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MÜNSTER

In search of model structures for non-equilibrium systems

April 24 – 28, 2023
Münster

Organizers

André Schlichting (University of Münster)
Uwe Thiele (University of Münster)
Oliver Tse (TU Eindhoven)
Johannes Zimmer (TU München)

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MM
Mathematics
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Cluster of Excellence

	Monday April 24	Tuesday April 25	Wednesday April 26	Thursday April 27	Friday April 28
09.00-09.30		Massimiliano Esposito	Brice Douet	Patricia Gonçalves	Mark Peletier
09.30-10.00		Alexander Mielke	Tanja Schilling	Tridib Sadhu	Artur Stephan
10.00-10.30		**Coffee**	**Coffee**	**Coffee**	**Coffee**
10.30-11.00		Moshir Harsh	Davide Gabrielli	Stefan Großkinsky	Giulia Pisegna
11.00-11.30		Rob Jack	Hugues Meyer	Dirk Peschka	Yuan Gao
11.30-12.00		Mario Ayala	Markus Bär	Stefano Olla	Raphael Wittkowski
12.00-14.00	**Registration and Opening**	**Lunch**	**Lunch**	**Lunch**	**Lunch**
14.00-14.30	*Survey Talks (45min each)*	Ramin Golestanian	Robert Großmann	Jaehyeok Jin	
14.30-15.00	Hartmut Löwen	Rishabh Gvalani	Aljaz Godec	Michiel Renger	
15.00-15.30	Milton Jara	Sabine Klapp	Horst-Holger Boltz	Michael te Vrugt	
15.30-16.15	**Coffee**	**Coffee**	**Coffee**	**Coffee**	
16.15-16.45	*Poster Pitch Talks*	Erwin Frey	*free afternoon for discussion*	Thomas Speck	
16.45-17.15	*and*	Jin Feng		Christian Maes	
	Posters				
18.30	**Reception**	**Conference Dinner Schloßcafé**			

General information

Venue. The main workshop venue is the MM-conference center located on the second floor of the Seminarraumzentrum (SRZ) at Orléans-Ring 12, 48149 Münster (see map on p. 4). You will find the registration there. Moreover, the coffee breaks and poster sessions take place in the lounge of the seminar building SRZ (second floor) right in front of the seminar room.

You can find the latest information on the webpage:
www.uni-muenster.de/MathematicsMuenster/go/non-equilibrium-systems

Wi-Fi access. If you are part of the eduroam community, you may connect to the network "eduroam" as usual. Otherwise you can connect to the SSID "GuestOnCampus" and start any web browser. You will automatically be redirected to the login page. Confirm the terms of use and click on "log in for free". 1 GB data volume is available per device and day. Please note that the connection is not encrypted.

Coffee break/Lunch. We provide coffee and snacks during the coffee breaks.

There are a couple of restaurants for lunch in the vicinity:

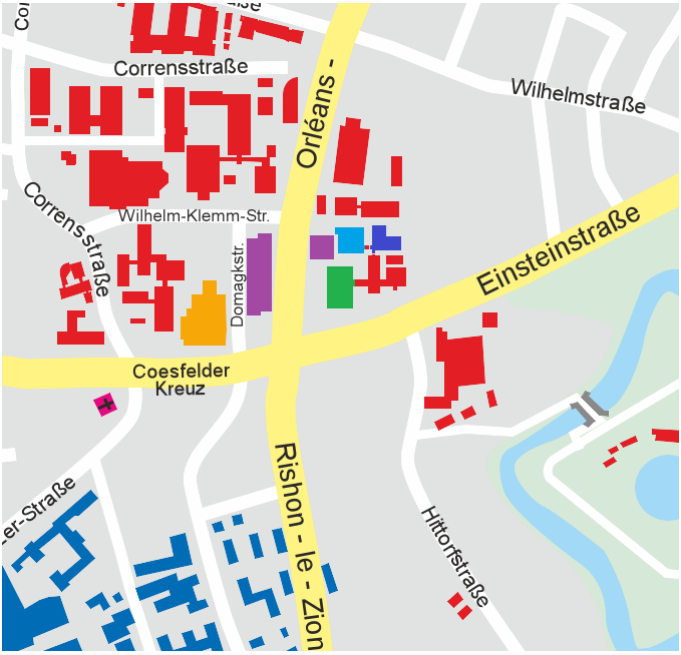
- Canteen – Mensa am Ring, Domagkstraße 61 (most convenient option, even if not the most idyllic place)
- Ristorante Milano (Italian), Wilhelmstraße 26 (closed Mondays)
- Il Gondoliere (Italian), Von-Esmarch-Straße 28 (closed Mondays)

- Buddha Palace (Indian), Von-Esmarch-Straße 18 (closed Tuesdays)
- La Gondola D'oro (Italian), Hüfferstraße 34
- Gustav Grün (Green Fast Food), Wilhelmstraße 1
- Áro (Green Fast Food), Neutor 3

Public transportation. You can check the bus schedule on the website of Stadtwerke-Münster (in German and English), or use Google maps.

Free afternoon on Wednesday. There will be a free late afternoon on Wednesday and here are some suggestions: Go see the castle, the park behind it and the embedded botanic garden. Visit a museum, e.g. the LWL Museum of Art and Cultural History or the Picasso-Museum. Have a walk around the lake 'Aasee' or make yourself familiar with European history at the Historical City Hall which is one of the two places where 1648 the Peace of Westphalia was signed.

Questions. In case of further questions, please use:
Email: nonequ23@uni-muenster.de
Emergencies via phone and various messenger: +49 173 / 947 56 49



SRZ (workshop venue, 2nd floor)
Math Department
canteen
multi-storey car park.

Book of abstracts

Condensation of SIP particles and sticky Brownian motion

Mario Ayala Tue 11:30

In this talk, we will first introduce the symmetric inclusion process (SIP) in the condensation regime. We will describe how to obtain an explicit scaling for the variance of the density field in this regime, when initially started from a homogeneous product measure, with the help of self-duality. This will provide new, relevant information on the coarsening dynamics of condensing interacting particle systems on the infinite lattice. Our result is obtained by proving convergence to sticky Brownian motion for the difference of positions of two SIP particles, in the sense of Mosco convergence of Dirichlet forms.

Modelling dynamics and control of turbulent vortices in cardiac systems and active fluids

Markus Bär Wed 11:30

Many relevant experimental systems and applications exhibit irregular dynamics such as spatiotemporal chaos or turbulence. In this talk, I will present two examples of such behavior where control of such states by transforming their dynamics into homogeneous or periodic steady states or regular periodic patterns is desirable. The specific applications are (i) defibrillation of cardiac tissue by periodic pacing and (ii) turbulence in active suspensions. For the cardiac system, we used simulations as well as data analysis not only to identify suitable conditions e. g. pacing strength and periods [1, 2], but also to determine the mechanism of defibrillation in this specific modus. For active

turbulence, a simple continuum model for an incompressible polar fluid was used for quantitative modelling of experimental findings in bacterial suspensions. Detailed investigations showed how and when the turbulent collective dynamics can be transformed into regular vortex lattices of different symmetries using periodic arrays of obstacles [3]. More recently, experiments in 2D monolayers of bacteria have prompted us to introduce a model for a compressible active fluid that exhibits formation and arrested coarsening of turbulent domains [4].

