International Conference NECD12

Nonequilibrium Collective Dynamics

Bridging the Gap between Hard and Soft Materials

October 1-4, 2012
Potsdam, Germany
International Conference NECD12

Nonequilibrium Collective Dynamics

Bridging the Gap between Hard and Soft Materials

October 1-4, 2012
Potsdam, Germany

An Event of the Research Training Group GRK 1558

“Nonequilibrium Collective Dynamics in Condensed Matter and Biological Systems”

Scientific and Organization Committee

Holger Stark (Chair)
Sabine Klapp (Co-chair)
Carsten Beta
Julia Eckert
Aljoscha Hahn
Andreas Knorr
Oliver Pohl
**Venue**

The conference takes place in the hotel “Seminaris Seehotel” in Potsdam, Germany. Potsdam is located about 30 km southwest of the center of Berlin.

Address: Seminaris Seehotel, An der Pirscheide 40, 14471 Potsdam, Germany

**Scope**

Collective dynamics under nonequilibrium conditions is ubiquitous in natural processes and technology, and of great current interest in experimental research as well as theoretical modeling. Different approaches to study nonequilibrium collective dynamics have been developed in different disciplines, in particular in hard and soft condensed matter and in biological physics.

The conference NECD12 aims at bringing together specialists in these fields and to stimulate an intensive exchange of methods and ideas among them.
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Opening remarks

9:00 – 9:35 **Kenneth Showalter** (West Virginia University, Morgantown)
Synchronization in populations of chemical oscillators

9:35 – 10:10 **Pietro Cicuta** (University of Cambridge)
Driving potential and noise level determine the synchronization state of hydrodynamically coupled oscillators

10:10 – 10:30 **Shashi Thutupalli** (Princeton University)
Chimera states in networks of coupled mechanical oscillators: the apathetic sympathy of clocks

Coffee break

11:00 – 11:35 **Peter Olmsted** (University of Leeds)
Fracture, instability, and shear banding in entangled polymers

11:35 – 11:55 **Andreas Zöttl** (Technische Universität Berlin)
Periodic and quasiperiodic dynamics of spherical and elongated microswimmers in poiseuille flow

11:55 – 12:15 **Giuseppe Gonnella** (University of Bari)
Self-propelled particles under shear

Lunch break

2:00 – 2:35 **Lyderic Bocquet** (University of Lyon)
Structure and dynamics of active colloidal suspensions

2:35 – 3:10 **Raymond Kapral** (University of Toronto)
Nanomotor dynamics and collective behavior in simple and active media

3:10 – 3:30 **Katrin Wolff** (Technische Universität Berlin)
Dynamics of active bottom-heavy particles in external fields

Coffee break

4:00 – 4:35 **Ignacio Pagonabarraga** (University of Barcelona)
Emergent patterns in internally driven suspensions

4:35 – 4:55 **Alexander Reinmüller** (Johannes-Gutenberg-Universität Mainz)
Swimming with many friends at low reynolds numbers

4:55 – 5:15 **Martin Trulsson** (ESPCI, Paris)
Transition from viscous to inertial regime in dense suspensions

6:00 – open Poster session and buffet
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Overview – Wednesday

9:00 – 9:35 Erwin Frey (Ludwigs-Maximillians Universität München)
Symmetry breaking and pattern formation in cellular systems

9:35 – 10:10 Igor Aronson (Argonne National Laboratory, Chicago)
Phase-field model of self-polarization and cell movement

10:10 – 10:30 Björn Stuhrmann (FOM Institute AMOLF, Amsterdam)
Nonequilibrium fluctuations of a remodeling in vitro cytoskeleton

Coffee break

11:00 – 11:35 Harry L. Swinney (University of Texas at Austin)
How bacteria in colonies can survive by killing siblings and reversibly changing shape

11:35 – 11:55 Matthias Theves (Universität Potsdam)
Motility statistics of swimming bacteria in confined microenvironments

11:55 – 12:15 Johannes Taktikos (Technische Universität Berlin)
Swimming strategies of bacteria

Lunch break

2:00 – 2:35 Tatsuo Shibata (RIKEN Center for Developmental Biology, Kobe)
Self-organization in the processes of inherent polarity formation, gradient sensing, and directional motility in eukaryotic chemotaxis

2:35 – 3:10 Julia M. Yeomans (University of Oxford)
Stirring by microswimmers

Coffee break

3:30 – 4:05 Andreas Engel (Carl-von-Ossietzky Universität Oldenburg)
Pattern formation and fluctuations in ferrofluids

4:05 – 4:25 Sebastian Jäger (Technische Universität Berlin)
The effects of external time-dependent fields on ferrofluids

5:30 – 9:30 Conference dinner on a boat on the river Havel
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<td>Michael Cates (University of Edinburgh)</td>
<td>Motility-induced phase separation in active brownian particles</td>
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<td>Hartmut Löwen (Heinrich-Heine-Universität Düsseldorf)</td>
<td>Clustering and turbulence in active colloidal fluids</td>
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<td>10:10 – 10:30</td>
<td>Paolo Malgaretti (Universitat de Barcelona)</td>
<td>Running faster, running together: molecular motors speed-up thanks to hydrodynamic coupling</td>
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<td>11:00 – 11:35</td>
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<td>Marc Neef (Universität des Saarlandes, Saarbrücken)</td>
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<td>Peter Hänggi (Universität Augsburg)</td>
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<td>Holger Stark (Technische Universität Berlin)</td>
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Non-equilibrium collective behavior of confined colloidal particles in a planar shear flow
Motional patterns of spherical colloids in a narrow microchannel
Space-resolved dynamic light scattering probing inhomogeneous dynamics in soft matter
Towards two-dimensional transport of paramagnetic colloids via an ac-induced ratchet
Brownian motion over curved manifolds
Structure and dynamics of suspensions of colloidal dumbbells
Simulation of non-equilibrium surface growth - first results for C60
Collective dynamics in driven granular suspensions
Glassy dynamics of brownian particles close to walls
The kinetics of crystallization and vitrification in colloidal hard spheres
Distorted structure in sheared dispersions as described by mode-coupling theory (mct)
Cooperative processes in restructuring gel networks
A mesoscopic model for cement gel
Polymer unfolding induced by spatially correlated noise
Strain rate (compressive & shear) dependent direct 3d observation of restructuring in colloidal gel
Front propagation during the sol-gel transition
Clustering and phase behaviour of active brownian particles
Structural features underlying supercooled dynamics and glass transition
Poster 35 **Aljoscha M. Hahn** (Technische Universität Berlin)
Active Brownian particles with state-dependent self-propulsion: effective dynamics and ratchet effect

Poster 36 **Andreas Kaiser** (Universität Düsseldorf)
How to capture active particles

Poster 37 **Francisco Alarcon** (University of Barcelona)
Collective motion in squirmer suspensions

Poster 38 **Juan Eduardo Sosa-Hernandez** (CINVESTAV Monterrey)
Chemotaxis of bacteria in highly restrictive microchannels

Poster 39 **Julian Bialke** (Universität Düsseldorf)
Clustering of self-propelled particles without alignment

Poster 40 **Oliver Pohl** (Technische Universität Berlin)
Recent experiments of active colloids show a coexistence of single

Poster 41 **Max Schmitt** (Technische Universität Berlin)
Swimming active emulsion droplets

Poster 42 **Jakob Löber** (Technische Universität Berlin)
Controlling the position of a front

Poster 43 **Jakob Löber** (Technische Universität Berlin)
Analytical approximations for spiral waves

Poster 44 **Mu-Jie Huang** (National Central University Jhongli)
Dynamics of rotating spirals in agitated wet granular matter

Poster 45 **Rodrigo Lugo-Frias** (Autonomous University of Querétaro)
Flow enhanced non-homogeneous nucleation: reaction diffusion equations and domain growth

Poster 46 **Alexander Dreher** (Universität des Saarlandes)
Spontaneous actin waves and their possible role for cell migration

Poster 47 **Dominic Jourdain** (Universität des Saarlandes)
Mechanical instabilities of tubular cellular protrusions

Poster 48 **Markus Baer** (PTB Berlin)
Modelling collective motion and cluster formation in myxobacteria

Poster 49 **Stefan Fruhner** (Technische Universität Berlin / PTB Berlin)
Electrical wave propagation in the human heart and the effect of mechanical motion
Book of Abstracts: Talks
Synchronization in populations of chemical oscillators
Kenneth Showalter
West Virginia University, Morgantown, WV USA

We have studied large, heterogeneous populations of discrete chemical oscillators (~100,000) to characterize two different types of number density dependent transitions to synchronized oscillatory behavior. For different chemical exchange rates between the oscillators and the surrounding solution, we find with increasing oscillator density (i) the gradual Kuramoto synchronization of oscillatory activity or (ii) the sudden quorum sensing “switching on” of synchronized oscillatory activity. We also describe the formation of phase clusters, where each cluster has the same frequency but is phase shifted with respect to other clusters, giving rise to a global signal that is more complex than that of the individual oscillators. Finally, we describe spatially distributed groups of excitable particles that diffusively exchange activator and inhibitor species with the surrounding solution. All particles are nonoscillatory when separated from the other particles; however, spatiotemporal oscillations spontaneously appear in groups above a critical size.

Driving potential and noise level determine the synchronization state of hydrodynamically coupled oscillators

Pietro Cicuta\textsuperscript{1}, Nicolas Bruot\textsuperscript{1}, Jurij Kotar\textsuperscript{1}, Marco Cosentino Lagomarsino\textsuperscript{2}

\textsuperscript{1} University of Cambridge
\textsuperscript{2} CNRS Paris

Motile cilia are highly conserved structures in biology, enabling motility and generating transport of fluid by periodic beating. Individual cilia are non-equilibrium and non-linear systems. However their internal degrees of freedom can be coarse grained, and represented by an effective force law that drives oscillations. Cilia are then phase oscillators: This is a helpful concept in addressing the higher level phenomenology of cilia synchronization, a key step towards understanding collective dynamics in many-cilia systems. Despite decades of observation, and recent advances, it is not known how collective waves emerge and what sets their properties. Here a synthetic model of phase oscillators, where colloidal particles are driven by optical traps, proves the role of the average force profile in establishing the strength of coupling and the type of synchronization. The predictive power of this approach is illustrated by successfully mapping the behavior of cilia in the alga \textit{Chlamydomonas} onto the coarse-grained model.
Chimera states in networks of coupled mechanical oscillators: the apathetic sympathy of clocks

Shashi Thutupalli¹,4, E. A. Martens²,4, A. Fourriere³, O. Hallatschek³

¹ Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany, and Princeton University, USA
² Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany, and Technical University of Denmark, Kgs. Lyngby, Denmark
³ Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany
⁴ Equal contribution

When the internal degrees of freedom of coupled non-equilibrium entities are taken into account, a rich tapestry of unexpected complex behavior is expected to emerge. Here, we explore this idea in the context of the classical experiment of Christiaan Huygens on the synchronization of mechanical clocks via the weak coupling through a common support. We utilize two populations of mechanical oscillators, where each population of oscillators is strongly coupled with itself, but with lesser strength with the neighboring population. This is reminiscent of adding many independent 'internal clocks' within each of two coupled 'master clocks' as in the classical Huygens' experiment as mentioned above. In such a setting, we find a range of collective behavior, the most striking of which is similar to a peculiar state that was predicted by Kuramoto and his co-workers in theoretical studies [1]: they studied a network of nonlocally coupled oscillators, i.e., oscillators that are coupled with a strength attenuating with distance, and discovered a state where synchronous and asynchronous oscillators co-exist, even though the oscillators are identical. Due to its incongruous nature, this surprising phenomenon was later dubbed as a chimera state, alluding to the ancient Greek monster with the same name. Since then, numerous theoretical studies have been carried out to study the emergence of this state in various network topologies [2, 3, 7, 8], different oscillator systems [2, 4, 5, 9], its stability [6, 8, 9, 10, 11] and bifurcation behavior [3, 7, 8]. Our setup mimics the topology studied previously by Abrams et al. [3] and Laing [4], which constitutes the simplest discretized version of nonlocal coupling and thus realise chimera states in a mechanical experimental setup for the first time. By variation of the oscillation frequency and the inter-population coupling strength, we establish a phase diagram for these chimera states. Further, we compare our experimental results with a mathematical model, which allows to study the nature of the chimera state in a physical context and is analyzed in more detail [12].


