Abstracts of oral contributions

in alphabetical order of the speakers

2

Polymer Folding Kinetics

Michael P. Allen, Štěpán Ružička, David Quigley, Michael Griggs

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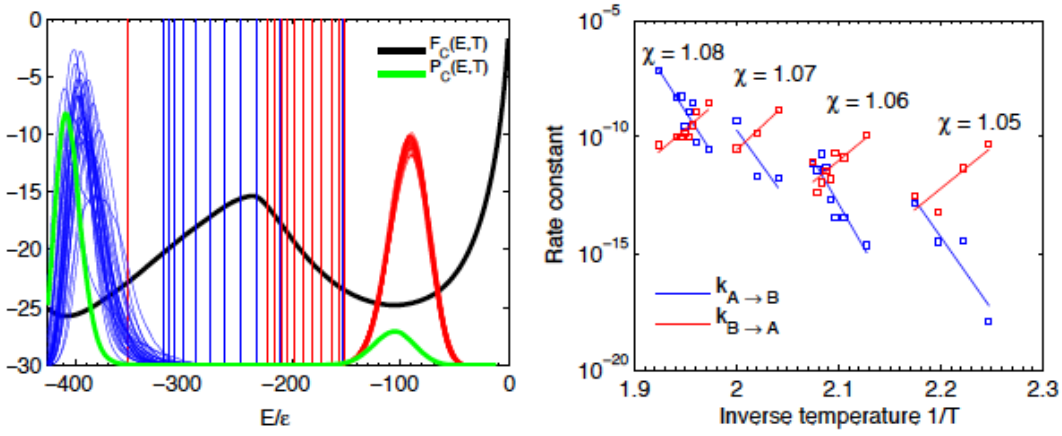
Flexible homopolymer chains with sufficiently short-ranged attractions have recently been proved to exhibit an all-in-one protein-like folding transition by Monte Carlo simulations. We have recently studied the kinetic properties of the transition using collision dynamics combined with forward flux sampling, using the potential energy as a reaction coordinate. This talk will discuss these results, and possible choices of additional reaction coordinates for this system. In addition, we have investigated the effects of hydrodynamic interactions on polymer collapse, using Brownian dynamics; recent simulation results will be presented, together with a discussion of the links with other simulation techniques.



Influence of hydrodynamics on the fluctuation theorem

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The fluctuation theorem is a fundamental result in physics. It quantifies the probability of observing a violation of the second law of thermodynamics [1, 2]. While its relevance on the mesoscopic level is well-known, its validity in the presence of hydrodynamic interactions was unclear [3].

We have tested the fluctuation theorem in the presence of hydrodynamic interactions in computer simulations employing the method of multi-particle collision dynamics. This method correctly describes both thermal fluctuations and hydrodynamic interactions [4, 5] even at very short time scales [6]. We demonstrate the validity of the fluctuation theorem in the presence of hydrodynamic interactions at all averaging (measurement) times [7] provided that a specific hydrodynamic scaling of the volume of measurement of entropy production is taken into account. This scaling arises since, in the presence of hydrodynamic correlations, entropy production is a collective process: we also verify that in the absence of hydrodynamics, no scaling is observed.

We discuss our results in the context of recent experimental investigations and provide insight essential for the analysis of the experimental results.

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[6] T. Franosch, M. Grimm, M. Belushkin, F. Mor, G. Foffi, L. Forró, S. Jeney, submitted (2011).
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The process of approach to equilibrium in the Fermi-Pasta-Ulam problem

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Universitá di Padova, Italy

As is well known, in 1954 Fermi, Pasta and Ulam started the field of molecular dynamics, by simulating on a computer the dynamics of a chain of masses connected by weakly nonlinear forces. Their aim was understanding the process of approach to statistical equilibrium in similar systems. Practically, they gave initially energy to only one or two low frequency normal modes, expecting to observe a rapid energy sharing among all normal modes, leading eventually to energy equipartition among all of them. But with great surprise, they observed no tendency at all to equilibrium: only a few low frequency modes were practically involved in the energy sharing, most modes being apparently excluded from it. Nowadays it is known that the state observed by FPU is metastable, i.e. it evolves, like a glassy state, on a much larger time scale.

The aim of the proposed talk is to illustrate the essence of what we know, at the moment, on the subject, with emphasis on some recent numerical results. Among them: denoting by N and ε respectively the number of particles and the energy per particle, at any fixed N the equilibrium time turns out to be a stretched exponential in $1/\varepsilon$ (large equilibrium times), but in the thermodynamic limit a crossover is observed to a power law (much shorter equilibrium times). Looking at the exponent in the power law, FPU models appear to be divided into universality classes, depending on the dimensionality and, in dimension one, on the "degree of tangency" of the considered model to the (integrable, no equilibrium at all) Toda model.

Lyapunov exponents in highly confined fluids

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The Lyapunov exponents measure the average rate of expansion and/or contraction of two initially nearby phase space trajectories of dynamical systems. They are one of the main tools for the characterization of chaos, providing also a quantitative measure. They have been used extensively to understand the chaotic properties of fluids in Molecular Dynamics (MD) and Non-Equilibrium Molecular Dynamics (NEMD) simulations and have proven to be a particularly useful tool for the characterization and theoretical analysis of systems far from equilibrium in thermostatted steady states. Until now the focus was on homogeneous systems in which the equations of motion were modified to include external forces and thermostatting terms and the dissipative character of the dynamics was distributed among all the degrees of freedom.

In this work we characterize Lyapunov spectra for inhomogeneous systems at a nonequilibrium steady state, thus obtaining an insight into what happens along different directions in the phase-space characterized by different dynamics with the use of NEMD. We show detailed results on the effect that real walls have on the Lyapunov spectra, computing the exponents for the phase space of both fluid and wall atoms. We show how the spectra reflects the presence of two different dynamics in the simulation cell: wall and fluid atoms are of the same species but the selective application of the thermostatting mechanism on one species only creates two dynamics, one Hamiltonian and one dissipative.

We also show how the different use of a thermostatting mechanism influences the properties of confined nanofluids. We accomplish that applying a thermostatting device to selectively to the wall or directly to the fluid, this modifies the pressure tensor across the pore and changes the Lyapunov spectra associated with the fluid particles' phase space. In particular, when the fluid is thermostatted, the Lyapunov spectrum is characterized by lower (in absolute value) maximal Lyapunov exponents, meaning that the fluid is intrinsically less chaotic than the system thermostatted by thermal conduction through the atomic walls. This is due to a reduced particle mixing both in velocity and coordinate phase space. The mechanical property results are also altered.

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Covariant Lyapunov vectors and local exponents for smooth and rough hard disk systems

Hadrien Bosetti

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The Oseledec splitting can be experimentally determined by computing covariant vectors. Using simple models (in and out of thermal equilibrium) we demonstrate how the time-reversal invariance affects the Gram-Schmidt and covariant vectors and the associated local Lyapunov exponents. We also show that the local covariant exponents vary discontinuously along directions transverse to the phase flow. Comparing the results for smooth and rough disks, we establish that the additional rotational degrees of freedom deeply affect the Oseledec splitting of the tangent space. In particular, we demonstrate that the rotations break the Hamiltonian character for the rough-hard-disk system.

This work was carried out in collaboration with Harald A. Posch (University of Vienna).