References

[1] P Buran, M Bär, S Alonso and T Niedermayer. Chaos 27, 113110 (2017).

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Quantitative kinetic theory of active particles with non-aligning interactions

Horst-Holger Boltz

Wed 15:00

We consider self-propelled particles with purely velocity-dependent interactions. The particles undergo apparent Brownian motion, even though the particle's equations are fully deterministic and no explicit noise terms are included in the model. We show that the interactions lead to internal, dynamical noise which can be interpreted as the noise of a network with time-dependent topology. Starting from the exact N-particle Liouville equation, a kinetic equation for the

one-particle distribution function is obtained. We show that the usual mean-field assumption of Molceular Chaos which involves a simple factorization of the N-particle probability leads to unphysical predictions. Going beyond mean-field by explicitly taking into account two-particle-correlations during interactions and using a first-principle, non-local closure of the BBGKY-hierarchy, we analytically calculate the scattering of particles. As a result we obtain explicit expressions for the colored network noise of an effective one-particle Langevin-equation and the corresponding self-diffusion.

Fluctuations in isotropic wave turbulence — a large deviation approach

Brice Douet Wed 9:00

In many physical systems, one is interested in writing the dynamics of mesoscopic or macroscopic variables describing the state of the system. Kinetic theories are examples where the average dynamics is known from classical theoretical works (eg. the Landau or the Balescu—Guernsey—Lenard equations in plasma physics, Boltzmann equation in kinetic gas theory, etc.). However, in general, fluctuations around the average are not described, or restrained to Gaussian fluctuations. Yet for many cases, rare events (ie. far from the typical trajectories) can be relevant, for instance when they lead to rare transitions, when they have a big impact, or when they are necessary to explain the irreversibility paradox of the kinetic equation [1] (ie. when the kinetic equation is time-irreversible whereas the dynamics is not). In this presentation, we consider a generic Hamiltonian system of nonlinear interacting waves with 4-wave interactions. In the kinetic regime of wave turbulence, we assume weak nonlinearity and large

system size. One can show the wave kinetic equation can naturally be regarded as the most probable evolution of the empirical spectrum, and that its distribution follows a large deviation principle [2, 3, 4]. The associated field theory, characterised by a large deviation Hamiltonian, can predict the probability of any dynamical path of the spectrum. However doing explicit computations of the fluctuations can be made difficult due to the functional equations which emerge. In this presentation, we will show that in isotropic wave turbulence, the large deviation Hamiltonian has a much simpler form. In the case where the interactions are local, we can compute the equations of the cumulants at higher order around the most probable state. These cumulants can then be computed explicitly or numerically. It sheds light on rarer fluctuations that were not described before in a general way.

Joint work with Fredddy Bouchet and Jules Guioth.

References

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[2] Guioth, J., Bouchet, F., Eyink, G.L.: Path large deviations for the kinetic theory of weak turbulence. Journal of Statistical Physics 189(20) (2022)

[3] Guioth, J., Onuki, Y., Bouchet, F.: Path large deviations for inhomogeneous weak wave turbulence. To be submitted to J. Stat. Phys.

[4] Guioth, J., Onuki, Y., Bouchet, F.: Dynamical large deviations for an inhomogeneous wave kinetic theory: linear wave scattering by a random medium. To be submitted to J. Stat. Phys.

Towards a Nonequilibrium Thermodynamics of Complex Systems

Massimiliano Esposito Tue 9:00

Equilibrium thermodynamics emerges from equilibrium statistical mechanics as the most likely behavior of a system in the macroscopic limit. Over the last two decades, enormous progress has been made in formulating statistical mechanics for small systems operating far-from-equilibrium. The resulting theory is called stochastic thermodynamics. I will show that taking the macroscopic limit of stochastic thermodynamics enables one to formulate a nonequilibrium thermodynamics of large systems typically described by nonlinear deterministic dynamics which can also capture macroscopic fluctuations around it [1]. This macroscopic stochastic thermodynamics gives rise to novel fundamental results (for instance, once can bound nonequilibrium steady state fluctuations using the entropy production along deterministic relaxation trajectories [2]) and enables to recover many classical phenomenological results in macroscopic irreversible thermodynamics within well controlled approximations. It also opens the way to study the energetics of many complex nonlinear phenomena in a broad range of systems such as chemical reaction networks (CRNs), nonlinear electrical circuits, and Potts models.

References

[1] G. Falasco and M. Esposito, "Macroscopic stochastic thermodynamics", to appear.

[2] N. Freitas and M. Esposito, "Emergent second law for non-equilibrium steady states", Nature Communications 13, 5084 (2022).

On a weak hydrodynamic limit (wHDL) theory

Jin Feng Tue 16:45

To understand mechanistic origin of probabilistic models in statistical and continuum mechanics, it is useful to study hydrodynamic limit for interacting particles following deterministic Hamiltonian dynamics. Traditional approach on such a program face many difficulties. One of them is about rigorous justification of canonical type ensembles. This is because relevant deterministic ergodic theory is still largely out of reach. Another huge barrier is on making sense of rigorous meaning of hyperbolic conservation law PDEs, which has been a way of describing $F = ma$ and thermodynamic relations in the continuum.

We expose a new approach by formulating the hydrodynamic limit program as a multi-scale abstract Hamilton-Jacobi theory in space of probability measures.

This talk will focus on derivation of an isentropic model. Through mass transport calculus, we develop tools to reduce the hydrodynamic problem to known results on finite dimensional weak KAM (Kolmogorov-Arnold-Moser) theory, showing sufficiency of using a weak version of ergodic results about micro-canonical ensembles, instead of the canonical ones. We will also reply on recent progress of viscosity solution theory for abstract Hamilton-Jacobi equation in space of probability measures (an example of Alexandrov space), and a calculus on Alexandrov spaces. These give a weak and indirect characterization on evolution of the limiting continuum model using generating-function formalism at the level of canonical transformation in calculus of variations, instead of hyperbolic systems of PDEs at the level of abstract Euler-Lagrange equations of the action functionals.

All together, these techniques enable us to realize a weaker but rigorous version of the hydrodynamic limit program.

This is work in progress with Toshio Mikami in Tsuda University, Japan.

