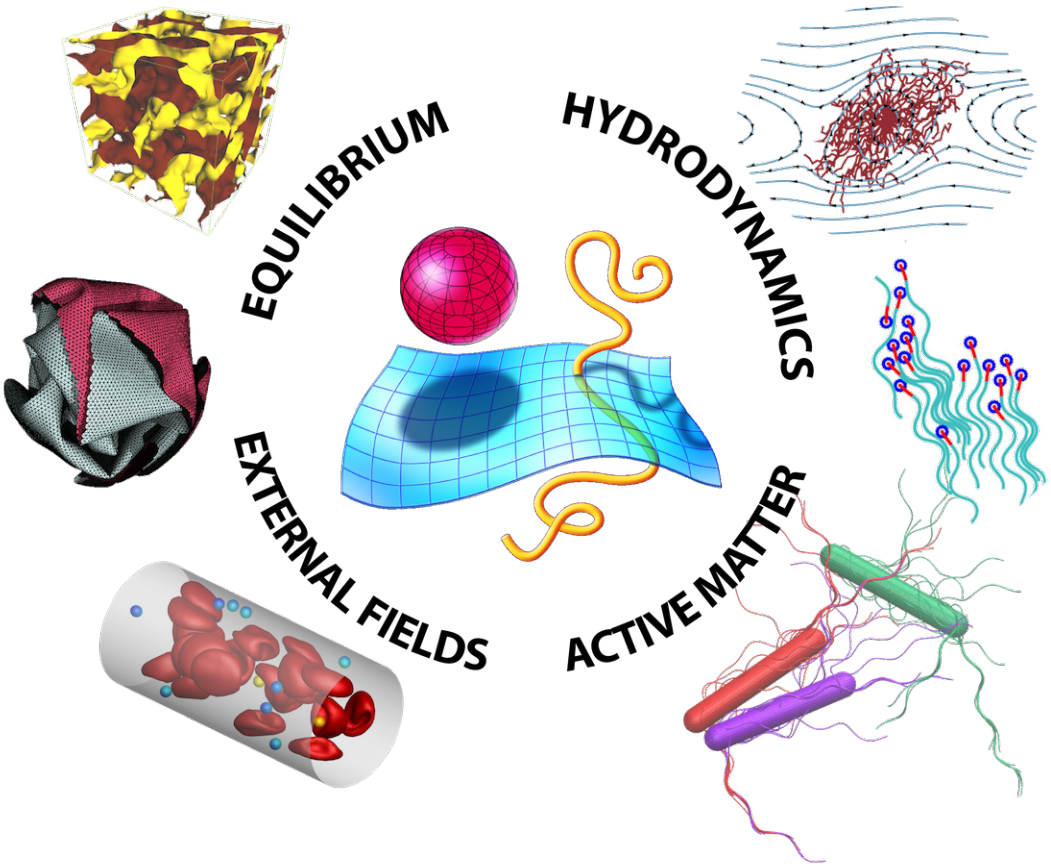
Symposium - From Membranes to Cells 2016

7 - 8 November 2016

Theoretical Soft-Matter and Biophysics (ICS-2)

Forschungszentrum Jülich

Abstracts of oral & poster contributions



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Scope

The symposium covers the structure and dynamics of complex fluids, soft matter, and biological systems, from colloids and (bio)polymers to the motion of cells, with emphasis on over 15 years of research at the Institute of Theoretical Soft Matter and Biophysics (ICS-2/IAS-2). This links fundamental aspects of statistical physics from membranes right up to complex biological structures, such as cells or swimming bacteria. Moreover, it provides a perspective on future developments in this dynamic field of research.

Monday, November 7

13.15	Bus leaves hotel	
14.00-14.15	Welcome	
		Chair: **Roland G. Winkler**
14.15-14.45	Michael Schick	**"Is the plasma membrane a two-dimensional microemulsion?"**
14.45-15.15	Ulrich Schwarz	**"Studying protein self-assembly with patchy particle models"**
15.15-15.45	Dmitry Fedosov	**"Fascinating red blood cell properties: non-equilibrium membrane fluctuations and intricate dynamics in flow"**
15.45-16.15	Coffee Break	
		Chair: **Thorsten Auth**
16.15-16.45	Erwin Frey	**"New Paradigms in Pattern Formation"**
16.45-17.15	Kurt Kremer	**"Polymeric Degrees of Freedom Do Matter: Polymer Melts, Elastomers, Collapsed Polymer Globules, Chromosome Territories etc"**
17.15-17.45	Roland Netz	**"A Highly Stretched Polymer in Water is an Energetic, not an Entropic Spring"**
17.45-18.15	Wim Briels	**"Coarse grain simulations of protein assemble: clathrin cages and alpha-synucleon fibers"**
18.30	Sebastian Schmidt	**"Over 15 years of Soft Matter and Biophysics"**
19.00-21.00	Poster session	
21.00		Bus to hotel

Tuesday, November 8

08.30	Bus leaves hotel	
		Chair: **Marisol Ripoll**
09.00-09.30	David Nelson	**"Thermalized sheets and shells: curvature matters"**
09.30-10.00	Reinhard Lipowski	**"From Membranes to Synthetic Cells"**
10.00-10.30	Friederike Schmid	**"Heterogeneous membrane structure and membrane-protein interactions: Insights from coarse-grained simulations"**
10.30-11.00	Thorsten Auth	**"Particle-membrane interaction: from model systems towards cells"**
11.00-11.30	Coffee break	
		Chair: **Dmitry Fedosov**
11.30-12.00	Siegfried Dietrich	**"Capillary forces on colloids at fluid interfaces"**
12.00-12.30	Hartmut Löwen	**"Colloidal particles in nonequilibrium: from nano-clutches to motility landscapes"**
12.30-13.00	Holger Stark	**"Hydrodynamics of active and passive colloids under confinement"**
13.00-14.30	Group Foto & Lunch break	
		Chair: **Gerrit Vliegenthart**
14.30-15.00	Benjamin Kaupp	**"In the realm of statistical physics - single-molecule sensitivity of sperm"**
15.00-15.30	Jens Elgeti	**"Swimming on the Edge"**
15.30-16.00	Joachim Krug	**"Genotypes, phenotypes, and Fisher's geometric model"**
16.00-16.30	Coffee break	
		Chair: **Jens Elgeti**
16.30-17.00	Udo Seifert	**"Biomolecular processes at steady state"**
17.00-17.30	Jan Dhont	**"Shear-gradient induced mass transport"**
17.30-18.00	Hansjörg Dittus	**"Search for Life beyond Earth - The Mainspring of Space Exploration?"**
18.15	Bus to hotel	
18.30	Bus to Burg Obbendorf	
18.30-22.00	Workshop dinner	
22.00		Busses to Rurtalbahn, hotel and Forschungszentrum

Poster contributions

P01	C. Abaurrea Velasco	Collective behavior of swimmers with density-dependent motility
P02	D. Alizadehrad	A nearly incompressible mesoscopic method for simulating complex fluids and flows
P03	H. Annepu	Dynamics of spheroidal squirmers in Poiseuille flow
P04	S. Das	Short time dynamics of crowded protein solution
P05	A. K. Dasanna	Interplay of adhesion and elasticity of infected erythrocytes during malaria life cycle
P06	Ö Duman	Dynamics of Collective Cell Motility
P07	T. Eisenstecken	Conformational properties of active semiflexible polymers
P08	N. Ganai	A Computer Simulation Study of Bulk Tissue Competition
P09	A. Ghavami	Polymer Dynamics of Microgel Particles: A Multiparticle Collision Dynamics Simulation Study
P10	E. Henry	Sorting red blood cells by their dynamical properties
P11	M. Hoore	von Willebrand factors and Platelets in Blood Stream: Margination and Adhesion
P12	R.Hornung	Simulating growing Sheets; Buckling and Folding
P13	A. Lamura	Dynamical behavior of vesicles in shear flow
P14	R. Li	Characterization of small anisotropic colloids by means of time-resolved flow Dichroism
P15	J. Mauer	Shape and Dynamics of Single Red Blood Cells in Shear and Tube Flows
P16	D. Niether	Thermophoretic accumulation in hydrothermal pores
P17	H. Noguchi	Membrane Shape Transformation Induced by Banana-Shaped Protein Rods
P18	A. Ravichandran	Cytoplasmic Rotation in a Coarse-Grained Model of Cortical Microtubules and Asymmetric Motor Composites
P19	J. Riest	Colloids with competing short-range attraction and long-range repulsion: Structure and dynamics
P20	B. Sabass	Collective bacterial migration is governed by two distinct force patterns
P21	G. M. Schütz	Slip of grip of a molecular motor on a crowded track: Modeling shift of reading frame of ribosome on RNA template
P22	K. Singh	Nanoparticle wrapping by receptor-mediated adhesion
P23	S. Sohn	A coarse-grained elastic model for cell deformation
P24	Z. Tan	Anisotropic Thermophoresis: Micro-geometry Matters
P25	M. Theers	Does hydrodynamics enhance phase separation of microswimmers?
P26	V. Vadhana	Confinement Induced Phase Transitions of a Soft Sphere Fluid: A Molecular Dynamics Study
P27	M. Wagner	Shape-Induced Hydrodynamic Effects in Thermophoretic Microswimmers
P28	M. Werner	Theory of Passive Polymer Translocation Through Amphiphilic Membranes
P29	Q.Yu	Nanoparticle uptake by vesicles

Abstracts of oral presentations

T01 - "Is the plasma membrane a two-dimensional microemulsion?"

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The "raft" hypothesis posits that the plasma membrane, which surrounds all cells, is heterogeneous consisting of regions of saturated lipids and cholesterol, which float in a "sea" of unsaturated lipids. The size of these rafts is thought to be on the order of 10 to 100 nanometers. The idea remains controversial, not only because the experimental evidence for such rafts is indirect, but also because there is little theoretical basis for their existence and for this particular size. I shall argue that it is likely that the plasma membrane is a two-dimensional microemulsion whose characteristic size emerges naturally from the elastic properties of the membrane.

T02 - Studying protein self-assembly with patchy particle models

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Supramolecular protein assemblies are central to many cellular processes and often can be reconstituted in the test tube, for example clathrin cages, virus capsids, the cartwheel of centrioles or the actin lamellipodium. Strikingly, these structures often have geometrically well-defined architectures, like filaments, rings, spherical capsules or branched networks, that relate to their specific function in the cell. We have explored several variants of patchy particles models that encode the architecture of the corresponding protein assembly in the definitions of the reaction patches. For purely geometrical patch definitions, we have developed a Brownian Dynamics scheme that ensures detailed balance and proper translational and rotational diffusion properties of the intermediates [1]. In order to study misformed structures, one can define reaction patches through anisotropic interaction potentials with appropriate rigidities. Moreover interaction with hydrodynamic flow can be investigated by embedding patchy particles in a solvent simulated with multi-particle collision dynamics (MPCD) [2]. We discuss several biologically relevant applications of the patchy particle approach. For virus self-assembly, we show that different assembly schemes and production rates are optimal for different molecular bond strengths [3,4]. For the SAS-6 rings forming the core of centrioles, we find that physiological protein concentrations are not sufficient to ensure ring formation, except in the presence of scaffolds [5]. For both rings and capsids, we find that shear flow can enhance protein self-assembly [2].