Fracture, instability, and shear banding in entangled polymers

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In the 1970’s Doi and Edwards predicted that entangled polymers could have a constitutive instability in which steady shearing flow becomes unstable. This was suggested to lead to shear banding, which could explain some instabilities in polymer processing. Although shear banding was not seen for many years in entangled polymers, it is well-established in wormlike micelles. Since 2006, a series of new experiments initiated by SQ Wang and co-workers have shown that shear banding may be prevalent in monodisperse entangled polymer solutions, and many interesting non-linear effects have been demonstrated thanks to extensive and innovative uses of particle imaging velocimetry (PIV). In this talk I will outline how a number of these instabilities can be understood based on current (and classic) constitutive models for entangled polymers.
Microorganisms in the human body have to respond to confining boundaries and fluid flow, like sperm cells in the Fallopian tube or pathogens in blood vessels. Also, artificial microswimmers would have to swim in narrow channels like arteries if in the future they may be used as drug deliverers in the human body. Due to vorticities in the flow field and hydrodynamic interactions with bounding surfaces, microswimmers change their swimming speeds and orientations.

To capture both effects of fluid flow and confinement, we analyze the dynamics of an elongated microswimmer in Poiseuille flow [1, 2]. We analytically and numerically study the swimmer trajectories in several microchannel geometries, namely between two infinitely extended parallel plates, and in a channel with circular and elliptical cross section. Neglecting the finite extent of the swimmer and its hydrodynamic interaction with the bounding wall, the dynamic equation for a spherical swimmer in 2D is given by a simple pendulum equation with the Hamiltonian as a constant of motion. Swimmers swing around the centerline of the channel while oriented upstream, or tumble when the flow is strong enough. For elongated microswimmers we also identify a Hamiltonian and qualitatively similar dynamics, but the swinging frequency is smaller as compared to spherical swimmers. For 3D trajectories in a channel with circular and elliptical cross section, the swimmer performs helical and helical-like trajectories. While the swinging and tumbling motion is periodic for swimming between two parallel plates and in a cylindrical channel, it becomes quasiperiodic for swimming in a channel with elliptical cross section due to a less symmetric channel geometry.

Accounting also for hydrodynamic interactions between the swimmer and the wall, we show that pushers such as sperm cells or bacteria and pullers like the algae Chlamydomonas show different behavior. We find that upstream motion in the center of the channel is stabilized for pullers but becomes unstable for pushers which move on a stable limit cycle.

Self-propelled particles under shear

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The study of active matter has been a growing topical field of research in recent years. A suspension of self-propelled particles, modeling for instance microbial or bacterial fluids, fish schools, or synthetic swimming microrobots, is a primary example of an active material. Differently from their passive counterparts, active and self-propelled particles continuously burn energy from their surroundings or from internal sources, typically to move and this drives them out of equilibrium even in steady state. Elucidating the possibly universal properties of such active and self-propelled matter has prompted physicists to consider highly simplified models, such as the Vicsek model, which has become a paradigm in this field. This model exhibits a transition from a disordered phase to an ordered one in which flocks of self-propelled particles form and move coherently, with long range order even in 2 dimensions.

In our recent work (Physical Review E, vol. 84 031930, 2011) we have extended the study of active materials to the case of externally driven, sheared, suspensions. We find that in the presence of shear (i) there is no order-disorder transition, and that (ii) coarsening of the domains is arrested so that clusters of particles assume an anisotropic shape with a well defined size decreasing with shear rate. Moreover, shear (iii) suppresses the so-called giant density fluctuations which are observed in the quiescent limit. Our results lead to a series of predictions for externally driven active systems, such as bacterial fluids, bird flocks, or even inanimate active matter such as vibrated granular rods.
Structure and dynamics of active colloidal suspensions

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Assemblies of self-propelling organisms, from bacteria to birds or fishes, generically exhibit a wide variety of collective behaviors, structures and patterns, such as flocks, swarms, and schools. The beauty of these patterns does not reflect the difficulty to understand these strongly out of equilibrium systems, which has been the object of an intense theoretical and numerical work over the last years. Following a different perspective, we explore the experimental behavior of this so-called ‘active’ matter on the basis of artificial (abiotic) swimmers, made of self-propelling colloids. In this talk, I will present various results obtained in our group in this context. While some of their behaviors can be understood on the basis of extensions of ”equilibrium” statistical descriptions – with the activity of the system described in terms of an effective temperature –, new phenomena are observed which depart from such equilibrium expectations. I will discuss in particular the observation of dynamic clustering occurring at moderate concentrations of the active suspension. This surprising behavior can be interpreted in the context a chemotactic aggregation scenario first introduced by Keller and Segel to account for bacterial aggregation, and accounting here for chemical interactions between colloidal swimmers. It suggests that chemical interactions between self-propelled colloids can mimic, on a purely physical basis, chemotactractivity and its consequences.
Nanomotor dynamics and collective behavior in simple and active media

Raymond Kapral

University of Toronto, Toronto, Canada

Sphere dimer motors are self-propelled objects built from linked catalytic and noncatalytic spheres which consume fuel in the environment and utilize the resulting self-generated concentration gradients to produce directed motion along their internuclear axes [1]. Chemical species in the environment that act as fuel or products can themselves undergo autocatalytic reactions leading to chemical waves and these can, in turn, influence motor dynamics [2]. In collections of such motors, the individual motors interact through forces that arise from concentration gradients, hydrodynamic coupling and direct intermolecular forces [3]. Under nonequilibrium conditions it is found that the sphere dimer motors self-assemble into transient aggregates with distinctive structural correlations and exhibit swarming where the aggregates propagate through the system. These phenomena will be illustrated by simulations of the dynamics of many-motor systems.


Dynamics of active bottom-heavy particles in external fields
Katrin Wolff\textsuperscript{1}, Holger Stark\textsuperscript{1}

\textsuperscript{1} Institut für Theoretische Physik, Technische Universität Berlin, Germany

It has been observed that active particles display an increased sedimentation length, which grows quadratically with the swimming speed, and the formation of polar order [1, 2]. Here, we investigate self-propelled particles which additionally are bottom-heavy, that is they feel a torque aligning them to swim against the gravitational field. We study their dynamics in an external gravitational field analytically and numerically using Brownian dynamics simulations. For bottom-heavy particles the gravitational field has the two opposite effects of i) sedimentation and ii) upward alignment of the particles’ swimming direction. Depending on the gravitational Peclet number $\alpha$, the active Peclet number $Pe$ and the particle excentricity $r_0$, we observe either effective sedimentation with increased sedimentation length (compared with the passive case but also the active case without bottom-heaviness) or inversion where particles concentrate at the top of the simulation box. We identify analytically the set of parameters for which these effects compensate such that the steady state density profile is constant in the bulk and quantify the relaxation to steady state numerically. For fixed particle properties, that is for fixed $Pe$ and $r_0$, we find the value of $\alpha$ resulting in maximum density inversion.


Emergent patterns in internally driven suspensions

Ignacio Pagonabarraga

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In this presentation I will analyze the collective dynamics of suspensions composed by self-propelling particles. These active systems cover a variety of systems of physicochemical and biological interest which are intrinsically out of equilibrium. I will describe how hybrid dynamic models can be exploited to assess the emergence of collective behavior in suspensions of self-propelling particles and also to discuss how heterogeneous colloids react to self-generated gradients in a chemical species. I will discuss the analogies and specificities of the patterns developed by these different kinds of active suspensions.
Swimming with many friends at low reynolds numbers

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Swimming at low Reynolds numbers - be it on one’s own or with a friend - is a fascinating scientific topic and of great interest for the biology of micro-organisms, but also for medical engineering and micro-fluidics. Special attention is paid to the capability of transporting cargo. But also fixed micro-swimmers acting as a pump are of importance. Dipolar particles moving diffusio-phoretically in self-generated solute gradients as well as objects propelling by periodic mechanical configuration and/or shape changes are studied extensively, as both circumvent Purcell’s fundamental ‘Scallop Theorem’.

We take a different approach to induce self-propulsion at low Reynolds numbers (Re < 10\textsuperscript{-4}): In this contribution, we present the experimental realization of self-organized micro-swimmers consisting of accumulations of multiple microscopic objects in a permanent non-equilibrium state. In particular, our swimmers consist of cation exchange resin fragments (CIEX) and colloidal particles on a charged glass surface. Autonomous self-propulsion occurs in very dilute aqueous suspensions at low background ion concentrations. It is intrinsically driven by electro-osmosis in the substrate surface plane, which is locally induced by the release of electrolyte by the CIEX. Motion is guided by the substrate. Typical velocities were 1 – 3\textmu m/s, while lifetimes were up to 25min. Of particular importance is self-organization and cooperation of the different components, which do not show self-propulsion on their own. Namely the colloidal particles are essential for symmetry breaking which leads to propulsion, as well as they resemble potential cargo.
Transition from viscous to inertial regime in dense suspensions

Martin Trulsson\textsuperscript{1}, Bruno Andreotti\textsuperscript{1}, Philippe Claudin\textsuperscript{1}

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Non-brownian suspensions present a transition from a newtonian behaviour close to the zero- shear limit to a shear thickening behaviour at large shear rate, none of which is clearly understood so far. We have carried out numerical simulations of such an athermal dense suspension under shear, at imposed confining pressure. Our set-up is conceptually identical to the recent experiments of Boyer and co-workers \cite{1}. Varying the interstitial fluid viscosities, we recover the Newtonian and Bagnoldian regimes and show that they correspond to a dissipation dominated by viscous and contact forces respectively. We show that the two rheological regimes can be unified as a function of a single dimensionless number, by adding the contributions to the dissipation at a given volume fraction.

\cite{1} F. Boyer, E. Guazzelli, and O. Pouliquen, Phys. Rev. Lett. 107, 188301 (2011)
Collective spontaneous emission from quantum dot arrays and ensembles

Pawel Machnikowski

Institute of Physics, Wroclaw University of Technology, 50-370 Wroclaw, Poland

In this presentation, I will discuss the results of the theoretical modeling of luminescence form systems composed of two quantum dots (QDs) and of large ensembles of QDs. The emission of light from such systems is affected by the collective interaction of the QDs with the modes of the electromagnetic field and by the coupling between the dots. It can also be influenced by occupation redistribution between the delocalized single-exciton states due to carrier–phonon coupling, which makes the optical properties of these structures markedly different from the usual exponential decay typical of single dots.

The numerical modeling is based on various kinds of Markovian Master equations describing the interaction of confined carriers with the modes of the electromagnetic field, augmented by non-Markovian terms accounting for the interaction with phonons, treated on the lowest-order level within the time-convolutionless formalism.

Our simulations show that formation of delocalized exciton states, with different strengths of the coupling to the electromagnetic field (that is, “darker” and “brighter” ones) leads to non-exponential decay of the exciton population and of the coherent luminescence signal from double QDs [1]. Collective effects can also lead to population trapping in dark states and to non-monotonic temperature dependence of the exciton life time [2], similar to that observed experimentally [3]. In the case of dense ensembles of QDs, the collective character of the spontaneous emission in the presence of inter-dot coupling leads to an enhanced emission rate [4], as indeed found in a recent experiment [5]. Our results indicate that the fundamental long-range (dipole) interactions via the common electromagnetic reservoir are not sufficiently strong to account for the experimentally observed effect. However, additional short-range interactions (which may arise due to a combination of tunnel coupling and Coulomb correlations) can indeed lead to faster radiative decay. Under the assumption that additional short range interactions are present, the model reproduces the observed dependence of the decay rate both on the number of emitting dots as well as on the spectral position of the detection.

Exciton and phonon dynamics in optically driven semiconductor quantum dot structures

Tilmann Kuhn
Westfaelische Wilhelms-Universitaet Muenster, Institut fuer Festkoerpertheorie

Due to the discrete nature of their electronic spectrum quantum dot structures are sometimes called semiconductor macro-atoms. In contrast to real atoms, however, in quantum dots electrons and holes are typically rather strongly coupled to the lattice degrees of freedom, i.e., to acoustic and optical phonons. On the one hand this restricts the possibility to perform coherent manipulations of the exciton system and therefore may limit possible applications, e.g., in the field of quantum information processing. On the other hand it opens up possibilities to manipulate in a controlled way the quantum state of phonons by optically addressing the exciton state in the quantum dot. The first part of the talk will be devoted to the role of phonons for the dynamics of the excitonic system. Motivated by recent experiments I will compare the cases of excitation by (i) a resonant, (ii) an off-resonant and (iii) a frequency-swept (chirped) pulse. When the two-level system is excited by a resonant laser pulse, the well known Rabi oscillations in the population as a function of the pulse area appear. In the presence of phonons, the Rabi oscillations are damped, but for sufficiently high pulse areas a revival of the Rabi oscillations is seen [1]. When the frequency of the laser pulse is detuned from resonance, no population inversion can be achieved without phonons. However, the excited state can become populated due to the simultaneous absorption or emission of phonons during the optical excitation. For low temperatures phonon absorption processes are unlikely, such that for positive detuning a population inversion can be achieved. In the third case, when the QD is excited by a chirped pulse, a population inversion can be achieved by making use of the process of adiabatic rapid passage. This can be understood in the dressed state picture: The system adiabatically follows the dressed states that change their character during the pulse. Phonon processes take place between the dressed states which, in contrast to the previous case, deteriorates the achievable population inversion. For low temperatures a strong asymmetry in the resulting inversion with respect to the sign of the chirp is found as phonon absorption processes are suppressed. For higher temperatures phonon absorption and emission processes become equally strong and a full inversion cannot be achieved anymore [2].

