetoelastic Materials
6:05 pm - 7:00 pm	**Konstantina Trivisa** (University of Maryland, USA) On a mechanical models for tumor growth -
7:00 pm - 8:30 pm	Dinner buffet

Tuesday, October 27, 2015

Session 5: Applied mathematics – Agnieszka Szwierczewska

9:00 am - 9:55 am	**Sarka Necasova** (Academy of Science Prague, Czech Rep) On the problem of singular limit in a Navier-Stokes-Fourier model with radiation
9:55 am - 10:10 am	**Marion Pfirsching** (University of Mannheim, Germany) Material flow problems on conveyor belts using a multi-scale model hierarchy
10:10 am - 10:30 am	Coffee break

Session 6: Applied mathematics – Anna Hundertmark

10:30 am - 11:25 am	**Fengyan Li** (Rensselaer Polytechnic Institute, USA) High order asymptotic preserving methods for some kinetic models
11:25 am - 11:55 am	**Christiane Helzel** (University of Düsseldorf, Germany) A kinetic model for the sedimentation of rod-like particles
12:00 pm - 1:30 pm	Lunch break

Session 7: Soft matter – Kirsten Martens

1:30 pm - 2:25 pm	**Eleni Katifori** (University of Pennsylvania, USA) Modeling and characterization of dynamically adaptive webs

2:25 pm - 2:40 pm	**Elisabeth Agoritsas** (University of Grenoble, France) Revisiting mean-field elastoplastic models at the mesoscopic scale
2:40 pm - 2:55 pm	**Silke Henkes** (University of Aberdeen, UK) Rigid cluster decomposition reveals criticality in frictional jamming
2:55 pm - 3:10 pm	**Sunita Kumari** (Banaras Hindu University, India) Reentrance phenomena in a binary mixture of liquid crystal: A role of inverse layer spacing
3:10 pm - 3:30 pm	Coffee break
3:30 pm - 5:00 pm	**Discussion panels**
5:00 pm - 5:10 pm	Refreshment
Session 8: Soft matter – Eleni Katifori	
5:10 pm - 6:05 pm	**Kirsten Martens** (University of Grenoble, France) Temperature concepts and out of equilibrium phase transitions in externally driven yield stress materials
6:05 pm - 7:00 pm	**Tanja Schilling** (Luxembourg University, Luxembourg) Percolation Revisited
7:00 pm - 8:00 pm	Dinner buffet
8:00 pm - 9:00 pm	**Olga Degtyareva** (Productivity for Scientists Ltd., Selkirk, UK) Productivity for Scientists - Coaching session

Wednesday, October 28, 2015

Session 9: Applied mathematics – Konstantina Trivisa

9:00 am - 9:55 am	**Agnieszka Swierczewska-Gwiazda** (University of Warsaw, Poland) Analysis of a viscosity model for concentrated polymers
9:55 am - 10:50 am	**Anna Hundertmark** (University of Mainz, Germany) Shear-dependent non-Newtonian fluids in hemodynamic modelling
10:50 am - 11:05 am	Coffee break

Session 10: Soft matter – Christine Peter

11:05 am - 12:00 pm	**Anne-Florence Bitbol** (Princeton University, USA) Multi-protein complexes: functions and constraints
12:00 pm - 12:15 pm	**Francesca Nerattini** (University of Vienna, Austria) Designing highly specific probes with tunable affinity
12:15 pm - 12:30 pm	**Rachel Bennett** (Oxford University, UK) Hydrodynamic models of microorganism behaviour
12:30 pm - 2:00 pm	Lunch break

Session 11: Soft matter – Tanja Schilling	
2:00 pm - 2:55 pm	**Christine Peter** (University of Konstanz, Germany) Simulating intrinsically disordered systems: assessing the sampling of conformational phase space
2:55 pm - 3:50 pm	**Marialore Sulpizi** (University of Mainz, Germany) Role of interfacial interactions in shaping the crystal growth
3:50 pm - 4:00 pm	**Maria Lukacova** (University of Mainz, Germany) Closing remarks
4:20 pm - 6:00 pm	**Olga Degtyareva** (Productivity for Scientists Ltd., Selkirk, UK) Productivity for Scientists II

Abstracts and list of participants

Talks

Posters

Abstracts: Talks

Modelling active nematics

Julia Yeomans * [1]

[1] University of Oxford – United Kingdom

We present numerical solutions of continuum equations of motion describing the behaviour of an active nematic in coexistence with a passive fluid and show how activity affects the properties of the active-nematic – isotropic interface. We compare activity due to motility and activity due to cell division and discuss our results in the context of experiments on bacterial colonies.

*Speaker

Fission and fusion scenarios for magnetic microswimmer clusters

Francisca Guzman-Lastra * [1], Andreas Kaiser [1], Hartmut Löwen [1]

[1] Heinrich-Heine University, Duesseldorf – Germany

Fission and fusion processes of particle clusters occur in many areas of physics and chemistry from subnuclear to astronomical length scales. Here we study fission and fusion of magnetic microswimmer clusters as governed by their hydrodynamic and dipolar interactions. Rich scenarios are found including scattering processes which are ubiquitous in nature. Those different scenarios depends crucially on whether the swimmer is a neutral swimmer, a pusher or a puller. Our predictions are obtained by computer simulations and they are verifiable in experiments on active colloidal Janus particles and magnetotactic bacteria.

*Speaker

Disclinations and defect patterns in n-atic liquid crystals

Oksana Manyuhina * [1], Mark Bowick [1]

[1] Syracuse University – Syracuse, NY 13244, United States

Liquid crystal materials exhibit long-range orientational order but no preferred distance between the constituent elements. Yet, they are elastic materials able to resolve geometric and topological frustration in a remarkable way by creating disclinations (discontinuities) in their continuous field. The strength and the nature of disclinations depend on the symmetry of elements forming liquid crystal phase. We propose a phenomenological description for unconventional triatic and tetratic phases, composed of triangles and squares, and construct the free energy invariant under the operations of the dihedral point symmetry group D3h and D4h, respectively. The found solutions for +1/3 and +1/4 disclinations in planar geometry can be used to construct defect textures with arbitrary number of topological defects. Confined to a surface of a sphere we require eight +1/4-disclinations for tetratic phase (or six +1/3-disclinations for triatic phase) giving the total charge +2 characteristic of a sphere. The interplay between the long-range defect-defect interactions, favouring high Gaussian curvature, and the bending energy of the underlying surface, results in flattening of the two-sphere towards rounded cube (or rounded octahedron). Cubic as well as octahedral building blocks pack perfectly in three dimensions and provide new possibilities for self-assembly by alignment or linking across functionalized flat faces.