Self-organisation of proteins in cells

Erwin Frey Tue 16:15

Protein pattern formation is essential for the spatial organisation of intracellular processes like cell division and flagellum positioning. A prominent example of intracellular patterns is the oscillatory pole-to-pole oscillations of Min proteins in E. coli, whose function is to ensure precise cell division. Cell polarisation, a prerequisite for processes such as stem cell differentiation and cell polarity in yeast, is also mediated by a diffusion-reaction process. More generally, these functional modules of cells serve as model systems for self-organisation, one of the core principles of life. Under which conditions spatiotemporal patterns emerge and how biochemical and geometrical factors regulate these patterns are major aspects of current research. In this talk, I will review recent theoretical and experimental advances in the field of intracellular pattern formation, focusing on general design principles and fundamental physical mechanisms.

Hidden temperature profile in the Kipnis-Marchioro-Presutti model

Davide Gabrielli Wed 10:30

Stationary non equilibrium states (SNS) have a rich and complex structure. The large deviations rate functionals for the empirical measure of a few one dimensional SNS of stochastic interacting systems have been computed, among wich the exclusion process and the Kipnis-Marchioro-Presutti (KMP) model. The corresponding rate functionals are not local due to the presence of long range correlations. We show for the KMP model that this can be explained introducing new hidden variables that can be interpreted naturally as the temperatures of the oscillators that are exchanging the energies. When two oscillators exchange energy they thermalize at the same time. We deduce that the invariant measure of the KMP model is a mixture of inhomogeneous product of exponential distributions, the law of the mixture is the invariant measure of the auxiliary temperature process.

Joint work with Anna De Masi and Pablo Ferrari.

Hamiltonian structure, Large deviation principle, Energy landscape and Transition path for non-equilibrium reactions

Yuan Gao Fri 11:00

Non-equilibrium chemical reactions can be modeled by random time changed Poisson process on countable states. The concentration of each species, defined as the molecular number over the size V of the

container, can be then regarded as a continuous time Markov chain. The large deviation principle (LDP), as V goes to infinity, gives a Hamilton-Jacob equation (HJE) and a Hamiltonian structure, which can be used to study the law of large number (LLN) type events and the rare events in non-equilibrium chemical reactions. The reaction rate equation is an ODE corresponding to the zero-cost trajectory(LLN-type path) in the Hamilton dynamics. Moreover, the LDP at finite t gives the rate of concentration on the zero-cost trajectory, while the LDP for invariant measures gives the energy landscape of a non-equilibrium reaction. The later is also proved to be a selected unique weak KAM solution to the corresponding stationary HJE. The LDP rate function also motivates a relative entropy type running cost in the stochastic optimal control formulation for the transition path theory. This formulation is used to compute the transition path and energy barrier for both non-equilibrium chemical reactions and drift-diffusion process.

Interfaces and dynamical transitions in strongly interacting many-body systems

Aljaz Godec Wed 14:30

Our understanding of collective phenomena out of equilibrium is still mostly based on mean-field ideas that neglect correlations, whose importance in turn grows with the strength of interactions. This raises doubts whether mean-field ideas sensibly describe the physical behavior of moderately to strongly interacting systems. I will describe our recent efforts to understand pair-correlation effects in classical many-body systems in and out of equilibrium, by accounting for pair correlations when evaluating thermodynamic limits. I will illuminate some a priori unexpected effects of correlations in the kinetics [1] and interfacial

phenomena [2], and show that they give rise to non-trivial global speed limits during non-equilibrium relaxation [3].

References

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Non-reciprocal active matter across the scales

Ramin Golestanian

Tue 14:00

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

References

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KPZ or Diffusive limits in multi-species exclusion

Patricia Gonçalves

Thu 9:00

In this talk, I will present a model which was introduced in [1] and consists of an exclusion process with different types of particles, let us say types A, B, and C. Depending on the interaction rate between the types of particles, the limiting density fluctuation fields end up in different universality classes: either they are governed by energy solutions of the stochastic Burgers equation or by the Ornstein-Uhlenbeck equation. These results match the predictions from the non-linear fluctuating hydrodynamics developed by Spohn, Schutz, and collaborators.

This is a joint work with G. Cannizzaro; A. Occelli, R. Misturini.

References

[1] Schuetz, Wehefritz-Kaufmann: Kardar-Parisi-Zhang modes in d-dimensional directed polymers, Phys. Rev. E 96, 032119 (2017).

Emergent pattern formation in communicating active matter

Robert Großmann

Wed 14:00

Inspired by trail formation as observed in colonies of driver ants, for example, we study ensembles of agent particles that communicate via deposition and sensing of pheromones. These chemical traces are produced by the agents themselves and encode their current position and walking direction. Other agents passing by will then tend to align with the orientation inscribed in the pheromone traces. In the limit of short pheromone lifetime, the dynamics of this system reduces to the seminal Vicsek model and, thus, yields the formation of transversally moving bands. In the opposite limit, the effective agent-agent interaction represents a form of delayed, non-reciprocal feedback and yields the spontaneous formation of macroscopic, persistent trails, which are followed and reinforced by the agents [1]. In this talk, we first discuss the phase diagram as function of the lifetime of pheromones. We rationalize our findings by analyzing mean-field equations that are systematically derived from the stochastic particle model. Numerical solutions of these order parameter equations show how transversal bands, common in the Vicsek model, are destabilized by chemical communication, eventually giving rise to the formation of "longitudinal", dynamic trails.

Joint work with Zahra Mokhtari, Robert I.A. Patterson and Felix Höfling.

References

[1] Mokhtari et al. (2022) New J. Phys. 24 013012

The thin-film equation with thermal noise

Rishabh Gvalani Tue 14:30

In this talk, we will study the lubrication approximation of the well-known fluctuating hydrodynamics model introduced by Landau and Lifschitz. The corresponding system is a fourth-order, degenerate, quasilinear singular PDE commonly referred to as the thin-film equation with thermal noise. We start by presenting an alternative derivation of the equation from thermodynamic principles using as inputs the correct invariant measure for the dynamics (the 1d Gaussian free field restricted to positive functions) and the correct dissipation mechanism (a weighted version of the H^{-1} inner product). Next, we propose a natural structure-preserving discretisation which preserves the strict positivity of the film height for large enough mobilities. Finally, we study the equation in the framework of the theory of regularity structures: we estimate (uniformly in the regularisation parameter) the appropriately renormalised centered model associated to the equation completing the first step in obtaining a solution theory for the equation.

This talk is based on two separate works with Benjamin Gess (MPI-MiS/Bielefeld), Florian Kunick (MPI-MiS), and Felix Otto (MPI-MiS) and with Markus Tempelmayr (MPI-MiS), respectively.

Accurate dynamics from self-consistent memory in stochastic chemical reactions with small copy numbers

Moshir Harsh Tue 10:30

Chemical reactions in the regime of small copy numbers can occur in gene regulation [1] and some protein interaction networks. Small copy numbers lead to large relative fluctuations, making mean field solutions as given by mass action kinetics unreliable [2]. Accurate calculations of the one and two-time quantities of these stochastic processes remain a challenging problem; numerical solutions of the master equation, for example, rapidly become infeasible as the number of molecular species grows, while stochastic simulations do not allow likelihood inference from dynamical trajectories.