In the second part of the talk I will concentrate on the quantum state of the phonons generated by an ultrafast optical excitation of the quantum dot exciton. Associated with the ultrafast excitation is an instantaneous shift of the equilibrium positions of the lattice ions resulting in a coherent oscillation around the new equilibrium position. A second ultrafast pulse can be used to efficiently control the quantum state of the generated phonons [3]. The resulting quantum dynamics of the phonons can be nicely visualized and interpreted in terms of a Wigner function representation [4]. It turns out that for suitable pulse parameters phononic Schrödinger cat states can be generated with properties that strongly depend on the delay and relative phase of the two exciting pulses. I will discuss the dynamics of these states as well as of the mean values and fluctuations of lattice displacement and momentum, in particular regarding the possibility to generate phonon squeezing.


Bunching and antibunching in electronic transport

Christina Pöltl$^1$, Clive Emary$^1$, Alexander Carmele$^1$, Julia Kabuss$^1$, Andreas Knorr$^1$ and Tobias Brandes$^1$

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In quantum optics the $g^{(2)}$-function is a standard tool to investigate photon emission statistics. We define a $g^{(2)}$-function of real time $\tau$ for electronic transport and use it to investigate the bunching and anti-bunching of electron currents [1]. Importantly, we show that super-Poissonian electron statistics do not necessarily imply electron bunching, and that sub-Poissonian statistics do not imply anti-bunching. We discuss the information contained in $g^{(2)}(\tau)$ for several typical examples of transport through nano-structures such as few-level quantum dots.

**Photocurrents in semiconductor nanostructures**

Huynh Thanh Duc\(^1\), Michal Pochwala\(^2\), Jens Förstner\(^2\), Torsten Meier\(^2\)

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Two concepts which have successfully been used to optically inject charge and spin currents on ultrafast time scales in semiconductor nanostructure without any external voltage are described. When exciting with two-color laser pulses the interference between to excitation pathways is used to coherently control the strength and the direction of the photocurrents. In this case, the direction into which the electrons flow is determined by a nonlinear excitation process. The purely optical excitation of photocurrents with one-color laser pulses is only possible in materials with a sufficient asymmetry. As an example GaAs quantum wells that are grown in the [110] direction are analyzed. The microscopic analysis of the optical current generation is based on the semiconductor Bloch equations.
**Contributed talk**

**Tuesday, 11:35 – 11:55 am**

**Full counting statistics for a single electron transistor strongly coupled to vibrations: a quantum master equation approach**

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Using a simple quantum master equation approach, we calculate the Full Counting Statistics of a single electron transistor strongly coupled to vibrations. The Full Counting Statistics contains both the statistics of integrated particle and energy currents associated to the transferred electrons and phonons. A universal fluctuation theorem, as well as an effective fluctuation theorem are derived for the general case where the various reservoirs temperatures and chemical potentials are different. The first relates to the entropy production generated in the junction while the second may be used as an electronic thermometer. The model recovers Franck-Condon blockade and potential applications to non-invasive molecular spectroscopy are discussed.
Jamming and glassy dynamics in driven granular systems: “melting a glass by freezing”

Claus Heussinger

University of Goettingen, Germany

The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. Structurally, these systems can all be viewed as dense assemblies of particles, and the particle volume fraction $\phi$ plays the role of the coupling constant that tunes the distance to the jamming transition. Apart from the industrial relevance of these materials, there is also a fundamental theoretical interest in the (athermal) jamming transition: as a new paradigm for structural arrest its relation to the (thermal) glass transition, the characterization of common and distinguishing features, remain to be elucidated.

In this contribution we present simulation results for a driven granular system in its glassy phase at high volume fraction. We show evidence of a remelting transition into a fluid phase, which occurs by reducing the amplitude of the driving. This transition is accompanied by superdiffusion, cooperative particle motion and a negative differential diffusivity. We will highlight the special role played by frictional interactions, which help particles to escape their glassy cages. Such an effect is in striking contrast to what friction is expected to do: make particles stick to reduce their mobility.
Studying mechanisms of ventricular fibrillation using an atomically accurate model of the human heart

Alexander Panfilov

Gent University, Belgium

Cardiac arrhythmias and sudden cardiac death is the leading cause of death accounting for about 1 death in 10 in industrialized countries. Although cardiac arrhythmias has been studied for well over a century, their underlying mechanisms remain largely unknown. One of the main problems in studies of cardiac arrhythmias is that they occur at the level of the whole organ only, while in most of the cases only single cell experiments can be performed. Due to these limitations alternative approaches such as mathematical modeling are of great interest.

In my talk I will report on development of anatomically accurate model of ventricles of the human heart that includes representation of electrical and mechanical function of the heart. Further, I will discuss several possible mechanisms of ventricular fibrillation which have been studied in our group using anatomically accurate modeling. The particular mechanisms are: negative filament tension, restitution induced breakup, mother rotor fibrillation and fibrillation due to deformation of cardiac tissue.
Properties of cardiac alternans

Blas Echebarria

Departament de Fisica Aplicada, Universitat Politecnica de Catalunya-BarcelonaTech, Barcelona, Spain.

In cardiac muscle, a change in transmembrane cellular potential produces a response known as action potential, that propagates along tissue. Many cardiac malfunctions are associated to problems in propagation, sometimes inducing the formation of rotors. When unstable, they can give rise to ventricular fibrillation, in which synchronous excitation is lost among different parts of the ventricle, impeding contraction, and causing death in a few minutes. Among the known precursors of life-threatening ventricular arrhythmias and sudden cardiac death are T wave alternans, defined as a periodic beat to beat change in the amplitude or shape of the ECG T wave. Although T wave alternans provide a global measure of the propagation at the whole heart level, they have been related to alternations in the duration of the excited phase (or action potential duration APD) at the single cell level, thereby establishing a causal link between electrical alternans and the initiation of ventricular fibrillation.

In this talk, I will review recent results regarding the origin and dynamics of cardiac alternans. At the cellular level, this rhythm often appears due to a steep relationship between the APD and the time elapsed from the end of the previous action potential. In other situations, it has been observed to be due to an instability in intracellular calcium dynamics. I will discuss different possibilities for the origin of this latter instability, including a nonlinear dependence of calcium release with calcium sequestration at the sarcoplasmic reticulum, or a slow recovery from refractoriness of release. In tissue, the oscillations at the single cell level can be spatially in or out of phase. This latter case is termed discordant alternates (DA) and is known to be related with the induction of reentry. Its origin can be related to the dispersion properties of the tissue. In this regard, recent developments will be presented, including the effect of anomalous dispersion, and tissue contraction.
A mechano-chemical model for contraction patterns in protoplasmic droplets of physarum polycephalum

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Protoplasmic droplets of the slime mold Physarum polycephalum show a variety of spatiotemporal contraction patterns such as spirals, traveling waves and synchronous oscillations. By coupling a two-phase poroelastic model for cytoplasm to a Ca-oscillator that regulates contraction of the actomyosin network, a continuum model is introduced that describes flow and deformation in addition to Calcium concentration in a physiologically realistic way. Cytoplasmic flow leads to a mechanical feedback extending the reaction diffusion mechanism by an advective term. The instabilities of this model are studied and numerical simulations are presented that are able to reproduce patterns seen in the experiments.
Chaos in nonlinear networks with time-delayed couplings

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Theoretical Physics, University Würzburg, Germany

Nonlinear units, interacting by time-delayed couplings, can develop chaos. In the limit of large delay times we distinguish two types of chaos: Strong chaos, where the maximal Lyapunov exponent is identical to the largest sub-exponent of the units, and weak chaos where it decreases with the inverse delay time. Strong chaos has a positive, and weak chaos a negative sub-exponent. For lasers and for some electronic circuits we find transitions from weak to strong to weak chaos by increasing the coupling strength. Networks of such units can synchronize to a common chaotic trajectory. The eigenvalues of the coupling matrix and the properties of a single unit with self-feedback determine the stability of complete synchronization. We find that only networks with weak chaos ā, i.e. with negative sub-exponents ā can synchronize in the limit of large delay times. If an eigenvalue gap exists, the network can synchronize completely. Otherwise, cluster synchronization is possible. The global loop structure of the graph of the network determines the patterns of synchronized clusters. If the greatest common divisor of all loop lengths is one, complete synchronization occurs for sufficiently weak chaos. Otherwise, the GCD gives the number of chaotic clusters. Physically, the GCD is related to mixing information about the trajectories of the individual units. Finally, we address the question of how many chaotic attractors are possible for a network of N units. Combining statistical mechanics of neural networks with nonlinear dynamics, we construct a model where the number of chaotic attractors increases exponentially with the size of the network.


Dynamics of rotating spirals in agitated wet granular matter

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Pattern formation of a thin layer of vertically agitated wet granular matter is investigated experimentally. Due to the strong cohesion arising from the capillary bridges formed between adjacent particles, agitated wet granular matter exhibits a different scenario as its dry counter-part. Rotating spirals with three arms, which correspond to the kinks between regions with different colliding phases, are the dominating pattern. This preferred number of arms corresponds to period tripling of the agitated granular layer, unlike predominantly subharmonic Faraday crispations in dry granular matter. The chirality of the spatiotemporal pattern corresponds to the rotation direction of the spirals. The meandering of the spiral core, the rotation speed and the shape of the spiral arms are quantified by image processing. The dependence of those quantities on the driving parameters will be presented.
Intracellular mechanochemical waves in an active poroelastic model

Sergio Alonso¹, Markus Radszuweit², Harald Engel², Markus Baer¹

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Many processes in living cells are controlled by biochemical substances regulating active stresses. The cytoplasm is an active material with both viscoelastic and liquid properties. We incorporate the active stress into a two-phase model of the cytoplasm which accounts for the spatiotemporal dynamics of the cytoskeleton and the cytosol. The cytoskeleton is described as a solid matrix that together with the cytosol as interstitial fluid constitutes a poroelastic material. We find different forms of mechanochemical waves including traveling, standing and rotating waves by employing linear stability analysis and numerical simulations in one and two spatial dimensions.
Symmetry breaking and pattern formation in cellular systems

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Ludwig-Maximilians-Universität München, München, Germany

Reaction-diffusion dynamics provide a versatile framework for intracellular self-organization phenomena. The Min system in E. coli employs such mechanisms to ensure precise cell division by its ability to dynamically adapt to cell geometry. Cell polarization, a prerequisite for processes such as stem cell differentiation and cell polarity in yeast, is also mediated by a diffusion-reaction process. Under which conditions patterns emerge, and how patterns are regulated by biochemical and geometrical factors are major aspects of current research. We will discuss general design principles of such cellular pattern forming systems and show how these are implemented for the respective specific biological function in cell division of E. coli and cell polarization in yeast.
Phase-field model of self-polarization and cell movement

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Modeling the movement of living motile cells on substrates is a formidable challenge; regulatory pathways are intertwined and forces that influence cell motion on adhesive substrates are not fully quantified. Additional challenges arise from the need to describe a moving deformable cell boundary and contact line dynamics. Here, we present a simple mathematical model coupling cell shape dynamics, treated in the framework of the Ginzburg-Landau-type equation for auxiliary mass density (phase field), to a partial differential equation describing the mean orientation (polarization of actin filaments) of the cell’s cytoskeletal network. In order to maintain the total area of the cell, the phase field equation is subject to a global conservation constraint. Correspondingly, the equation for mean polarization incorporates key elements of cell mechanics: directed polymerization of actin network at the cell membrane, decay of polarization in the bulk of the cell, and formation of actin bundles (stress fibers) in the rear. The model successfully reproduces the primary phenomenology of cell motility: discontinuous onset of motion, diversity of cell shapes and shape oscillations, as well as distribution of traction on the surface. The results are in qualitative agreement with recent experiments on the motility of keratocyte cells and cell fragments. The asymmetry of the shapes is captured to a large extent in this simple model, which may prove useful for the interpretation of recent experiments and predictions of cell dynamics under various conditions.
Nonequilibrium fluctuations of a remodeling in vitro cytoskeleton

Björn Stuhrmann\textsuperscript{1}, Marina Soares e Silva\textsuperscript{1}, Martin Depken\textsuperscript{1}, Frederick C. MacKintosh\textsuperscript{1}, Gijsje Koenderink\textsuperscript{1}