Time-dependent non-equilibrium molecular dynamics

Giovanni Ciccotti

Dipartimento di Fisica Universitá di Roma "La Sapienza"
and School of Physics University College of Dublin

We present a way to extend stationary state (equilibrium and nonequilibrium) Molecular Dynamics to time dependent nonequilibrium situations, including the dynamical processes of response and relaxation. The procedure, which we have called Dynamical Non-Equilibrium Molecular Dynamics (D-NEMD), to distinguish it from standard NEMD, only used to simulate stationary nonequilibrium states, is based on a generalization of linear response theory. The idea has been formulated by Onsager in the thirties in metaphysical language; given a solid foundation in the fifties by Green and Kubo (in the linear and nonlinear regime); and adapted to MD simulations by the present author (in collaboration with G. Jacucci and I.R. Mac Donald) in the seventies. It has been called the nonlinear Kubo-Onsager relation, connecting dynamical nonequilibrium averages or dynamical relaxations to stationary probability distribution functions (initial distribution) suitably sampled. To show the power of the method we apply it to study the onset of nonlinear behavior in transport processes of simple fluids, by looking at the convective circulation in liquids which establishes, as stationary asymptotic state, convective rolls. Moreover we will also apply the method to get the hydrodynamic relaxation of an interface between two immiscible liquids.

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Heat fluctuations in an out of equilibrium bath

Sergio Ciliberto

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We measure the energy fluctuations of a Brownian particle confined by an optical trap in an aging gelatin after a very fast quench (less than 1 ms). The strong nonequilibrium fluctuations due to the assemblage of the gel are interpreted - within the framework of the fluctuation theorem - as a heat flux from the particle towards the bath. We derive an analytical expression of the heat probability distribution, which fits the experimental data and satisfies a fluctuation relation similar to that of a system in contact with two baths at different temperatures.

Projection operator methods in nonequilibrium response theory

Matteo Colangeli

Politecnico di Torino, Italy

Because of the dissipation, phase space volumes contract, on average, therefore one may assume that the dynamical system has a fractal attractor. The corresponding invariant measure is singular with respect to the Lebesgue measure, hence one might conclude that the approach of [1], does not apply. Indeed, various authors have pointed out difficulties, which may prevent the validity of standard response functions, in low dimensional dynamics [2, 3]. We tackle the response problem from the point of view of physics, which may capitalize on the large number of degrees of freedom. Indeed, although certain structures are common in low dimensional phase spaces, especially in connection with the possibility of considering the response of arbitrarily chosen "observables" physics is mainly concerned with projections of the dynamics from high dimensional systems to small ones [4], and on rather simple kinds of observables and perturbations. Thus, our approach greatly reduces the possibility of encountering pathological situations in applications and also permits to characterize the special kind of reduction occurring when passing from a deterministic to a stochastic description of dynamical systems [4].

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Nonequilibrium issues in macroscopic experiments

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Gravitational wave (GW) detectors are macroscopic instruments with displacement sensitivity approaching the limit set by the uncertainty principle. To this end, reducing the thermal noise down to negligible levels is often a major challenge to the experimentalists. Moreover, making a detector with noise of pure stationary Gaussian statistics has proven to be as difficult as making a very sensitive one, these two requirements often being contrasting. From the thermodynamic viewpoint, GW experiments are usually modeled as equilibrium systems, but it is doubtful that this description is justified. We discuss the potential impact of non-equilibrium statistics on the performance of GW detectors. We also outline the research plan of the RareNoise project, which addresses this issue, and show some experimental results on non-equilibrium macroscopic oscillators.

Non-equilibrium and equilibrium molecular dynamics of nanoconfined fluids and nanostructured materials

Peter T. Cummings

Department of Chemical and Biomolecular Engineering, Vanderbilt University, and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

In this talk, I will review a line of my research that began with using non-equilibrium molecular dynamics (NEMD) to predict the transport properties of real fluids, progressed to understanding experimental data on the viscosity of nanoconfined fluids, and then led to using simulation to understand phase transitions in nanoconfined fluids. Branching off this line of research, we investigated friction in oscillating multi-wall carbon nanotubes and simulated the structure, dynamics and electron transport in gold nanowires. Intertwined with this will be some reminiscences from 30+ years of professional and personal interaction with Denis Evans.

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Nonequilibrium molecular dynamics study of permeation through a polymer membrane

Peter J. Daivis

RMIT University, Melbourne, Australia

Flow through a simplified model polymer membrane is simulated by nonequilibrium molecular dynamics methods. We use an external field in the microscopic equations of motion to drive the solvent flow, and compute the flux as a function of the driving field. The relationship between the external field and the membrane permeability coefficient is derived. We find that the flux is directly proportional to the field, yielding a permeability coefficient. The solvent permeability coefficient is computed as a function of the membrane thickness and density. We also compute the solute permeability for various solute particle sizes and different values of the solute-membrane interaction parameters. Membrane fouling is studied by including a polymeric solute, and the effect of cross-flow is simulated by including a component of the external field parallel to the membrane surface. These results show that this method constitutes a viable and well-defined technique for studying polymer membrane permeability.

Modelling nonequilibrium macoscopic oscillators of interest to experimentalists

Paolo De Gregorio

Politecnico di Torino, Italy

Recent developments in experimental Gravitational Waves (GW) detection have led to the emergence of concerns regarding the inconsistency of treating the apparati as equilibrium systems. Nonequilibrium considerations surface, for example, in examining the electronic feedback machinery that is used to damp and to stabilize GW oscillator-bar detectors, or when considering temperature gradients produced by high-powered lasers used in interferometric GW detectors. Either way, the experimental apparatus often consists of an oscillator with a very high quality factor, subjected to some power supply, and capable of extraordinary sensitivity in length displacement. Two theoretical paradigms (with their advantages and disadvantages) are presented: one in which the oscillator is described by an ad hoc Langevin equation with memory, and one in which it is modelled by a deterministic one-dimensional chain of anharmonic oscillators. Within both, it is seen that GW experiments suggest entirely novel problems to theorists.

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Diffusion processes in molecular dynamics

Carl Dettmann

University of Bristol, UK

Recently a hybrid thermostat incorporating desirable features of both Nose-Hoover deterministic and Langevin stochastic thermostats has been proposed in joint work with M. Chaplain and A. Samoletov. Subsequent quantitative tests have shown it to be efficient in comparison with alternatives. This work follows from a general scheme based on (for example configurational) temperature definitions, and the relation between deterministic and stochastic diffusions, leading to a wide variety of existing and new thermostats. Following discussion of stochastic thermostats, an example of purely deterministic dynamics will be given, quantifying the effects of periodic boundary conditions on deterministic diffusion in molecular dynamics simulations.

A Langevin dynamics for systems immersed in a linear, nonequilibrium flow

Matthew Dobson, Frédéric Legoll, Tony Lelièvre, Gabriel Stoltz

Ecole des Ponts, Paris Tech, France

In this work, we derive a Langevin dynamics for sampling a system embedded in a steady, non-uniform flow. We consider flows, where the velocity is a linear function of the space variable $\mathbf{Q}$: $u_{\text{background flow}} = A\mathbf{Q}$ for some traceless matrix A. Following and adapting the arguments of Dürr, Goldstein, and Lebowitz (1981), where a single large particle interacting with a microscopic heat bath model is considered, we arrive at the system

$$\begin{aligned} d\mathbf{Q} &= \mathbf{V}dt, \\ d\mathbf{V} &= -\gamma(\mathbf{V} - A\mathbf{Q})dt + \sigma dW, \end{aligned} \tag{1}$$

where $(\mathbf{Q}, \mathbf{V})$ are the large-particle position and velocity, W(t) is a standard Brownian motion, and γ and σ are constants satisfying the fluctuation-dissipation relation. Note that the friction term depends on the relative velocity of the large particle with respect to the background flow. Hence, Equation (1) is a way to take into account both thermal fluctuations and a background flow which is not at equilibrium.

