Scientific report on the conference

Nonequilibrium processes: the last 40 years and the future

August 29 - September 2, 2011

Venue: University Centre Obergurgl, Austria, operated by the University of Innsbruck, Austria.

Organizers:
Debra J. Bernhardt (Searles), Griffith University, Brisbane, Australia
Harald A. Posch, University of Vienna, Austria
Lamberto Rondoni, Politecnico di Torino, Italy

1) Summary

Statistical physics pervades all areas of physics. For systems in thermodynamic equilibrium there exists an impressive theoretical understanding, which, to some extent, is still lacking for systems out of equilibrium. Recently, significant progress has been achieved by the formulation of fluctuation relations for nonequilibrium systems, and this discovery has revolutionized our thinking about nonequillibrium processes. Thus, the time was ripe for an overview of this subject, and the conference in Obergurgl provided just that. It was attended by a significant fraction of the leading scientists in the world, who were responsible for this new approach. From the discussions at the conference one gets the impression that the field now has reached some maturity, combining experimental, theoretical and mathematical approaches. The wide spectrum of topics discussed at the conference included both fundamental problems such as the foundation of statistical mechanics and the Second Law of thermodynamics, and very applied topics such as a kinetic model of rain-drop formation, or the fluctuations of huge macroscopic objects designed for the detection of gravitational waves.

The conference lasted from Monday morning (August 29, 2011) to Friday noon (September 2, 2011), and was attended by 65 participants. Almost every participant gave a talk or presented a poster. Altogether, there were 49 lectures (of 25 to 30 minutes each) and 6 posters. The poster session took place on Tuesday evening (August 30, 2011) and lasted for almost two hours. There were no lectures on Wednesday afternoon (September 31). Instead, on the invitation of the Australian National University, Canberra, a conference dinner took place at a mountain restaurant near Obergurgl, which provided an excellent setting for celebrating the 60th birthday of Professor Denis J. Evans, one of the leading scientists in nonequilibrium physics.

2) Scientific Content

Stimulated by ever more sophisticated numerical simulation techniques and novel mathematical tools, nonequilibrium science has experienced a tremendous boost over the last forty years. It resulted in the formulation of a whole family of relations, which include the Fluctuation Theorem for systems in nonequilibrium stationary states (NESS-FT) [1, 2], the Transient Fluctuation Theorem (TFT) for systems driven away from thermal equilibrium [3], and the Jarzynski equality [4] and the nonequilibrium work relations of Crooks [5]. They provide exact results and, consequently, reflect various aspects of the Second Law of thermodynamics. They are the focus for active research presented by many speakers at the conference. For example, J. Kurchan [6] introduced an infinite family of generalized Second Law-like inequalities, which may be used to approximate the probability distribution for a driven out-of-equilibrium system by thermodynamic (stationary) trial distributions. Using a variational procedure, this allows for optimization. R. Klages examined whether TFTs existed for models exhibiting anomalous diffusion. It was found that the conventional TFT is not recovered for a subdiffusive system, whereas it holds for a superdiffusive case.

D.J. Evans, in the final talk of the conference, addressed the foundations of statistical mechanics and provided an overview of the fluctuation theorems and relations for the special class of systems with time-reversible deterministic dynamics. In particular, considering thermostated systems to which a periodic external perturbation is applied, a derivation of Clausius' theorem was given, which is based on these fluctuation theorems. Interestingly, the proof does not make direct use of the Second Law as was the case in the original work by Clausius [7]. At this point it is worth mentioning that Pusz and Woronowicz in their celebrated paper [8] introduced the notion of "passivity" and "activity". Loosely speaking, an *isolated* system is passive, if its energy generally increases due to periodic perturbations. Only active systems, for which the opposite were true if they existed, are candidates for a *perpetuum mobile* of the second kind. Thus, passivity is another way of formulating Clausius' theorem. If this concept is applied to specific states, one may show for an analytically solvable example - an ensemble of periodically-perturbed independent harmonic oscillators - that the *active* states (violating the Second Law) are located in phase space on a Cantor-like set and, consequently, are of measure zero [9], whereas the passive states dominate in accord with the Second Law. [1]

Small systems embedded in a heat bath may be treated within the recently developed framework of statistical thermodynamics. U. Seifert explained in his talk, how the basic quantities - applied work, dissipated heat, and entropy production - may be identified on the level of an individual stochastic trajectory. For NESS states, a fluctuation theorem may be derived for the total entropy production. Also a general fluctuation-dissipation theorem as well as generalized Green-Kubo relations may be obtained in this case. Based on these concepts, universal expressions for the efficiency of autonomous nano machines

[1] Just as an aside, the possibility of such spontaneous discussions, which otherwise would rarely occur, is a point in case for organizing a conference such as the one in Obergurgl.

have been derived [10]. In a related contribution, Z.C. Tu talked about the efficiency at maximum power of the Feynman ratchet as a heat engine.

The importance and applicability of the fluctuation theorems and relations to nonequilibrium processes may be inferred from the following examples presented in Obergurgl. It was observed by Belushkin that the NESS-FT also holds for mesoscopic systems in the presence of hydrodynamic interactions, if a proper scaling of the measurement volume is applied. This scaling is a consequence of the collective processes mediated by the hydrodynamic interactions [11]. Another talk by H. Touchette was concerned with the dynamics of a solid object, which moves over a vibrating solid surface and experiences solid friction in addition to a constant force. The probability distribution of the work done on the object by the force was derived, and a fluctuation relation for the mechanical work fluctuations incorporating the solid friction was obtained [12]. The experimental situation in connection with the fluctuation relations was addressed by S. Ciliberto, who considered energy fluctuations of a Brownian particle confined by an optical trap in an aging gelatin after very fast temperature quenches. The existence of a fluctuation relation similar to that of a system in contact with a bath at different temperatures was experimentally confirmed.