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The cytoskeleton is a highly dynamic biopolymer network which spans the interior of a living cell and provides it with mechanical stability. Molecular motors embedded in the cytoskeleton convert chemical energy into mechanical work by sliding filaments past each other. Elucidating ensuing nonequilibrium collective dynamics is essential for a physical understanding of cytoskeletal self-organization into functional architectures that drive cell functions such as migration, division, and tissue morphogenesis. To investigate the intricate interplay of stress generation and network remodeling we have developed an in vitro model system of a contractile cytoskeleton which is heterogeneous and evolves structurally over time. We quantify by video microrheology the temporal evolution of motor-driven probe particle fluctuations. At early evolution times, the fluctuation spectrum is dominated by strong non-Gaussian fluctuations which arise from large directed displacements reflecting motor-driven network contractions. At later times, directed displacements are infrequent and finally disappear, while the time scale of activity decreases considerably. We show that these effects are due to contractile coarsening of the motors into large foci. Our work provides insight into the self-organization of nonequilibrium motor-driven networks which are relevant to living cells and which provide inspiration for material science.
How bacteria in colonies can survive by killing siblings and reversibly changing shape

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A few bacteria on a surface (e.g., skin or a medical instrument) can grow into a colony consisting of a billion bacteria and spanning several centimeters. What happens when neighboring colonies of bacteria grow and approach one another? Studies of Paenibacillus dendritiformis (a bacterium found commonly in soil) reveal that neighboring bacterial colonies mutually inhibit growth through secretions of a lethal protein. An immediate question is why doesn’t this toxin kill the bacteria secreting it? A mathematical model helps answer this question. Further, sub-lethal concentrations of the toxin are found to induce the rod-shaped P. dendritiformis bacteria to switch shape to cocci, a spherical shape that is resistant to the toxin and to other antibiotics. But if the cocci encounter persistent favorable growth conditions, they switch back to rods. Thus the bacteria adapt to adverse environmental conditions by a reversible change in form.
Motility statistics of swimming bacteria in confined micro-environments

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Biofilms (BFs) are communities of sessile bacteria, embedded in an extracellular polymeric structure (EPS), which form at solid-liquid or liquid-air interfaces. We use microfluidic channels of varying height and geometry in combination with high speed imaging to study the swimming patterns of bacteria that coexist with surface attached clusters of sessile bacteria during the early stage of BF-formation. In shallow microchannels, our model organism, the soil bacterium \textit{Pseudomonas putida}, performs a random walk with a strong anti-correlation in its direction of propagation between two subsequent runs, indicating a run-reverse behavior. Using microchannels of different height and with varying densities of obstacles, we study the dependence of the swimming pattern on the geometrical parameters of the micro-environment. The tracking experiments are complemented by high speed fluorescence recordings to monitor the reorientation of a bacterium’s flagellae during a turn event.
Swimming strategies of bacteria

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There are several types of bacteria whose characteristic swimming patterns can be described in terms of random walks. For the bacterium *E. coli* that performs the well-known run-and-tumble motion, the (long-time) diffusion coefficient has been calculated [Lovely & Dahlquist, J. Theor. Biol. 50 (1975)]. In contrast to *E. coli*, most marine bacteria completely reverse their direction of motion after a tumble event; for the marine bacterium *V. alginolyticus* it has been shown recently that its swimming strategy is described by sequences of run, reverse-run, and randomizing flick events [Xie et al., PNAS 108 (2011)]. For this random walk we determine the diffusion coefficient analytically and compare it to *E. coli*.

It has been reported that the chemotactic drift speed with which the bacteria approach a food source is about three times larger for *V. alginolyticus* compared to *E. coli*. Whereas the chemotactic drift speed of *E. coli* in a small gradient has already been computed [Locsei, J. Math. Biol. 55 (2007)], we performed an analogous calculation of the drift speed for the run-reverse-flick strategy of *V. alginolyticus*. For small gradients, it turns out that there is no significant change in the chemotactic drift between both random walk strategies.
Self-organization in the processes of inherent polarity formation, gradient sensing, and directional motility in eukaryotic chemotaxis

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The ability of cells to sense an external chemical gradient is essential to cellular functions such as chemotaxis and other diverse processes. To sense a chemical gradient, eukaryotic cells have to detect differentials in the concentration of chemicals along the periphery of cells without rapid motile translocation. A concentration differential of a few percent across a cell body of a few tens of micrometers can be sufficient to induce directional migration. What mechanism can afford such astonishing sensitivity? In addition, the gradient information must be maintained in the presence of noise in signaling network and amplified sufficiently for downstream processes to produce directional migration. In eukaryotic cells, such as Dictyostelium discoideum and other mammalian cells, the phosphatidylinositol (PtdIns) lipids reaction is a key transmembrane signaling event responsible for gradient sensing for eukaryotic cell chemotaxis. The self-organization activity of the PtdIns lipids reaction induces an inherent polarity even in the absence of an external chemoattractant gradient by producing a localized domain of PI(3,4,5)P3 on the membrane [1]. The enzymes phosphatase and tensin homolog (PTEN) and phosphoinositide-3-kinase (PI3K), which are regulators for PtdIns lipid concentrations along the membrane, were essential for the self-organization behaviors whereas functional actin cytoskeleton was not. Defects in these enzymes inhibited such a behavior. We then developed a statistical method to reconstruct a phase portrait of the characteristic dynamics of the PtdIns lipids system from the noisy time-lapse data of fluorescent images of each single cell. On the basis of the experimental results and the reconstructed dynamics, we developed a theoretical model for the self-organization of the PtdIns lipids signaling system. Further analysis indicates that this self-organized system responds sharply to a shallow external gradient. These results imply that the self-organized activity, independent of external cues, is the basis for sensitivity to shallow chemoattractant gradients.

**Stirring by microswimmers**

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Because of their size bacteria and fabricated micro-swimmers swim at low Reynolds number, a regime where the effect of hydrodynamics can be counterintuitive. Moreover micro-swimmers provide experimentally accessible examples of active systems that create their own energy and operate out of thermodynamic equilibrium.

The mechanisms by which bacteria interact with particles in their environment are relevant to their feeding strategies and may contribute to oceanic mixing. We discuss how passive tracers are advected by swimmers, and hence estimate the diffusion constant of particles in a bacterial suspension.

We also examine encounters between a swimming bacterium and an inert spherical particle across a range of particle sizes, from tracers, through particles of intermediate size that are capable of deflecting the paths of the bacteria, to particles much larger than the swimmer that effectively behave as curved surfaces as a swimmer approaches.
Pattern formation und fluctuations in ferrofluids

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Colloidal suspensions of nano-sized ferromagnetic grains exposed to time-dependent magnetic fields show unusual hydrodynamic behaviour at the macroscale as well as intriguing cooperative effects at the microscale. As examples of the former we present the stabilization of a Rayleigh-Taylor unstable stratification of liquids [1] and the generation of cylindrical Korteweg-de-Vries solitons around a current-carrying wire [2], both realized in recent experiments [4, 5]. As example of the latter we discuss the role of interactions between ferromagnetic particles in a ferrofluid ratchet rectifying thermal fluctuations under non-equilibrium conditions.

The effects of external time-dependent fields on ferrofluids

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We investigate suspensions of colloidal dipolar particles that are exposed to external time-dependent fields. Mainly, we are interested in the dynamic behavior, the structure formation phenomena, and the phase behavior that colloidal particles exhibit under the influence of rotating fields. This includes synchronization and desynchronization effects of the particles with the external field, layer and cluster formation, and the relation of the latter to a first order vapor-liquid phase transition. Additionally, we investigate the behavior of dipolar particles that are exposed to oscillating fields. Surprisingly, such fields can lead to a noise induced rotation of the dipolar particles, which can be strongly influenced and enhanced by the dipolar interactions. Our methods of choice to look into these questions are Langevin dynamics simulations, Brownian dynamics simulations with hydrodynamic interactions and Monte-Carlo simulations.
Motility-induced phase separation in active brownian particles

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Active Brownian particles (ABPs, such as self-phoretic colloids) swim at fixed speed $v$ along a body-axis $\mathbf{u}$ that rotates by slow angular diffusion. Run-and-tumble particles (RTPs, such as motile bacteria) swim with constant $\mathbf{u}$ until a random tumble event suddenly decorrelates the orientation. We show that when the motility parameters depend on density $\rho$ but not on $\mathbf{u}$, the coarse-grained dynamics of interacting ABPs and RTPs are equivalent. In both cases, a steeply enough decreasing $v(\rho)$ causes phase separation in dimensions $d = 2, 3$, even when no direct forces act between the particles. This points to a generic role for motility-induced phase separation in active colloids.
Clustering and turbulence in active colloidal fluids

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We explore the dynamics and transport properties of strongly interacting active colloidal particles by computer simulation and dynamical density functional theory. Brownian dynamics simulations are used to study the nonequilibrium dynamics of concentrated self-propelled rods which are interacting via a Yukawa segment model.

In a linear channel, transient hedgehog-clustering at the system boundaries is found [1]. An wedge-like confinement is shown to be a very efficient trap for active particles [2]. In the two-dimensional bulk, anomalous turbulence emerges [3] in agreement with recent experimental data on bacterial motion [4].

Finally we study the freezing transition for very dense self-propelled particles and find significant differences to equilibrium freezing [5]. Simulation data are compared to a recent field-theoretical approaches of freezing based on the phase-field-crystal model which is extended towards active systems.

Running faster, running together: molecular motors speed-up thanks to hydrodynamic coupling

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We present simulations that reveal a surprisingly large effect of hydrodynamic coupling on the speed of thermal ratchet motors. The model that we use considers particles performing thermal ratchet motion in a hydrodynamic solvent. Using a particle-based, mesoscopic simulations that maintain local momentum conservation, we analyze quantitatively how the coupling to the surrounding fluid affects stepper motion. We find that coupling can increase the mean velocity of the stepping particles by almost two orders of magnitude, precisely because ratchet motion has both a diffusive and a deterministic component. The resulting coupling also leads to the formation of stepper-aggregates at longer times. The correlated motion that we describe increases the efficiency of stepper-delivered cargo transport and we speculate that the mechanism that we have uncovered may play a key role in speeding up molecular motor-driven intracellular transport.
Self-phoretic colloids: individual and collective motion

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I will talk about our current theoretical work on phoresis and taxis of catalyst-coated particles immersed in a reactant medium, with emphasis on the route from single-particle dynamics to collective equations of motion.
The taylor-couette motor: spontaneous flows of active polar fluids between two coaxial cylinders

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We study the dynamics of active polar fluids in a Taylor-Couette geometry where the fluid is confined between two rotating coaxial cylinders. This system can spontaneously generate flow fields and thereby set the two cylinders into relative rotation either by spontaneous symmetry breaking or via asymmetric boundary conditions on the polarization field at the cylinder surfaces. In the presence of an externally applied torque, the system can act as a rotatory motor and perform mechanical work. The relation between the relative angular velocity of the cylinders and the externally applied torque exhibits rich behaviors such as dynamic instabilities and the coexistence of multiple stable steady states for certain ranges of parameter values and boundary conditions.
Numerical simulations on the basis of a simple elastic-network (EN) model of the actin protein show that this macromolecule essentially behaves as a strain sensor, responding by well-defined domain motions to mechanical perturbations. We identify several sensitive residues within the nucleotide-binding pocket (NBP) which are able to translate local perturbations into the characteristic motions of the actin protein domains, i.e. flattening of the molecule and closing of the cleft between the two mobile domains. Extending the EN model by introducing of a set of breakable links which become effective only when two domains approach one another, it was observed that G-actin possesses a metastable state corresponding to a closed conformation. A transition to this state can be induced by appropriate perturbations in the NBP region. The ligands were roughly modeled as a single particle (ADP) or a dimer (ATP), which were placed inside the NBP and connected by elastic links to the neighbors. Our approximate analysis suggests that binding of ATP stabilizes the closed conformation of actin, which may play an important role in the explanation why the polymerization process is highly accelerated in the presence of ATP.
Stochastic thermodynamics and the fluctuation-dissipation theorem
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for non-equilibrium steady states Stochastic thermodynamics provides a framework for describing systems embedded in a heat bath and externally driven to non-equilibrium. Examples are colloidal particles in time-dependent optical traps, single biomolecules manipulated by optical tweezers or AFM tips, and motor proteins driven by ATP excess. Non-equilibrium steady states are characterized by time-independent driving.

I will review our recent work for such systems concerning the form of the fluctuation-dissipation theorem for such NESS [1, 2] and illustrate the general relations with results for specific systems like a sheared colloidal suspension [3] or a simple model for the rotary motor F1-ATPase [4]. The first systems allows to discuss the emergence of an “effective temperature” and the second one to draw a relation between the FDT and efficiency of a motor.