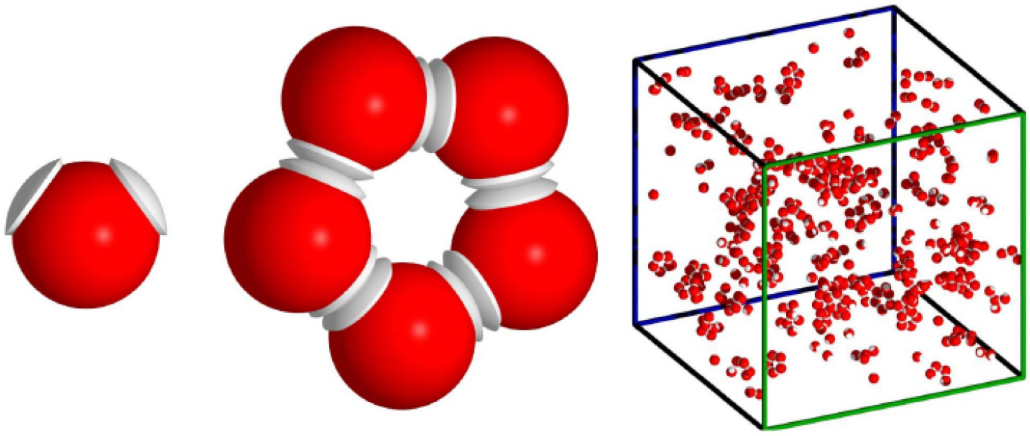

Fig. 1: *Assembly of five-fold rings from patchy particles in a Brownian Dynamics simulation with detailed balance [1].*

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T03 - Fascinating red blood cell properties: non-equilibrium membrane fluctuations and intricate dynamics in flow

J. Mauer[1], H. Turlier[2], S. Mendez[3], L. Lanotte[4], T. Auth[1], J.-F. Joanny[5], T. Betz[6], M. Abkarian[4], G. Gompper[1], and D. A. Fedosov[1]

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Red blood cells (RBCs) constitute the major cellular part of blood and are mainly responsible for the transport of oxygen. They have a biconcave shape with a membrane consisting of a lipid bilayer with an attached cytoskeleton formed by a network of the spectrin proteins. The RBC membrane encloses a viscous cytosol (hemoglobin solution), so that RBCs possess no bulk cytoskeleton and organelles. Despite this simple structure in comparison to many other cells, RBCs exhibit fascinating properties and behavior in flow. One such example is membrane flickering, which can be easily observed under optical microscopy. This phenomenon has been initially attributed to pure thermal fluctuations of the cell membrane, and later followed by several suggestions about the possible involvement of non-equilibrium processes [1], without definitively ruling out equilibrium interpretations. Our recent study has rigorously shown the involvement of non-equilibrium processes through a violation of the fluctuation-dissipation relation, which is a direct demonstration of the non-equilibrium nature of flickering [2]. Another interesting example is the behavior of RBCs in flow, which show complex deformation and dynamics. Current simplified understanding of RBC behavior in shear flow is that they tumble or roll at low shear rates and tank-tread at high shear rates. This view has been mainly formed by a number of experiments performed on RBCs dispersed in a viscous solution, which is several times more viscous than blood plasma [3]. However, under physiological conditions with increasing shear rates, RBCs successively tumble, roll, deform into rolling stomatocytes, and finally adopt highly-deformed poly-lobed shapes [4]. This behavior is governed by RBC elastic and viscous properties and it is important to consider it under relevant physiological conditions.

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T04 - New Paradigms in Pattern Formation

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What does ``self'' in self-organisation refer to? Is there a physical process mediating this ``self''-organisation? In this talk I will explain how these questions can be similarly addressed for diverse system classes which are based on interactions that conserve some quantity, such as mass in chemical dynamics, strategies in zero-sum games, or prices in transactions on liquid markets. I will start from the observation that lateral instabilities in reaction-diffusion systems generically induce movement of local equilibria. Using a well-established model for biological pattern formation as a paradigmatic example, I will show that such shifts can destabilise local equilibria endogenously, driving the system into a turbulent state. Remarkably, this shows that order can re-emerge from the turbulent state when distinct unstable modes work in concert to control local destabilisation.

T05 - Polymeric Degrees of Freedom Do Matter: Polymer Melts, Elastomers, Collapsed Polymer Globules, Chromosome Territories etc

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The role of topological constraints on conformational as well as relaxational and dynamical properties of open linear and closed ring polymers as well as mixtures thereof is discussed. In the case of polymer melts the conformational statistics can be used to directly determine the entanglement molecular weight in excellent agreement to experiment. By manipulating the entanglements through non-equilibrium processes in long chain melts materials with new rheological properties can be obtained. For ring polymers the situation is completely different. While linked rings act like DeGennes' Olympic gels, we find that non concatenated polymer rings segregate and form individual "collapsed" objects. I discuss some details of their conformations, which not only is related to one of the very basic problems in polymer science but also has far reaching consequences from the collapse of gels to chromosome territories. Furthermore chain length effects play a decisive role when it comes to structure formation in driven systems.

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T06 - A Highly Stretched Polymer in Water is an Energetic, not an Entropic Spring

Susanne Liese and Roland R. Netz

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In many applications, a polymer's elastic response against conformational deformations is key to its function. According to text book knowledge, a polymer reacts to the stretching of its end-to-end separation by an increase in entropy that is due to the reduction of available molecular conformations. This is why polymers are commonly called entropic springs. By a combination of single-molecule force spectroscopy experiments with molecular dynamics simulations in explicit water, we show that PEG in fact turns from an entropic into an energetic spring at moderate stretching. The thermodynamic analysis of our simulation trajectories reveals that the conformational entropy price of chain stretching is compensated by the entropy gain associated with the release of water molecules forming double hydrogen bonds with the PEG backbone in the low-stretching state. As a consequence, the stretching response of PEG is predominantly of energetic, not of entropic, origin and caused by the release of strongly energetically bound water upon stretching. These findings not only challenge a basic notion of polymer science but also constitute a case example that sheds light on the antagonistic interplay of conformational solute and solvent degrees of freedom.

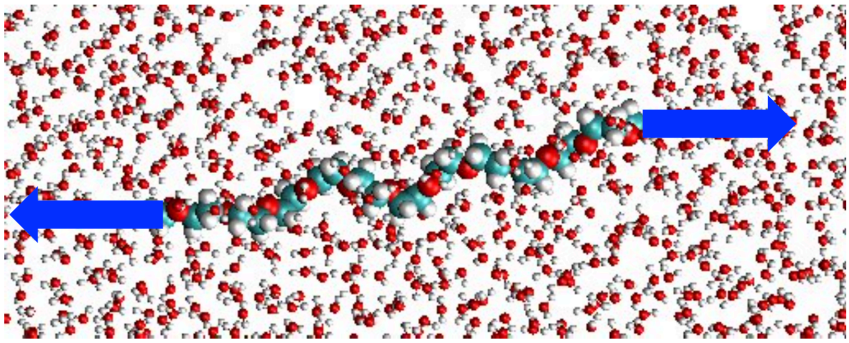

Fig. 1: *Snap shot of the MD simulation for a PEG chain with N = 11 segments at a stretching force of f = 120pN.*

T07 - Coarse grain simulations of protein assemble: clathrin cages and alpha-synucleon fibers

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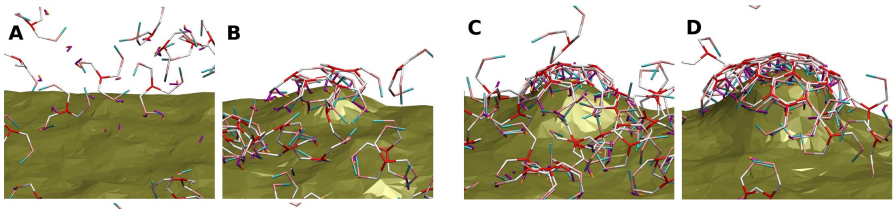
Under favorable conditions clathrin triskelia have the ability to self assemble into cages, predominantly those consiting of sixty clathrins. The triskelion molecule consists of three legs, each containing several proteins, and attached to a central point. We have developed a coarse grain model for these molecules and extracted the interaction energy between neighboring legs from experimental data on the critical self assembly concentration. The main function of clathrins is to self assemble near a membrane and by this construct a bag wrapped around cargo on the other side of the membrane. We have managed to simulate the first stages of this process.



As a second example of the use of coarse grain protein models I will present simulations of the self-assembly of the amyloidogenic core of alpha-synucleon into long fibers. These long fibers are assumed to play an important role in the development of Parkinson's disease. In our simulations the protein is modelled as a short chain of chameleonic particles able to change their structure from elongated cylinders forming beta sheets to spherical beads (representing disordered and alpha helix configurations).

T08 - Thermalized sheets and shells: curvature matters

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Understanding deformations of macroscopic thin plates and shells has a long and rich history, culminating with the Föppl-von Karman equations in 1904, characterized by a dimensionless coupling constant (the "Föppl-von Karman number") that can easily reach FvK = 10^7 in an ordinary sheet of writing paper. However, thermal fluctuations in thin elastic membranes fundamentally alter the long wavelength physics, as exemplified by experiments from the McEuen group at Cornell that twist and bend individual atomically-thin free-standing graphene sheets (with FvK = 10^{13}!) We review here the remarkable properties of thermalized sheets, where enhancements of the bending rigidity at T = 300K by factors of ~5000 have now been observed. We then move on to discuss thin amorphous spherical shells with a uniform nonzero curvature, accessible for example with soft matter experiments on diblock copolymers. This curvature couples the in-plane stretching modes with the out-of-plane undulation modes, giving rise to qualitative differences in the fluctuations of thermal spherical shells compared to flat membranes. Interesting effects arise because a shell can support a pressure difference between its interior and exterior. Thermal corrections to the predictions of classical shell theory for microscale shells diverge as the shell radius tends to infinity.