The equations of motion (1) are the limit of a family of mechanical systems containing a single distinguished particle immersed in an infinite bath of small atoms that have a consistent mean velocity gradient A, and random initial conditions. The large particle interacts with the bath atoms via elastic collisions, and feels no other external forces. In the limit as the mass of the individual bath atoms approaches zero, we find that the large particle evolves according to the stochastic dynamics (1).

Numerical experiments will also be presented, where we consider several (large) particles evolving according to

$$\begin{aligned} d\mathbf{Q}_i &= \mathbf{V}_i dt, \\ d\mathbf{V}_i &= -\nabla_i \varphi(\mathbf{Q}) - \gamma_i(\mathbf{V}_i - A\mathbf{Q}_i)dt + \sigma dW_i, \end{aligned} \tag{2}$$

where φ is the system's potential energy. The equilibrium measure of (2) is not analytically known. We will show numerically that it is consistent with the imposed background flow and temperature.

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Rattling and freezing in a 1-D transport model

Jean-Pierre Eckmann

Departement of Theoretical Physics and Department of Mathematics, University of Geneva

With Lai-Sang Young, I considered a heat conduction model which is an open system in which particles exchange momentum with a row of (fixed) scatterers without recoil.

The main phenomenon for this model is freezing, which is the slowing down of particles with time although there is no dissipation. Most results evade rigorous mathematical analysis, but several features shed light on the intriguingly slow convergence to a steady state, in which all but one particle remain active.

Dissipation and the foundations of classical statistical mechanics

Denis J. Evans

The Australian National University, Canberra, Australia

Over the last 15 years we have discovered a group of related theorems that enable us to prove the "laws" of thermodynamics. Each of these "laws" is provable for time reversible, deterministic equations of motion that satisfy a mathematical condition called T-mixing. The axiom of causality is also required. These proofs involve a new mathematical quantity first defined in 2000, namely dissipation. Dissipation, not entropy, turns out to be the central quantity for the fluctuation theorems, the dissipation theorems, linear and nonlinear response theory, and the relaxation theorem. Using dissipation, we can also derive Clausius' Inequality and Equality, without assuming the Second "Law" of thermodynamics.

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Current fluctuations at a phase transition

Antoine Gerschenfeld

Ecole Normale Supérieure, Paris, France

Some one-dimensional systems are known to exhibit anomalous Fourier's law when considered out of equilibrium. This has been observed numerically in mechanical models which conserve momentum, such as the Fermi-Pasta-Ulam chain, or the hard-rod gas.

We have observed a similar anomalous Fourier's law in the ABC model, a nonequilibrium diffusive system, which undergoes a phase transition when considered on a ring. While current fluctuations obey Fourier's law both above and below the critical point, they diverge and become anomalous in the critical regime. This talk will present the predictions of the macroscopic fluctuation theory and compare them to the results of numerical simulations, as well as some results on the critical-point space and time correlations.

Spin-coupling in nanofluidics

J. S. Hansen[1], B. D. Todd[2], Peter J. Daivis[3], and Henrik Bruus[4]

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In the fluid dynamical description of macroscopic systems, the coupling of the fluids molecular degree of freedom to the hydrodynamical degrees of freedom is usually disregarded. However, the coupling does exist [1], and recently it has been shown that the coupling between the molecular intrinsic angular momentum (spin) and the fluid translational momentum becomes important on small length scales [2, 3].

The effect of the coupling is governed by the extended Navier-Stokes equations and involves four transport coefficients for isotropic incompressible fluids, namely, the shear viscosity, the rotational viscosity and the two spin viscosities. As shown by Evans and Streett [4] and Evans and Hanley [5] these are defined via the corresponding constitutive relations and can be evaluated using the correct fluctuation-dissipation expressions.

In this talk I show molecular dynamics results for the transport coefficients of liquid water. The calculated values are then used in the extended Navier-Stokes equations that includes the microscopic details. I analyze two different systems: (i) a planar Poiseuille flow and (ii) a flow generated by a rotating electrical field. It is shown that for the Poiseuille flow the coupling effect has significant impact on the flow profile and by comparing the continuum description with nonequilibrium molecular dynamics simulations it is concluded that the extended Navier-Stokes equations are valid down to very small length scales. The coupling also enables conversion of rotational electrical energy into fluid linear momentum [2]. It is shown that in order to generate measurable flow rates in nanogeometries the field strength must be of the order of 0.1 MVm^{-1} and must rotate with a frequency of more than 100 MHz.

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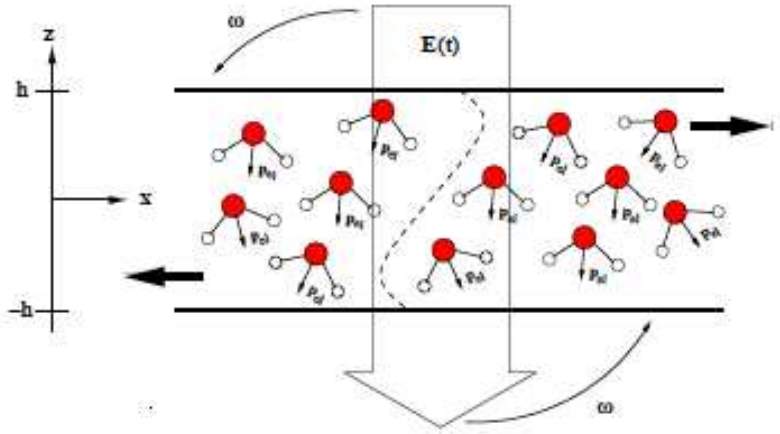

Figure 1: Schematic illustration of flow generation using a rotating electrical field, $\mathbf{E}(t)$. The water molecules have a permanent electrical dipole, here denoted $\mathbf{p}_{el}$ (which is not perfectly aligned with the field due to thermal fluctuations). The velocity profile is indicated by the dotted line and illustrates the opposite flow directions as shown by the thick black arrows.

1952.

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[3] J.S. Hansen, Henrik Bruus, B.D. Todd, and Peter J. Daivis. Rotational and spin viscosities of water: Appli- cation to nanofluidics. J. Phys. Chem., **133**, 144906, 2010.

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Rotating molecules and polymers subjected to a shear flow, thermostats and twirler

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Nonequilibrium molecular dynamics computer simulations give insight into the dynamic processes underlying the complex rheological behavior of chain molecules [1], of polymer melts [2] and polymer solutions [3]. Chain molecules rotate, stretch and change their shape in a periodic and sometimes in a chaotic manner. In the nonlinear flow regime, the average angular velocity of a molecule decreases strongly with increasing shear rate. A ratio of components of the gyration tensor displays a similar behavior. So we may ask: can this apparent interrelation between the average angular velocity and a quantity characterizing the average shape of a molecule already be seen and analyzed in the dynamics of a single stretchable dumbbell molecule subjected to shear flow with a time-reversible thermostat? The Gaussian and the Nose-Hoover thermostats change the magnitude of the angular momentum, but do not reverse its direction, as it does occur in many-particle systems. One way out is to extract the data from the shear-induced difference of the relevant quantities of two independent identical dumbbells which start with exactly opposite angular momentum [4]. For a single dumbbell, the information of interest can be obtained from its dynamics when a standard thermostat is supplemented by a twirler [5]. The twirler exerts a kind of a Lorentz force, whose strength is controlled by an additional equation of motion. Essential features of the many-particle system are already found in the simplest time-reversible dynamics involving just 5 first-order differential equations for a two-dimensional elastic dumbbell subjected to a shear flow with a Gaussian thermostat and coupled with a twirler.