Effective fluctuation theorems in experiments
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Fluctuation theorems (FT) are one of the few exact relations that are valid for systems driven out of equilibrium. One of the most prominent examples is certainly the FT for entropy production. So far, experimental studies concentrated only on simple systems with one degree of freedom. By combining paramagnetic colloidal particles and rotating laser tweezers, we study two nonequilibrium steady states which can be coupled by an externally controlled magnetic field. We use digital video microscopy to follow both particles' nonequilibrium fluctuations with high accuracy. As derived from stochastic thermodynamics, all degrees of freedom have to be taken into account to maintain the FT. In experiments a subtle situation occurs if not all degrees of freedom are accessible, i.e., when in our system only the fluctuations of one particle are observed. We show that for the prevailing majority of experimental cases the inferred entropy production, which now is only an apparent one, obeys an effective FT. Beyond that, there exist extreme cases for which not even an effective FT is preserved.
Molecularly derived effective free energies and constitutive equations for complex fluids from thermodynamically guided simulations

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Deriving reliable effective free energies and constitutive equations for flowing complex fluids from the microscopic dynamics still presents major challenges to date [1, 2]. Here, we address this issue within a systematic coarse-graining method that is able to efficiently bridge the time- and length scale gap between the microscopic and macroscopic level of description. The proposed method is illustrated for nematic liquid crystals as well as low-molecular polymer melts subjected to homogeneous flow fields. We work within the framework of nonequilibrium thermodynamics and obtain the effective free energy via thermodynamic integration within a generalized canonical ensemble [3]. In order to obtain also the dynamics of the coarse-grained model, we use a hybrid Monte-Carlo-molecular dynamics iteration scheme [4]. We establish the functional form of the macroscopic constitutive model by reconstructing the thermodynamic building blocks from our simulations [5]. For low-molecular polymer melts, the constitutive model we propose shows shear thinning, stress overshoots, normal stress coefficients and elongational viscosities in agreement with reference results.


Experimental study of particle dynamics in random energy landscapes

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Energy landscapes provide a theoretical framework which has proven to be very powerful, e.g., for understanding the phenomena of protein folding or the dynamics of glass-forming systems. We experimentally studied the dynamics of individual as well as interacting colloidal particles in random energy landscapes[1, 2], which were optically generated by laser light fields. The particle dynamics were extracted using video microscopy and characterised using, e.g., the mean squared displacement, the van Hove function and the non Gaussian parameter. In both, one and two dimensions, the dynamics are initially diffusive and then, at intermediate times, show an extended sub-diffusive regime before diffusive motion is recovered at long times. These effects are less pronounced in two dimensions as compared to one dimension since local maxima can easily be circumvented.


Thermodynamics of detection

Massimiliano Esposito

University of Luxembourg, Luxembourg

Monitoring the dynamics of a small device always requires some sort of interaction with the system. This means that the measured system will be biased by the measurement. I will analyze the thermodynamic implications of this observation and present detailed results obtained for the study of charge transfer through a quantum junction monitored by a quantum point contact.
Doing small systems: fluctuation relations and the arrow of time

Peter Hänggi

University of Augsburg, Augsburg, Germany

This talk is aimed at highlighting issues that relate to doing thermodynamics and statistical physics of finite size systems. This theme gained considerable importance in view of fascinating advances in nanotechnology and system biology. While the fathers of thermodynamics developed the famous 5 Laws of Thermodynamics (incl. a $-1^{st}$ Law), having in mind macroscopic systems, these grand concepts need to be inspected anew in view of the fact that the fluctuations grow with decreasing size to a level where they even may play the dominant role. This holds true particularly for the inter-relationships between fluctuations and, importantly, the measurements of work, heat & heat flow and thermodynamic equilibrium quantifiers such as (non-fluctuating) free energy changes or production of thermodynamic entropy. – Subtleties occur in equilibrium thermodynamics for small systems, such as the role of finite size for quantities like (possibly negative-valued) canonical heat capacitance in presence of strong system-environment coupling.

I further elaborate on recent, timely results for nonequilibrium classical and quantum fluctuation relations. An attempt is made to outline pitfalls and still open issues (relativistic and others) together with those inherent difficulties that likely do emerge with the experimental validation scenarios of such relations. Finally, a connection between Fluctuation Relations, nonlinear Response and its feasible relation with the ever-lasting intriguing challenge in detecting the origin of an ”Arrow of Time” will be elucidated.

This presentation is based on joint work with Michele Campisi, Gert-Ludwig Ingold and Peter Talkner, all at the University of Augsburg. – Own pertinent recent works that apply for the theme of this talk are:


Book of Abstracts: Posters
Dissipation-assisted multiple exciton generation in semiconductor nanocrystals

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The population dynamics of single- and bi-exciton states in semiconductor nanocrystals is modeled numerically in order to study the transient bi-exciton population that occurs in an optically excited semiconductor nanocrystal in the presence of Coulomb coupling between single- and two-exciton state and a dissipation channel. In this way, we show that dissipation plays an important role in the multiple exciton generation (MEG) process.

We consider a subset of nanocrystal states composed of 4 levels, including the ground state (empty nanocrystal), two single exciton states and a bi-exciton state. Only the single exciton state which has a higher energy is assumed to be optically active (bright). We assume that the bi-exciton state is coupled only to the bright state by a Coulomb coupling on the order of 1meV. The other single exciton state represents all the possible states to which the exciton can relax from the bright state. Band mixing and other Coulomb interaction between electrons and holes are neglected. Our modeling is performed in the density matrix formalism by numerically solving a Markovian master equation. Dissipation is included via Ohmic spectral densities with the Gaussian cut off.

We study the dynamics of the dissipative (MEG) process for various energetical alignments of the states in about zero temperature. The results show that the system evolution strongly changes if the dissipation is included. In the case of ultra-fast coherent excitation, one always initially has a one-exciton state; without dissipation there would only be oscillations of the exciton number [1] but in the presence of dissipation the oscillations are damped and the number of excitons can grow close to 2 due to a dissipation-assisted impact ionization process, which is followed by Auger decay back to the value of 1. For incoherent excitation, the initial number of excitons can exceed 1. In the absence of dissipation, it would remain constant but in the presence of dissipation it can grow considerably to a maximum value and then decay, which is consistent with experimental observation [2]. In a certain range of parameters, the growth of the exciton number (MEG process) is fast (on picosecond time scale) and the following decay (Auger process) is much slower (on the time scale of hundreds of picoseconds). In some cases, the maximum occupation of the bi-exciton state increases when dissipation is included. To obtain the dynamics of an ensemble of nanocrystals with certain size dispersion, we average our results over the energy of the bi-exciton state which can be different for each single nanocrystal. We use a Gaussian distribution for the value of the bi-exciton energy. We show that the role of dissipation remains important also for the ensemble-average dynamics.


Impact of band structure and α-factor on locking dynamics of optically injected quantum dot laser – an analytical approach

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We study the influence of the band structure and of the linewidth-enhancement factor (α-factor) on the locking dynamics of a quantum dot (QD) laser under optical injection. In a QD laser the carrier lifetimes in the discrete QD levels determine the damping rate of the relaxation oscillations, which in terms crucially effects the dynamics of the QD laser. Therefore we derive the carrier lifetimes by microscopical calculations of the Coulomb interaction between the discrete QD levels and the surrounding quantum well acting as a carrier reservoir. QD devices with different sizes of the QDs, i.e. with different band structures, can be modeled by varying the energy spacing between the quantum well and the QD levels.

The dynamics is investigated in terms of injection strength $K$ and input frequency detuning $\Delta \nu_{\text{inj}}$ between the injecting laser (master laser) and the QD laser (slave laser). For small $K$ the synchronization region (Arnold’s tongue) is limited by saddle-node on an invariant cycle bifurcations, i.e. Adler’s type locking. In the locking region the QD laser exhibits stable frequency locked continuous wave operation with the frequency of the master laser.

At a critical value $K_c$ and positive $\Delta \nu_{\text{inj}}$ the saddle-node line transversely intersects with a Hopf-bifurcation line in a codimension-2 zero-Hopf (ZH) point. Thus for $K > K_c$ the locking tongue is for positive detuning bordered by a supercritical Hopf-bifurcation leading to undamped relaxation oscillations.

By taking advantage of the time-scale separation between the fast photon equations and the slower carrier equations, we find analytical approximations for the bifurcation lines limiting the locking tongue and for the ZH-point. Further an analytical expression is presented for the critical value of the injection strength, below which no Hopf-bifurcation can occur. The analytical expressions reveal the dependence of the bifurcation lines on the α-factor and on the damping of the relaxation oscillation (and thus on the band structure).

A stronger damping of the relaxation oscillations shifts the ZH-point to higher $K$ enlarging the range of stable frequency locked continuous wave operation. To obtain strong damping there exists an optimal energy spacing between the quantum well and the QD levels and thus an optimal band structure.

To proof the validity of the analytical approximations we compare them with numerical results obtained by direct numerical integrations and path continuation techniques.
Solitary pulses in semiconductor quantum dot media with simultaneous gain and absorption

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The propagation of conservative and dissipative optical solitons in semiconductor quantum dot media is investigated theoretically. We derive a nonlinear Schrödinger equation and a saturable gain/absorber equation from microscopic optical Bloch equations. These resulting wave equations exhibit conservative and dissipative soliton solutions, respectively. For the case of dissipative solitons the influence of dissipation and pumping on the solutions is taken into account microscopically, by means of phonon assisted quantum dot–wetting layer interaction, which exhibits a significant temperature dependence. We conclude on the possible existence of soliton solutions for realistic material parameters of a semiconductor quantum dot system.
Criticality in transport through the quantum Ising chain

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We consider thermal transport between two reservoirs coupled by a quantum Ising chain as a model for non-equilibrium physics induced in quantum-critical many-body systems. By deriving rate equations based on exact expressions for the quasiparticle pairs generated during the transport, we observe signatures of the underlying quantum phase transition in the steady-state energy current already at finite reservoir temperatures.

\[1\] preprint: http://arxiv.org/abs/1208.5989
Signature of carrier multiplication in the optical emission of quantum dots

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Carrier multiplication (CM) in quantum dots has been proposed as one possible technique to further increase the efficiency of photovoltaic conversion [1, 2, 3]. Hereby, the absorption of an high energy photon leads to the creation of a high energy single exciton, which can then further decay via Auger-channels into multiple low energy excitons. As multiple competing relaxation channels exist, it is not easy to confirm impact ionization as the dominating one. To allow the identification of such relaxation channels, we model the electron dynamics using a quantum kinetic equation of motion approach. With that we are able to calculate time-resolved emission spectra [4]. Here we find qualitatively different dynamical behaviors on an ultrafast time scale under variation of the length of the exciting light pulse. Using the electron dynamics, we are able to clearly attribute this signature in the emission spectrum to the Auger-type relaxation channels, therefore opening a way to experimentally verify CM in quantum dots.

Finally we extent our results to colloidal CdSe quantum dots using realistic quantum states and electron-phonon coupling.

Line narrowing of excited state transitions in nonlinear polarization spectroscopy

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Coupled nanostructures can exhibit very fast dephasing and energy relaxation times down to tens of femtoseconds, often obscured by inhomogeneous broadening. While there exists line-narrowing methods to retrieve these times, they only work for the lowest excitonic state. We show that the relaxation times of the higher excitonic states can be extracted by non-linear polarization spectroscopy performed in the frequency domain (NLPF). Using a Bloch equation approach \cite{1}, we present a microscopic theory to calculate NLPF spectra, which we then apply to photosynthetic light-harvesting complexes. Hereby, we use self-consistent structural data for the excitonic couplings of pigments and the spectral density of exciton-vibrational coupling \cite{2}. The results show that NLPF is suited to compensate effects of inhomogeneous broadening \cite{3}.

\begin{thebibliography}{9}
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Synchronization of self-sustained oscillators due to hydrodynamic interaction

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Synchronization of a collection of interacting dynamical elements is observable in many physical, chemical, biological, as well as social systems. A particularly impressive example for synchronization is the formation of so-called metachronal waves in a carpet of cilia on the surface of many microorganisms. There is strong evidence that this collective behavior is caused by hydrodynamic interactions. It means that the beating of a cilium is altered by the flow field induced by the motion of the other cilia. Based on our previous work [1], we study the emergence of metachronal waves in an open linear chain of one-dimensional driven phase oscillators coupled by hydrodynamic interactions only. In particular, we investigate how a variation of the driving force parameters and of geometrical parameters like oscillator spacing or the distance of the oscillator chain to a bounding wall influence synchronization. Moreover, we discuss the robustness of metachronal waves against thermal noise and when the intrinsic frequencies of the oscillators are chosen from a distribution mimicking biological systems.