Here, we present a path integral based method that captures the fluctuations beyond mean field using self-consistently determined memory: by integrating information from the past we can systematically improve our approximation for the dynamics of chemical reactions [3]. This memory is not added ad-hoc, but can be shown to arise naturally by considering the effective action of the Doi-Peliti field theory of chemical reactions. The effective action is treated perturbatively but we can self-consistently re-sum a very large class of diagrams resulting in a stable expansion.

We can treat any general network of chemical reactions by deriving an analytical expression for the corrections to the mean-field free energy, analogous to the Plefka expansion [4] that leads to the TAP equations. This correction is then regularized, inspired by the diagrammatic perturbation theory calculations. We demonstrate this method and its accuracy on single and multi-species binary reactions across a range of parameter values [3]. We show how this approach also opens a route to making inferences from experimentally measured dynamics.

This is joint work with Peter Sollich.

References

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[2] Schnoerr, D., Sanguinetti, G. & Grima, R. Approximation and inference methods for stochastic biochemical kinetics - a tutorial review. J. Phys. A: Math. Theor. 50, 093001 (2017).

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Examples of hydrodynamic behaviour in two-species exclusion processes

Rob Jack

Tue 11:00

We discuss several different results for simple exclusion processes with two species of particles. We first show numerical results where inhomogeneous states appear in two-dimensional systems in which the species are driven in opposite directions, and we explain how these results can be rationalised by considering hydrodynamic PDEs for the density [1]. We then discuss how hydrodynamic equations in such models can be characterised, including a systematic analysis based on the method of matched asymptotics [2]. Finally, I will present some results [3] for large deviations in the hydrodynamic limit, associated with fluctuations of the entropy production in a simple model of active matter [4].

References

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NESS and Markov chains

Milton Jara Mon 14:45

Non-equilibrium stationary states (NESS) are ubiquitous in nature, and their description presents striking challenges to mathematicians. Roughly speaking, NESS are stationary states on which the presence of currents prevents the system to be in (statistical) equilibrium. A possible way to describe NESS is through Markov chains. We say that the invariant measure of a Markov chain is a NESS if it is not reversible. Therefore, we can restate the study of NESS as the study of non-reversible Markov chains and their invariant measures. Donsker-Varadhan theory of large deviations of Markov chains is an example of a general theory that can be used to achieve this goal. One successful example of application of this strategy is the Macroscopic Fluctuation Theory (MFT) of Bertini, De Solé, Gabrielli, Jona-Lasinio and Landim, which describes the large fluctuations of NESS for driven-diffusive systems in terms of certain thermodynamic variables. In recent works, we have developed a theory of quantitative hydrodynamics that allows us to describe the CLT fluctuations of NESS for driven-diffusive systems, that confirms the prediction of MFT also at the level of the CLT.

Systematic coarse-graining of microscopic molecules for predictive field-theoretical modeling

Jaehyeok Jin Thu 14:00

While microscopic particle-based simulation can elucidate the underlying mechanisms of molecular processes, it is not practical for simulating long-time dynamics, and a field-theoretical approach can be utilized here to resolve such a computational bottleneck. For spatiotemporal scales longer than the molecular level, both hydrodynamic interactions and fluctuations are two central quantities for modulating the long-time dynamics of molecular fluids. Despite advances in mesoscopic fluctuating hydrodynamics, which is the phenomenological realization of the Navier-Stokes equation, the underlying microscopic interactions of molecules are often missing.

In this talk, we present a bottom-up, systematic approach for incorporating important microscopic physics into the field-theoretical level at a molecular to mesoscopic scale. In order to accurately account for thermal fluctuations and microscopic interactions that are essential for long-time dynamics, we utilize the Dean-Kawasaki dynamics, which correctly describes the density function for interactions of the Langevin processes. Despite being physically rigorous, the Dean-Kawasaki model is mathematically ill-defined and fails to be renormalized due to the multiplicative structure of the noise in divergence form. Therefore, our framework is based on the mathematically regularized description of the Dean-Kawasaki dynamics with the microscopic interactions at the particle level. Then, the interaction potential and dynamic coefficients in a non-linear stochastic partial differential equation can be faithfully derived from the particle-level simulation by employing bottom-up coarse-graining methods. We will show that our approach can correctly model the role of microscopic interactions in the fluctuating fields of

fluids. Altogether, the present approach provides a new protocol for the bottom-up design of predictive field-theoretical models and enables a better understanding of the behavior of complex systems at different length scales.

Chiral motion and vortex states in active fluids

Sabine Klapp Tue 15:00

In this talk I will discuss recent results on the collective behavior of active systems exhibiting chiral- or vortex like motion. To this end we use a scale-bridging approach combining particle-based equations, continuum (field) equations and linear stability analysis. The first example concerns systems with intrinsic chirality (circle swimmers) and non-reciprocal alignment coupling. Numerical solution of the field equations provides an overview of the complex collective dynamics that involves, beyond flocking and motility-induced phase separation, also frustrated states induced by non-reciprocity. The results turn out to be fully consistent with those of a linear stability analysis [1]. In addition, I will present first results characterising these states microscopically based on numerical simulations of the underlying Langevin equations.

The second example concerns suspensions of microswimmers exhibiting mesoscale turbulence. Using a continuum-theoretical approach (which can be derived microscopically [2]), we explore the transition from a vortex state to mesoscales turbulence in an ordered array of obstacles. We find an intriguing similarity with a continuous second-order equilibrium phase transition in the 2D Ising universality class [3]. We then discuss the transport of advected tracer particles, which show a diffusion maximum related to the interplay of various dynamical time scales.

References

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Fundamentals and applications of classical dynamical density functional theory

Hartmut Löwen

Mon 14:00

Classical dynamical density functional theory (DDFT) has been proven to be a vital and flexible modeling tool for non-equilibrium phenomena, for a recent review see [1]. In this talk I shall first propose dynamical density functional theory and comment on its validity. Then various applications of DDFT will be discussed. They include colloidal crystallization on imposed crystallization seeds [2], colloidal flow driven through constrictions and over barriers [3] and DDFT for active systems [4]. Finally the relation to more phenomenological phase-field-crystal (PFC) modelling will be discussed including recent results on active systems [5,6]. A final example is bacterial growth in colonies governed by mechano-sensing [7].

References

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What makes a good nonequilibrium model?

Christian Maes Thu 16:45

We discuss the nature and derivation of local detailed balance (with an application to nonequilibrium calorimetry), and we add ideas on the fluctuation dynamics of a probe in an active bath.