*Speaker

Asymptotic preserving simulations of kinetic systems for chemotaxis

Alina Chertock * [1]

[1] Department of Mathematics, North Carolina State University (NCSU) – Department of Mathematics, NCSU Campus Box 8205, Raleigh NC 27695, United States

We consider numerical approximations of the kinetic equations describing a collective behavior of bacteria and their interaction with both nutrients and chemoattractant. We introduce a non-dimensional small parameter (epsilon=the ratio of the mean free paths corresponding to isotropic and chemotactic reorientation) and by choosing a diffusion scaling we obtain a transport equation in nondimensional form depending on this parameter. In [Chalub et al. (2004)] the conditions have been derived under which the drift-diffusion limit of this Fokker-Planck system yields the Keller-Segel model. With respect to this result our aim is to investigate asymptotic preserving schemes for the corresponding kinetic chemotaxis equations.

*Speaker

A macro-scale flow solver for 3D heterogeneous multi-scale simulations using discontinuous Galerkin FEM

Nehzat Emamy *† [1], Maria Lukacova-Medvidova [1], Florian Kummer [2]

[1] Numerical Mathematics, Johannes-Gutenberg University Mainz – Germany
[2] Chair of Fluid Dynamics, Technical University of Darmstadt – Germany

A macro-scale flow solver is developed to be used for 3D heterogeneous multi-scale numerical simulations of polymers. Within the macro-scale solver, the Cauchy momentum equations are discretized using a high-order accurate discontinuous Galerkin Finite Element Method (dG). The stress tensor will be computed for the non-Newtonian fluid by performing molecular dynamics simulations. Therefore, an explicit time integration of the viscous terms in the momentum equations is required.
To integrate the momentum equations efficiently, the projection scheme is employed, where by solving a Poisson equation for the pressure the mass conservation is enforced. Solving the Poisson equation is the most computationally expensive step of the method. Therefore, to reduce the computational cost of solving the Poisson equation, we reduce the degrees of freedom by performing a transformation from the dG space to continuous Galerkin (cG) space for the pressure.
To show the stability and convergence rates of the macro-scale solver, we consider Newtonian fluids as a first step, where analytical solutions of the Stokes and Navier-Stokes equations are available. Preliminary results show the same accuracy for the equal degrees of the velocity and pressure, when the Poisson equation is solved in the cG space rather than dG. For the mixed-order scheme, where the degree of the pressure is one less than the velocity, dG shows a slightly higher accuracy. However, solving the Poisson equation in the cG space is still advantages because of solving a smaller system of equations.

*Speaker
†Corresponding author: emamy@uni-mainz.de

Mathematical Model of Pulsatile Flow of a Dusty Fluid through a symmetrical constricted tube

Anju Saini * [1], V.k. Katiyar [1]

[1] IIT Roorkee – India

The present work is concerned to study the pulsatile flow behavior of particulate suspensions through a tube with sinusoidal wall vibrations. Finite difference method has been used to solve the unsteady nonlinear Navier–Stokes equations in cylindrical coordinate system assuming axial symmetry under laminar flow condition so that the problem efficiently turns into two-dimensional form. An extensive quantitative study is performed through numerical computations of the preferred quantities having physiological importance through their graphical demonstration so as to authenticate the applicability of the current model. Results for velocity of fluid and dust particles and wall shear stress distribution have been discussed.

*Speaker

Collective Mechanics of Epithelial Cell Layers

M Cristina Marchetti * [1]

[1] Syracuse University, Physics Department – United States

The transmission of mechanical forces among cells and between cells and their environment plays a crucial role in regulating the materials properties and organization of tissues and the collective migration of cell groups, which are in turn important in a variety of developmental processes, from wound healing to morphogenesis and cancer metastasis. In this talk I will present physical models that account for long-range force generation and transmission in collections of living cells. I will show that by the interplay between individual cell motility and contractility, and cell-cell interactions, is key for understanding both the spatial organization of forces exerted by cell colonies on their environment and the propagating stress waves that control the coordinated dynamics of expanding cell monolayers.

*Speaker

Caveats of mean first-passage time methods applied to the crystallization transition

Swetlana Jungblut * [1]

[1] University of Vienna – Austria

Using the crystallization transition in a Lennard-Jones fluid as example, I will show that mean first-passage based methods may underestimate the reaction rates. The reason of this deficiency can be traced back to the non-Markovian character of the dynamics caused by the projection to a poorly chosen reaction coordinate. The non-Markovianity of the dynamics becomes apparent in the behavior of the recurrence times.

*Speaker

Mathematical Modeling and Analysis of Magnetoelastic Materials

Anja Schlömerkemper * [1] Barbora Benešová [2], Jing-Mei Qiu [3], Tao Xiong [4] Chun Liu [5]

[1] Universität Würzburg, Institute for Mathematics

Abstract: Magnetic materials have the special property that they react to applied external fields in remarkable ways and have therefore many technological applications. They can not only be found in medical applications, but, for example, also in loud speakers and shock absorbers. We propose a model for micromagnetic materials in the framework of complex fluids. The system of PDEs to model the flow of the material is derived in a continuum mechanical setting from variational principles including the least action principle and the maximum dissipation principle. In this talk, we outline the process of modeling and the energetic variational approach. Moreover, we highlight the coupling between the elastic and the magnetic properties of the material. The obtained model is a general model of micromagnetic materials, but is rather complex from the analytical point of view. Therefore, we provide also simplified versions of the model for which we show existence of weak solutions.
This is joint work with Barbora Benešová and Johannes Forster (Institute of Mathematics, University of Würzburg, Germany) as well as with Carlos García-Cervera (Mathematics Department, University of California, Santa Barbara, USA) and Chun Liu (Department of Mathematics, Penn State University, University Park, USA).

*Speaker

On a mechanical models for tumor growth

Konstantina Trivisa *† [1], Franziska Weber

[1] Department of Mathematics – Mathematics Building University of Maryland College Park, MD 20742-4015, United States

Mechanical models for tumor growth are used extensively in recent years for the analysis of medical observations and for the prediction of cancer evolution based on imaging analysis. This work presents a variational framework appropriate for simulations for the numerical approximation of a mechanical model for tumor growth and the analysis of its dynamics. The system under investigation is given by a multi-phase flow model: the densities of the different cells are governed by a transport equation for the evolution of tumor cells, whereas the velocity field is given by a Brinkman regularization of the classical Darcy's law.
Theoretical and numerical results are presented, An efficient finite difference scheme is proposed and shown to converge to a weak solution of the system. Our approach relies on convergence and compactness arguments in the spirit of Lions-Feireisl.

*Speaker
†Corresponding author: trivisa@math.umd.edu

On the problem of singular limit in a Navier-Stokes-Fourier model with radiatio

Sarka Necasova * [1], Bernard Ducomet [2]

[1] Institute of Mathematics, Academy of Sciences (IM ASCR) – Zitna 25, 11567 Praha 1, Czech Republic
[2] CEA DAM DIF, Arpajon – CEA – France

We consider relativistic and "semi-relativistic" models of radiative viscous compressible Navier-Stokes-Fourier system coupled to the radiative transfer equation extending the classical model introduced in [1] and we study some of its singular limits (low Mach and diffusion) in the case of well-prepared initial data and Dirichlet boundary condition for the velocity field. In the low Mach number case we prove the convergence toward the incompressible Navier-Stokes system coupled to a system of two stationary transport equations. In the diffusion case we prove the convergence toward the compressible Navier-Stokes with modified state functions (equilibrium case) or toward the compressible Navier-Stokes coupled to a diffusion equation (non equilibrium case). Moreover, the coupling with magnetic field and singular limit will be described.