Fluctuations in a nanoscopic carnot cycle

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We present a model of a generalized Carnot cycle containing only one particle. This simple model allows for a detailed analysis of the fluctuations of work and heat for an operation far from the equilibrium and for the quasi static case. While for macroscopic motors a deterministic description is sufficient, on the scale of molecular motors fluctuations play a crucial role. Recently, several theoretical models of stochastic motors – heat engines [1] as well as isothermal motors [2, 3] – have been studied in the framework of stochastic thermodynamics. Using our model, we show that fluctuations are important not only in situations far from equilibrium, but also in the quasi static limit.

Orientational dynamics of nematic liquid crystals under shear flow: stability and growth of dynamical modes in inhomogeneous systems.

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We study the nonequilibrium dynamics of rodlike nematic polymers under shear flow. We employ a mesoscopic description, and use the alignment tensor as an order parameter. Five coupled partial differential equations describe the dynamics of the alignment tensor. The rheological phase diagram with respect to the shear rate and reduced temperature are investigated for the homogeneous case. Contrary to earlier work, we employ numerical continuation methods, to obtain and classify the boundaries between different dynamic states. We check the validity of the results for the 1D inhomogeneous case and discuss differences to the homogeneous case. In our contribution we also discuss results of the investigation of domain growth of dynamic states.
Effective confinement as origin of the equivalence of kinetic temperature and fluctuation-dissipation ratio in a dense shear-driven suspension

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In thermal equilibrium, correlation and response functions are related by the fluctuation-dissipation theorem such that the so-called fluctuation-dissipation ratio (FDR) equals the thermal energy for any time. Driven into a nonequilibrium steady state, this property is generally lost and the FDR becomes time-dependent. For the velocity autocorrelation and the corresponding response functions of a tagged particle in a shear-driven colloidal suspension, however, we still find this ratio to be approximately time-independent and equal to the kinetic temperature in a broad density range. This a priori surprising result can be understood using the idea of an effective confinement in dense suspensions. Employing a time-scale separation, we can deduce an approximate fluctuation-dissipation relation connecting the correlation and response via the kinetic temperature as a constant scaling factor plus a correction term containing cross-correlations. In numerical simulations we show that this correction is negligible in a wide parameter range. Additionally, we show that a similar behavior can be found in a simple model system consisting of a single colloidal particle, trapped in a harmonic potential, subjected to shear flow.
Colloidal crystallization in quasi-2d induced by electrolyte gradients

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In this contribution, we present a crystallization effect of colloidal model systems under quasi two-dimensional confinement exploiting impurity-induced non-equilibrium conditions [1]. In particular, we use aqueous suspensions at low background salt concentrations confined between two charged walls. Gradients of ions released by seed particles intrinsically induce electro-osmotic currents which lead to particle transport along the substrate surface plane. This enhances the local particle concentration out of a thermodynamically stable monolayer fluid. Subsequently crystallization in a triangular monolayer structure occurs. Crystallites with one or more domains grow centered around the seeds with a saturating temporal growth behavior. Growth slows exponentially in time and finally ceases after the crystallites having reached their final size. Our results indicate a relation between the seed geometry and the resulting morphology. In our study we combine optical real-space microscopic experiments and Brownian dynamics computer simulations. We anticipate that efficient modeling together with convenient substrate fabrication will facilitate flexibly designing thin crystalline colloidal material of specified micro-structure.

Diffusion of particles at dense cellular flow in microvessels
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Individual cell motion in small blood vessels and microfluidic devices play an important role in the mixing and transport of substances. In blood flow a micron-scale flow field of red blood cells (RBCs) enhances the diffusion of particles to several orders greater than simple Brownian diffusion. An RBC is a deformable biconcave cell with a high surface-to-volume ratio, in which a Newtonian solution of hemoglobin is enclosed by a thin membrane. Experimental techniques for particles tracking in dense suspensions still encounter difficulties owing to opaque images (light scattering by RBCs and light absorption by hemoglobin). We study the spreading of fluid particles in blood flow at physiologically relevant hematocrits using a large-scale simulation. We developed a numerical model of micro-scale cellular flow based on a particle method. The elastic membrane deformation was modeled by a spring network of vertices. Herein, we quantified radial dispersion coefficient in microvessels by tracking many tracer particles. Effect of flow parameters on particle diffusion was analyzed. Results yielded a nearly linear dependency of particle dispersion on hematocrit and shear rate. We developed a non-dimensional dispersion coefficient by performing a scaling analysis, which provided an effective tool to predict the particle dispersion at dense cellular flow and a good insight into transport phenomena in microcirculation.
A century since Einstein’s theoretical formulation of Brownian motion, the subject remains an active area of research in the scientific community. While various generalizations of the isothermal Brownian motion has been formulated, we present results for a non-equilibrium generalization, namely hot Brownian motion, which has a high relevance in science and industry. In hot Brownian motion, a nanoparticle is kept at a higher temperature than the ambient solvent—a scenario often encountered in trapping and tracking experiments [3]. We demonstrate, using fluctuating hydrodynamics and molecular dynamics simulations, that the asymptotic dynamics of the heated colloid can be described by an effective Langevin equation supplemented by effective transport coefficients [1, 2, 3]. Further, we illustrate that these effective parameters are different for different degrees of freedom, and as well as for different modes of motion. Our analysis is highly relevant for numerous application of symmetrically and asymmetrically heated colloids, such as the self-propulsive motion of a Janus particle and paves the way for a deeper understanding of these non-equilibrium situations.


Dynamical signature of freezing in colloidal hard sphere like fluids

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The particle dynamics of a metastable liquid differs significantly from a liquid in the equilibrium state, giving the possibility to define the freezing point of the system of interest. A hard sphere (HS) system is the simplest model system showing a fluid crystal phase transition. We here focus on the dynamics of concentrated HS suspension around the fluid-crystal phase transition point using dynamic light scattering. Dynamic light scattering gives access to the intermediate scattering function (ISF) which measures particle number density fluctuations. Another aspect of the dynamics is the correlation of particle currents dictated by conservation of particle number density, which can be obtained by numerically differentiating the ISF [1, 2]. Recently it was shown that it is possible to define a dynamic freezing criterion in colloidal hard sphere systems (PMMA in decaline) by a careful analysis of the space time correlation function of longitudinal particle currents (CCF) [3]. We used highly cross-linked polystyrene (PS) microgel colloids dispersed in a good solvent 2-ethylnaphthalene to obtain a gravity matched colloidal model system with hard sphere like interaction. We studied the dynamics of the colloidal fluid around the main structure factor peak (1.7<qR<5) over a wide concentration range crossing the freezing transition. For the equilibrium fluid we observe an universal scaling of the CCF in good agreement with PMMA hard sphere systems. Significant deviations from the scaling were found for qR-values around the structure factor peak once the suspension is in the metastable state while scaling still works for qR values in front and behind the structure factor peak. In the equilibrium fluid state the CCF can be well described fitting a stretched exponential to the data. The number of high frequency modes increases with increasing volume fraction. This process immediately stops crossing the freezing volume fraction. Furthermore it is observed that the decorrelation of the CCF becomes nonmonotonic at the structure factor peak for particular delay times if the fluid becomes overcritical. This slowing down of the decorrelation of the CCF can be interpreted as a resistance to free momentum diffusion on a particular length scale.

Rotational hot brownian motion

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We establish an effective Markov theory for the rotational Brownian motion of hot nanoparticles. Compact analytical expressions for the effective temperature $T_{HBM}$ and friction $\zeta_{HBM}$ are derived from the fluctuating hydrodynamic equations of motion and verified by large-scale molecular dynamics simulations over a wide temperature range. This provides unique insights into the physics of hot Brownian motion and an excellent starting point for the experimental tests and applications involving laser-heated nanorods and Janus particles.
Controlling inertial focussing: a numerical study with multi-particle collision dynamics

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At intermediate Reynolds numbers, rigid particles in a cylindrical microfluidic channel position themselves at a fixed distance from the channel axis and channel walls, an effect first discovered by Segré and Silberberg \cite{Segre1961}. The Segré-Silberberg effect can be understood in terms of an effective lift force acting in radial direction on the particles. Devices utilizing inertial focusing for particle separation have recently been demonstrated \cite{Hur2009}.

Here we use the method of multi-particle collision dynamics (MPCD) to investigate the motion of a spherical colloid in a pressure driven flow at intermediate Reynolds numbers. MPCD is a mesoscale simulation technique to solve the full Navier-Stokes equations \cite{Kapral2008} and has successfully been applied to colloidal dynamics in previous studies.

We first investigate the spatial probability distribution of a colloidal particle and discuss its dependence on particle size and Reynolds number \cite{Prohm2012}. Second, we identify the momentum transfer from the MPCD fluid on the particle with a radial lift force and use this lift force to set up a Langevin equation describing the thermal motion of the colloid. We demonstrate that in steady-state the radial distribution functions follow from the Boltzmann distribution for the potential connected to the lift force.

Finally, we discuss feedback control schemes using additional radial or axial forces to localize the colloid at a fixed radial position within the channel. We discuss the application of these control to particle sorting and their optimization.


\cite{Hur2009} Hur et al., \textit{Lab Chip}, \textbf{10}, 274 – 280 (2009).


Non-equilibrium collective behavior of confined colloidal particles in a planar shear flow

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Sheared fluids are fundamental examples of non-equilibrium soft-matter systems. In this contribution we consider specifically a film of colloidal particles under planar Couette flow. As a framework for solving the equation of motion we employ overdamped Brownian Dynamics simulations. Being interested in the collective dynamics we investigate the impact of the shear flow and confinement focusing on structure formation and time-dependent behavior of our system. Trying to understand and to describe the behavior of observed structures we use e.g. order parameters, pair correlation function, density profiles and other evaluation tools.
Motional patterns of spherical colloids in a narrow microchannel

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Microfluidic devices have emerged as powerful tools for manipulating, controlling, and analyzing various processes in chemistry, physics, and biology. With the help of such devices one can perform controlled studies on the influence of confinement of colloidal particles and one can easily drive suspended objects out of equilibrium using a pressure driven Poiseuille flow. Thereby novel and intriguing dynamic structure formation in complex fluids occurs whose knowledge is essential, e.g., for developing tools to transport and sort particles on the micron scale.

We study the motional patterns of spherical colloids under the influence of a pressure driven flow, which are confined between two planar parallel walls. The colloids are neutrally buoyant and interact hydrodynamically via the solvent. For this situation, we determine the grand mobility matrix using a multipole expansion of the force densities on the spheres and taking into account the applied Poiseuille flow and the no-slip condition at the walls \cite{1}. We show that different initial conditions lead to different motional patterns, e.g., where particle trains either form a propagating wave or one particle oscillates back and forth between its neighbors, similar to observations in recent experiments \cite{2}. We analyze the stability of these patterns and investigate how they depend on the number and relative positions of the colloids.

\begin{thebibliography}{9}
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Space-resolved dynamic light scattering probing inhomogeneous dynamics in soft matter

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Dynamic light scattering (DLS) is the most powerful tool determining the dynamic properties in soft matter giving the possibility to monitor the particle movement over a huge time interval of 11 decades. Using standard techniques the ensemble averaged dynamics can be determined in ergodic media. In nonergodic samples (e.g. glasses) the measured time-averaged and the ensemble-averaged one differ. Special techniques have been developed (Interleaved sampling [1], Echo technique [2], multispeckle analysis [3]), measuring the intensity autocorrelation function (ICF) of many different coherent areas (speckles) simultaneously, in order to obtain ensemble averaged data. We here present a new designed multispeckle DLS experiment. In order to measure many speckles simultaneously we map the sample onto a fast charge-coupled device as a detector, which allows us to monitor the intensity of more than 1000 speckles simultaneously and to connect each speckle with its origin scattering volume. Due to the simultaneously monitored speckles we get a much better statistic than in standard DLS-Experiments. Furthermore the multispeckle setup allows us to measure time-resolved as well as space-resolved ICFs to probe differences in spatially separated subensembles. The spatial resolution can be used to probe the phenomenon of dynamical heterogeneities in metastable colloidal fluids. The frequency distribution of the ICFs for a colloidal liquid with a volume fraction of 0.4826 is symmetric and can be described by a Gaussian function. In comparison the frequency distribution for a metastable fluid with a volume fraction of 0.5744 is no longer symmetric and can be described by two Gaussian functions.

Towards two-dimensional transport of paramagnetic colloids via an ac-induced ratchet

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Magnetic garnet films autonomously form a striped magnetization which can be adjusted through an external magnetic field. Paramagnetic particles, which float in a certain distance above the film, align parallel to the magnetization stripes. An oscillating external magnetic field brings the colloids to a non-equilibrium state and induces a ratchet in the magnetic garnet film so that the system behaves as a Brownian motor.