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[2] M. Kröger, W. Loose and S. Hess: *Rheology and structural changes of polymer melts via nonequilibrium molecular dynamics*, J. Rheology **37** (1993)1057-1080 ; M. Kröger and S. Hess: *Rheological evidence for a dynamical crossover in polymer melts via nonequilibrium molecular dynamics*, Phys. Rev. Lett. **85** (2000) 1128-1131.
[3] C. Aust, S. Hess, and M. Kröger: *Rotation and deformation of a finitely extendable flexible polymer molecule in a steady shear flow*, Macromolecules **35** (2002) 8621-8630.
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and polymers, Eds. P. Pasini, C. Zannoni, S. Zumer (Kluwer Dordrecht), (2005) 269-294.
[5] S. Hess: *Construction and Test of Thermostats and Twirlers for Molecular Rotations*, Z.Naturforsch. **58a** (2003) 377-391.

Swarms with canonical active Brownian motion

Helmuth Hüffel

Faculty of Physics, University of Vienna, Austria

We present a swarm model of Brownian particles with harmonic interactions, where the individuals undergo canonical active Brownian motion, i.e., each Brownian particle can convert internal energy to mechanical energy of motion.We assume the existence of a single global internal energy of the system. Numerical simulations show amorphous swarming behavior as well as static configurations. Analytic understanding of the system is provided by studying stability properties of equilibria.

This is joint work with Alexander Glück, University of Vienna, and Saša Ilijíc, University of Zagreb.

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Deterministic thermostats, theories of nonequilibrium systems, and parallels with the ergodic condition

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In this presentation, we will discuss our recent and on-going work on the disambiguation of various Fluctuation-Relation results that appear ostensibly the same, but differ in subtle yet crucial ways. In this regard we find useful analogies with the development of notions of ergodicity in equilibrium theories. We consider the important role that simulation thermostats [pioneered by Evans *inter alios*] have played in the development of nonequilibrium theories, permitting connections between entropy production and the underlying dynamics. We elaborate on the purpose and limitations of deterministic thermostats in the context of irreversible thermodynamics and the development of theories of nonequilibrium phenomena. Finally, we reflect on recent developments, particularly in the context of small systems, the connection between dynamics and initial states, and the passage from transience to the steady state. Such reflections are important in view of the ever-growing relevance of these theories to nanotechnological systems.

Fluctuation relations for anomalous dynamics

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[2] Queen Mary University of London, School of Mathematical Sciences, Mile End Road, London E1 4NS, UK

We consider work fluctuation relations (FRs) for three generic types of dynamics generating anomalous diffusion: Lévy flights, Gaussian stochastic processes, and time-fractional kinetics. By combining Langevin and kinetic approaches we calculate the probability distributions of mechanical, respectively thermodynamical work in the two paradigmatic nonequilibrium situations of a particle subject to a constant force, and a particle in a harmonic trap dragged by a constant force. We check the transient FR for two models exhibiting superdiffusion, where a fluctuation-dissipation relation does not exist, and for two other models displaying subdiffusion, where there is a fluctuation-dissipation relation. In the two former cases, the conventional transient FR is not recovered, whereas in the latter two it holds either exactly or in the long-time limit [1].

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An infinite family of Second Law-like inequalities

Jorge Kurchan

École Supérieure de Physique et de Chimie Industrielles, Paris, France

An infinite number of inequalities may be derived for out-of-equilibrium systems, having the Hatano-Sasa as a particular case. I will show that with the aid of these, one may obtain a variational estimate of the out-of-equilibrium distribution.

Negative temperature states in the Discrete Nonlinear Schrödinger Equation

Roberto Livi

University of Florence, Italy

We describe, how negative temperature states may appear in the form of breathers coupled to a background in the Discrete Nonlinear Schrödinger Equation. We shall also discuss, how transport properties are affected by the presence of such a kind of nonlinear excitation.

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Going beyond Navier-Stokes to describe strong shock waves in fluids

Michel Mareschal[1], **Brad L. Holian**[2], **and Ramon Ravelo**[2]

[1] Universite Libre de Bruxelles and ZCAM, University of Zaragoza
[2] Los Alamos National Laboratory, USA

Shock waves in fluids have already been investigated by Molecular Dynamics simulations during early non-equilibrium studies in the late seventies, showing surprisingly good agreement with Navier-Stokes equations for weak shocks. Once the Mach number increases beyond 2-3, linear-laws based hydrodynamics becomes insufficient: the origin of this discrepancy lies in the departure from local equilibrium for fluid states in the shock front with an important non-equipartition of kinetic energy. This, in turn, leads to the necessity of including a relaxation process in the continuous modeling.

We have reinvestigated this problem by introducing new variables in the continuous description, and using a generalized version of the Fourier law as proposed, in another context, by Cattaneo. We will present, how we have applied this generalization to the shock wave problem, and show, how this has permitted to obtain quantitative agreement between the two levels of description, atomistic and continuous, in the case of strong shocks.

Lyapunov exponents and modes for a quasi-one-dimensional system

Gary Morriss

University of New South Wales, Sydney, Australia

We review the existing knowledge of Gram-Schmidt Lyapunov vectors and then describe the advances made in the last couple of years towards a complete understanding of their origin. The introduction of a method to calculate covariant Lyapunov vectors has lead to numerical studies and an interpretation of the information that they give.

We demonstrate the preservation of the Lyapunov modes in a system of hard disks by the underlying tangent space dynamics. We propose a modified Gram-Schmidt procedure based on orthogonality with respect to the centre (zero) space that produces the exact numerical mode. This Gram-Schmidt procedure can also exploit the orthogonality between conjugate modes in order to find a simple relation that determines the Lyapunov exponent from the Lyapunov mode.

We construct a field theory for a system, where the number of particles is large enough so that the Lyapunov mode contributions from each particle can be considered to change continuously with particle position. The solution of the partial differential (wave) equation gives the observed functional forms for all modes. The wave speed of the LP modes is predicted to reasonable accuracy for the full range of densities and system sizes.

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The role of external electric fields in enhancing ion mobility, drift velocity and drift-diffusion rates in aqueous electrolyte solutions

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Molecular simulations have been carried out using the method of molecular dynamics to investigate the role of external electric fields on the ion mobility, drift velocity and drift-diffusion rate of ions in aqueous electrolyte solutions. These properties are critical for a range of processes including electro-dialysis, electro-deionization, electrophoresis and electro-osmosis. Our results show that external electric fields relax the hydrated ion structure at significantly larger time scales (between 300 - 800 ps), than most other relaxation processes in solutions (generally of the order of 1 ps). Previous studies that did not account for the much longer relaxation times did not observe this behavior for ions even with very high electric fields. External electric fields must also overcome several (at least two or more) activation energy barriers to significantly change the structure of hydrated ions. As a result, the dynamic behavior changes almost in bands as a function of electric field strengths, rather than linearly. Finally, the effect of the field is much less dramatic for water than for the ions. Thus electric fields will be of more significance in processes that involve the transport of ions (such as electro-deionization), than the transport of water (electro-osmosis).