References

[1] B. Ducomet, E. Feireisl, S. Necasova: On a model of radiation hydrodynamics. Ann. I. H.
Poincare-AN 28 (2011) 797–812.
[2] B. Ducomet, S. Necasova: Low Mach number limit in a model of radiative flow, Journal of Evolution equations, 14 (2014) 357–385.
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[4] B. Ducomet, S. Necasova: Singular limits in a model of radiative flow, J. Math. Fluid Mech. 17
(2015), 2, 341–380.
[5] B. Ducomet, S. Necasova: Non-relativistic limit in a model of radiative flow. Analysis (Berlin) 35 (2015), no. 2, 117–137.

*Speaker

Material flow problems on conveyor belts using a multi-scale model hierarchy

Marion Pfirsching * [1]

[1] Department of Mathematics and Computer Science Mannheim – Germany

Conveyor belts are used in a wide field of industrial application, for example in bottling plants. Here the collision between the material is an intentional part of the transportation process. With an increasing number of particles on the belt, microscopic models are too long to calculate. Therefore we work with a macroscopic model wherever it is possible. The loss of accuracy is compensated with a decrease of computation time. It can be shown that the result of the macroscopic model is quite similar to the result calculated by a microscopic model with a large number of particles. Also after optimizing over both models, the optimization results are quite similar.

*Speaker

High order asymptotic preserving methods for some kinetic models

Juhi Jang [1], Fengyan Li * [2], Jing-Mei Qiu [3], Tao Xiong [4]

[1] University of Southern California – United States
[2] Rensselaer Polytechnic Institute – United States
[3] University of Houston – United States
[4] Université de Lyon – France

Many problems in science and engineering involve parameters in their mathematical models. Depending on the values of the parameters, the equations can differ greatly in nature. Asymptotic preserving (AP) methods are one type of methods which are designed to work uniformly with respect to different scales or regimes of the equations when the parameters vary.
In this talk, I will present our work in developing high order AP methods for some kinetic models, including discrete-velocity models in a diffusive scaling and the BGK model in a hyperbolic scaling. When the Knudson number approaches zero, the limiting equations of the former model can be heat equation, viscous Burgers' equation, or porous medium equation, while the limiting equations for the latter are the compressible Euler equations. When the Knudson number is very small, the BGK model also leads to compressible Navier-Stokes equations. The proposed methods are built upon a macro-micro decomposition of the equations, high order discontinuous Galerkin (DG) spatial discretizations, and the stiffly accurate implicit-explicit Runge-Kutta (IMEX-RK) temporal discretizations. Theoretical results are partially established for uniform stability, error estimates, and rigorous asymptotic analysis. Numerical experiments will further demonstrate the performance of the methods.

*Speaker

A kinetic model for the sedimentation of rod-like particles

Christiane Helzel * [1]

[1] Heinrich-Heine-University Düsseldorf – Germany

We will present a coupled multi-scale system consisting of a kinetic equation that is coupled to a macroscopic flow equation. The reciprocal coupling leads to the formation of clusters: The buoyancy force creates a macroscopic velocity gradient that causes the microscopic particles to align so that their sedimentation reinforces the formation of clusters of higher particle density. Furthermore, we will present several macroscopic models which can be derived from the kinetic model and which also describe the formation of clusters. Results of numerical simulations will be used to validate these macroscopic models. This is recent joined work with A.E.Tzavaras from KAUST.

*Speaker

Modeling and characterization of dynamically adaptive webs

Eleni Katifori * [1]

[1] Department of Physics and Astronomy, University of Pennsylvania (UPenn) – 209 South 33rd Street, 19104 Philadelphia PA, United States

Transport networks play a key role across four realms of eukaryotic life: slime molds, fungi, plants, and animals. In addition to the developmental algorithms that build them, many also employ adaptive strategies to respond to stimuli, damage, and other environmental changes. We model these adapting network architectures using a generic dynamical system on weighted graphs and find in simulation that these networks ultimately develop a hierarchical organization of the final weighted architecture accompanied by the formation of a system-spanning backbone. We quantify the hierarchical organization of the networks by developing an algorithm that decomposes the architecture to multiple scales and analyzes how the organization in each scale relates to that of the scale above and below it. The methodologies developed in this work are applicable to a wide range of systems including the slime mold physarum polycephalum, human microvasculature, and force chains in granular media.

*Speaker

Revisiting mean-field elastoplastic models at the mesoscopic scale

Elisabeth Agoritsas * [1], Eric Bertin [1], Kirsten Martens [1], Jean-Louis Barrat [1]

[1] Laboratoire Interdisciplinaire de Physique (LIPhy) – Université Joseph Fourier - Grenoble I, CNRS : UMR5588 – France

Encompassing very dissimilar systems (such as foams, pastes, or metallic glasses), amorphous materials are composed of particles that can have very different shapes and sizes, such as grains of sand in a sandpile or bubbles in a soap foam. Lacking a crystalline structure, they exhibit a structural disorder that turns out to play a determinant role in their mechanical properties, while challenging their very description. Several elasto-plastic models have been developed at the mesoscopic scale, in order to account for the plasticity in such amorphous systems, such as the Soft-Glassy-Rheology (SGR) model [1] and the Hébraud-Lequeux (HL) model [2]. These two mean-field models have proven to be rather successful in reproducing certain features observed in amorphous systems, but not all at once. Moreover, a consistent picture connecting these models is still missing.
Here we discuss the physical ingredients that are put in those two mean-field models, distinguishing between thermal and mechanical noises in the mean-field dynamics of such amorphous materials. We focus in particular on the role of structural disorder, implemented by means of a distribution of energy barriers for the system to overcome when an external constant shear rate is applied to the material, and discuss specifically its implications for a generalization of the HL model [3].

References

[1] P. Sollich, F. Lequeux, P. Hébraud, & M. Cates, Phys. Rev. Lett. 78, 2020 (1997), P. Sollich, Phys. Rev. E, 58, 738 (1998).
[2] P. Hébraud & F. Lequeux, Phys. Rev. Lett. 81, 2934 (1998).
[3] E. Agoritsas, E. Bertin, K. Martens, & J.-L. Barrat, Eur. Phys. J. E 38, 71 (2015).