Projection operators, linear GLE and active baths : an attempt to derive compact and meaningful coarse-grained equations of motion

Hugues Meyer Wed 11:00

Reducing the complexity of a system composed of many degrees of freedom can be made by deriving self-consistent equation of motion for a small set of variables that capture its main features. This task is usually referred to as a coarse-graining procedure, one of the most well-known example being the Langevin equation and its generalized version which is nowadays heavily used in computer simulations to generate system trajectories at a cheap computational cost. Systematic coarse-graining procedures can be derived using projection operator techniques, which have recently been developed for numerical coarse-graining procedures of non-equilibrium processes. Using simple projectors, we show that a structure similar to the Generalized Langevin Equation can always be derived under very light assumptions. One striking result is the validity of a identity relating the effective memory kernel and the fluctuating force of the process which has the structure of a fluctuation-dissipation relation. As most non-equilibrium processes do not fulfill standard fluctuation-dissipation relations, the physical interpretation of such an identity must be challenged. This is noticeably true for active systems which are known to break such relations. We propose here a route to try to resolve this conflict in the coarse-grained description of the active bath. Using a 2-step projection procedure, we propose to split the usual memory/friction kernel into a so-called passive contribution and an active one.

Non-Equilibrium Steady States and EDP-convergence for slow-fast gradient systems

Alexander Mielke Tue 9:30

A new saddle-point characterization is for a special class of Non-Equilibrium Steady States (NESS) is derived. It relates to gradient systems $(X_{\rm slow} \times X_{\rm fast}, E, R)$ where the state u decomposes into a slow part U and a fast part w, i.e. $u = (U, w)$. Under natural conditions w will fast converge to a NESS that depends in U that only moves slowly. The corresponding w can be found as null saddle point for the Lagrangian

$$X_{\rm fast} \times X_{\rm fast}^* \ni (w, \zeta) \ \mapsto \ R^*(U, w; \Xi, \zeta) - R^*\big(U, w; -{\rm D}E(U, w)\big).$$

We show that this saddle-point structure appears naturally in the theory of EDP-convergence of families of gradients systems $(X, E_\varepsilon, R_\varepsilon)$, i.e. convergence in the sense of the "Energy-Dissipation Principle", if we consider slow-fast gradient systems which arise in chemical reaction-diffusion systems. For a scalar diffusion equation with a thin membrane region with low mobility we show that the arising transmission is generated by a nonlinear kinetic relation.

The research is partially joint work with Th. Frenzel, M. Peletier, and A. Stephan.

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Diffusive behavior in completely integrable infinite dynamics

Stefano Olla Thu 11:30

We investigate the macroscopic behaviour of the density fluctuations of a one dimensional dynamics of hard rods with random length. After recentering on the effective velocity the density fluctuations of particles of a given velocity v on the diffusive space-time scaling will evolve driven by a browian motion with a diffusivity depending on v. This rigid evolution of fluctuations is expected in other completely integrable systems (Box-Ball, Toda Lattice,..), in contrast with the behavior in chaotic dynamics where space-time white noise appears in the evolution equations.

Joint work with Pablo Ferrari (U. Buenos Aires).

How GENERIC arises from upscaling a Hamiltonian system

Mark Peletier Fri 9:00

In this talk, on joint work with Alexander Mielke and Johannes Zimmer, I want to explain our recent insights in how irreversibility arises out of coarse-graining reversible systems. In this context, 'irreversibility' means a system in GENERIC form, and 'reversible system' is a Hamiltonian system. The big question is how and why entropy and the Onsager operator appear.

The mathematical version of this question consists of taking a Hamiltonian system, doing some 'coarse-graining' and then proving that, miraculously, the irreversible parts of GENERIC appear. We study a particular example, in which many calculations can be done by hand, and in which one can trace the origins of entropy and the Onsager operator back to the Hamiltonian system. This talk will be informal, because some of the steps have not been made rigorous yet, and there still is much to be learned. But I hope it will at least be interesting.

Multiscale limits of thin-film models with moving support

Dirk Peschka Thu 11:00

In this talk, we will be exploring some intriguing features of thin-film models. Despite their simple appearance, these models have proven to be both mathematically challenging to analyze and physically sensible for predicting flows of viscous fluids with free boundaries. These

degenerate fourth-order equations exhibit a gradient flow structure and have a rich structure of possible structure formation process.

Typically, thin-film problems are solved by considering a regularized problem with a precursor that lifts the degeneracy of the parabolic equation. However, in this talk, we will present an alternative approach that treats the thin-film equation as a coupled PDE for the film height h, which is coupled to the evolution of its support in a free boundary problem. This approach also utilizes a gradient flow structure with a coupling of bulk and interfacial forces, naturally represented with a saddle-point structure. We'll explore natural discretization schemes and consider the limit of vanishing and infinite (interfacial) mobility, along with physically relevant examples and mathematically interesting phenomena.

This talk is based on joint work with Luca Heltai [1], Lorenzo Giacomelli and Manuel Gnann [2] and also features some experimental/theoretical results from [3].

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Dynamical Renormalization Group approach to the collective behavior of swarms

Giulia Pisegna Fri 10:30

Recent data on strongly correlated biological systems showed the validity of scaling laws as one of the fundamental traits of collective behaviour. Field theoretical techniques, such as the Renormalization Group, thus became useful tools to describe living systems as bird flocks, cell colonies and insect swarms. Experiments unveiled traces of critical dynamics in the latter system, exhibiting an inertial dynamics in the velocities and a dynamical critical exponent $z \approx 1.2$ [1]. To rationalize this evidence, we develop an inertial active field theory in which the velocity is coupled to its generator of internal rotations, namely the spin, through a mode-coupling interaction [2]. Supported by the indication of weak density fluctuations in insect swarms, we study its near-critical regime with a one-loop Renormalization Group approach under the assumption of incompressibility. The presence of friction in the dynamics of the spin rules a paramount crossover between two fixed points: the unstable nderdamped fixed point with $z = 1.3$ and the stable overdamped fixed point with $z = 1.7$, where dissipation takes over. We show how finite-size systems with weak dissipation, such as swarms, can actually exhibit the critical dynamics of the unstable fixed point thus providing a theoretical result which is in good agreement with experimental data [2].

Joint work with A. Cavagna, L. Di Carlo, I. Giardina, T.S. Grigera, M. Scandolo.

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New perspectives in Macroscopic Fluctuation Theory

Michiel Renger Thu 14:30

One major challenge of non-equilibrium (=non-detailed balance) thermodynamics is the possible occurrence of divergence-free fluxes. In Macroscopic Fluctuation Theory (MFT) one studies these divergence-free flux through flux large deviations. MFT is originally developped for systems that are (approximately) driven by white noise, with quadratic large deviations. This already breaks down for very basic models of particles that hop around on a 3-state space; these are essentially jump processes, hence driven by Poisson noise and have non-quadratic large deviations. We (among others) developped a generalisation of MFT that encompasses such systems, and even allows a decomposition into gradient flow dynamics and Hamiltonian dynamics.

If time allows, I will also present a few new insights into 'generalised orthogonality' between entropic and Hamiltonian forces, linearised structures and/or relations with GENERIC.