Heat conduction in the hard point chain

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I discuss heat transport in a chain of point particles that interact elastically whenever they hit one another, and when they reach a maximal distance. Although the model is not chaotic, in the case of diatomic chains it behaves very much like typical chaotic nonlinear models. In this context its study allows for a clean study of the role of the thermodynamic pressure on the scaling behavior of heat conductivity. Very interesting is also the equal-mass, zero-pressure limit: in spite of being integrable, nontrivial sub and superdiffusive features can be found in equilibrium and off-equilibrium simulations.

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Non-equilibrium statistical mechanics of granular fluids: from experiment to theory

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I will present results from a recent experiment on quasi-2D granular material fluidized on a vibrating plate, where spatial velocity correlations are directly related to non-conservative properties of the dynamics. A non-equilibrium fluctuating hydrodynamics approach allows to interpret such results in terms of a velocity correlation length, which grows as the packing fraction is increased, and which separates two ranges of space-time scales where *different* temperatures act. Deviations from the equilibrium Fluctuation-Dissipation relation and connections with the Fluctuation-Relation for entropy production will also be discussed.

Simultaneous material and structural optimization in the spider web attachment disk

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Spider webs are a fascinating example of natural structural engineering, part of the class of non-living structures produced externally to the body of an animal, which are essential for its survival. The webs are optimally designed for their evolutionary pressures, both structurally and materially, and through several hierarchical levels [1]. The structural and material levels are inseparable from one another; the material properties govern the structure and vice versa [2].

We explore the possibility of holistic optimization of the two quantities. We consider the case of the attachment disk, the gooey structure used to anchor the orb web to its physical surroundings. The attachment disk is an example of a natural structure which shows remarkable adhesive properties. Woefully little is known about the intricate, lace-like structure of the attachment disk or the mechanical properties of the piriform silk of which it is fabricated [3]; although we know that piriform spigots are present in most - if not all - orb-weaving species [4], and recent studies have identified its protein structure for some species [5,6]. We propose to study the attachment disk with a new elastica peeling model of a two-branched adhesive anchorage [7] and optimize it materially and structurally. We conclude with the results of some Molecular Dynamics simulations and consider their applications for the design of super-tough materials [8].

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Hyperbolicity and effective degrees of freedom of extended dynamical systems

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Lyapunov exponents and vectors are important characteristic quantities of nonlinear dynamical systems. Recently, efficient algorithms for the calculation of covariant Lyapunov vectors and the associated instantaneous Lyapunov exponents were established. These allow to probe various aspects of hyperbolicity of high-dimensional dynamical systems.

Our recent results in this respect for dissipative extended systems will be reviewed and the relation to the finite number of effective degrees of freedom of infinite-dimensional systems will be discussed. These results are elaborated for prototypical systems of spatio-temporal chaos such as Coupled Map Lattices, the Kuramoto Sivashinsky and the Complex Ginzburg-Landau equation [1,2].

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An optically trapped particle and the fluctuation relations: applying two decades of developments to one simple system

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Since Evans, Cohen, and Morriss first proposed a fluctuation theorem in 1993, there has been a proliferation of new fluctuation relations. While the two main relations, the Evans-Searles Fluctuation Theorem and the Jarzynski equality, are well studied, many of the other relations are not as well known, and the connection between these relations is obscure. In this presentation we provide a short review by application of these many relations. We do this by applying a significant number of these relations to a simple system based on one of the early experimental demonstrations of the FT, the optical trapping experiment.

Directed diffusion in complex social networks

Farinaz Roshani

Alzahra University, Iran

If we model an individual as a vertex within a network that represents the society, we can then define a degree of influence of each vertex on its neighbours, and define a propagation function which characterizes the simultaneous connectedness of each vertex with its neighbours. This constitutes a generalized model for directional propagation of rumour. The degree of influence and the propagation function define parameters, which decide, what fraction of the society have heard the rumour after the rumour has run its course.

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The nature of the glass and gel transitions: structural and dynamic insights from colloids

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We identify structural and dynamic data signatures, which clearly distinguish gels and glasses for the first time. We use a colloidal model system of hard and sticky spheres and base our results on time-resolved single-particle tracking with confocal microscopy, and confirm our findings with molecular dynamics simulation.

Since gels are identified with arrested spinodal decomposition, gelation in sticky sphere systems appears first-order-like in effective temperature. We measure discontinuities both in long-term dynamics and a novel local structural measure. By contrast, dynamic and structural measures show that the glass transition in hard spheres and sticky spheres at very high density is continuous. An important consequence of our criteria for gelation/vitrification finding is that states thermodynamically defined as gels may persist up to very high packing fractions, around $\gtrsim 0.58$. We further show that gelation is intrinsically coupled to pressure, and argue that constant volume experiments are required for gelation and this, along with the relevant timescales, is why gels are found in soft matter, almost without exception.

Nonequilibrium phenomena in liquid crystals

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Nonequilibrium phenomena and transport phenomena are much richer in liquid crystals than in ordinary isotropic liquids due to the lower symmetry of the former. In particular, various alignment phenomena take place, for example, the director of a nematic liquid crystal attains different orientations relative to an external field such as a temperature gradient or a velocity gradient. A particularly interesting phenomenon occurs when a nematic liquid crystal is subjected to a planar Couette velocity gradient. Then the director either comes to rest at a constant alignment angle relative to the stream lines, *i.e.* the system is flow stable, or it starts rotating, *i.e.* the system is flow unstable. The alignment angle and the rotation rate are determined by the balance between the rotational and irrotational part of the Couette velocity field.

Results will be presented of a simulation of the Gay-Berne fluid undergoing planar Couette flow, starting at high temperatures in the nematic phase where the liquid crystal is flow stable, and continuing to lower temperatures towards the nematic-smectic A phase transition where the liquid crystals becomes flow unstable. The viscosity coefficients that determine the alignment angle and the director rotation rate have been obtained both by Green-Kubo relations and by nonequilibrium molecular dynamics methods, and they give consistent results that agree with the alignment angle and the director rotation rate that are actually obtained in a direct shear flow simulation. Close to the nematic-smectic A transition point, the linear relations between the velocity gradient and the shear stresses break down, and the flow becomes non-Newtonian.

Space-time correlations in the ASEP conditioned on carrying a large flux

Gunter Schuetz

Forschungszentrum Jülich, Germany

We show that in the asymmetric simple exclusion process (ASEP) on a ring, conditioned on carrying a large flux, the particles experience an effective long-range potential which is similar to the effective potential between the eigenvalues of the circular unitary ensemble in random matrices. We obtain the quasi stationary measure, transition probabilities and spatio-temporal correlations using the Bethe ansatz and determinantal free fermion techniques.

Stochastic thermodynamics of nonequilibrium steady states

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University of Stuttgart, Germany

Stochastic thermodynamics provides a framework for describing small systems embedded in a heat bath and externally driven to non-equilibrium [1]. 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. A first-law-like energy balance allows to identify applied work, dissipated heat and entropy production on the level of an individual stochastic trajectory.

For non-equilibrium steady states (NESSs), total entropy production obeys a detailed fluctuation theorem even for finite times [2]. As an alternative to the phenomenological approach of introducing an effective temperature in order to adjust the equilibrium form of the fluctuation-dissipation theorem (FDT) to a NESS, we have derived a transparent general form of the FDT in a NESS [3]. Finally, generalized Green-Kubo relations hold true in NESSs under the weak assumption of local detailed balance [4]. Under the same condition, universal results for the efficiency of autonomous nano-machines can be derived [5]. Where available, these theoretical results will be illustrated using data from experimental model systems.