T09 - From Membranes to Synthetic Cells

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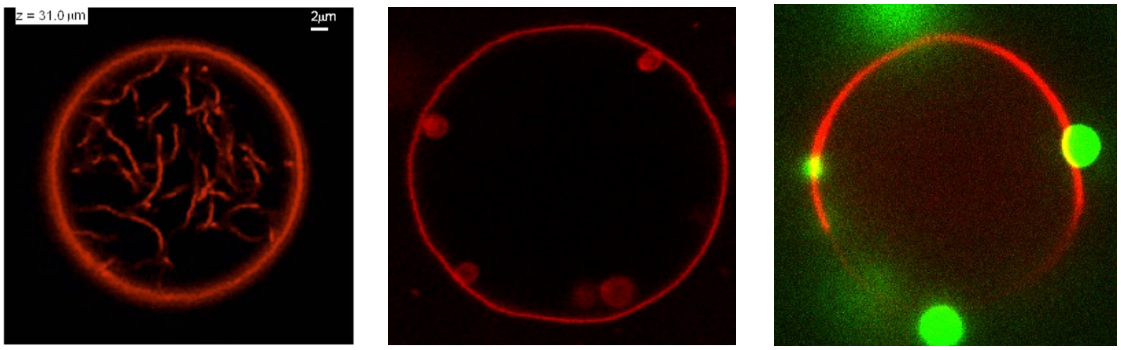
The spatial architecture of biological cells is based, to a large extent, on fluid membranes that separate space into separate compartments. These compartments are flexible and can be remodeled with respect to their morphology and composition. Analogous remodeling processes can be studied using giant unilamellar vesicles (GUVs) as shown in Fig. 1. This figure displays examples for spontaneous tubulation, [1, 2] protein-induced budding, [3, 4] and partial wetting by protein-enriched droplets [5]. The last example is intimately related to the recent discovery that cells contain membrane-less organelles that behave like liquid droplets.

Because of their fluidity, the membrane-bound and droplet-like compartments are highly dynamic and can change their topology via fusion and fission. For membrane compartments, these topology-changing processes can be spatially localized to intramembrane domains. Both types of fluid compartments provide useful modules for a bottom-up approach to synthetic biology. The talk will end with a brief outlook on this emerging research field as currently pursued in the MaxSynBio consortium.



(a) (b) (c)

Fig. 1: *Three remodeling processes of GUV membranes (red):* **(a)** *Spontaneous tubulation of a membrane that has acquired a large spontaneous curvature by polymer adsorption [2];* **(b)** *Membrane budding induced by membrane-bound proteins [3]; and* **(c)** *Partial wetting of a membrane by liquid droplets enriched in intrinsically disordered proteins (green) [5].*

Acknowledgements

The MaxSynBio consortium is cofunded by the Max Planck Society and the Federal Ministry of Education and Research, Germany.

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T10 - Heterogeneous membrane structure and membrane-protein interactions: Insights from coarse-grained simulations

Friederike Schmid

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We have used coarse-grained simulations of a generic molecular model for lipid membranes to gain insights into physical mechanisms that influence the structure and phase transitions of lipid membranes and the interactions between lipids and proteins. Here I focus on two aspects: (i) The interactions of membranes with inclusions and the comparison with a simple elastic theory. (ii) The formation of nanoscale domains in multicomponent membranes and a possible explanation in terms of the same elastic theory. Similar domains have been observed experimentally in binary and ternary model membranes. In an outlook, I report on ongoing work on the interactions of membranes with fibril-forming peptides.

T11 - Particle-membrane interaction: from model systems towards cells

S. Dasgupta[1,2], K. Singh[1], Q. Yu[1], T. Auth[1], and G. Gompper[1]

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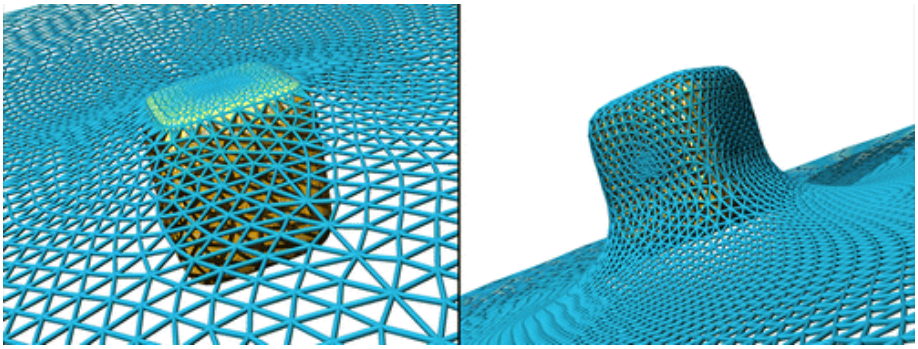
Shape and surface properties crucially determine the interactions of particles with lipid-bilayer membranes [1-3] and fluid interfaces [4]. Recent advances in nanotechnology have made a zoo of engineered particles with different shapes available for applications, and a wide variety of shapes is also found for viruses and parasites. Membrane or interface deformations caused by adhered particles lead to deformation-mediated interactions and self-assembly.

For particles at membranes, the relevant energy contributions are deformation and adhesion energy. Particle shape strongly influences the deformation energy and therefore the wrapping state of a particle. Non-spherical particles experience an increased stability of membrane-bound states compared with spherical particles [1,2]; for cube-like and rod-like particles, two partially-wrapped membrane-bound states are found that are separated by an energy barrier. Egg-shaped malarial parasites that invade erythrocytes are a very interesting special case where the wrapping phase diagram even has a critical point [3]. The wrapping phase diagrams that we calculate for model systems systematically characterize particle-membrane interaction, which helps to understand the interaction of nanoparticles with biological cells. Towards the interaction of particles with biological cells, we have recently started to also investigate specific, receptor-ligand binding between nanoparticles and cells in addition to adhesion via homogeneous van-der-Waals interaction. We find a partially-wrapped states for high receptor-ligand bond energies and for low receptor densities, as well as Langmuir-like binding isotherms.



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T12 - Capillary forces on colloids at fluid interfaces

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Colloidal particles, which are trapped at fluid interfaces, deform them. This gives rise to effective lateral interactions among such colloids. Under favorable conditions this capillary interaction resembles two-dimensional gravity or electrostatics. Accordingly, these systems can be described in terms of permanent or induced capillary multipoles. This provides a simple interpretation of numerous experimental observations.

In a further analogy, the presence of thermally excited capillary waves generates Casimir-like forces between the colloidal particles, but with a larger variety of possible boundary conditions as compared with the case of the standard Casimir force.

The capillary attraction among the colloids drives their collective dynamics. This dynamics exhibits an instability which is formally analogous to the gravitational instability on cosmological scales. Corresponding analytic and simulation studies are discussed.

T13 - Colloidal particles in nonequilibrium: from nano-clutches to motility landscapes

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Colloidal suspensions are ideal model systems for confinement effects on the submicron scale [1]. In this talk, some recent advances in understanding effects of adaptive and flexible confinement which is steered externally are summarized. The idea of a colloidal corral is proposed which encircles and confines passive Browian particles. This corral enables to measure the osmotic pressure directly by steering the confinement [2]. The adaptivity induces a unfamiliar multiple relaxation scenario close to the kinetic glass transition [3] and can finally be rotated realizing a colloidal "washing machine" which acts like a clutch and can be used to transmit torque [4]. Finally active Brownian articles in externally steered motility landscapes will be adressed [5].

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Nature Communications **7**, 12828 (2016).

T14 - Hydrodynamics of active and passive colloids under confinement

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Confining soft matter helps to explore the full range of inherent properties of a specific system. In this talk we mostly use hydrodynamic simulations with multi-particle collision dynamics, a technique pushed forward at the FZ Jülich, to explore how passive colloids and microswimmers behave under strong confinement.

First, simulations of dense colloidal suspensions under pressure-driven flow in narrow microchannels reveal self-organized rarefaction pulses traveling upstream similar to experimental observations. Force chains span between the channel walls and create transiently jammed regions, which are unjammed by the rarefaction pulses. Frictional contacts between colloids and most importantly between colloids and walls are necessary for the pulses to occur. We rationalize the traveling pulses in a phenomenological model.

Second, we use squirmers as model swimmers to explore phase separation of active systems in a quasi-two-dimensional geometry. For sufficiently large swimming speed the squirmers, strongly confined between two plates, indeed phase-separate into a dilute and a dense phase. However, strangely enough, the binodal of the dilute phase depends on the mean density. We explain this feature by studying the mechanical pressure balance in the system. In addition to active and steric pressure, we need to include a hydrodynamic pressure, which explicitely results from the flow field generated by the squirmers, in order to fulfill pressure balance.

Lastly, I demonstrate how different types of self-propelled particles, such as active Brownian and run-and-tumble particles (bacteria), behave differently in a regular maze.

Acknowledgements

Our work is funded by the DFG through the priority program SPP 1726, *Microswimmers - from Single Particle Motion to Collective Behaviour,* and the research training group GRK 1558 *Nonequilibrium collective dynamics in condensed and biological system,* as well as the VW foundation within the program *Computational Soft Matter and Biophysics* and the Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen (HLRN).

T15 - In the realm of statistical physics – single-molecule sensitivity of sperm

U.B. Kaupp

Sperm must find the egg during fertilization. The egg assists fertilization by releasing chemical factors that attract sperm. The sperm flagellum serves both as antenna that registers the chemoattractant, as motor that propels the cell, and as rudder for steering. Sperm are exquisitely sensitive: they can register the binding of a single molecule of chemoattractant and respond with a Ca^{2+} signal. Ca^{2+} controls the flagellar beat and, thereby, the steering response. I will discuss the cellular signaling pathway that endows sperm with single-molecule sensitivity and controls navigation in a chemical gradient. During navigation, sperm perform a surprisingly rich variety of computational operations; they can count, differentiate, integrate, and they can reset their signaling pathway. We use a variety of kinetic, opto-chemical, and photonic techniques to delineate the sequence of signaling events and to control navigation in a chemical gradient. Using Digital Inline Holographic Microscopy, we follow 3D navigation of sperm in a complex 3D landscape of the chemoattractant.

T16 - Swimming on the Edge

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Both, in their natural environment and in a controlled experimental setup, microswimmers regularly interact with surfaces. These surfaces provide a steric boundary, both for the swimming motion and the hydrodynamic flow pattern. These effects typically imply a strong accumulation of microswimmers near surfaces. While some generic features can be derived, details of the swimmer shape and propulsion mechanism matter, which give rise to a broad range of adhesion phenomena and have to be taken into account to predict the surface accumulation for a given swimmer. Over the past decade, we studied many different forms of surface adhesion, ranging from relatively detailed sperm models with full hydrodynamic interactions to idealized self-propelled Brownian spheres. In this talk, I demonstrate how numerical simulations and analytic theory can be used to predict the accumulation statistics for different systems, with an emphasis on swimmer shape, hydrodynamics interactions, and type of noise.

Acknowledgements

Over twelve years of fruitful collaborations with Gerhard Gompper is highly appreciated

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T17 - Genotypes, phenotypes, and Fisher's geometric model

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Biological evolution can be conceptualized as a dynamical process in the space of gene sequences guided by the *fitness landscape*, a mapping that assigns a measure of reproductive value to each genotype [1]. The relationship between genotype and fitness is generally complex, as it is mediated by the multidimensional organismic phenotype that interacts with the environment and thereby determines reproductive success. A simple mathematical framework for exploring this relationship is provided by *Fisher's geometric model* (FGM), which describes the phenotype as a vector in an n-dimensional Euclidean trait space with a unique optimum located at the origin [2]. Genetic mutations are encoded as random phenotypic displacements, and complex fitness landscapes arise from the projection of the discrete network of genotypes onto the continuous trait space (Fig. 1). The talk will discuss the properties of these fitness landscapes from the viewpoint of statistical physics, and describe a recent analysis of interactions between beneficial mutations in the fungus *Aspergillus nidulans* based on FGM [3].