Large deviations in the non-equilibrium stationary state of diffusive systems: Microscopic and hydrodynamic solutions

Tridib Sadhu Thu 9:30

I shall present our exact results [1] for the large deviations function of the density profile and of the current in the non-equilibrium stationary state of a one-dimensional symmetric exclusion process coupled to boundary reservoirs with slow rates. Our results extend the earlier exact results [2, 3], where rates at the boundaries are comparable to the bulk ones, to the regime where boundary-rates are significantly slower. I shall then show how these new results can be reproduced [4] using the fluctuating hydrodynamics description of the macroscopic fluctuation theory [5]. In describing this hydrodynamic approach I shall present a solution [4] of the variational problem for density large deviations in certain diffusive systems.

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How to make noise

Tanja Schilling Wed 9:30

One widely used effective equation of motion for coarse-grained variables is the Langevin equation, a stochastic differential equation, in which the effect of the neglected degrees of freedom is encoded in friction terms and stochastic noise. We will review the steps of derivation and approximation that are required to obtain the Langevin equation from a system's microscopic description, and we will recall how to extend these derivations to the case of explicitly time-dependent microscopic dynamics. We will discuss the interplay between the potential of mean force and the memory kernel, the range of validity of the second fluctuation dissipation theorem, and the stochastic interpretation of the fluctuating force, i.e. the noise.

How much heat is dissipated in active fluids?

Thomas Speck Thu 16:15

Entropy production and heat dissipation are quantitative hallmarks of non-equilibrium systems. The thermodynamic efficiency determines the fraction of energy spent to drive the system that is recoverable as useable work. While stochastic thermodynamics allows to calculate entropy production and dissipation rates from dynamic particle data, a full quantification requires to resolve all microscopic degrees of freedom participating in the dissipative processes, which is typically unfeasible in complex many-body systems. A paradigmatic example is motile active matter, which is characterized by the directed motion of its constituents that needs to be sustained by supplying (free) energy,

constantly driving the system away from thermal equilibrium. I will describe how the true dissipated heat in a simplified model, active Brownian particles, can be recovered from particle trajectories. I will then discuss an isothermal cyclic machine using a colloidal active particle as its working medium, showing that its thermodynamic efficiency is negligible. Finally, I will sketch some ramifications for the modeling of synthetic and living active matter.

On time-splitting methods for gradient flows with two dissipation mechanisms

Artur Stephan Fri 9:30

A gradient system $(X, \mathcal{E}, \mathcal{R})$ consists of a state space X (a separable, reflexive Banach space), an energy functional $\mathcal{E} : X \to \mathbb{R} \cup \{\infty\}$ and a dissipation potential $\mathcal{R} : X \to [0, \infty[$, which is convex, lower semicontinuous and satisfies $\mathcal{R}(0) = 0$. The associated gradient-flow equation is then given by

$$0 \in \partial\mathcal{R}(u'(t)) + \mathrm{D}\mathcal{E}(u(t)) \quad \text{or equivalently} \quad u'(t) \in \partial\mathcal{R}^*(-\mathrm{D}\mathcal{E}(u(t))).$$

In my talk we are interested in the case where the dual dissipation potential $\mathcal{R}^*$ is given by the sum $\mathcal{R}^* = \mathcal{R}_1^* + \mathcal{R}_2^*$ for two dissipation potentials $\mathcal{R}_j : X_j \to [0, \infty[$, $X_j \subset X$. This splitting provides also a decomposition of the right-hand side of the combined gradient-flow equation $u'(t) \in \partial(\mathcal{R}_1^* + \mathcal{R}_2^*)(-\mathrm{D}\mathcal{E}(u(t))) = \partial\mathcal{R}_1^*(-\mathrm{D}\mathcal{E}(u(t))) + \partial\mathcal{R}_2^*(-\mathrm{D}\mathcal{E}(u(t)))$, and enables to construct solutions via a split-step method. Assuming that both gradient systems $(X, \mathcal{E}, \mathcal{R}_j)$ define gradient-flow equations $u'(t) \in \partial\mathcal{R}_j^*(-\mathrm{D}\mathcal{E}(u(t)))$ on $[0, T]$, the split-step method is defined by

[1] fixing a time step $\tau = T/N$ and solving on the semi-intervals of length $\tau/2$ alternatingly the gradient-flow equations corresponding to $(X, \mathcal{E}, 2\mathcal{R}_j)$,
[2] concatenating the solutions N-times to a trajectory on the interval $[0, T]$.

In my talk I will show that in the limit $N \to \infty$, the concatenated solutions indeed converge to the solution of the combined gradient-flow equation. The analysis relies on methods from the calculus of variations, and the usage of the energy-dissipation principle for gradient flows.

This is joint work with Alexander Mielke (Berlin) and Riccarda Rossi (Brescia).

Orientation-dependent propulsion of active Brownian spheres: from self-advection to programmable cluster shapes

Michael te Vrugt Thu 15:00

Applications of active particles require a method for controlling their dynamics. While this is typically achieved via direct interventions, indirect interventions based, e.g., on an orientation-dependent self-propulsion speed of the particles, become increasingly popular. In this work [1], we investigate systems of interacting active Brownian spheres in two spatial dimensions with orientation-dependent propulsion using analytical field-theoretical modeling and Brownian dynamics simulations. It is found that the orientation-dependence leads to self-advection, circulating currents, and programmable cluster shapes. We show that the presence of an orientation-dependent propulsion breaks the vatiational structure that the field theory would otherwise have at second order in derivatives.

Joint work with Stephan Bröker, Jens Bickmann, Michael E. Cates and Raphael Wittkowski

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Deriving predictive field theories with the interaction-expansion method

Raphael Wittkowski Fri 11:30

Field theories are a very powerful tool for understanding systems of interacting active particles. By systematic coarse-graining of a microscopic model, one can derive predictive field theories. Compared to phenomenological field theories, predictive field theories provide analytical expressions that predict the values of the parameters involved in the field theories in terms of the parameters of the underlying microscopic model. In this talk, I given an overview about the interaction-expansion method and its recent applications.

Poster

On symmetric polyconvexity conditions of quadratic forms

Omar Boussaid

We are interested on finding conditions on the coefficients of a quadratic form to be symmetric polyconvex. A fully characterization of symmetric polyconvex quadratic forms and more generally of arbitrary functions is given in the 2d and 3d Cases by Boussaid et all where they show that a quadratic form in 2d (3d) is symmetric polyconvex if by adding some positive constant by the determinant (cofactor matrix), the result is convex. In this contribution we want to give conditions on the coefficients of the quadratic form to be symmetric polyconvex. We treat first the case of 2d and then the 3d case.