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Interpreting force spectroscopy of soft matter using dynamic umbrella sampling

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Soft Matter is a sub-discipline of condensed matter physics that focusses upon chemical and biological matter that is easily deformed by thermal forces or fluctuations. These materials show their most interesting behaviour/properties at energy scales on the order of k_BT, where classical (as opposed to quantum) physics dominates. Soft matter, such as single DNA molecules and self-assembled micelles, are characterised by many internal degrees of freedom and weak enthalpic interactions. Consequently, these can be highly responsive to external fields, and they can respond slowly in comparison to enthalpy-dominated systems. These long relaxation times can be problematic when trying to characterise the equilibrium states of soft matter, as the measurement perturbs the equilibrium state of the soft system.

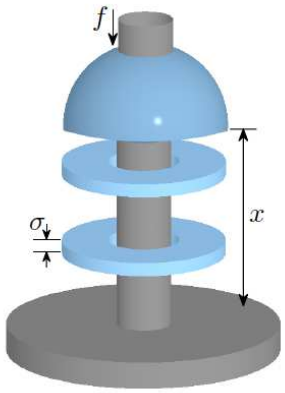

Figure: Schematic of a piston-rotaxane molecule showing $N = 2$ free rings threaded onto an axle that is end-tethered to a surface. The top-most ring, referred to as a piston-ring, is optically-trapped and controlled in force spectroscopy. Such experiments provide distributions of the measured force, f, as a function of the position optical trap centre, x_0: As only a close analogue of this molecule has been synthesized, we resort to stochastic simulation to construct distributions of measured force.

Here we demonstrate a method to extract equilibrium averages of state properties from experiments of soft matter that are not at equilibrium and, indeed, can be far from equilibrium. This method, a dynamic version of umbrella sampling, has its origins in computer simulation of equilibrium states [1] which was recently ex-

tended to non-equilibrium using concepts central to Fluctuation Theorems [2,3]. Here we demonstrate the utility of this method in determining equilibrium information from experimental force spectroscopy of soft systems that are not at equilibrium. We experimentally demonstrate this with a model soft system, a colloidal bead fluctuating in an optical trap, and we extend this demonstration to a complex soft molecule, a piston–otaxane that behaves as a molecular version of an automobile shock absorber [4,5], using simulated force spectroscopy [6].

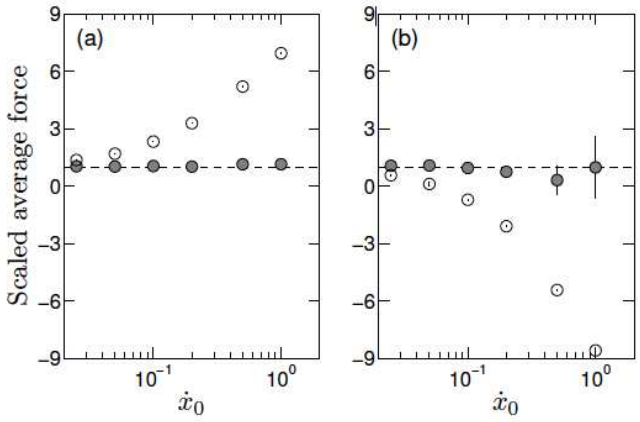

Figure: Scaled average force on the piston ring at the completion of (a) compression and (b) expansion at different rates, $\dot{x}_0$, of the piston rotaxane. Open circles are scaled non-equilibrium averages of the force, $\langle f \rangle_{noneq}/\langle f \rangle_{eq}$; filled circles are scaled equilibrium averages constructed from dynamic umbrella sampling, $\langle f \rangle_{noneq}^{unbiased}/\langle f \rangle_{eq}$.The compression/expansion rate is given as the speed of the optical trap centre, $\dot{x}_0$, dimensionally scaled by the ring thickness and the diffusion time for a ring to diffuse a mean distance equal to its thickness. That the non-equilbrium average forces (open circles) are rate dependent proves that the molecule is out of equilibrium upon measurement. Note that when the dynamic bias is removed from this force data, the average forces (filled circles) are independent of rate and coincide with the equilibrium average force.

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The formation and annihilation of solitons and standing strainwave superstructures in a two-dimensional colloidal crystal: A new non-equilibrium state?

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Confining a colloidal crystal within a long narrow channel produced by two parallel walls can be used to impose a mesoscale superstructure of a predominantly mechanical elastic character. When the crystal is compressed in the direction perpendicular to the walls, we obtain a structural transition when the number of rows of particles parallel to the walls decreases by one. All the particles of this vanishing row are distributed throughout the crystal. If the confining walls are structured (say with a corrugation along the length of the walls), then these extra particles are distributed neither uniformly nor randomly; rather, defect structures are created along the boundaries resembling soliton staircases, inducing a nonuniform strain pattern within the crystal. Here, we study the conditions of stability, formation, and annihilation of these solitons using a coarse grained description of the dynamics. The processes are shown by comparing superimposed configurations as well as molecular animations obtained from our simulations. Also, the corresponding normal and shear stresses during the transformation are presented.

We also obtain the effective interaction between the solitons and use a Lindemann criterion that shows the reduction in dimensionality causes the finite soliton lattice to readily melt as the temperature is raised. A study of these dynamical processes should be useful for controlling strain wave superstructures in the self-assembly of various nano- and mesoscaled particles.

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The motion of 1D driven interfaces: exact solutions of the KPZ equation

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A widely studied nonequilibrium interface dynamics considers a stable phase in contact with a metastable phase. If the order parameter for the bulk phases is not conserved and mixes rapidly, the effective equation of motion for the interface was proposed by Kardar, Parisi, and Zhang some time ago. We explain some recent exact solutions of this equation in the case of a 1D interface and their connection to the thin film turbulent liquid experiment by Takeuchi and Sano. In particular, the unanticipated role of replicas will be emphasized.

Accurate predictions of fluid slip

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In this presentation we provide a derivation to predict the slip velocity for a fluid flowing in the near vicinity of solid walls. In particular we present results for a system consisting of an atomic fluid confined by atomistic walls at the nano-scale. Our derivation is based upon forming equilibrium time correlation functions of relevant measurable fluid properties. These correlation functions are formed for increasingly fine-grained slabs of fluid adjacent to the walls. By computing the various correlation functions, we are able to extract the slab friction coefficient adjacent to the wall for a limiting slab width, and, hence, the slip velocity for the fluid, to very high accuracy. We present numerical results from non-equilibrium molecular dynamics (NEMD) simulations to verify our theoretical predictions. We demonstrate the model's high accuracy and robustness by presenting excellent agreement between predicted and NEMD slip lengths for several flow geometries and fluid-wall interaction potentials that mimic hydrophobic and hydrophilic behaviour. Results for fluids such as methane and water confined to graphene nanochannels will also be presented, and we demonstrate convincingly the super-lubricating properties of graphene surfaces.

Fluctuations of a Brownian particle with dry friction

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This talk will discuss a Langevin equation, first studied by the late Pierre-Gilles de Gennes, in which there is a solid-solid or dry friction force acting on a Brownian particle in addition to the viscous friction usually considered in the study of Brownian motion. Exact and approximate solutions for the time-dependent propagator, velocity correlation function, frequency spectrum, and optimal fluctuation paths of this equation will be presented. The large deviations of a work-like quantity will also be discussed in the context of fluctuation relations.

This is joint work with W. Just, E. Van der Straeten (QMUL), A. Baule and E. G. D. Cohen (New York).