*Speaker

Rigid cluster decomposition reveals criticality in frictional jamming

Silke Henkes *† [1], David Quint [2], Yaouen Fily [3], Jennifer Schwarz‡ [4]

[1] University of Aberdeen - ABDN (UNITED KINGDOM) – United Kingdom
[2] Stanford University [Stanford] – Stanford 450 Serra Mall, Stanford, CA 94305. (650) 723-2300, United States
[3] Brandeis University – Brandeis University 415 South St. Waltham, MA 02453, United States
[4] Syracuse University – Syracuse, NY 13244, United States

The interplay of constraints, forces, and driving gives rise to the jamming transition in granular media. While the jamming transition in frictionless systems displays features of a mixed first- and second-order phase transition, the more experimentally relevant case of systems with friction appears to be different: there is no single jamming point but a generalized isostaticity line of transitions and observed hysteresis has led to interpretations as a first-order phase transition along this line. Here, we investigate the nature of the frictional jamming transition using the framework of rigidity percolation theory. We decompose slowly sheared frictional packings into rigid clusters and floppy regions through a generalization of the pebble game that includes frictional contacts. We then discover a second-order transition controlled by the emergence of a system-spanning rigid cluster accompanied with a critical distribution of rigid cluster sizes slightly below the generalized isostaticity line. In contrast, in frictionless jamming, a space-filling, system-spanning rigid cluster emerges accompanied with a non-critical rigid cluster size distribution slightly below isostaticity. The transition location, in both cases, signifies that spatial correlations in the constraints are important. We also correlate rigid clusters with other microscopic measures of rigidity.

*Speaker
†Corresponding author: shenkes@abdn.ac.uk
‡Corresponding author: jmschw02@syr.edu

Reentrance phenomena in a binary mixture of liquid crystal: A role of inverse layer spacing

Sunita Kumari * [1], Shri Singh [1]

[1] Department of Physics, Banaras Hindu University, Varanasi, India – India

The occurrence of reentrant phenomena in a binary mixture of liquid crystals under pressure is observed in high-pressure experimental studies [1, 2] has been explained within the framework of Landau de Gennes theory. In this phenomenological theory, the free energy density expansion is written in terms of nematic, smectic A order parametrs. The most important feature of the work is that the role of inverse layer spacing q, which mimics an order parameter, becomes coupled to the order parameters. The influence of concentration on reentrant behaviour is also discussed by varying the coupling between the concentration variable and the order parameters. We found that the order parameters coupling terms and inverse of layer spacing play important role and that the present analysis is in good qualitative agreement with the available experimental results.

References

[1] P.E. Cladis, R.K. Bogardus, W.B. Daniels and G.N. Taylor, Phys. Rev. Lett. 39, 720 (1977).
[2] P.E. Cladis, R.K. Bogardus and D. Aadsen, Phys. Rev. A 18, 2292 (1978).

*Speaker

Temperature concepts and out of equilibrium phase transitions in externally driven yield stress materials

Kirsten Martens * [1]

[1] Laboratoire Interdisciplinaire de Physique (LIPhy) – Université Joseph Fourier - Grenoble I, CNRS : UMR5588 – France

Steadily sheared disordered systems that yield in an athermal way (like foams or granular systems) provide excellent examples for the study of driven disordered systems reaching an out-of-equilibirium steady state. The interesting feature of these type of systems is that fluctuations are solely introduced through the mecanical response itself. And the challenge is thus to describe this mecanical noise in a selfconsistent correct manner. In this talk I will show that in this situation usual effective temperature based concepts, like Arrhenius type dynamics, should in our opinion not hold [1].
Even more interestingly these systems exhibit non-equilibrium phase transitions, that can be both continuous [2] and discontinuous [3], and are again not governed by usual temperature considerations, but other yielding dynamics related concepts. For the continuous transisition we observe dynamical heterogeneities with diverging length and time scales, whereas in the discontinuous case we could show the existence of a phase coexistence between two dynamical phases. The existence of critical dynamics leads us to the question whether it will be possible to define different universality classes for the flow of yield stress materials, similar to what has been done in the field of the depinning transition [4].

References

[1] Rheology of athermal solids: Revisiting simplified scenarios and the concept of mechanical noise temperature, Alexandre Nicolas, Kirsten Martens and Jean-Louis Barrat, EPL, 107, 44003 (2014).
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*Speaker

Percolation Revisited

Tanja Schilling * [1]

[1] University of Luxembourg (UL) – 162 a, avenue de la faiencerie, 1151 Luxembourg, Luxembourg

Connectivity percolation is the transition in which isolated clusters of solid particles in a fluid (or of voids in a solid) become connected in some sense to form a system-spanning network. This network has a significant effect on the mechanical and transport properties of the material on a macroscopic scale. If, for example, an electrically insulating polymer is mixed with conductive fibres such as carbon nanotubes, the conductivity of the composite increases by many orders orders of magnitude near the percolation transition of the filler material. We investigate percolation in suspensions of fibres by means of connectedness percolation theory and by specialized Monte Carlo simulations. Our study covers the entire range of aspect ratios from spheres to extremely slender rods. The theory and the simulations agree very well for aspect ratios down to values as low as 10. The percolation threshold for both hard and ideal rod-like particles of aspect ratios below 1000 deviates significantly from the inverse aspect ratio scaling prediction, thought to be valid in the limit of infinitely slender rods and often used as a rule of thumb for fibres in composite materials. Hence, most fibres that are currently used as fillers in composite materials cannot be regarded as practically infinitely slender from the point of view of percolation theory. Comparing percolation thresholds of hard rods and new benchmark results for ideal rods, we find that (i) for large aspect ratios, they differ by a factor that is inversely proportional to the connectivity distance between the hard cores, and (ii) they approach the slender rod limit differently. We also study the effects of polydispersity on the percolation transition. We discuss length and diameter polydispersity as well as dispersity in the connectedness criterion. The main result is that the percolation threshold shows universal behaviour, i.e._˜it depends only on certain cumulants of the size distribution.

*Speaker

Analysis of a viscosity model for concentrated polymers

Agnieszka Swierczewska-Gwiazda * [1]

[1] University of Warsaw (UW) – Banacha 2, 02-097 Warszawa, Poland

We will concentrate on a class of mathematical models for polymeric fluids, which involves the coupling of the Navier-Stokes equations for a viscous, incompressible, constant-density fluid with a parabolic-hyperbolic integro-differential equation describing the evolution of the polymer distribution function in the solvent, and a parabolic integro-differential equation for the evolution of the monomer density function in the solvent. The viscosity coefficient, appearing in the balance of linear momentum equation in the Navier-Stokes system, includes dependence on the shear-rate as well as on the weight-averaged polymer chain length. The system of partial differential equations under consideration captures the impact of polymerization and depolymerization effects on the viscosity of the fluid. Such system well captures polymer flows in concentrated regime.

*Speaker

Shear-dependent non-Newtonian fluids in hemodynamic modelling

Anna Hundertmark * [1], Mária Lukáčová [1]

[1] Johannes Gutenberg University, Mainz (JGU Mainz) – Institut of Mathematics, Staudingerweg 9, Mainz, Germany

Shear-dependent fluids are characterized by a nonlinear dependence of the viscosity on the shear rate —D(v)—. In the shear-thinning (pseudo-plastic) fluids the viscosity is reduced with the shear rate, in the shear-thickening (dilatant) fluids the viscosity is an increasing function of the shear rate. Experimental investigations reveal that blood is a non-Newtonian fluid exhibiting in particular shear-thinning properties. This phenomenon starts to be more profound in small blood vessels or if local flow phenomena are important, but several reports in the literature demonstrate that even in large blood vessels the non-Newtonian models yield more accurate results.
Besides the nonlinear rheological dependence in the mathematical model, the interaction of the compliant vessel with the blood leads to the geometrical nonlinearity, since the geometry of the moving computational domain depends on the solution. Thus our hemodynamic fluid flow model presents a complex problem coupling the non-Newtonian fluid with the elastic structure. We analyse the underlying system of equations from the theoretical point of view and show the existence of weak solution for a shear-dependent power-law fluid coupled viscoelastic structure modelled by generalized string equation, see [1].