Fluctuating Hydrodynamics for a dilute gas of active particles

Quassim Feliachi

Hydrodynamics equation are often used to describe active systems in a coarse-grained way. For a lot of applications, the particle number is not big enough to totally discard finite number of particles effect. That is why physicists have been adding noise terms in hydrodynamics equations to take into account graininess. As a statistical physicist, I am interested in how to derive this noise term from the microscopic dynamics. In this talk, I will show how to derive a fluctuating kinetic theory, and the corresponding fluctuating hydrodynamics, for a dilute gas of aligning self-propelled particles. The result is a set of stochastic

partial differential equations for the density field and orientation field that describe the collective motion of active particles at the macroscopic level. The noise term is derived from the microscopic dynamics, through the use of large deviation theory.

Persistence in Brownian motion of an ellipsoidal particle in two dimensions

Anirban Ghosh

We investigate the persistence probability $p(t)$ of the position of a Brownian particle with shape asymmetry in two dimensions. The persistence probability is defined as the probability that a stochastic variable has not changed its sign in the given time interval. We explicitly consider two cases—diffusion of a free particle and that of a harmonically trapped particle. The latter is particularly relevant in experiments that use trapping and tracking techniques to measure the displacements. We provide analytical expressions of $p(t)$ for both the scenarios and show that in the absence of the shape asymmetry, the results reduce to the case of an isotropic particle. The analytical expressions of $p(t)$ are further validated against numerical simulation of the underlying overdamped dynamics. We also illustrate that p(t) can be a measure to determine the shape asymmetry of a colloid and the translational and rotational diffusivities can be estimated from the measured persistence probability. The advantage of this method is that it does not require the tracking of the orientation of the particle.

Reducing cloud-climate uncertainties with Maximum Entropy Production

Benjamin Hernandez

Clouds are a vital component of the Earth's climate system, playing a significant role in its energy budget and water cycle. Stratocumulus clouds, in particular, are challenging to incorporate into climate models but have a tremendous impact on predicting future climate. Their global presence is so influential that even a small change of a few percentage points in their reflectivity could offset the doubling of CO2.

Stratocumulus clouds exist in two organized states, each with different effects on their surrounding environment. The Maximum Entropy Production Principle provides a powerful tool for studying this multi-stable system with a high-level perspective, shedding light on its behaviour and impact on the Earth's climate. To better understand this complex system, we are mainly interested in using techniques from Non-Equilibrium Statistical Mechanics, with a focus on the Maximum Entropy Production principle. This concept, firstly introduced by Paltridge (1975) in Climate Science and later formalised by Jaynes (1979) in terms of Shannon's entropy, has, in the recent years, been applied successfully to various disciplines. The principle, whose efficacy is still a hot topic in the community, holds the promise of being able to predict steady-state behaviour without requiring a detailed understanding of the microscopic details of the system's dynamics, but only knowledge of the boundary conditions.

This is a joint work with Franziska Glassmeier and Pier Siebesma Department of Geoscience & Remote Sensing, Delft University of Technology.

Can Monte Carlo methods be used to simulate active-matter systems ?

Juliane Klamser

A central question in the field of active matter concerns the emergent collective phenomena when individual particles have the ability to move persistently, i.e. when particles overcome a characteristic finite distance without changing their direction of motion. Although considerable effort has been put to develop analytical approaches to describe the statistical physics of active matter, the state of the art is far from comparable to equilibrium statistical physics. Our advances therefore strongly rely on numerical studies where many active-matter models have been proposed and simulated. However, little attempts have been made to develop an algorithmic toolbox for those models. In equilibrium, the detailed-balance condition allows to exploit the unphysical moves of Monte Carlo (MC) approaches to efficiently simulate large systems. As there is no analog of detailed balance for active matter, the construction of MC algorithms that faithfully capture continuous-time active-matter models is not straight forward. I will present a realisation of kinetic MC analogues of the work-horse models of self-propelled particles, namely Active-Ornstein Uhlenbeck, Active Brownian, and Run-and-Tumble particles.

The long-time behaviour of interacting particle systems: A Lyapunov functional approach

Jonas Köppl

We study the long-time behaviour of possibly non-reversible interacting particle systems on the d-dimensional hypercubic lattice, which admit at least one Gibbs measure as a time-stationary measure. Under some mild non-degeneracy conditions on the rates and the specification, we prove that one can use the relative entropy density as a Lyapunov functional and thereby show that all possible limits of the associated measure-valued dynamics are also Gibbs measures if the initial condition is translation-invariant.

In the special case of reversible interacting particle systems on one and two-dimensional lattices, we extend the method to non-translation invariant initial distributions and completely determine the phase portrait of the dynamics. This answers open questions on the possibility of time-periodic behaviour in two dimensions and on the connection between uniqueness of the invariant measure and ergodicity.

Variational convergence from mean-field stochastic particle systems to the exchange-driven growth model

Chun Yin Lam

We consider the hydrodynamic limit of mean-field stochastic particle systems on a complete graph. The evolution of occupation number at

each vertex is driven by particle exchange with its rate depending on the population of the starting vertex and the destination vertex. In particular, models having condensation phenomena, like the zero-range process, are included. This mechanism is fundamental in many applications, like cloud formation, polymerization, migration and wealth exchange.

Under detailed balance conditions, the evolution equation of the law of the particle density can be seen as a generalised gradient flow equation with a gradient structure motivated by the Large Deviations Principle (LDP) of the Markov process. To pass to the limit in the equation, we use a variational formulation based on a suitable energy-dissipation functional, which coincides with the LDP rate function in the finite system. The convergence of the system in this variational sense is established based on compactness of the density and flux and Γ-lower-semicontinuity of the energy-dissipation functional along solutions to the continuity equation. The driving free energy is shown to converge to that of the hydrodynamic limit, after taking possible condensation phenomena into account.

This is a joint work with André Schlichting.

Chromatin as an active poroelastic system: understanding its out-of-equilibrium thermodynamics

Clara Luque-Rioja

Living systems dissipate energy constantly as they carry out essential functions. These dynamics frequently produce complex behaviors that can be classified as non-thermal processes since they are ordered and

self-organized. Nonetheless, it can often be challenging to tell whether a process' dynamics are significantly different from those of a thermally driven process. Undoubtedly, non-equilibrium activity is required for the survival of life, but it is uncertain how to identify and quantify these dynamics in biological systems.

Here, we present an active-poroelastic theoretical framework to represent chromatin as an active-elastic solid coupled to a permeating fluid. We incorporate the active stress into a two-fluid model that accounts for the spatiotemporal dynamics of the nucleus based on experimental data that suggests large-scale correlated mobility of chromatin inside the nuclei of live differentiated cells. Both passive thermal fluctuations and active scalar events, such as condensation and decondensation, which we refer to as spikes, have an impact on this system. The coupled set of equations showing the presence of emergent processes is simulated in this instance.