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Fragmentation of liquid droplets

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Fragmentation is an example of material failure. It is a problem with widespread applications including: fracture of brittle solids, break-up of oil shale, destruction of armor and exploding munitions. A complete mathematical and physical understanding of material fragmentation is currently beyond reach given the complexity involved. Modelling provides the best hope for making progress in this area. A useful starting point for numerical work is to study the fragmentation of liquid droplets following adiabatic expansion.

In this work we have studied the break-up of 2-dimensional liquid droplets using two different non-equilibrium expansion methods: the Holian-Grady method (homogeneous expansion within periodic boundaries) and the Hoover-Blink method (expansion with free boundaries). The expansions have been performed at a range of different initial thermodynamic states, chosen once the phase diagram had been constructed (for the simple short-ranged pair potentials used). Results are discussed in terms of the fragment size distributions and the local properties of the clusters, including their shape, various measures of temperature and energy). Comparisons are made between the statistical properties of clusters obtained using both NEMD methods.

Efficiency at maximum power of Feynman's ratchet as a heat engine

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The maximum power of Feynman's ratchet as a heat engine and the corresponding efficiency η_* are investigated. When a perfect ratchet device (no heat exchange between the ratchet and the paw via kinetic energy) works between two thermal baths at temperatures $T_1 > T_2$, its efficiency at maximum power is found to be $\eta_* = \eta_C^2/[\eta_C - (1-\eta_C)\ln(1-\eta_C)]$, where $\eta_C \equiv 1 - T_2/T_1$. This efficiency is slightly higher than the value $1-\sqrt{T_2/T_1}$ obtained by Curzon and Ahlborn [Am. J. Phys. **43** (1975) 22] for macroscopic heat engines. It is also slightly larger than the result $\eta_{SS} \equiv 2\eta_C/(4-\eta_C)$ obtained by Schmiedl and Seifert [EPL **81** (2008) 20003] for stochastic heat engines working at small relative temperature difference.

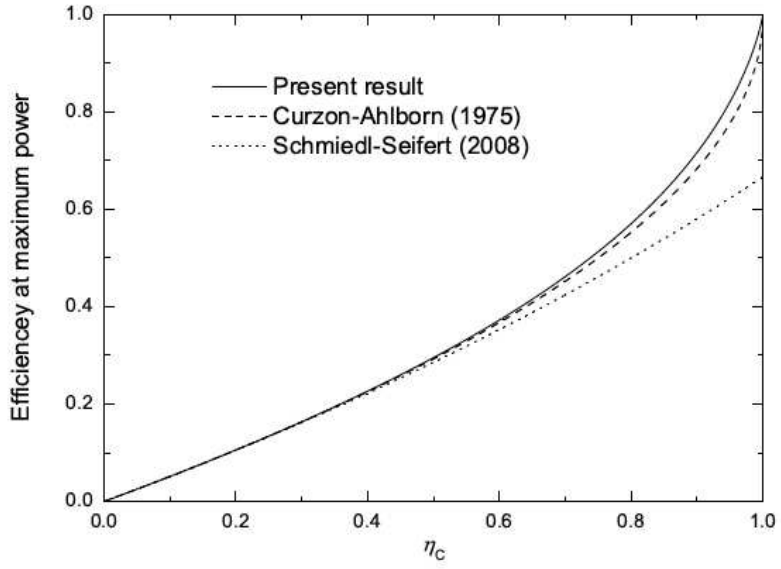

Figure 1. Efficiency at maximum power for different model system [Tu, J. Phys. A **41** (2008) 312003].

The anomalous dynamics of one-dimensional hamiltonian systems

Henk van Beijeren

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The dynamics of generic one-dimensional hamiltonian systems with translation invariant short-ranged interaction potentials are shown to be in the Kardar-Parisi-Zhang universality class. Scaling functions obtained by Prähofer and Spohn by solving the polynuclear growth model [1] can be used to obtain exact expressions for the long-time behavior of the Green-Kubo integrands for heat diffusion and sound attenuation, as well as for system-size dependent coefficients of heat conduction and sound damping. The Green-Kubo integrands decay with time as $t^{-2/3}$; the sound mode damping constant diverges with system size as $L^{1/2}$, and the heat conduction coefficient as $L^{1/3}$. The coefficients can be obtained exactly from the Prähofer-Spohn scaling functions combined with mode-coupling amplitudes as obtained by Ernst, Hauge and Van Leeuwen [2]. Due to the presence of three conserved densities (mass, momentum and energy), giving rise to three hydrodynamic modes with different propagation velocities (+ or $-c_0$, the adiabatic sound velocity for the sound modes and zero for the heat mode), there are important and still superdiffusive corrections to the asymptotic long time respectively large size behaviors. By using mode coupling techniques, one can estimate these corrections as well.

Previous results by Delfini et al. [3] provide a correct one-loop mode coupling approximation to these exact results for weakly anharmonic chains. However, these results require corrections as soon as c_p/c_v deviates appreciably from unity.

Exceptions to these results occur in case some of the mode coupling amplitudes are vanishing. The condition for this is $\left(\frac{\partial c_0 n}{\partial n}\right)_s = 0$. This is satisfied for a number of exactly solvable models such as harmonic chains and Toda lattices, but it may also happen in special points, lines etc. of the phase diagrams of not exactly solvable models.

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Scaling of the current time correlation function of fluids of hard sphere particles: exposing the difference between thermodynamic stability and metastability

Bill van Megen

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The current correlation function is determined from dynamic light scattering measurements of a suspension of particles with hard sphere-like interactions. For suspensions in thermodynamic equilibrium, we find scaling of the space and time variables of the current correlation function. This finding supports the notion that the movement of suspended particles can be described in terms of uncorrelated Brownian encounters, i.e., a configuration-space-only description. However, in the metastable fluid, at volume fractions above freezing, this scaling fails; a dynamical discontinuity is exposed at the freezing density. Experimental results are complimented by molecular dynamics on hard sphere fluids. The limited scaling found exposes the space-time window where momentum and configuration spaces are statistically orthogonal.

Notions of entropy and entropy production in non-equilibrium systems

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In the physics literature the notion of entropy has been defined in a number of different frameworks:

- The thermodynamic entropy due to Clausius is a thermodynamic state variable of a system in (local) thermodynamic equilibrium;
- The Boltzmann entropy, which is defined in the single-particle phase space, was introduced to characterize the decay of a system towards equilibrium;
- The Gibbs entropy characterizes an ensemble in phase space;
- In stochastic thermodynamics the entropy characterizes ensembles of small systems subjected to a bath.

In order to highlight differences in the predictions of the various entropy notions we will work out these functionals for a simple transport model. Fluctuations will also be considered.

Test-tube rain

Michael Wilkinson

Open University, Milton Keynes, England

I shall report on experiments on a test-tube model for rainfall, in which a steady rate of temperature change of partially miscible liquids induces periodic cycles of turbidity and droplet precipitation. The droplet growth is modelled by a period of Ostwald ripening, followed by a finite-time runaway growth of droplet sizes due to larger droplets sweeping up smaller ones. This theory predicts that the period T and the temperature sweep rate R are related by $T = \text{const} \cdot R^{-3/7}$, in good agreement with the experiment. The theory is a benchmark model for rainfall, applicable to warm clouds in a convectively stable atmosphere, and it resolves an apparent bottleneck in the kinetics of rain droplet growth.

This is joint work with Jürgen Vollmer, Tobias Lapp, Max-Planck Institute for Dynamics and Self-organisation, Göttingen, Germany.