In the numerical simulations the so called added mass effect of the fluid on the light cardiovascular structure leads to difficulties, additional iterations between the fluid flow and the structure equations are used to stabilize the system (strongly coupled schemes). We use the so called global iterations with respect to the domain to approximate the system, see [2]. Moreover we investigate a novel and efficient, loosely (weakly) coupled method of kinematic splitting [3], which avoid the necessity of additional stabilization and sub-iterations. We compare the numerical results and the convergence of both FSI methods for some non-Newtonian and Newtonian models. The significance of the non- Newtonian rheology and the fluid-structure interaction has been confirmed in the hemodynamic wall parameters such as the wall shear stress and the oscillatory shear index as well, see also [4].

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*Speaker

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Multi-protein complexes: functions and constraints

Anne-Florence Bitbol * [1]

[1] Princeton University [Pinceton] – Princeton University Princeton, NJ 08544 USA, United States

Self-assembled multi-protein complexes play key roles in cells, e.g., as molecular motors, enzymes, channels, and receptors. Functional interactions between proteins forming these complexes impose constraints on their evolution, on their sequences and on their abundances. We investigate theoretically some aspects of this fundamental link between functions and constraints in multi-protein complexes, from the population scale to the molecular scale.
Proteins that form a complex are evolutionarily coupled by the need to preserve functional interactions. This coupling can lead to the existence of fitness valleys, which hinder further evolution. Fitness valley crossing can be facilitated by specific population structures. Using a minimal model, we quantitatively determine when, and to what extent, population subdivision accelerates fitness valley crossing.
Besides, the evolutionary coupling between proteins that interact together is reflected in their sequences, which allows to infer specific interaction partners from sequence data.
At the cellular scale, function can impose constraints on the abundances of proteins. We investigate these constraints in the case of the proteins involved in E. coli chemotaxis. We show that the requirements of fast signaling impose lower bounds on the abundances of these proteins, and we demonstrate that the gain of the chemotaxis signaling pathway saturates when protein abundances are increased beyond physiological levels.
Hence, functional interactions impose constraints on proteins at multiple levels. Fundamental features of the self-assembly process, such as nucleation barriers, can in turn serve a particular biological function. The enzyme CTP synthetase forms long polymers in cells, and this polymerization is coupled to negative feedback by the product of the enzyme. We show that coupling enzyme activity to polymerization with a nucleation barrier enables ultrasensitive enzymatic regulation.

*Speaker

Designing highly specific probes with tunable affinity

Francesca Nerattini * [1]

[1] Computational Physics Group, University of Vienna – Austria

Finding ligands able to bind with high specificity and tunable affinity to a target protein is one of the major challenges in medical research [1]. To this aim we develop a computational protocol based on the coarse-grained protein model "Caterpillar" [2] that has proven to be quantitative for design and folding simulations. We apply the model to design proteins that bind specifically to a simple pocket. The generated pocket specific sequences can be tuned with different biding free energies, computed using the Caterpillar and verified with all atom MD simulations.

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*Speaker

Hydrodynamic models of microorganism behaviour

Rachel Bennett * [1], Ramin Golestanian

[1] University of Oxford (UK) – Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, United Kingdom

Many of the observed features in the behaviour of microorganisms emerge from hydrodynamics. Two minimal models are presented which show experimentally observed behaviours. The first model considers the synchronisation between the two flagella of Chlamydomonas. Rotation of the cell body modifies the hydrodynamic friction felt by each flagellum and provides a synchronisation mechanism. The stability of synchronisation is sensitive to the flagellar beat pattern and when intrinsic noise is added run-and-tumble behaviour emerges. The model steers phototactically when the beat pattern is coupled to light intensity, and we use the simplicity of the model to understand the mechanism of phototactic steering. The other model considers motility of bacteria at a surface. We show how hydrodynamics lead to a variety of behaviours depending on how much of the flagellum becomes attached to the surface. We show how interesting motility modes arise in free-swimming cells due to hydrodynamic friction between cell appendages and the surface.

*Speaker

Simulating intrinsically disordered systems: assessing the sampling of conformational phase space

Christine Peter * [1]

[1] University of Konstanz – Germany

Disordered proteins are of increasing interest in biomedical and biomaterials applications with severe challenges to both experiment and theory. These systems show very little and at best partial and transient structuring, they are highly dynamic, with equilibria between multiple conformations of similar stabilities. Characterization of these equilibria and the identification of states is significantly more complex compared to systems with few well-defined folded conformations. This characterization, however, is a prerequisite to assess methods to overcome sampling limitations, such as advanced sampling methodologies or dual-scale approaches with reduced-resolution models. I will show different examples which illustrate how dimensionality reduction methods can be successfully applied to describe the phase space sampled by intrinsically disordered systems in atomistic and coarse grained simulations, to judge the success of elevated sampling techniques or to guide further simulations. One example are early stages of biomineralization, where simulations can give mechanistic insight into how the pre-alignment of ions from solution by additives may steer the crystallization of calcium rich minerals into different polymorphs. We have used Hamiltonian replica exchange and automated projection of the configurational space to sample and analyze the complex multidimensional configurational space of aqueous solutions of oligo-glutamate and calcium ions.

*Speaker

Role of interfacial interactions in shaping the crystal growth

Marialore Sulpizi * [1]

[1] Condensed Matter Theory Group (KOMET 331) – KOMET 331, Institute of Physics, Johannes Gutenberg-University, D-55099 Mainz, Germany

Liquid-solid interfaces are ubiquitous and responsible for a number of phenomena encountered in biological, chemical and physical processes. Surface-induced changes of material properties are not only important for the solid support but also for the liquid itself.

Among properties controlled by the specific interactions at solid/liquid interface is crystallization and shape selective crystal growth. This is fundamental for example to the synthesis of nanoparticles with specific tailored shape/size. In biomineralization the interaction between soft (proteins/solution) and hard matter (mineral) which occurs at the interface is the key do develop unique structural properties. Atomistic simulation can provide a powerful tool to understand interfacial phenomena. They can provide a microscopic interpretation of the experiments and identify which are the key interactions controlling a given phenomena allowing for a tailored intervention to shape and tune the material properties.

I will present a few examples from my research activity where we use atomistic simulations, also including electronic
structure, in order to address the properties of solid/liquid interfaces. In particular I will discuss the role of interfacial interactions in controlling the anisotropic growth of gold nanorods and calcium acetate crystals.