The Brownian motion of the paramagnetic colloids is assumed to be overdamped. As a framework for solving the equation of motion for the time-dependent probability density, we employ the Dynamical Density Functional Theory (DDFT) where the microscopic particle interactions enter via a free energy functional.

First investigations are done in an one-dimensional cut perpendicular to the stripes, with a simplified two-dimensional model and in similar one-dimensional systems. Transport properties such as mean flow, density profiles, mean-squared displacement and the diffusion coefficient are investigated in dependence of the driving frequency and the particle’s magnetic susceptibility.
Brownian motion over curved manifolds

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The general covariance of the diffusion equation is exploited in order to study the curvature effects appearing in Brownian motion over a d-dimensional curved manifold (and sub-manifold). It is emphasized that on curved spaces there are several manners to define the displacement of a Brownian particle, which are compatible between them. Three physical observables are considered; namely, the geodesic displacement, the ambient spatial displacement, and the projected displacement. Their expectation values measure the curvature effects. For instance, it is shown that for the classical minimal surfaces, the ambient spatial displacement does not have curvature effects, whereas the geodesic displacement does it. Furthermore, the same expectation values are also studied over spheres, and development surfaces. Our findings are corroborated through a Langevin formalism on curved spaces.
Structure and dynamics of suspensions of colloidal dumbbells

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We investigate the static and dynamic structure of suspensions of colloidal dumbbells using Brownian dynamics computer simulations. The particular focus is the study of bulk structure and linear response transport coefficients at different densities and anisotropy parameters. In our work, the dumbbells are modelled by fused spheres interacting via a short-ranged hard-core-like repulsive Yukawa pair interaction. Crystal structures in the plastic crystal (PC) phase are identified and the PC-liquid transition is investigated. We present structural properties of the suspensions in form of static and dynamic structure factors $S(q,\omega)$ and pair distribution functions $g(r)$. Furthermore we calculate transport coefficients from auto-correlation functions in equilibrium. This includes the frequency-dependent rotational and translations self-diffusion as well as suspension shear viscosities.
Simulation of non-equilibrium surface growth - first results for C60

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Kinetic Monte Carlo simulation methods allow the simulation of non-equilibrium epitaxial surface growth over experimentally realized time spans of minutes and growth of multiple layers of particles. Through variation of simulated temperature and adsorption rate the structures formed can be manipulated and predictions for experimental methods such as molecular beam epitaxy can be made. We apply the method to simulate multilayer growth of C60. The material parameters are obtained through comparison with grazing-incidence X-ray spectroscopy measurements [1].

Collective dynamics in driven granular suspensions

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Suspensions of 0.2 mm glass spheres, driven by the water flow in a fluidized bed, show several hallmarks of glassy behavior like dynamical heterogeneities and a diverging viscosity. We present experimental results gained by a torsion pendulum and fast X-ray tomography performed at the ESRF synchrotron in Grenoble.
Glassy dynamics of brownian particles close to walls

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By using Brownian dynamics simulations, we study the slowdown of the dynamics of spherical particles at small temperatures or high densities. In our model system, the particles interact via finite-ranged repulsive interactions. In the limit of small overlaps the dynamics of our soft spheres corresponds to the overdamped dynamics of hard spheres. We determine the relaxation time as a function of temperature and pressure. The dynamics in the vicinity of a wall is compared to the dynamics in bulk. Furthermore, we add a structure to the wall that is build up by a pattern of attractive Gaussian traps.
The kinetics of crystallization and vitrification in colloidal hard spheres

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A complete understanding of the solidification process is one of the long standing problems in condensed matter physics. There are two possible scenarios: In crystallization the metastable melt rearranges into a long range ordered solid state (crystal) while in vitrification the short range order is maintained (glass) and the melt does not reach the equilibrium state. The use of colloidal model systems provides an ideal controlled experimental system to reduce this lack of knowledge. We investigated the solidification scenario in suspensions of gravity matched colloidal hard spheres (HS) using time resolved static light scattering as well as dynamic light scattering techniques. Solidification kinetics were measured using an advanced time resolved laser light Bragg scattering setup, averaging over the whole Debye-Scherrer cone to allow access to data with a good statistic even at early times of the solidification process. From the time evolution of the measured static structure factor we were able to determine characteristic quantities of the solidification process: the amount of solid material X, mean size of the crystalline/solid clusters $L_{xtal}$, volume fraction of the crystalline phase and number density of crystals $n_{xtal}$. A detailed analysis of these quantities shows that solidification is originated by precursors (compressed, structurally heterogeneous clusters) during the induction stage. In crystallization these objects convert into highly ordered crystals in a fast, activated process. This kind of precursor mediated crystallization of a system with hard sphere interaction has been confirmed by simulation work (T. Schilling et al. PRL 105 (2011)). In the case of vitrification these conversion is hindered and the system is locked in the metastable precursor state. Following the same processes over a range of volume fractions from near freezing to above the glass transition allows to systematically link the mechanisms involved in HS crystallization to those of the HS glass transition. In addition to this we measured the evolution of the intermediate scattering function (ISF) as function of waiting time giving us the possibility to quantify the time evolution of the α-relaxation. In the crystallizing sample the Debye-Waller factor increases significantly during the main crystallization process while in the vitrifying sample a constant increase of this quantity is observed. Furthermore there is an evidence of a quantitative correlation of the dynamic and the kinetic properties.
Distorted structure in sheared dispersions as described by mode-coupling theory (mct)

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The structure of a hard sphere supercooled liquid, like dense colloidal suspensions or metallic glasses, becomes anisotropic and distorted under shear. Within a transient regime, stress autocorrelation functions show a non-monotonous behaviour between linear response and steady flow. This can be observed macroscopically in stress overshoots or microscopically in super-diffusive particle motion. We use microscopic mode-coupling theory and molecular dynamics simulations to investigate the anisotropic, time-dependent change of structure in the structure factor and pair correlation function. Both, k space and real space are considered in order to evaluate the physical background of transient non-monotonicity in glass forming liquids under shear.
Cooperative processes in restructuring gel networks

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We have carried out a comparative study of restructuring and non-restructuring gel networks, by means of molecular dynamics. The networks arise from self-assembly of colloidal particles, whose effective interactions yields local rigidity necessary to make thin network structures at low volume fractions mechanically stable. The localization of particles in the network, akin to some extent to caging in dense glasses, appears to be determined only by the network topology and displays the same features in restructuring and non-restructuring networks. Nevertheless, bond-breaking processes induce cooperative processes that are not present in the non-restructuring networks and we are able to relate them to the presence of regions where bond-breaking is more likely to occur. Interestingly, such regions are not characterized by more mobile particles: because the mesoscale organization of the network is not disrupted by single bond-breaking events, such events can instead change significantly the mobility of regions further away.
A mesoscopic model for cement gel

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Calcium-silicate-hydrate (CSH) is the primary hydration product of Portland cement. It precipitates and solidifies into a nano-scale gel, which literally glues together the different parts of cement and it is responsible for its mechanics. To investigate the connection between the evolution of the CSH gel microstructure and its rheological properties, we model the CSH as a mesoscale gel. The nano-scale particles, which form the CSH gel, set the resolution length of our model and it does not account for the atomistic details of the CSH, below the length of few nanometers. However, the cohesive effective interaction of the nano-particles is determined by the atomistic structure of CSH. We follow the nano-particles trajectories with Molecular Dynamics. Analyzing the trajectories, we study the structure and the dynamics of the CSH gel. A very important effect in the evolution of the CSH gel is the continuous hydration reaction. To incorporate in our model the formation of new CSH hydrates, we introduce Monte Carlo events of addition and deletion. The competition between effective interactions and particle formation allows cooperative motion and rearrangement, which leads to complex microstructures with variable rheological behavior.

Polymer unfolding induced by spatially correlated noise

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Understanding the diffusive behavior in complex environment is crucial for the molecular biophysics. Numerous advances have been already contributed to this field, i.e. the development of subdiffusion formalism [1] and relating it to the microscopic model [2] which provide a framework for modeling systems with time-correlated noise. However, while this theory sheds light upon the temporal aspect of the diffusion in complex media, little work has been done to understand its spatial counterpart and its consequences.

In my presentation, I would like to report our findings regarding the influence of spatially correlated Gaussian noise on a 2D polymer-like particle. By means of Langevin equations, we have simulated a bead-spring chain, where the nearest neighbors interact via the harmonic potential and every node interacts globally by Lennard-Jones potential, which provides excluded volume. We have also introduced a harmonic interaction between beads \( i \) and \( i + 2 \) which resulted in a saw-like conformation of the chain. This system has been forced by the spatially correlated Gaussian noise, which amplitude and the correlation length can be varied.

Our results on the noise induced chain stiffening have been already reported in [3]. In this presentation, I will discuss several new effects introduced by the spatial correlations in noise, namely: beads motion synchronization, increased time-correlation of the nearest neighbors distance, and, most notably, chain unfolding due to the rise in the correlation length.

Strain rate (compressive & shear) dependent direct 3d observation of restructuring in colloidal gel

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Colloidal gels are nonergodic disordered states of soft matter. Due to weak aggregation of the colloidal particles a sample spanning percolated network forms. The heterogeneous gel microstructure is time dependent as it undergoes restructuring depending on many factors, e.g. sample history, external stress, gravitational compression due to its own weight, interstitial fluid pressure, etc. Understanding the link between microstructure and mechanical response of colloidal gels under external deformation is relevant for their applications, e.g. pastes, coating, lubricants, inks, etc. The strain rate dependent mechanical response reflects the time scales involved in restructuring the microstructure [1, 2]. Still, there is little evidence of direct observation of the 3D microstructure at particle level and corresponding strain rate dependent mechanical response [3].

We present data of a study on silica colloidal gel (particle size ~ 700 nm) obtained using laser scanning confocal microscopy synchronized with an indenter to apply strain. Attraction among the silica particles are induced by chemisorbing the surfactant N,N-dimethyl-N-octadecyl-3-amino-propyltrimethoxysilyl chloride (DMOAP) on the particle surface. The particles are suspended in the organic solvent cis-decalin to match closely the particle refractive index allowing high quality optical imaging and visualizing deep within the sample. This in-house built experimental set-up allows us for simultaneous 3D imaging of microstructure while applying strain (at different rates) in different directions (compressive & shear) [4] and tracking of the motion of the individual colloids forming the gel. We will be discussing the findings of direct observation of 3D structural configuration at a single particle level obtained while applying the deformation at different strain rates. Results will be analyzed based on the detailed analysis of the change in particle connectivity, average nearest contact number, number of interparticle bond breakage and bond formation. The global structural analysis will be presented using structural correlation length of the particle aggregates in the gel.

Front propagation during the sol-gel transition
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We study the microrheology of a micron-sized sample of a thermoreversible gel during the sol-gel transition after a fast temperature quench. We identify two different mechanisms responsible for the gelation of the quenched sol phase: a fast process associated to the local formation of the gel network and a slower process induced by presence of the already formed network at the boundaries. We interpret the latter as a the propagation of a gel front which accelerates the aging rate of the sol-gel transition.
Clustering and phase behaviour of active brownian particles

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Using large-scale Brownian dynamics simulations, we investigate the collective dynamics and structure of self-propelled particles in 3 dimensions. As a minimal model of an active system we use purely repulsive spherical particles with a constant propulsion speed $v_0$, whose direction diffuses in a Brownian fashion. We investigate how the effective diffusivity $D_{\text{eff}}$ depends on $v_0$ as well as on the volume fraction $\phi$ of particles in the system. Furthermore, the prevalence of activity-induced phase transitions and clustering of the colloids, as has been theoretically predicted \cite{Tailleur2008} and shown to occur in 2 dimensions \cite{Fily2012}, is investigated. Finally, we examine the implications on the above-mentioned properties of adding a passive component to the active system. In particular, we assess what effect the presence of active particles has on the diffusivity of the passive ones.


Structural features underlying supercooled dynamics and glass transition.