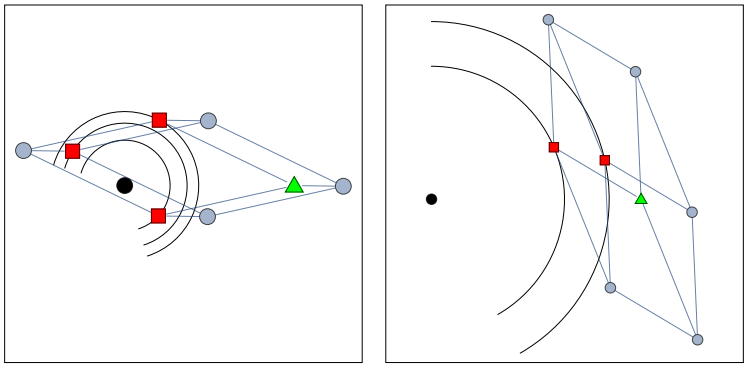

Fig. 1: *Illustration of the relationship between phenotypes and genotypes in FGM. The genotype space is spanned by three random mutational vectors originating from the wildtype phenotype (triangle), and the circles are lines of constant fitness. Although the phenotypic optimum is unique (black dot), there are multiple genotypic fitness maxima (squares).*

Acknowledgements

This work has been supported by DFG within SFB 680 *Molecular basis of evolutionary innovations* and SPP 1590 *Probabilistic structures in evolution*.

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T18 - Biomolecular processes at steady state

U. Seifert

Conceptually, a non-equilibrium steady state is arguably one of the simplest paradigms of statistical physics. Within the framework of stochastic thermodynamics [1], they allow for quite universal statements. After a brief review of the foundations, I will introduce a couple of our recent results for biomolecular processes. In particular, I will discuss the inevitable costs of precision in any such process in terms of a thermodynamic uncertainty relation [2]. As an example how an effective temperature can emerge in a steady state, I will present our joint experimental and theoretical investigation of mechanically excited DNA hairpins [3].

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T19 - Shear-gradient induced mass transport

Non-uniform flow of glasses and gels

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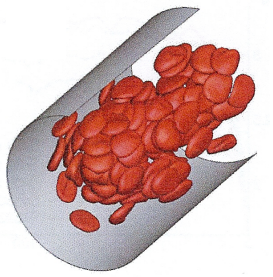
In many systems under flow conditions (like granular matter, blood [see the figure], and macromolecular solutions) with inherent spatial gradients of the shear rate, direct interactions lead to transport of matter from regions of high to low shear rate. In this presentation, the origin of such shear-induced mass fluxes resulting from direct interactions will be discussed, and an explicit expression for the corresponding transport coefficient is derived. The mechanism through which shear-gradient induced mass transport leads to non-uniform, shear-banded flow profiles in colloidal glasses and gels is discussed. The advection-diffusion equation that includes shear-gradient induced mass transport, together with an appropriate equation of motion for the flow velocity, including non-local stresses, are solved numerically. The resulting shear-banded flow profiles will be compared to experiments on hard-sphere colloidal glasses.



Red blood cells in a cylindrical tube. The cells migrate to the center. From: *D. Katanov, G. Gompper, D.A. Fedosov Microvasc Res. 2015,* ***99****, 57.*

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T20 - Search for Life beyond Earth - The Mainspring of Space Exploration?

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The idea to explore the world beyond earth became a serious desire at the the end of the 19th century when technique lead to an industrial revolution. It became obvious that humans will be able to go to space one day. The tremendous progress which space technology underwent within the last 60 (!) years led to a new picture of the cosmological history but also changed our sight to life and its evolution.

Abstracts of poster presentations

P01 - Collective behavior of swimmers with density-dependent motility

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Microswimmers span from bacteria to human-made nanorobots [1]. To simulate collective behavior, generic models allow to study a large number of particles and to still maintain certain characteristics, such as the aspect ratio. Because many biological swimmers are anisotropic, we use self-propelled rods in two dimensions that interact with a soft repulsive potential. Our capped interaction potential allows rods to cross each other [2]. This makes our simulations suitable for studying quasi-2D experiments, such as microtubule motility assays or a thin layer of swimming bacteria.

The phase behavior of monodisperse rods with constant self-propulsion has been characterized systematically [2, 3]. While for low densities cluster formation is observed, at high densities laning is found. However, many biological swimmers show density-dependent motility, such as quorum sensing phenomena in bacteria [4]. Density-dependent self-propulsion can be characterized by the ratio of the propulsion velocity of a single rod and a rod in a dense environment, and by and exponential dependence with the number of neighboring particles. We study for the first time self-propelled rods with physical interactions and a density dependent propulsion force. We show that by decreasing the self-propulsion of the rods with the local density of swimmers the polar alignment and phase segregation are favored. Enhanced phase segregation helps bacterial colonies in biofilms become more compact, which increases their resistances against external chemical agents.

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P02-A nearly incompressible mesoscopic method for simulating complex fluids and flows

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Numerical simulation and theoretical modeling of mesoscopic processes, ranging from microorganisms in biofilm formation to flow of dense suspensions of small deformable particles and macromolecules in complex environment, are constantly challenged by the large separation of time scales and length scales. Recently, to address some drawbacks of previous methods, smoothed dissipative particle dynamics (SDPD) was established[1, 2]. The aim of this work is to provide a general framework and efficient set of SDPD parameters including liquidlike macroscopic transport coefficients for simulating mesoscopic complex fluids. We consider the effect of weight function, temperature, SDPD parameters, and most importantly the equation of state on the speed of sound as well as on other SDPD fluid properties such as viscosity, structure, and diffusion coefficient. Modifying the equation of state, we show that the speed of sound can be controlled, while radial distribution function (RDF) and Schmidt number correspond to liquid state.

Performing reverse-Poiseuille flow simulations, we have considered viscosity and RDF variation versus shear rate. The RDF in equilibrium and in shear flow remains same and independent of shear rates. This is an advantage in modeling of structures and boundaries either rigid or deformable. Furthermore, for appropriate course-graining parameters measured viscosity shows very slight changes (around 1-2 percent) over several orders variation of shear rates. The averaged mean-square displacement (MSD) of the solvent particles shows liquidlike diffusive motion ($\langle R^2 \rangle \propto t$), even for low temperatures. We also show an analytical approximation for diffusion coefficient, which agrees very well with that determined from MSD. Finally, we present the applicability of the method to modeling cellular blood flow as an example of complex fluid in irregular geometries. Density variation either inside the fluid or close to wall-surface remains smaller than one percent and the velocity field satisfies well the divergence-free condition, indicating that the simulated fluid is nearly incompressible. In conclusion, our results demonstrate the true nearly continuum liquid behavior of the defined course-grained system, which reproduces the Navier-Stokes solutions, and thereby provides a powerful approach for the quantitative analysis of complex mesoscopic processes.

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P03 - Dynamics of spheroidal squirmers in Poiseuille flow

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Bacteria such as *E. coli* exhibit a remarkable rheological behavior. On the one hand, the viscosity exhibits a Newtonian plateau at low shear rates, which decreases with increasing concentration. On the other hand, the bacteria exhibit positive rheotaxis, i.e., they swim preferentially upstream next to surfaces. This points toward an intriguing interplay between the swimmer flow field with the surface [1]. An understanding of this behavior is important, for example, for biofilm formation and may also be helpful in applications with bacteria as viscosity modifiers. To analyze the properties of microswimmers in channel flows, we consider spheriodal squirmers [2] with a rotlet dipole embedded in a MPC fluid [3] and study their flow-induced structure and dynamics. Depending on where the thrust is generated, the squirmers are classified as pullers (thrust is generated in front of the organism), pushers (thrust is generated behind the organism), and ciliates (symmetric velocity field). The no-slip boundary condition at a surface combined with the swimmer characteristics (puller, pusher) leads to a preferential alignment parallel (pusher) or perpendicular (puller) to the wall. This applies to both, spherical as well as spheroidal squirmers as long as they are not to close to a surface and the hydrodynamics is determined by the far field. We want to shed light on the influence of near-field hydrodynamic interactions on the swimming behavior of spheroidal squirmers close to surfaces. Our simulations reveal a dependence of the swimming behavior under flow on the shape of the microswimmer. We find positive rheotaxis for spheroidal pushers in narrow channels, which disappears in the limit of zero rotlet dipole strength.

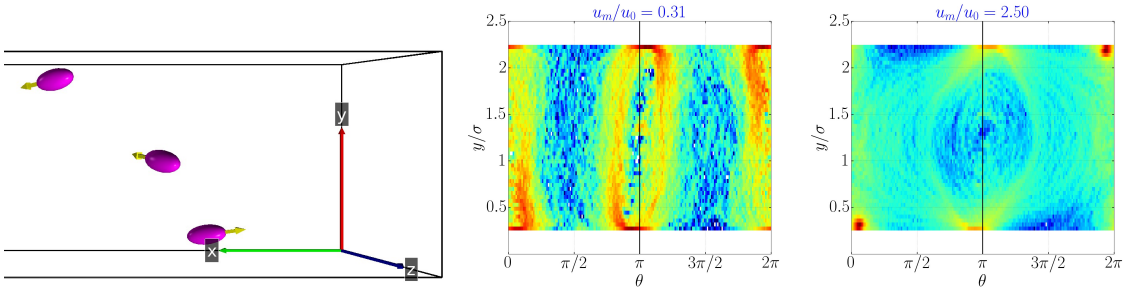

Fig. 1: *Spheroidal pushers displaying upstream motility (swimming in $x-$ direction) in a channel at low shear rates. Probability density function for the pushers' position y/σ within the channel and alignment angle θ along flow direction for low (left) and high (right) flow rates.*

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P04 - Short time dynamics of crowded protein solution

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Proteins in aqueous solution can organize into complex structures which effect the diffusive behaviour of the protein. For example, mammalian eye-lens proteins can form gel-like structures when suspended in water and exhibit dynamical arrest in crowded conditions [1]. We investigate the static and dynamical properties of such attractive globular proteins using a hybrid coarse-grained simulation approach. The proteins are modelled as colloidal particles and treated by molecular dynamics simulations. The surrounding fluid is described by the multiparticle collision dynamics method, a mesoscale hydrodynamic technique [2-5]. Colloids with isotropic interaction are studied, as well as colloids with additional attractive patchy interactions. We observe a space-spanning percolating network of the patchy colloids with a considerable influence on their dynamics. We analyze the properties of the network-like arrangement to get insight into the structure of the colloidal aggregates. Thus, we conclude that the complex "patchy" interactions of proteins give rise to a dynamic behaviour in crowded environments which differs drastically from that of spherical colloids.