Quasi-equilibrium and the emergence of solid behaviour in amorphous materials

Stephen Williams

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Amorphous solids are not in a state of equilibrium, rather they are in quasi-equilibrium. A fluid cannot support a stress. If we subject a fluid to a sudden change in strain, a nonequilibrium stress results that then relaxes to zero. This relaxation cannot be understood in terms of equilibrium statistical mechanics. In contrast, if we subject a solid to the same protocol, initially a nonequilibrium stress results, which then relaxes to some perturbed equilibrium or quasiequilibrium non-zero stress. Even if the solid-like material is able to flow on some much longer time scale, we can still accurately quantify the observed non-zero stress on a relevant time scale using equilibrium or quasi-equilibrium statistical mechanics. We will assume that this is the fundamental difference between a solid and a fluid.

Recently, we have developed quasi-equilibrium statistical mechanics for the case of planar shear. This work shows, how solid behaviour emerges in amorphous materials from microscopic considerations. Here, the relevant quasi-equilibrium statistical mechanics will be reviewed. It will be shown, how the response in the stress, to a change in the strain, is qualitatively different for a quasi-equilibrium solid relative to a supercooled fluid. New molecular dynamics simulation results will be presented. These show convincingly, how this qualitative change emerges very sharply, upon crossing from a supercooled fluid to a history dependent quasi-equilibrium solid.

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Abstracts of posters

in alphabetical order of the main authors

A new paradigm for (steady-state) coarse graining of stochastic dynamics

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It has been recently pointed out [http://arxiv.org/pdf/1105.2178] that cyclic fluxes are essential for understanding non-equilibrium steady states in stochastic thermodynamics. Such fluxes are driven by affinities. The product of a cyclic flux with its driving affinity is related to its entropy production and therefore with dissipation of energy in the system. We present a new paradigm for complexity reduction using a coarse-graining procedure based on cyclic fluxes, affinities and locality.

Thermodynamic fluctuations in actively cooled resonators

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A system must not be necessarily as small as a pollen particle to be dominated by microscopic fluctuations: also a ton-size resonant metal bar can be used as a test bench for statistical mechanics theories. We analyze the thermodynamic balance of the gravitational wave detector AURIGA, modeled as a macroscopic electromechanical oscillator in contact with a thermal bath, $T_0 = 4.6$ K, and further cooled by an active feedback system, equivalent to a viscous force. The oscillator is driven to a non-equilibrium steady state, at the fictitious "effective temperature" $T_{\rm eff} = 21$ mK $\ll T_0$. The discrepancy between $T_{\rm eff}$ and the thermal bath temperature reveals the nonequilibrium nature of the phenomenon. The energy flow in the system shows that the feedback circuit is actually extracting energy from the thermal bath by making use of its knowledge of the physical state of the oscillator.

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Lyapunov instability of rough hard disks

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The phase-space instability of a classical dynamical system is most naturally defined in terms of the time evolution of a set of specified perturbation vectors in tangent space. Two such sets are commonly used, the orthonormal Gram-Schmidt vectors, and the covariant vectors. Both sets provide complementary information on the chaotic dynamics. The Gram-Schmidt vectors are intimately related to the eigen-subspaces of the Oseledec matrix, whereas the covariant vectors constitute a practical realization of the Oseledec splitting of the tangent space into a hierarchy of stable and unstable subspaces at any point visited by the trajectory. The latter are also unique in the sense that they may be readily converted from one coordinate representation to another.

Here we also analyze two-dimensional systems of smooth and rough hard disks. We show that the additional rotational degrees of freedom for rough hard disks have a strong influence on the Oseledec splitting. In particular, the rough-hard-disk systems are not strictly hyperbolic and not symplectic.

Modeling non-equilibrium properties in nuclear waste vitrification

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The Thermal Oxide Reprocessing Plant (THORP) at Sellafield in Cumbria is the UKs only site for the recycling of spent light-water reactor fuel. Its cessation of operation scheduled for 2014 will generate a backlog of high-level nuclear waste requiring safe intermediate storage, before it can be interred in a long-term disposal facility for geological timescales. Immobiliser materials serve as the first line of defense against radioisotope leeching from nuclear waste facilities, functioning as a stable matrix in which the waste can be fixed and maintain its integrity both under radiation damage and environmental exposure.

Lithium borosilicate glass vitrification is the principal waste immobilisation strategy in the UK. Because the costs are so high, and the safety procedures so stringent, it is desirable to develop glass compositions specific to individual waste streams so as to maximize waste loading while simultaneously minimizing the practical melting temperature.

Reliable values and models for transport properties, including shear viscosity and thermal conductivity, are lacking. There is a need to develop a fundamental understanding of the variation of these transport properties with both composition and temperature, in order to inform better predictive models.

As part of a larger programme of work aimed at closing the gap, we intend to conduct computational modeling of glass flow properties as a function of radioisotope content. The simulation work will provide us with pseudo-experimental data to test semi-empirical models as well as enlarging the information databases for temperatures and compositions relevant to the nuclear waste industry.

In particular, in this presentation we focus on a comparison of equilibrium and non-equilibrium methods for estimating glass viscosity as a function of temperature.

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The evolution of covariant Lyapunov modes

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We have explained the evolution of the covariant vectors (CV) in the quasi-one-dimensional system completely, starting from the CV modes identical to the original Gram-Schmidt (GS) vectors, to their final stable values as a linear combination of these modes. From the description of the nature of the dynamics we have been able to find the exact values, or distributions and means, of the angles between the CV modes.

Piston-rotaxanes as molecular shock-absorbers

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A rotaxane is a molecule that is architecturally similar to some baby rattles: one or more ring-like molecules threaded onto a molecular axle that is capped on both ends with stoppers to prevent the rings from falling off. These materials were first synthesised only 40 years ago. One of the most interesting features of these rotaxanes is the ability of a ring to slide along the axle. For example, by tuning strong enthalpic interactions within the molecule, chemists can entice a ring to cover specific portions of the axle - this can be used to shield particular chemical groups so as to impart a changeable molecular hydrophobicity or reactivity. However these rings don't need to be enthalpically localised: these rings can shuffle along the axle and their translational entropy leads to an array of interesting soft properties. In this talk we describe soft properties of entropy- dominated rotaxane molecules, specifically a piston-rotaxane (P-R) which behaves as a scaled-down version of automobile shock-absorber. These include predictions of (i) the equilibrium thermo-mechanical response of a single piston-rotaxane [1], and (ii) the micro-valve behaviour of a surface grafted with these molecules [2], as well as predictions of (iii) the molecule's non-equilibrium response that is comparable with single molecule force spectroscopy [3] and which characterises the shock-absorbing properties.

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Relevance of sampling schemes in light of Ruelle's linear response theory

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We reconsider the theory of the linear response of non-equilibrium steady states to perturbations. We first show that by using a general functional decomposition for space-time dependent forcings, we can define elementary susceptibilities that allow to construct the response of the system to general perturbations. Starting from the definition of SRB measure, we then study the consequence of taking different sampling schemes for analysing the response of the system. We show that only a specific choice of the time horizon for evaluating the response of the system to a general time-dependent perturbation allows to obtain the formula first presented by Ruelle. We also discuss the special case of periodic perturbations, showing that when they are taken into consideration the sampling can be fine-tuned to make the definition of the correct time horizon immaterial. Finally, we discuss the implications of our results in terms of strategies for analyzing the outputs of numerical experiments by providing a critical review of a formula proposed by Reick.