*Speaker

Abstracts: Posters

P1: Creep dynamic in soft matter

Raffaela Cabriolu * [1]

[1] Laboratoire Interdisciplinaire de Physique (LIPhy) – Université Joseph Fourier - Grenoble I, CNRS : UMR5588 – 140 rue de la physique BP 87 F-38402 Saint Martin d'Hères, raffaela.cabriolu@ujf-grenoble.fr, France

Detecting any precursors of failure in Soft Matter Systems (SMS) is an inter-disciplinary topic with important applications (e.g. prediction of failure in engineering processes). Further it provides ideal benchmark to understand how mechanical stress and failure impacts the flow properties of amorphous condensed matter. Furthermore, some SMS are viscoelastic, flow like viscous liquids or deform as solids depending on the applied forces. Often SMS are fragile and local rearrangements trigger catastrophic macroscopic failure. Despite the importance of the topic little is known on the local creep dynamics [1,2] before the occurrence of such catastrophic events [3,4]. To study creep and failure at an atomic/molecular level and at time scales that are not easily accessible by experiments we chose to setup microscopic simulations. In this work we present the response of a colloidal system to stress and shear applied in different environmental conditions and we compare our results to experimental works and existing theories.

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*Presenting author

P2: Computational study of aggregation of PCPDTBT in presence of a solvent

Nancy C. Forero-Martinez * [1], Tristan Bereau [1], Bjoern Baumeier [2], Kurt Kremer [1]

[1] Max Planck Institute for Polymer Research – Ackermannweg 10 55128 Mainz, Germany
[2] Eindhoven University of Technology – P.O. Box 513, 5600 MB Eindhoven, Netherlands

Conjugated donor-acceptor polymers exhibit characteristic charge transport properties that are exploited by using them as donor materials in organic photo-voltaic devices. In particular, low-band-gap polymers such as PCPDTBT have been designed to broaden the spectral range of absorbed photons. However, PCPDTBT-based optimised cells show no significant improvement in the device performance [1]. Some studies suggest that this behaviour is related to the microstructure of the system [2,3]. For example, the change in morphology of side chains, when going from linear to branched alkyl side groups, reduces the tendency of PCPDTB to crystallise thus compromising its absorption properties [4]. Evidently, the processing solvent affects both, the morphology of thin films and the absorption properties of PCPDTBT [5]. To complicate matters even further and to the best of our knowledge, there is no definite consensus about the crystalline structure of PCPDTBT [3,6].
To contribute to this ongoing discussion, we are developing a computational model aimed at studying the dynamics of PCPDTBT aggregation in presence of a solvent. We started with a simplified model of the polymer system, where only CPDT monomers are taken into account. An atomistic description of the potential energy has been developed and tested against the crystal structure of CPDT observed experimentally. We study structure and dynamics of CPDT monomers in solvent in order to characterise the interactions between polymer and solvent, and to identify the forces promoting aggregation. We intend to use these results as an input for more sophisticated computations and larger scale simulations.

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*Presenting author

P3: On the asymptotic behavior of trajectories of essentially nonlinear systems with resonance frequencies

Victoria Grushkovskaya * [1]

[1] Institue for Systems Theory and Automatic Control (IST) – Pfaffenwaldring 9 70550 Stuttgart, Germany

This talk is devoted to the study of the decay rate of solutions for systems in critical cases. The practical interest to such systems is motivated by their frequent occurrence in physics and many engineering systems, from the simplest mechanisms to the motion of celestial bodies. This study presents the method for obtaining asymptotic estimates and constructing Lyapunov functions for systems with q pairs of purely imaginary eigenvalues. As resonances have the high influence on the stability and decay rate of oscillations, we admit that frequencies of the system satisfy resonance relations. The main methods used in the study are the center manifold reduction and normal form theory. The results obtained are applied to a mechanical system with partial dissipation.

*Presenting author

P4: Freezing dynamics of hard colloidal cubes

Carina Karner * [1], Christoph Dellago [1]

[1] University of Vienna, Faculty of Physics – Austria

Currently, research on hard anisotropic colloids is receiving a lot of attention from various experimental and theoretical groups in the soft matter community, partly due to the availability of new fabrication techniques making it possible to produce colloidal particles with various anisotropic shapes or interactions [1]. Recent results obtained from computer simulations and theory indicate that many three dimensional hard anisotropic particles of polyhedral shape exhibit a first order phase transition from an unordered fluid to an ordered crystal. Hard colloidal cubes belong to this class of particles and have recently been studied numerically [2] as well as experimentally [3]. Unlike isotropic particles, cubic particles have to assume not only positional but also orientational order as they crystallize. Therefore the natural question to ask is how the interplay of orientatioanl and translational degrees of freedom influences the course of the transition. In order to gain insight into the dynamics of the freezing transition, we employed kinetic Monte Carlo in combination with rare event sampling methods. Using free energy and nucleation rate calculations, we show that even at low over-pressuring, cubic colloids transition extremely fast from the metastable liquid to the cubic crystal. Our findings provide further evidence that hard colloidal cubes assume first orientational order, whereas translational cubic order only emerges in sufficiently large clusters of orientational order. Despite its simplicity, the hard cube system clearly exhibits an intricate pathway to nucleation, suggesting that other anisotropic particle systems might show similarly complex kinetic behaviour.

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*Presenting author

P5: Motility of active fluid drops on surfaces

Diana Khoromskaia [*†] [1], Gareth Alexander [1,2]

[1] Centre for Complexity Science, University of Warwick – Centre for Complexity Science, Zeeman Building, University of Warwick, Coventry CV4 7AL, UK, United Kingdom
[2] Department of Physics, University of Warwick – University of Warwick Gibbet Hill Road Coventry CV4 7AL, United Kingdom

Drops of active liquid crystal have recently shown the ability to self-propel, which was associated with topological defects in the orientation of active filaments [Sanchez *et al.* , Nature 491, 431 (2013)]. Here, we study the onset and different aspects of motility of a three-dimensional drop of active fluid on a planar surface. We analyse theoretically how motility is affected by orientation profiles with defects of various types and locations, by the shape of the drop, and by surface friction at the substrate. In the scope of a thin drop approximation, we derive exact expressions for the flow in the drop that is generated by a given orientation profile. The flow has a natural decomposition into terms that depend entirely on the geometrical properties of the orientation profile, i.e. its bend and splay, and a term coupling the orientation to the shape of the drop. We find that asymmetric splay or bend generates a directed bulk flow and enables the drop to move, with maximal speeds achieved when the splay or bend is induced by a topological defect in the interior of the drop. In motile drops the direction and speed of self-propulsion is controlled by friction at the substrate.