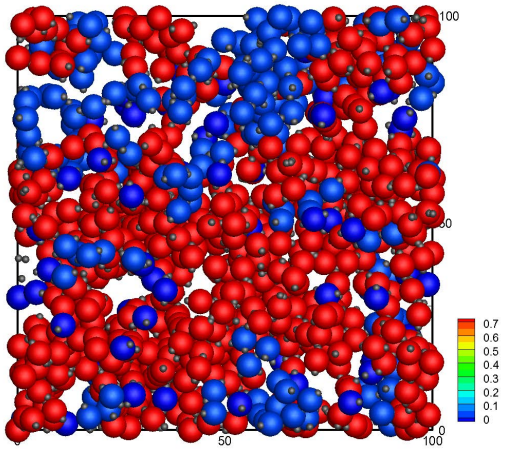

Fig. 1: *Configuration of colloids with patch attraction for volume fraction $\phi = 0.1$. The color code indicates the cluster size distribution.*

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P05 - Interplay of adhesion and elasticity of infected erythrocytes during malaria life cycle

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One of the most severe forms of malaria is caused by the unicellular parasite *Plasmodium falcipuram*. During the blood stage of the malaria life cycle, infected red blood cells (iRBCs) develop supramolecular adhesive protrusions on their surface, so-called *knobs*. The number of the knobs increases over the 48 hours infectious life cycle and leads to adhesion of the iRBCs to the endothelial cells in the microvasculature. This in turn results in capillary obstruction and contributes to the symptoms of the disease.
Here we report measurements of the adhesion strength of infected erythrocytes during the blood stage of malaria. Adhesion strength is characterized by contact area of adherent cells to a substrate coated with CSA (chondroitin sulfate A) ligands. Quantitative understanding of how adhesion strength is modified by elasticity and knob density is achieved by combining both experimental data and mesoscopic modelling [1, 2]. We show that the interplay between adhesion and elasticity leads to interesting morphological behavior (see Fig.1) of red blood cells during the life cycle of the malaria. This complements recent measurements of volume and surface area of iRBCs in suspension [3].

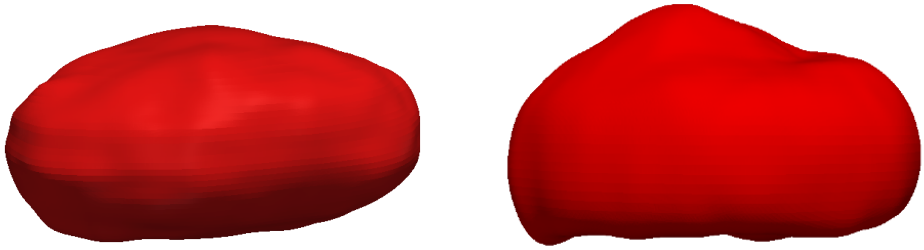

Fig. 1: *Typical three dimensional shapes of non-adherent (left) and adherent (right) cells of malaria-infected red blood cells after around* 28 *hours post infection.*

Acknowledgements

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P06 - Dynamics of Collective Cell Motility

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Collective cell migration plays a driving role in various phenomena spanning from pattern formation during embryonic development to wound healing and tumor invasion in cancer. Recent experiments have shown that, during the collective migration of cells, as cell density increases due to proliferation, migration slows down and yet the fastest cells move together in an increasingly cooperative manner, reminiscent of glassy dynamics [1, 2]. These glass-like dynamics, which has been observed in the behaviour of motile tissues at high densities, is accompanied with caging and dynamical heterogeneities [3]. In this work, we develop a model of deformable, motile cells to study confluent monolayers. We analyse the properties of cell monolayers to gain insight into the dynamics of collective cell behaviour. We observe a slowing down of dynamics, as a function of cell density, accompanied with increasingly cooperative motion at higher densities in accordance with the experimental results reported in the literature.

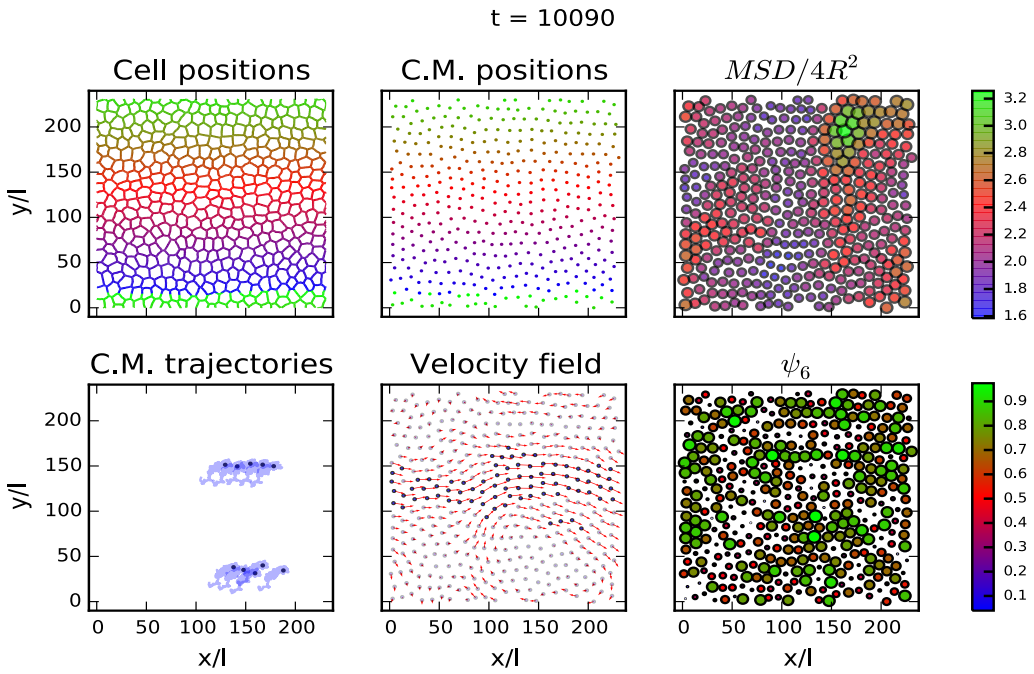

Figure: Behaviour of the cell monolayer at a packing fraction of 0.97.

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P07 - Conformational properties of active semiflexible polymers

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Active motions of filamentous biopolymers are prevalent in living cells and are mainly driven by various types of molecular motors [1]. Such motors often move and transfer forces along biopolymers, which are well described as semiflexible polymers.
Here, we present analytical results for the conformational properities of flexible and semiflexible polymers exposed to active noise. For the description of the polymer, we adopt the continuous Gaussian semiflexible polymer model. Activity is incorporated by adding a self-propulsion velocity such that every point of the polymer is independently propelled in directions changing in a diffusive manner (cf. Fig. 1). Furthermore, the finite polymer extensibility is taken into account which turns out to be essentially for the polymer conformations [2]. Our calculations predict a strong dependence of the polymer internal relaxation times on the activity. The conformational properities of semiflexible polymers, determined via the relaxation times, exhibit a crossover from a bending elasticity dominated dynamics to the flexible polymer dynamics with increasing activity. This leads to a significant noise-induced polymer shrinkage over a large range of self-propulsion velocities (cf. Fig. 1) [3]. For large activities, the polymers swell and their mean square end-to-end distance approaches $L^2/2$, where L is the polymer contour length.

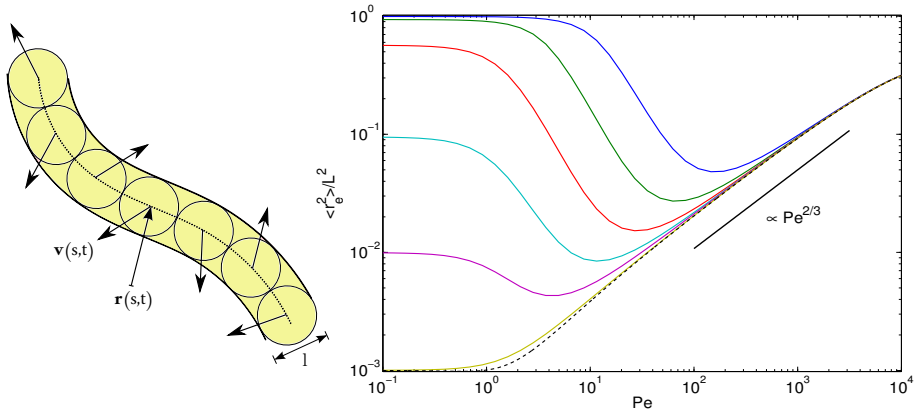

Fig. 1: *Active polymer model and the mean square end-to-end distances as function of the Péclet number Pe for the polymer stiffnesses $pL = 10^3$, 10^2, 10, 1, 10^{-1}, and 10^{-2} (bottom to top at $Pe = 10^{-1}$). Here, L is the polymer length and $l_p = 1/2p$ is the persistence length. The dashed line represents the flexible limit, $pL \to \infty$, with an asymptotic of $\langle r_e^2 \rangle \propto Pe^{2/3}$ for moderate Pe.*

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P08 - A Computer Simulation Study of Bulk Tissue Competition

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In the case of cancer, there is a competition for space within a biological system between a cancerous tumour and healthy host tissue. It has been proposed, that the homeostatic pressure [1] plays a crucial role in tissue competition. The homeostatic pressure is the steady state pressure of a tissue for which cell division and cell death (or apoptosis) rates balance. Indeed, Ref. [2] suggests that when two tissues with different homeostatic pressure are growing in competition on a substrate, the tissue with the higher homeostatic pressure invades the other one. The interface separating the two tissues propagates with constant velocity, which grows linearly with the difference of their homeostatic pressures. Here, we study three dimensional tissue competition using a minimalistic mesoscale simulation model [3, 4]. Again, we find that the tissue with higher homeostatic pressure wins the competition. However, for non-identical adhesion strengths the results are surprising. We find that two different tissues can coexist though they have different homeostatic pressures, if the cross-adhesion strength between the two competing tissues is lower than their self-adhesion strengths. The steady state pressure of the mixture is higher than the homeostatic pressure of both competing tissues. Our results suggest a mechanical explanation for tumour heterogeneity.

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P09 - Polymer Dynamics of Microgel Particles: A Multiparticle Collision Dynamics Simulation Study

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Microgels consist of a cross-linked polymer network that exhibit different swelling behaviors in response to external stimuli like change of temperature, pH, or ionic strength. Such responsive particles are possible candidates for a broad range of applications, like drug delivery, sensing, purification, etc. A detailed understanding of both their structural and dynamical properties is a key requirement for an application-based design of microgel systems.

In order to study the dynamics of microgel systems in presence of hydrodynamic interactions, we perform hybrid mesoscale simulations, combining the multiparticle collision dynamics approach for fluids with molecular dynamics simulations of the polymer [1]. First, the dynamic structure factor $S(q,t)$ for a neutral microgel is determined which shows a scaling relation $S(q,t) = S(q,0) f[((ql)^{\alpha}t)^{\beta}]$ (see Fig. 1), with the values $\alpha = 2.7$ and $\beta = 0.74$. These values are in reasonable agreement with the theoretical prediction $\alpha = 3$ and $\beta = 2/3$ for a single polymer [2].