Gelation and hydrodynamic limits in a spatial Marcus-Lushnikov process

Elena Magnanini

A coagulation process describes the behavior of a particle system where families of particles merge (or coagulate, or coalesce) as time passes. The coagulation mechanism is regulated by a kernel, that is typically a positive symmetric function of the two masses (and not of the space). When it grows sufficiently fast, as the size of the particles gets large, infinite particles could emerge in finite time; this kind of phase transition is known as gelation.

In the present work we consider a spatial coagulation model where the spatial interaction is driven by the kernel, and starting from the

generator of the process, we provide conditions under which gelation occurs. In some special cases the coagulation process can be coupled with an inhomogeneous random graph; in this context we are able to identify an upper bound for the gelation time in terms of the critical parameter that determines the appearance of a giant component in the inhomogeneous random graph. Our analysis is complemented by the characterization of the limiting behavior of the coagulating particle systems with a nonlinear kinetic equation, a spatial version of the Flory equation. This is a system of differential equations that describes the evolution in time of the density of particles with a given size and position.

Joint work with L. Andreis and T. Iyer.

Nanoparticle Taylor Dispersion Near Charged Surfaces with an Open Boundary

Joshua D. McGraw

The arrangement of colloidal particles in the sub-micrometric space above an interface is typically described by the Gibbs-Boltzmann distribution, taking into account a conservative interaction between particles and the boundary. These distributions in turn may have a major effect on the transport of such microscopic particles in the near-surface region, with a hallmark example being Taylor dispersion. In this dispersion, particles' diffusive motions along velocity gradients amplify the dispersive spreading in the streamwise direction, as compared to pure diffusion. We recently showed, in a combined experimental and theoretical work [1], that introducing a reactive or particle-consuming boundary strongly modifies the aforementioned dispersive transport,

with a striking order of magnitude reduction as compared to the non-interacting case. The equilibrium Gibbs-Boltzmann distribution is no longer complete in this situation and must be supplanted with a steady, non-equilibrium distribution accounting for particle loss. Our experimental data is well captured by an advection-diffusion model incorporating both a conservative electrostatic interaction and particle loss. These results demonstrate the need to properly account for particle-surface interactions in the aim of quantitatively describing nanoscale particle transport.

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Modelling dynamic AFM force measurements of complex liquids

Simone Riva

We study the theory of Direct AFM (atomic force microscopy) force measurements of complex liquids. An AFM force measurement is a useful tool for studying the dynamics of complex liquids – dispersions of several different phases, such as suspensions, emulsions, and foam, which may react to external stimuli such as mechanical stress, pressure, and temperature. However, the measurement provides a force per time curve. It must be translated to the physics in the liquid, which is enclosed between a hard surface and the AFM cantilever translating along the liquid, to yield meaningful and accurate description of the physics of the system. There are several challenges in such a theory, foremost of which is capturing the connection between the liquid microscopic structure and macroscopic strain and stress. Other

challenges are to translate the stress in the liquid to the force on the AFM cantilever and to model the response of the AFM cantilever to the former, for obtaining accurate prediction of the measurement. We use the principles of classical density functional theory to obtain the strain-stress relationship of a complex liquid film, comprising micelles in an electrolyte solution that support electrostatic and micelle steric interactions. Moreover, we minimize a descriptive energy functional of the complex liquid to obtain its structure. The corresponding local chemical potential of the system translates to the near equilibrium dynamics of the film, which we use to simulate the dynamically changing spatiotemporal thickness of the liquid film under the strain induced by the AFM cantilever.

Symmetry-breaking, motion and bistability of active drops

Fenna Stegemerten

Cell crawling crucially depends on the collective dynamics of the actomyosin cytoskeleton. However, it remains an open question to what extent cell polarization and persistent motion depend on continuous regulatory mechanisms and autonomous physical mechanisms. Experiments on cell fragments and theoretical considerations for active polar liquids have highlighted that physical mechanisms induce motility through splay and bend configurations in a nematic director field. Here, we employ a simple model, derived from basic thermodynamic principles, for active polar free-surface droplets to identify a different mechanism of motility. Namely, active stresses drive drop motion through spatial variations of polarization strength. This robustly induces parity-symmetry breaking and motility even for liquid ridges (2D drops) and adds to splay- and bend-driven pumping in 3D geometries.

Intriguingly, then, stable polar moving and axisymmetric resting states may coexist, reminiscent of the interconversion of moving and resting keratocytes by external stimuli. The identified additional motility mode originates from a competition between the elastic bulk energy and the polarity control exerted by the drop surface. As it already breaks parity-symmetry for passive drops, the resulting back-forth asymmetry enables active stresses to effectively pump liquid and drop motion ensues.

Joint work with Karin John and Uwe Thiele.

Understanding probability and irreversibility in the Mori-Zwanzig projection operator formalism

Michael te Vrugt

Explaining the emergence of stochastic irreversible macroscopic dynamics from time-reversible deterministic microscopic dynamics is one of the key problems in philosophy of physics. The Mori-Zwanzig (MZ) projection operator formalism, which is one of the most important methods of modern nonequilibrium statistical mechanics, allows for a systematic derivation of irreversible transport equations from reversible microdynamics and thus provides a useful framework for understanding this issue. However, discussions of the MZ formalism in philosophy of physics tend to focus on simple variants rather than on the more sophisticated ones used in modern physical research. In this work [1], I close this gap by studying the problems of probability and irreversibility using the example of Grabert's time-dependent projection operator formalism. This allows to better understand how general proposals for understanding probability in statistical mechanics, namely

(a) quantum approaches and (b) almost-objective probabilities, can be accomodated in the MZ formalism.

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Length-minimizing interface flow in mass-conserving reaction–diffusion systems

Henrik Weyer

Intracellular protein patterns are described by reaction–diffusion systems that conserve the total protein number. Driven by a chemical fuel, concentration patterns form in these systems by proteins switching between different conformational states which diffuse differently rapidly, typically representing membrane-bound and cytosolic states. Intriguingly, two-component mass-conserving reaction–diffusion (2cMcRD) systems modeling cell polarization have been argued to show pattern dynamics reminiscent of phase separation approaching thermodynamic equilibrium: The pattern wavelength grows continuously in a process termed coarsening. To analyze highly nonlinear patterns formed in two-dimensional 2cMcRD systems, we derive a geometric flow describing the motion of the pattern-interface line. We show that the flow preserves the enclosed area while minimizing the length of the interface line. Moreover, it interpolates between the two-sided Mullins–Sekerka flow describing Cahn–Hilliard dynamics and the area-preserving mean-curvature flow, the interface flow of conserved Allen–Cahn systems. Coarse-graining to an interface flow thereby uncovers connections between 2cMcRD systems far from equilibrium and classical models of phase separation approaching thermodynamic equilibrium.

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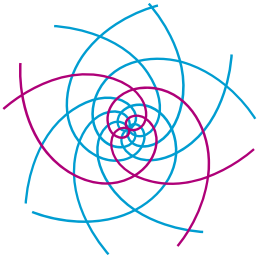

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