*Presenting author
†Corresponding author: D.Khoromskaia@warwick.ac.uk

P6: Improved Transferability of Coarse Grained Models for Polymer Crystallization Using Machine Learning

Chan Liu *† [1], Christine Peter [2], Kurt Kremer [1], Tristan Bereau [1]

[1] Max Planck Institute for Polymer Research – Ackermannweg 10 55128 Mainz, Germany
[2] University of Konstanz – Germany

Molecular dynamics simulations are a potentially powerful tool to study polymer crystallization. Coarse-grained (CG) models, which combine a number of atoms into superatoms or beads, can significantly speed up the simulations and provide reasonable resolution for studying polymer crystallization. One of the major challenges in CG modeling is the reduction of the number of degrees of freedom, making the resulting coarse models state point dependent; that is, they cannot easily be transferred to a range of temperatures, densities, system compositions, etc. Thus the force fields developed from the structures of an atomistic melt is not guaranteed to transfer to crystalline structures. The problem is, however, that most common strategies to derive CG models apply to liquids, not crystalline systems. In this work, we introduce a Machine Learning approach to improve an existing CG model parametrized for a different phase by predicting the deviation between CG and atomistic forces, which can be seen as an external force added on the original CG force field. This model predicts a force on each bead based on the surrounding geometry without projecting it onto pairwise potentials such that it can potentially reproduce many-body contributions. As a test case, the approach is applied to syndiotactic polystyrene. We evaluate the transferability of the new CG model by comparing structural parameters (e.g. order parameter, radial distribution functions, the distribution of the centers of molecules) in different phases with the atomistic model, which is obtained by using a backmapping method and running replica exchange molecular dynamics. This approach opens the perspective to modeling many-body interactions in CG simulations and thus improve the transferability and accuracy of its force field.

*Presenting author
†Corresponding author: liuchan@mpip-mainz.mpg.de

P7: Numerical analysis of the diffusive Peterlin viscoelastic model

Hana Mizerova * [1]

[1] Institute for Mathematics, Johannes Gutenberg University in Mainz – Germany

A mathematical model describing the unsteady behaviour of some incompressible polymeric fluids is studied. Polymers are treated as two beads connected by a spring. By the Peterlin approximation of the nonlinear spring force it is possible to obtain a closed system of equations for the conformation tensor. The macroscopic dumbbell-based model for dilute polymer solutions can be derived. More precisely, we have the conservation of mass, momentum and time evolution of the positive definite conformation tensor, where the diffusive effects are also taken into account. The existence and uniqueness of a weak solution, in two space dimensions, can be shown using the energy estimates, see [1]. For the Oseen-type Peterlin model we propose a linear pressure-stabilized characteristics finite element scheme that preserves the positive definiteness of the discrete conformation tensor. For the P1/P1/P1 finite element approximation of the velocity, pressure and conformation tensor we get the first order error estimates, cf. [2]. Experimental order of convergence is confirmed numerically. The results of the cavity flow problem for some viscoelastic fluids are presented. The present work has been supported by the German Science Foundation (DFG) under IRTG 1529 "Mathematical Fluid Dynamics" and TRR 146 "Multiscale Simulation Methods for Soft Matter Systems". It has been realized in collaboration with M. Lukáčová, Š. Nečasová, M. Renardy, M. Tabata, H. Notsu and B. She.

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*Presenting author

P8: Influences of biopolymers on calcium oxalate crystal growth

Leila Salimi Parvaneh * [1,2], Davide Donadio [2], Marialore Sulpizi [1]

[1] Institut für Physik – D 55099 Mainz, Germany
[2] Max Planck Institute for Polymer Research (MPIP) – Germany

Calcium oxalate occurs widely in kidney stones and among a variety of living organisms[1]. The presence of bio-polymers such as polyacrylate, polyaspartate or polyglutamate during the formation of calcium oxalate crystal has a great impact on the crystalline phase, morphology and growth rate[2-4]. In spite of advances in the experimental characterization of the influence that these bio-polymers exert on the crystallization, a full understanding of the processes that occur on a molecular scale has not yet been accomplished. First principle and classical Molecular dynamics simulations give detailed information on such processes and thus offer a valuable tool to complement the experimental investigations. In our work, we have applied a combination of these two methods in order to understand how polyglutamate affect the growth inhibition of calcium oxalate.
We have performed DFT-based Born-Oppenheimer Molecular dynamics (BOMD) simulations [5] to study the structural and dynamical properties of the interfaces between calcium oxalate dihydrate (COD) (100) and (101) and water. Our study reveals differences in the coordination of calcium ions at the surface with water. We also characterize the interaction between different surfaces of COD and biomolecules. As a first step we consider acetate as an analogue for the carboxylate group of glutamate side chains, and we estimate its binding structure and free energies on different COD surfaces at different coverage. Preferential binding of carboxylate to the (100) surface is found, providing a rational for recent experimental results on anisotropic growth of COD crystals in the presence of biopolymers [2].

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*Presenting author

P9: Integral equations for contact interaction problems

Ganna Shyshkanova * [1]

[1] Zaporizhzhya National Technical University (ZNTU) – 69063, Zaporizhzhya, Zhukovskyi st., 64 / Applied Mathematics Department, Ukraine

Mathematical modeling of three-dimensional contact interaction problems leads to solving of equations containing double integrals with weak singularity of the simple layer Newtonian potential or Reisz potential types with unknown density and unknown domain of integration. The unknown functions of the problem are a function, which characterizes the distribution of normal pressure, and functions of the domain boundaries. It is assumed that these functions depend on several parameters characterizing the geometry of contact bodies geometric shape and surface roughness. The contact problem solution gets particular relevance in the research of interaction of roughness surfaces taking into account losses on friction, contact rigidity of movable and unmovable joints, etc.

Analytic dependences for the potential calculation over ring are received, expressing integral operator kernels by Gegenbauer's polynomials. The technique based on expansion by small parameter is developed for doubly-connected contact domain reduction to the sequence of problems for ring domain. The expansion of simple layer potential is obtained when density has no circular symmetry. With use of it in every approximation, integral operators are transformed to Frechet differentiable operators. Taking into account roughness leads to Fredholm integral equations of 2nd kind. Coefficient of roughness deformation could be used as a parameter of regularization. Influences of the bodies shape geometry, type of loading, roughness and friction coefficients values are analyzed.

The advantages of the proposed method are easy possibility to receive simple formulae in closed form for each approximation, the formulae are convenient for qualitative analysis and durability calculations.

*Presenting author

P10: Numerical Study of transport and deposition of aerosols within human lungs bifurcation tubes

Sarita Singh * [1], Vinod Katiyar [2]

[1] Uttarakhand Technical University Dehradun, Uttarakhand India – WIT-Uttarakhand Technical University Dehradun, Dehradun-248001 Uttarakhand India, India
[2] Indian Institute of Technology Roorkee, India – Department of Mathematics, Indian Institute of Technology Roorkee, India, India

A deposition characteristic of aerosol particles within human upper airways is to be significant importance in two main applications. (i) Effect of assessment of potential on health. (ii) Deposition of drug. The human respiratory system, working in conjunction with the cardiovascular system, supplies oxygen to, and removes carbon dioxide from, the cells of the body. The respiratory system conducts air to the respiratory surfaces of the lungs. There, the bloods in the lung capillaries readily absorb oxygen and gives off carbon dioxide gathered from the body cells. The circulatory system transports oxygen-laden blood to the body cells and picks up carbon dioxide. The term respiration describes the exchange of gases across cell membranes both in the lungs (external respiration) and in the body tissues (internal respiration). The model of transport and deposition of aerosol within human lung bifurcation tubes will be solved numerically and a comparison will also discussed with the available experimental data.