Second, we study the polymer dynamics of coreshell microgels, where the dynamic structure factor exhibits two distinct behaviors on short and long-time scales [3]. On short-time scales, the $S(q,t)$ is similar to that of a neutral microgel, while on the longer-time scales, the behavior is more similar to a microgel in bad solvent (collapsed state). A similar behavior is observed in experiments.

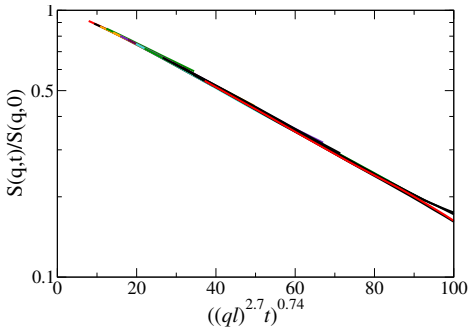

Figure 1: Normalized dynamics structure factor of a microgel.

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P10 - Sorting red blood cells by their dynamical properties

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A combination of mesoscale hydrodynamic simulations and microfluidic experiments are used to explore the use of cells' mechanical and dynamical properties as biomarkers for separation. The dynamic behaviour of red blood cells (RBCs) within deterministic lateral displacement (DLD) devices is investigated within various array geometries and for different viscosity contrasts between the intra-cellular fluid and suspending medium. We find that the viscosity contrast and associated cell dynamics clearly determine RBC trajectories through DLD devices. Simulation results compare well to experiments and provide new insights into the physical mechanisms which govern the sorting of non-spherical and deformable cells in DLD devices.

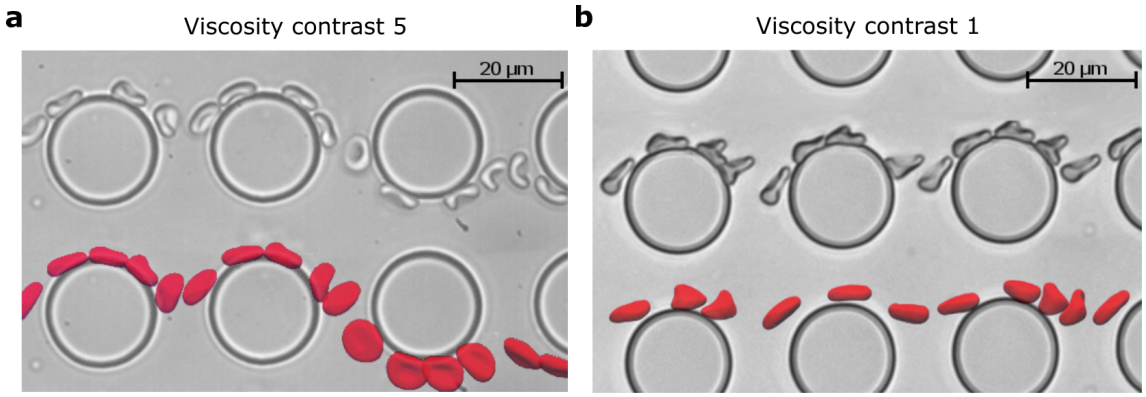

Fig. 1: *Stroboscopic images of RBCs in a DLD device taken from simulations and experiments at different viscosity contrasts.* **(a)** *At a physiological viscosity contrast between intracellular medium and suspending medium, row swapping is promoted by tumbling behaviour.* **(b)** *For intracellular and suspending mediums of equal viscosity, tank-treading type dynamics occur and the RBC favours the dis-*

Keywords: Cell sorting, deterministic lateral displacement, red blood cell, cell dynamics

Acknowledgements
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P11 - von Willebrand factors and Platelets in Blood Stream: Margination and Adhesion

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To stop bleeding, platelets must adhere to the injured endothelium and plug the opening. Although platelet adhesion to the injured substrate is effective in low shear rates, they are unable to firmly adhere to the surface by their own in shear rates higher than $900\ \mathrm{s}^{-1}$ [**?**]. In such conditions, von Willebrand factors (VWFs), the largest soluble proteins in blood stream play the crucial role [**?**]. They unwrap in high shear rates and adhere to the injured site; at the same time, they adhere to platelets and tether them from flowing in the blood flow. VWFs are long concatemers of VWF dimers bound to each other end to end [**?**]. The conformation of VWF polymer is such that in the absence of shear stress, the polymer remains globular, thus hiding its adhesive sites (A1 domains) for binding platelet receptors (Glycoprotein Ibα) or collagen. At sufficiently high shear rates, the VWF stretches making the interaction of its adhesive domain with platelet receptors or collagen possible.
For adhesion to occur, the platelets and VWFs must migrate to the proximity of tha injured walls. Indeed, the presence of red blood cells (RBCs) in blood stream facilates it by a process called margination. Accordingly, RBCs move to the center of the vessel and leave a RBC free layer near the walls. Then, the other micro-scale components such as ultra-large VWFs and platelets are pushed to this layer and populate in there making hemostasis more probable. In addition, VWFs must be stretched to be hemostatically active since their adhesive domains are shielded from platelet receptors if the VWF polymer is coiled. Since VWFs are known to be coiled in low shear rates and stretched critically in sufficiently high shear rates [**?**], their adhesion occurs only in high shear rates.
By using meso-scale simulations, we study the behavior of VWFs and platelets in blood flow. It is shown that although platelets margination is enhanced by either increasing volume fraction of RBCs or by increasing shear flow, the margination of VWFs is non-trivially dependent on these two properties. It is also shown that VWF-platelet adhesion and aggregation are critically dependent on shear flow. It is found that the presence of ultra-large micro-scale VWFs is necessary in this process.

Acknowledgements

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P12 - Simulating growing Sheets; Buckling and Folding

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Mechanical stresses have been shown to play an important role in growth and development. In thin, sheet-like tissues, the build up of stress can trigger buckling events which then give rise to the specific morphology of the tissue itself. Examples for this process are the formation of villi and crypts (in- and outward folded domains) in the mammalian intestine or the folding of the cerebral cortex during embryo development [1,4]. We extend an existing tissue growth model to describe growth phenomena of tissue sheets, where feedback between growth and mechanics emerges naturally from the microscopic dynamics [2]. The model tissue is kept in a locally flat geometry with a meshless membrane model [3]. Together, this results in a growing membrane with finite bending rigidity. Starting from a flat configuration, growth creates stress, leading to buckling (see Fig. 1, left). The coupling of growth stress and buckling results in a finite wavenumber, non-trivial wrinkling pattern . We use Föppl-von Kármán theory and a homeostatic pressure approach for growth [4] to describe quantitatively the early time development (see Fig. 1, right).

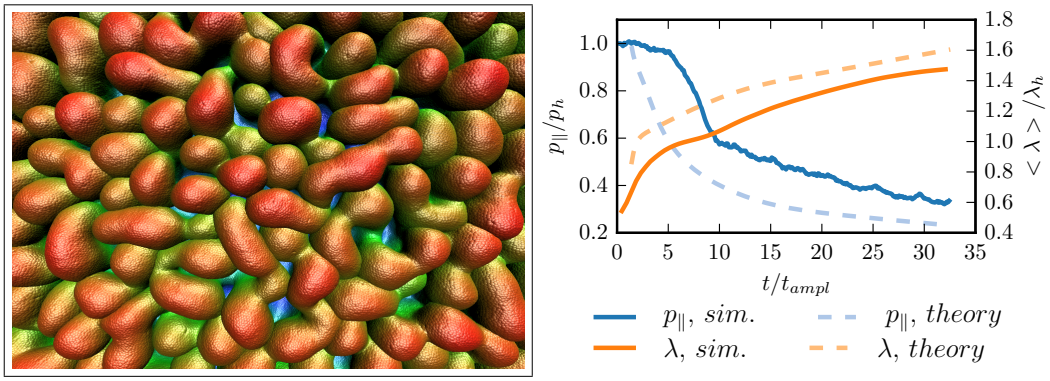

Fig. 1: *Left: Snapshot of a growing membrane which shows typical crypt-like structures. Right: Average wavelength and in-plane pressure of the growing membrane during wrinkling. Comparison between theoretical and simulation results.*

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P13 - Dynamical behavior of vesicles in shear flow

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A deep understanding of the dynamics and rheology of suspensions of vesicles, cells, and capsules is relevant for different applications, ranging from soft glasses to blood flow [1]. The study of confined fluid vesicles under shear flow will be presented by using a combination of molecular dynamics and mesoscale hydrodynamics simulations (multi-particle collision dynamics) in two dimensions [2]. The flow behavior is studied as a function of the shear rate, the volume fraction of vesicles, and the viscosity ratio between inside and outside fluids. Results are obtained for the dynamics of vesicles, for the intrinsic viscosity of suspensions, and for the formation of cell-free boundary layers near the confining walls [3-5].

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P14 - Characterization of small anisotropic colloids by means of time-resolved flow Dichroism

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The average size and size-polydispersity of suspensions of anisotropic colloids that are much smaller than the wavelength of visible light can be determined by means of time-resolved dichroism measurements by applying step-up shear flow [1] to an isotropic and dilute suspension. The time-period of the alternating orientation angle with respect to flow direction, as well as the decay of its amplitude are sensitive to size and polydispersity. Flow dichroism measurements offer a sensitive method for their characterization. We extend previous work [1,2] to rod-like particles of *arbitrary aspect ratio* by a numerical solution of the rotational Smoluchowki equation with shear flow. The developed algorithm allows us to fit the time-dependent flow dichroism data with respect to the average size and polydispersity of the anisometric colloids in the sample. Experimental data on tumbling of small anisotropic colloids will be presented together with the results of the fits with this new algorithm. These small rods are CdSe-CdS rods, $CuInS_2$ tiles, and CdSe, quantum dots with average dimensions on the order of O(10 nm).

Acknowledgements

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P15 - Shape and Dynamics of Single Red Blood Cells in Shear and Tube Flows

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The dynamics, deformation, and orientation of red blood cells (RBCs) in microcirculation affect the flow resistance and transport properties of whole blood [1],[2]. We investigate the shape and dynamics of single RBCs in shear and tube flows via mesoscopic hydrodynamic simulations. We use the smoothed dissipative particle dynamics method with angular momentum conservation [3]. The simulations are performed in narrow slits or microtubes at the scale of microvessels. This study is motivated by our previous simulations [2], where the viscosity ratio between the RBC cytosol and suspending media was equal to one. Now, a realistic viscosity ratio of five is employed and its effect on the dynamics, shapes, and transition between various types of motion is investigated. Simulations for different shear rates and confinements lead to a phase diagram of shapes and dynamics differing from the previously predicted diagrams [2]. In agreement with the previous studies, the parachute shape of RBCs occurs at high confinements and shear rates, whereas at low confinements, an unstable slipper shape occurs. The slipper may experience strong deformations depending on the shear rate. At low shear rates, a snaking dynamics is obtained. We will discuss the importance of the viscosity contrast on the flow resistance, and the effect of different stress-free shapes of the RBC [4], [5] on its dynamics in flow.