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We have studied the supercooled liquid state response to an instantaneous shear deformation, in terms of the correlations between the soft modes of the inherent structure belonging to the initial and final configurations, the quench vectors and the isoconfigurational Debye-Waller factors of the initial thermal configuration, as a function of the temperature and of the strain amplitude. The spatial distributions of non-affine displacements characterizing such response are not only strongly correlated to the dynamical heterogeneities of the supercooled liquid but also to the low energy soft modes of the inherent structure, responsible for the onset of plasticity in the amorphous solid.
Active Brownian particles with state-dependent self-propulsion: effective dynamics and ratchet effect

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We investigate the nonequilibrium statistics of a suspension of overdamped free Brownian particles with spatially varying active velocity, i.e. self-propulsion. Our numerical and analytical investigations show that the particles accumulate in regions of low activity, accompanied by the emergence of polar ordering, i.e. position-dependent average orientation. By adiabatic elimination of the orientational degrees of freedom, we derive an effective dynamics of the particles, yielding a stochastic process with multiplicative noise. This is corroborated by an appropriate asymptotic expansion of the Smoluchowsky Equation. Further, we consider the ratchet effect for active particles \cite{1, 2} supplemented by external forces. Assuming again a comparatively fast rotational dynamics, we show that the active Brownian ratchet resembles Büttiker’s “hot-spot ratchet” \cite{3}, which induces directed transport by a spatially periodic temperature profile along a periodic potential.


How to capture active particles

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In many applications, it is important to catch collections of autonomously navigating microbes and man-made microswimmers in a controlled way. Using computer simulation of a two-dimensional system of self-propelled rods we show that a static chevron-shaped wall represents an excellent trapping device for capturing self-motile particles. Its catching efficiency can be controlled by varying the apex angle of the trap which denotes the sharpness of the cusp. Upon decreasing the angle we find a sequence of three emergent states: no trapping at wide angles followed by a sharp transition towards complete trapping at medium angles and a crossover to partial trapping at small cusp angles. A generic trapping 'phase diagram' maps out the conditions at which the capture of active particles at a given density is rendered optimal.
Collective motion in squirmer suspensions
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Collective motion in out-of-equilibrium systems composed of a large number of interacting individuals can be seen as a self-assembly phenomenon, which gives rise to intriguing emergent patterns. Due to their kinetic origin, the spontaneous structures these system give rise to are far more complex than equilibrium self-assembly in traditional metals, ceramics and polymers, with many levels of functionality, hierarchical organization, and compartmentalization [1]. Non-equilibrium materials must actively consume energy and remain out of equilibrium to support their structural complexity and functional diversity [2, 3]. In Biology flocking birds, fish schools, and insect swarms constitute examples of collective motion that plays a role in a range of problems, such as spreading of diseases [4]. In particular, micro-swimmer suspensions at low Reynolds number, such as bacterial colonies [5], exhibit fascinating collective behavior, including the possibility of non-equilibrium phase transitions between disordered and ordered states, novel long-range correlations, and pattern formation on mesoscopic scales [6]. Using a simple model in which the effect of the internal metabolism of the micro-organism can be described through the effective fluid flow the particle generates on its surface, making use of the squirmer model [7], and adding a Lennard-Jones (LJ) interaction between the swimmers as a model of the communication between the micro-organisms, we have fully characterized the clusters and the collective coherent orientation of the swimmers movement which emerge for some cases. We analyze the transition of the spontaneously formed structures as a function of the relative strength of the LJ interactions and hydrodynamic interactions

Chemotaxis of bacteria in highly restrictive microchannels

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The present research evaluates the impact of physical constriction to the chemotactic phenomena of Escherichia coli MG1655 by measuring physical parameters such as speed, turn angle and trajectories. This phenomenon is tested into a microfluidic device that provides the physical constriction and generates a chemotactic linear gradient. We used a hydrogel-based gradient generator that provides the chemical diffusion between three channels; sink, test and source. The bacteria are confined in 10µm square channels. This device allows measuring the dynamic behavior of bacteria under the constriction with a very good time resolution using confocal microscopy. This let us to find differences in the speed and angle distribution for the microorganism with two conditions, with and without the chemoattractant alpha-methylaspartate.
Clustered of self-propelled particles without alignement

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We study analytically and numerically a two dimensional system of self-propelled particles which interact through an isotropic pair potential. Starting with the Smoluchowski equation we perform a stability analysis to gain insight in which regime particles form clusters and predict a non-equilibrium phase diagram. In the second part of this work we perform Brownian dynamics simulations for three different pair potentials: the Yukawa potential, the Gaussian core model, and a harmonic pair potential known from modelling granular media. We show excellent agreement between numerical and analytical results despite the approximations and closures made in the analytic part.
Recent experiments of active colloids show a coexistence of single particles and clusters [1]. In such a "hot cluster phase" the clusters are themselves mobile and their size varies in time. Our model incorporates two phoretic effects which determine the colloid's dynamics. Self-electrophoresis on the one hand leads to active motion. On the other hand each particle depletes a certain chemical which causes diffusiophoretic motion of nearby colloids, similar to bacteria moving along gradients of nutriants. In our case however, both, translational motion and reorientation towards the gradient contribute to the overall dynamics. A hot cluster phase is reproduced which may collaps to a single cluster system. This depends on two parameters controlling chemotactic interaction and activity. We define a cluster persistence quantity, which diverges in the collapsed phase and determine cluster size distributions close to the transition.

Swimming active emulsion droplets

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In a recent attempt to build a spherical self-propelling microswimmer, a so-called squirmer, micron-sized droplets of water and bromine were placed into a surfactant rich oil medium [1]. These droplets then started to swim in a directed swimming motion. The reason for the swimming motion lies in a chemical reaction of the bromine with the surfactant monolayer at the droplet interface. The reaction product is a surfactant with a higher surface tension. As a consequence, local gradients in surface tension will lead to a fluid flow in the adjacent fluid inside and outside of the droplet. Due to this so-called Marangoni effect, the resting state of the droplet becomes unstable and the droplet starts to move. A study of the collective motion of many droplets revealed a swarming behavior, which is believed to arise purely due to hydrodynamic interactions.

A rigorous theoretical model, based on a free energy functional for the droplet interface, is presented and simulated. The simulations confirm the directed swimming motion of a single droplet. Additionally, stopping and oscillating solutions were found. By calculating the squirmer 'stirring' parameter $\beta$, we could then characterize the swimming droplet to be a pusher. Since these swimmers are known to show polar velocity correlations, our results are in perfect agreement with the swarming behavior found in experiments.

Controlling the position of a front
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We present a method to control the position as a function of time of a one-dimensional front solution of a one-component reaction-diffusion system according to a specified protocol of movement. Given this protocol, the control function is found as the solution of a perturbatively derived Fredholm integral equation of the first kind. Two cases are considered. First, we derive an analytical expression for the space ($x$) and time ($t$) dependent control function $f(x, t)$ valid for arbitrary protocols and arbitrary bistable reaction kinetics. Second, for stationary control of the Schlögl model we present an analytical solution of the problem to stop a front at a specified position. The analytical results are in good agreement with numerical simulations of the underlying reaction-diffusion equations.
Analytical approximations for spiral waves

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Using a simple ansatz, we obtain an approximate analytical solution of the linear eikonal equation for a rigidly rotating spiral wave in an excitable medium. From the equation for the wave front, we find a universal expression relating the rotation frequency $\Omega$ and the core radius $R_0$ of the spiral. The equation for the wave back gives a relation $\Omega (B)$ between $\Omega$ and the single parameter $B$ that characterizes the excitability of the medium. We find properly shaped spiral waves for all possible values of $\Omega$ and $B$, however, there are significant deviations between the analytically and numerically determined $\Omega$ over $B$ dependence.
Coarse-grained simulations of active protein machines in biological membranes with a solvent

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Protein machines, cyclically changing their conformations, play a fundamental role in the living cells; many of them are found in cellular membranes. Since the cycles of the machines are in the millisecond range, approximate coarse-grained descriptions are needed. Recently, entire operation cycles of some protein machines could already be reproduced by using coarse-grained models, with solvent included. Here, we proceed further and demonstrate that dynamical cycle simulations of machines immersed into a membrane are possible. Our approach combines the elastic-network description for a machine with the multiparticle-collision modeling for the solvent and a reduced description for the lipids. Membrane-mediated synchronization of machine cycles has been found in our simulations.
Flow enhanced non-homogeneous nucleation: reaction diffusion equations and domain growth

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We follow the scheme of classical nucleation theory to describe the aggregation of particles in solution. The non-monotonic effects of flow and elastic stresses in within the nuclei are introduced by performing a local thermodynamic analysis of energy contributions. This allows us to derive an expression for the non equilibrium Gibbs free energy of the process and then to describe the dynamics of nucleus formation in the presence of flow.

We study the growth of the domain of nucleation using the Becker-Döring scheme of bimolecular reactions and considering spatial inhomogeneities by means of a diffusion term in the reaction equations. The reaction diffusion equations we obtain are analyzed in several cases, one of them leading to the well know Fisher-Kolmogorov equation. Domain growth dynamics is analyzed in terms of reaction fronts in the absence and presence of flow.
Spontaneous actin waves and their possible role for cell migration

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The crawling of eukaryotic cells on substrates is driven by the cytoskeleton. How the cytoskeleton is organized in this process is still poorly understood. It has been suggested that spontaneous polymerization waves provide a possible answer to this question. We examine this possibility theoretically by analyzing a system of treadmilling filaments in a deformable domain. It is known that treadmilling filaments can spontaneously generate polymerization waves [1]. The domain boundary is characterized by a surface tension and a bending rigidity and evolves due to interactions with the filaments. We find spiral waves as well as states with a net directional motion of the system’s geometric center of mass. In contrast to [2], we solve the full system of dynamic equations and consider a more realistic length regulation of the filaments.

Mechanical instabilities of tubular cellular protrusions

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Cellular systems present a multitude of tubular protrusions, e.g., filopodia, axons or stereocilia. These structures are essentially cylinders delimited by a lipid membrane and filled with cytoskeletal filaments. The intrinsic activity of such protrusions can induce mechanical instabilities. For example, peristaltic shape transformations of axons have been observed subsequent to osmotic perturbations [1]. To further understand possible mechanical instabilities of tubular protrusions, we study the dynamics of active gels inside cylindrical membrane tubes. A multi-component hydrodynamic theory is used to describe cytoskeletal dynamics on a continuum level and on macroscopic length and time scales.

Modelling collective motion and cluster formation in myxobacteria

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Experiments on collective motion of different strains of myxobacteria (wild type, two mutant species) are interpreted with the help of a simple model for cluster formation of self-propelled particles. In the two mutant species a transition to motion in large clusters is observed, that can be quantified with the analysis of the cluster size distribution. The model of cluster formation reproduces the qualitative transition from an exponentially decaying to a biomodal cluster size distribution found in experiments and in simulations of self-propelled particles and rods. The transition point is characterized by a power-law cluster-size distribution with a finite size cutoff. The exponents of the power law are shown to be non-universal and depend crucially on the fragmentation and collision rates of individual clusters.

Electrical wave propagation in the human heart and the effect of mechanical motion

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Modelling electrical activity in the human heart is a challenging task from different point of views. The mathematical description needs to accurately account for anatomical details like fibre orientation or heterogeneity of the heart tissue. A precise physiological description demands for a large number of cells in computer simulations. To reduce the computational burden mechanical motion often is neglected. On the other hand it might be essential for a deeper understanding of the mechanisms of arrhythmias like tachycardia and fibrillation.

In this work we incorporate experimentally estimated motion into computer simulations. Time-resolved magnetic resonance images (MRI) were recorded in order to create finite element meshes that allow to map mechanical motion on statically performed simulations [1]. A tagged acquisition protocol was chosen so that cardiac motion can be extracted for a set of distinct points within the myocardial region. The orientation of the muscle fibres was allocated algorithmically [2] since this information is not present in MRI recordings. The intra- and extracellular domains are treated separately utilizing a bidomain approach – a set of partial differential equations for the extracellular potential \( \phi_e \) and the transmembrane potential \( V_m = \phi_e - \phi_i \)

\[
\nabla \cdot (\sigma_i \nabla V_m) = -\nabla \cdot \left( (\sigma_i + \sigma_e) \right) \nabla \phi_e ,
\]

\[
\nabla \cdot (\sigma_i \nabla V_m) + \nabla \cdot (\sigma_i \nabla \phi_e) = \beta \left( C_m \frac{\partial V_m}{\partial t} + I_{ion} \right),
\]

where \( \beta \) is the dimensionless surface-to-volume ratio and \( C_m \) is the membrane capacitance. \( \sigma_{e,i} \) denotes the conductivity tensor. The ionic models enter via the ionic currents \( I_{ion} \). In this work two of them were applied to the simulations: a 4-variable minimal model by Bueno-Orovio, Cherry and Fenton (BOCF) [3] and a 14-variable model by ten Tusscher (TNNP) [4]. Each of these models is tuned to fit the ionic dynamics to epicardial, myo- and endocardial cells.

The impact of cardiac motion on artificially generated biosignals like the electrocardiogram (ECG) or the magnetocardiogram (MCG) is demonstrated by drawing comparisons to statically performed simulations. Our approach also offers the opportunity to calculate the mechanical stresses during cardiac contraction from experimental data.

References


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(ii) collective dynamics in dispersions of colloidal particles and molecular machines;

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