*Presenting author

P11: Interplay between geometrical constrains and alphabet size in the design of patchy polymers

Chiara Cardelli *† [1], Valentino Bianco , Ivan Coluzza , Lorenzo Rovigatti

[1] Computational Physics Group University of Vienna – Sensengasse 8 1090 Wien Austria, Austria

Patchy polymers can be designed to self-assemble into specific structures. The aim of polymer design is to find a sequence of particles along the chain that will fold into a target structure, according to a given "alphabet" of interacting particles [1-2]. The alphabet size and the geometrical constraints introduced by the patches affects the designability of the polymer.
Here we study, via Monte Carlo simulation, how the alphabet size and the number of patches determine the phase space of the sequences and make the polymer designable.

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*Presenting author
†Corresponding author: chiara.cardelli@univie.ac.at

List of participants

- **Agoritsas, Elisabeth**, Université Grenoble Alpes, France, *elisabeth.agoritsas@ujf-grenoble.fr*
- **Annou, Karima**, Centre de Développement des Technologies Avancées, Algeria, *annoukarima@yahoo.fr*
- **Bennett, Rachel**, Oxford University, UK, *rachelcreedon@btinternet.com*
- **Bereau, Tristan**, Max Planck Inst. for Polymer Research, Germany, *bereau@mpip-mainz.mpg.de*
- **Bitbol, Anne-Florence**, Princeton University, USA, *anneflorencebitbol@gmail.com*
- **Cabriolu, Raffaela**, Université Grenoble Alpes, France, *raffaela.cabriolu@ujf-grenoble.fr*
- **Cardelli, Chiara**, University of Vienna, Austria, *chiara.cardelli@univie.ac.at*
- **Chertock, Alina**, North Carolina University, USA, *chertock@math.ncsu.edu*
- **Degtyareva, Olga**, Productivity for Scientists Ltd., UK, *olgandegtyareva@gmail.com*
- **Emamy, Nehzat**, Joh. Gutenb. University Mainz, Germany, *emamy@uni-mainz.de*
- **Eskandari, Zahra**, Max Planck Inst.for Polymer Research, Germany, *zahrascan@gmail.com*
- **Forero Martinez, Nancy C.**, Max Planck Inst. for Polymer Research, Germany, *forero@mpip-mainz.mpg.de*
- **Grushkovskaya, Victoria**, University of Stuttgart, Germany, *vi.grushkovskaya@gmail.com*
- **Guzman-Lastra, Francisca**, University of Düsseldorf, Germany, *francisca.guzman@thphy.uni-duesseldorf.de*
- **Helzel, Christiane**, University of Düsseldorf, Germany, *christiane.helzel@hhu.de*
- **Henkes, Silke**, University of Aberdeen, UK, *shenkes@abdn.ac.uk*
- **Hundertmark, Anna**, Joh. Gutenb. University Mainz, Germany, *hundertm@uni-mainz.de*
- **Jabbari Farouji, Sara**, Joh. Gutenb. University Mainz, Germany, *sjabbari@uni-mainz.de*
- **Jungblut, Swetlana**, University of Vienna, Austria, *swetlana.jungblut@univie.ac.at*
- **Karner, Carina**, University of Vienna, Austria, *carina.karner@univie.ac.at*
- **Katifori, Eleni**, University of Pennsylvania, USA, *katifori@gmail.com*
- **Kössel, Fabian**, Joh. Gutenb. University Mainz, Germany, *fkoessel@uni-mainz.de*

- **Kumari, Sunita**, Banaras Hindu University, India, *sunitabhu02@gmail.com*
- **Li, Fengyan**, Rensselaer Polytechnic Institute, USA, *lif@rpi.edu*
- **Liu, Chan**, Max Planck Inst. for Polymer Research, Germany, *liuchan@mpip-mainz.mpg.de*
- **Lukacova, Maria**, Joh. Gutenb. University Mainz, Germany, *lukacova@uni-mainz.de*
- **Manyuhina, Oksana**, Syracuse University, USA, *omanyuhi@syr.edu*
- **Marchetti, M. Cristina**, Syracuse University, USA, *mcmarche@syr.edu*
- **Martens, Kirsten**, Université Grenoble Alpes, France, *kirsten.martens@ujf-grenoble.fr*
- **Maskey, Sabina**, Clemson University, USA, *smaskey@g.clemson.edu*
- **Mizerova, Hana**, Joh. Gutenb. University Mainz, Germany, *mizerova@uni-mainz.de*
- **Morozova, Tatiana**, Lomonosov Moscow State University, Russia, *morozova.tatjjana@physics.msu.ru*
- **Necasova, Sarka**, Academy of Science Prague, Czech Republic, *matus@math.cas.cz*
- **Nerattini, Francesca**, University of Vienna, Austria, *francesca.nerattini@gmail.com*
- **Peter, Christine**, University of Konstanz, Germany, *christine.peter@uni-konstanz.de*
- **Pfirsching, Marion**, University of Mannheim, Germany, *mpfirsch@mail.uni-mannheim.de*
- **Prsha, Marija**, University of Zagreb, Croatia, *marija.prsha@gmail.com*
- **Rudzinski, Joseph**, Max Planck Inst. for Polymer Research, Germany, *rudzinski@mpip-mainz.mpg.de*
- **Saini, Anju**, Indian Institute of Technology Roorkee, India, *anju.iitr@gmail.com*
- **Salimi Parvaneh, Leila**, Joh. Gutenb. University Mainz, Germany, *salimi@uni-mainz.de*
- **Schilling, Tanja**, Luxembourg University, Luxembourg, *Tanja.Schilling@uni.lu*
- **Schlömerkemper, Anja**, University of Würzburg, Germany, *anja.schloemerkemper@mathematik.uni-wuerzburg.de*
- **Shyshkanova, Ganna**, Zaporizhzhya University, Ukraine, *shganna@yahoo.com*
- **Singh, Sarita**, Uttarakhand Technical University Dehradun, India, *saritamath@gmail.com*
- **Schmid, Friederike**, Joh. Gutenb. University Mainz, Germany, *friederike.schmid@uni-mainz.de*
- **Statt, Antonia**, Joh. Gutenb. University Mainz, Germany, *statt@uni-mainz.de*
- **Sulpizi, Marialore**, Joh. Gutenb. University Mainz, Germany, *sulpizi@uni-mainz.de*
- **Swierczewska-Gwiazda, Agnieszka**, University of Warsaw, Poland, *aswiercz@mimuw.edu.pl*
- **Trivisa, Konstantina**, University of Maryland, USA, *ktrivisa@gmail.com*
- **Virnau, Peter**, Joh. Gutenb. University Mainz, Germany, *virnau@uni-mainz.de*
- **Yeomans, Julia**, Oxford University, *julia.yeomans@physics.ox.ac.uk*
- **Zhang, Shuangshuang**, Joh. Gutenb. University Mainz, Germany, *zss1223@hotmail.com*
- **Zhou, Jiajia**, Joh. Gutenb. University Mainz, Germany, *zhou@uni-mainz.de*

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