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P16 - Thermophoretic accumulation in hydrothermal pores

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The thermophoretic properties of aqueous formamide solutions as a function of concentration and temperature are studied by means of Infra-Red Thermal Diffusion Forced Rayleigh Scattering. Comparing the results with empirical concepts to describe the temperature dependence of aqueous solutions [1] and molecular dynamics simulations of formamide water mixtures [2] it becomes apparent that the system only adheres to the empirical equation in a dilute state and deviates when formamide-formamide interactions take place at higher concentrations.
Formamide is of special interest in the *'origin-of-life'* concept as it has been shown that a number of prebiotic molecules such as purine, adenine, cytosine and 4(3H)-pyrimidinone form from formamide under catalytic conditions and at sufficiently high concentrations [3]. For nucleotides and short DNA strands it has been shown with numerical finite-element calculations that a high degree of accumulation in hydrothermal pores occurs [4]. Using our thermophoretic data on the formamide/water system, we show that the same combination of thermophoresis and convection in hydrothermal pores leads to accumulation of formamide up to concentrations where nucleobases are formed. The high degree of formamide accumulation is due to an unusual temperature and concentration dependence of the thermophoretic behaviour of formamide. Starting with a formamide concentration of 10^{-3} wt%, estimated to be typical in shallow lakes on early earth [5], the accumulation-fold in part of the pores increases strongly with increasing aspect ratio of the pores, and saturates to highly concentrated aqueous formamide solutions of approximately 85 wt% at large aspect ratios.

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P17 - Membrane Shape Transformation Induced by Banana-Shaped Protein Rods

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In living cells, morphology of biomembranes is regulated by various proteins. Many of these proteins contain a banana-shaped binding module called BAR (Bin-Amphiphysin-Rvs) domain. We have studied how anisotropic spontaneous curvatures of banana-shaped protein rod induce effective interaction between the proteins and change membrane shapes by using implicit-solvent meshless membrane simulations [1-4].

We found that the self-assembly of the rods is divided to two directional assemblies at the low rod density [1] and polyhedral vesicles and polygonal tubes are formed at the high density [2]. We also revealed that a small spontaneous curvature perpendicular to the rod can remarkably alter the tubulation dynamics at high rod density whereas minor effects are only obtained at low density [3]. A percolated network, which suppresses tubule protrusion, is intermediately formed for negative perpendicular curvatures. For high rod density, high rod stiffness, and/or low line tension of the membrane edge, the rod assembly induces vesicle rupture, resulting in the formation of a high-genus vesicle and membrane inversion [4].

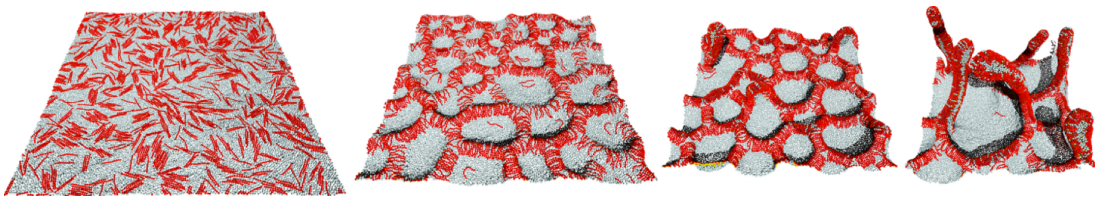

Fig. 1: *Sequential snapshots of tabulation from a flat membrane induced by protein rods.*

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P18 - Cytoplasmic Rotation in a Coarse-Grained Model of Cortical Microtubules and Asymmetric Motor Composites

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Motor proteins, such as kinesins, are molecular machines that hydrolyse ATP to perform mechanical work on microtubules (MTs) to drive motility in cells. This is important for processes such as cytokinesis, localization of organelles, and cytoplasmic streaming [1]. The recent work of Lu *et al.* has shown in vivo that microtubule sliding, induced by kinesin-1 is important for normal oocyte cytoplasmic rotation, a process required for efficient localization of mRNAs and proteins during oogenesis in Drosophilia [2]. Namely, free microtubules are observed to move against cortically anchored microtubules generating forces that contribute to cytoplasmic streaming.

To elucidate the relation of microscopic mechanisms to the macroscopic properties, we use a two dimensional Brownian dynamics model [3]. Circularly confined polar filaments are modelled as a linear rigid chain of penetrable beads that mutually attract each other by depletion forces. Motors are harmonic force dipoles that move on the filaments in the direction of MT polarisation, and pull cross-linked filaments with them [4]. In this work we study the effect of both, tetrameric and dimeric motors. Tetrameric motors have two motile arms that cross-link two neighbouring MTs, while dimeric motors have one motile arm, and another anchored arm, similar to kinesin-1.

We show that tetrameric motors bundle MTs, and do not lead to motility. Unlike tetrameric motors that induce relative tangential stress only in the case of aligned MTs, kinesin-1-like, dimeric motors induce stresses in the case of both anti-aligned and aligned MTs. This leads to perpetual motility in a layer of MTs close to the confinement edge, where filaments are distinctly more anti-aligned than the center of the confinement. Higher densities of motors do not change the organization of filaments, but induce more stress and propel filaments faster. The structures consist of large nematically aligned droplets with point defects at the boundary.

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P19 - Colloids with competing short-range attraction and long-range repulsion: Structure and dynamics

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The dynamic clustering of globular particles in suspensions exhibiting competing short-range attraction and long-range repulsion such as in protein solutions has gained a lot of interest over the past years. We investigate theoretically the influence of clustering on the dynamics of globular particle dispersions [**?**]. To this end, we systematically explore various pair potential models by a combination of state-of-the-art analytic methods in conjunction with computer simulations where the solvent-mediated hydrodynamic interactions are likewise included. Our results show that the cluster peak (intermediate-range-order peak) is present also in the hydrodynamic function characterizing the short-time dynamics. Enhanced short-range attraction leads to a smaller self-diffusion coefficient and a larger dispersion viscosity. The behavior of the (generalized) sedimentation coefficient is more intricate depending on the selected interaction parameters. Our results are relevant also for technological applications, such as the ultrafiltration of proteins.

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P20 - Collective bacterial migration is governed by two distinct force patterns

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Many bacteria have the ability to generate mechanical forces. When coordinated, these forces allow migration, aggregation, and host infection. To understand how forces are coordinated during migration of M. xanthus, we perform the first systematic measurements of bacterial cell-substrate traction. We find very distinct traction patterns for two migration modes called twitching and gliding. In groups, twitching leads to local, transient adhesion, while gliding allows for collective emergence of directional force. These two force organization principles can play complementary and essential roles for bacterial life.

P21 - Slip of grip of a molecular motor on a crowded track: Modeling shift of reading frame of ribosome on RNA template

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We develop a stochastic model for the programmed frameshift of ribosomes synthesizing a protein while moving along a mRNA template. Normally the reading frame of a ribosome decodes successive triplets of nucleotides on the mRNA in a step-by-step manner. We focus on the programmed shift of the ribosomal reading frame, forward or backward, by only one nucleotide which results in a fusion protein; it occurs when a ribosome temporarily loses its grip to its mRNA track. Special "slippery" sequences of nucleotides and also downstream secondary structures of the mRNA strand are believed to play key roles in programmed frameshift. Here we explore the role of an hitherto neglected parameter in regulating -1 programmed frameshift. Specifically, we demonstrate that the frameshift frequency can be strongly regulated also by the density of the ribosomes, all of which are engaged in simultaneous translation of the same mRNA, at and around the slippery sequence. Monte Carlo simulations support the analytical predictions obtained from a mean-field analysis of the stochastic dynamics [1].

Acknowledgements

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P22 - Nanoparticle wrapping by receptor-mediated adhesion

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Biological cells internalize cargo via different pathways. In all cases, the cargo is encapsulated within a carrier that interacts with the plasma membrane of a cell via wrapping. Understanding the mechanisms involved in this internalization process is important both from a fundamental science and from an application point of view. For example, in drug delivery and nanomedicine, nanoparticles can be used as carriers. Furthermore, nanoparticles are used for food processing and in technological applications, therefore a better understanding of their toxicity is required. Towards understanding the complex wrapping process, we study wrapping of a spherical nanoparticle decorated with ligands that interacts with a lipid-bilayer membrane via receptor-ligand bonds.

Theoretical calculations have shown that the wrapping state of nanoparticles depends both on particle properties, such as size and shape, the membrane properties, such as bending rigidity and tension, and the strength of the adhesive interaction [1-3]. We calculate the deformation energy of the fluid membrane using the Helfrich curvature Hamiltonian. We take into account receptor-ligand binding energy and receptor entropy [4]. For a given fraction of a particle being wrapped by the membrane, we obtain an optimum number of bound receptors at equilibrium. For low-receptor densities and high receptor-ligand bond energies, we find stable partial-wrapped states. We show that in this regime the kinetics of receptor-mediated wrapping can determine the number of nanoparticles that attach to a cell, which is important to understand dosage effects for nanoparticle-cell interaction.

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P23 - A coarse-grained elastic model for cell deformation

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A broad range of *in silico* models (e.g. liquid or viscoelastic drop models) has been introduced to reproduce the complex mechanical properties of various cell types [1]. These models are used to understand and quantify experimental measurements. In this work, we employ a coarse-grained cell model which incorporates the membrane properties similar to the RBC-model [2] and an elastic inner mesh to include the cytoskeletal properties. The model is formulated in the framework of the dissipative particle dynamics simulation method and can include multiple cell compartments with different mechanical properties. We perform various mechanical tests that are similar to experiments [1] to determine the mechanical properties of a single cell. We also investigate the deformation of this cell in fluid flow. We expect that this model will help us better understand the contribution of different cell compartments to overall cell deformation.

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P24 - Anisotropic Thermophoresis: Micro-geometry Matters

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When a thermal gradient meets colloid-solvent interface, local pressure gradients around colloid will be generated which result in colloidal migration. This transport phenomenon is referred to as colloidal thermophoresis. In contrast to particles with spherical shape, elongated colloids may have a thermophoretic response depends on colloid orientation, and more interestingly a non-vanishing thermophoretic force can be induced in a direction perpendicular to the temperature gradient [1]. By means of mesoscale hydrodynamic simulations, we investigate anisotropic thermophoresis of rod-like colloids.

As an analogy to friction of rods, the anisotropic thermophoresis can be characterized by two orthogonal thermal diffusion factors, which determine the thermal diffusion factor in arbitrary orientation (Fig.1, *Top*). In dilute limit, this linear combination relation explains that the temperature gradient induces no alignment in the rods, and shows that the thermophoretic force increases linearly with the rod length. Rods are constructed by the so-called 'shish-kebab' model what allows us to vary the surface geometry. Remarkably, the amplitude and direction of anisotropy can be changed by tuning rugosity (Fig.1, *Bottom*). This can be understood since both different rugosities and solid-liquid interactions induce various interfacial temperature gradients what result in diverse anisotropic effects. Our study shows that anisotropic thermophoresis may be quantitatively controlled by interfacial tunability [2]. In practical, this anisotropic effect of thermophoresis has shown to be the basic mechanism that allows the construction of thermophoretic turbines, which move in the presence of an external temperature gradient [1].

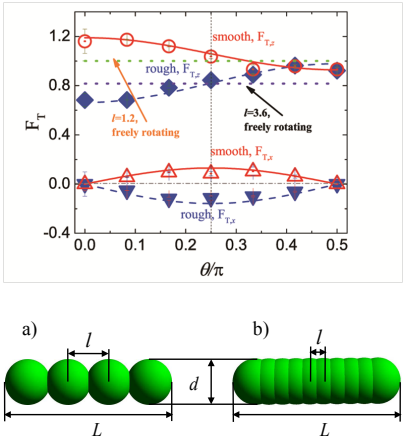

Fig. 1: *Top: Thermophoretic forces of rods with different orientations. Bottom: Schematic representation of model of rods with different rugosities.*

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P25 - Does hydrodynamics enhance phase separation of microswimmers?

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In contrast to passive colloids, microswimmers can exhibit phase-separation into a cluster-phase and a gas-like-phase without any attractive interactions. This motility-induced phase separation has received considerable attention recently [1]. For simplicity, theoretical studies typically exclude hydrodynamic interactions and apply the model of active Brownian particles. Recent simulation studies have addressed the role of hydrodynamics, but contradictory results have been found [2, 3, 4]. We present a simulation study of spheroidal squirmers [5] in a quasi-2D system and resolve said contradictions. We find that hydrodynamics tends to suppress phase separation for spherical swimmers, while it enhances phase separation for elongated swimmers (see Fig. 1). Furthermore, so-called pullers, which are swimmers with a negative force-dipole coefficient, show cluster formation at lower packing fractions, while so-called pushers (positive force-dipole coefficient) need considerably higher packing fractions to form clusters.

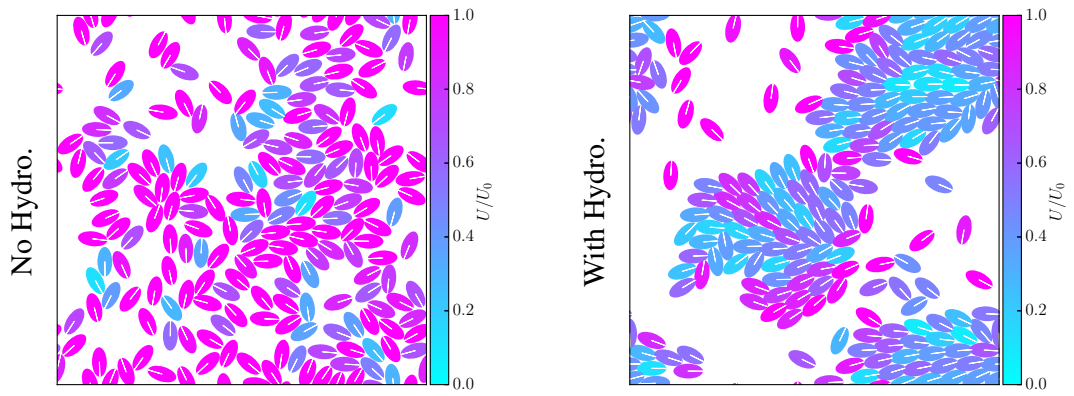

Fig. 1: *Snapshots of spheroidal swimmers with Péclet number* $Pe_r = 12$ *at area packing fraction* $\phi_{2D} = 0.5$. *Left: Active Brownian particles; Right: Neutral squirmers.*

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P26 - Confinement Induced Phase Transitions of a Soft Sphere Fluid: A Molecular Dynamics Study

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Molecular dynamics (MD) simulations were carried out for a pure component, monatomic Lennard-Jones fluid confined between mica surfaces. When the surface separation is an integral multiple of the molecular diameter, the fluid forms distinct layers whereas, jammed layers are formed for intermediate surface separations. The in-plane pair correlation function (PCF) analyzed for contact as well as inner layers begins to exhibit long range translational ordering when the separation distance between the mica surfaces is decreased below four molecular diameters. We also observed a transformation of contact layers from square symmetric structures to a state when square and triangular symmetric structures coexist as the surface separation is decreased below four molecular diameters. The self-intermediate scattering function (SISF) $F_s(k,t)$, a powerful tool to probe molecular dynamics exhibits a gamut of rich dynamics such as distinct two-step relaxation processes indicative of glassy dynamics as predicted by the mode coupling theory (MCT), three-step relaxation processes characterized by jump dynamics and hopping events[1] as well as a striking transition to non-ergodic states characterized by a non-relaxing SISF for specific surface separations even beyond 500 ns. Although a Lennard Jones fluid has no glass transition temperature by itself and can undergo freezing under extreme confinement[2], this study reveals that, confinement introduces new relaxation processes and length scales that a confined LJ fluid is found to exhibit multiple relaxation regimes different from its corresponding bulk counterpart.

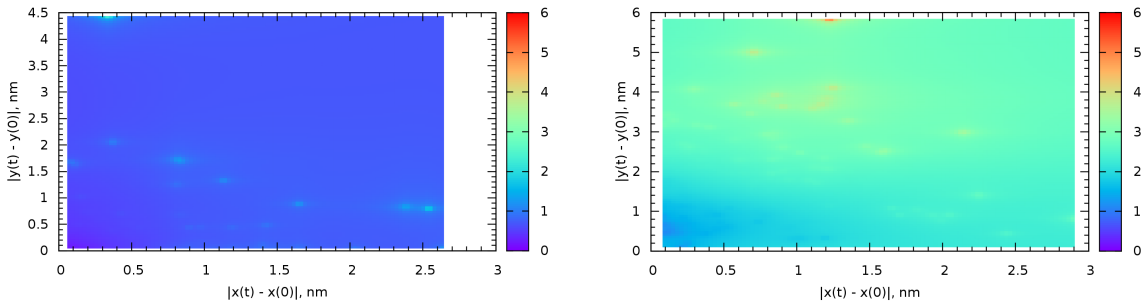

Fig. 1: *In-plane $(x-y)$ mobility map for a 3 layered system at 100 ns illustrates dynamic heterogeneities in the confined system wherein the inner layer (right) is more mobile than the contact layer (left).*

Acknowledgements

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P27 - Shape-Induced Hydrodynamic Effects in Thermophoretic Microswimmers

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Thermophoresis refers to the drift motion experienced by particles immersed in a fluid with an intrinsic gradient of temperature. In thermophoretic swimmers a local temperature gradient is generated due to the existence of a material that can quickly absorb heat from a heating source such as irradiating light. An asymmetric distribution of the heated material on the particle surface translates into a persistent particle motion [1]. The motion direction is determined by the thermophoretic character of the particle, whether thermophobic or thermophilic [2]. Experimentally, these particles have been synthesized as Janus spherical particles being half coated with gold [1]. Other shapes such as dimer swimmers have already been investigated resulting in a significantly different hydrodynamic behaviour [3, 4].
In this work, we first study the effect of the swimmer shape by means of computer simulations. We employ a well-established mesoscale simulation technique that couples multi-particle collision dynamics (MPC) as a coarse-grained description of the fluid with molecular dynamics for an adequate resolution of fluid-colloid interactions [5]. This methodology offers an efficient inclusion of hydrodynamics, thermal fluctuations, and the sustainability of temperature gradients. Moreover, the tunable fluid-solvent interactions allow us to explore various thermophoretic behaviors. We characterize the swimming behavior as a function of the swimmer shape, *e.g.* self-propelled dimers with asymmetric sizes, or rod-like swimmers with parallel and perpendicular propulsion.
Interaction between pairs of swimmers is investigated as well. Thermophoretic self-propelled particles interact with each other not only through direct pair interactions, but they will react as well to each other's temperature gradients and to their hydrodynamically induced flow fields. Whether and how pairs of swimmers form persistent geometric structures, or swim independently, will determine the collective behavior of large assemblies of these swimmers.

Acknowledgements

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P28 - Theory of Passive Polymer Translocation Through Amphiphilic Membranes

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We propose a theoretical framework for examining translocation of flexible polymers through amphiphilic membranes: A generic model for monomer-membrane interactions is formulated and the Edwards equation is employed for calculating the free energy landscape of a polymer in a membrane environment [1]. By the example of homopolymers it is demonstrated that polymer adsorption and the symmetry of conformations with respect to the membrane's mid-plane trigger passive polymer translocation in a narrow window of polymer hydrophobicity. We demonstrate that globular conformations can be taken into account by means of a screening of the external potential, which leads to excellent agreement of predicted translocation times with dynamic lattice Monte Carlo (MC) simulations [2]. The work opens a theoretical road-map on how to design translocating flexible polymers by referring to universal phenomena only: adsorption and conformational symmetry. As confirmed by MC simulations on amphiphilic polymers [3], promising candidates of translocating polymers in practice are short-block amphiphilic copolymers, which in the limit of small block sizes resemble homopolymers on a coarse grained level.

Acknowledgements

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P29 - Nanoparticle uptake by vesicles

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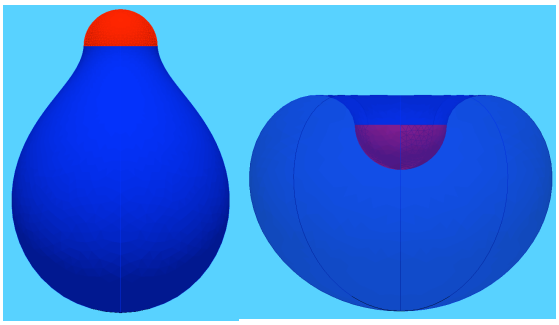
Nanoparticles are used for a variety of biomedical applications, such as drug delivery, biological markers and intracellular transport [1]. Nanoparticles are able to go through the lipid bilayer membrane, but the mechanism of their entry into cells is hotly debated. Previous studies have revealed that nanoparticle adsorption and wrapping by cell membrane depends not only on particle size and shape, but also on the interaction of the particle with the membrane and on the membranes' mechanical properties [2-4]. Our work focuses on the uptake of nanoparticles by vesicles using a curvature-elastic description by a continuum model for membranes, where the membrane deformation energy is given by the Helfrich Hamiltonian. We use triangulated surfaces and numerically minimize the deformation energy for various sizes and shapes of vesicles and particles. For spherical vesicles, partially-wrapped states have lower bending energies for nanoparticles that exit vesicles than for nanoparticles that enter vesicles. Our calculations may help to gain a better understanding of endocytosis and exocytosis for biological cells.



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