Another topic much discussed at the conference were systems with reduced geometries. In an illuminating review, G. Benettin discussed the present status of our understanding of the famous Fermi-Past-Ulam problem based on extensive recent simulation results [13]. Let N denote the number of particles and ϵ the specific energy, and let the total energy be initially concentrated in a few small wavenumber (k) modes. For finite N and small ϵ, the $\alpha+\beta$-FPU system first relaxes towards a quasi-stationary state, with an exponential decay with k (similar to the integrable Toda system, for which no equilibrium state exists). But there exists another much longer time scale T_e for the system to reach equipartition of the mode energies. For finite N, T_e turns out to be a stretched exponential in $1/\epsilon$ (very large T_e), which crosses over to a power law (much shorter T_e), when the thermodynamic limit is approached ($N \to \infty$). There seems even the possibility of the existence of a third time scale. Another very thorough theoretical study on the anomalous dynamics of one-dimensional Hamiltonian systems was reported by H. van Beijeren. Exploiting the analogy of these systems with the Kardar-Parisi-Zhang equation and the exact solutions of the polynuclear growth model by Prähofer and Spohn, the application of mode-coupling theory provides exact expressions for the long-time behavior of heat diffusion and sound attenuation as a function of system size L. Some of the results carry over also to exactly solvable models such as harmonic chains and Toda chains. A. Politi studied heat conduction in another one-dimensional system consisting of pairs of point particles. Whenever point particles hit each other, or when the particles of a pair reach a maximum separation, an elastic collision occurs. Although the model is not chaotic, its behavior is very similar to that of chaotic nonlinear systems. The role of the pressure on the scaling behavior of the heat conductivity was studied by compute simulation. In the zero-pressure limit sub- and superdiffusive features are found [14].

Rheological problems constituted another topic of widespread interest. K. Travis modeled the fragmentation of two-dimensional liquid droplets and studied the fragment size

distribution and other cluster properties. S. Hess reported on computer simulations of a system of stretchable dumbbell molecule subjected to shear flow and a Gaussian computer thermostat supplemented by a twirler [15]. With such a simplified model many features of much more complicated systems may be studied such as the relation between the angular velocity and the shape of a chain molecule or of a polymer molecule in melts or polymer solutions, a problem of great significance for industrial applications [16]. In another talk by P.T. Cummings simulation results for nanoconfined fluids and nonostructured materials were provided. The aim of this study is to understand experimental data of the viscosity and of phase transitions of real nanoconfined fluids. Furthermore, friction in oscillating multi-wall carbon nanotubes, and the structure, dynamics and electron transport in gold nanowires were studied.

The application of dynamical system theory, and the computation of Lyapunov spectra and covariant Lyapunov vectors in particular, were the topic of a number of talks and posters. Taking a quasi-one-dimensional system of hard disks as example, G. Morriss introduced a modified Gram-Schmidt procedure, based on the required orthonormality of the perturbation vectors with respect to the null space in tangent space, to generate the Lyapunov modes. The null space is a consequence of the intrinsic continuous symmetries such as invariance of the Lagrangian with respect to time and/or space translations. From the orthogonality between conjugate modes also the Lyapunov exponents for this pair of modes may be determined. From a field theory for large systems also the propagation speed of the modes may be predicted with reasonable accuracy. H. Bosetti compared the properties of covariant and Gram-Schmidt vectors for planar systems of smooth and hard disks [18]. Surprisingly, it was shown that rough hard disks, which conserve the total energy but allow an exchange of energy between translational and rotational degrees of freedom, are not symplectic. Furthermore, the set of covariant Lyapunov vectors were shown to be unique in the following sense: once obtained for a particular frame of reference, it may be easily converted to another representation, say from Cartesian coordinates to polar coordinates [19]. They are time-reversal invariant and have a well-defined physical meaning, which is not the case for the Gram-Schmidt vectors. Finally, G. Radons applied the covariant Lyapunov vectors to the study of prototypical systems of spatiotemporal chaos such as Coupled Map Lattices, the Kuramoto-Sivashinsky and the Complex Ginzburg-Landau equations [20]. It is shown that the tangent space may be split into two hyperbolically decoupled subspaces. Only one of these subspaces, which is spanned by a finite number of entangled modes, carry the relevant physical information for the trajectory, whereas the other subspace contains trivial spurious modes, which decay quickly.

L. Conti reported about the first (and so far unique) verification of a fluctuation relation in an experiment concerning a macroscopic object: a resonant bar, which weighs two tons and which is kept at liquid helium temperature and acted upon by a feedback mechanism. This device acts as a gravitational wave detector. Nicola Pugno reported on one intriguing application of molecular dynamics, to understand adhesion, in particular of biological nature. Andrea Puglisi talked about experiments and theory of fluctuations concerning granular matter.

This short description of some of the activities at the conference in Obergurgl is by no means complete. There were numerous interesting talks throwing light onto various other aspects of nonequilibrium systems, but there is not enough room here to give due credit to all this work. But the examples should already convey the feeling of the participants that the conference succeeded to provide a most valuable survey of the current activities in this field by many leading groups from all over the world.

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3) Outlook

The conference brought together a significant fraction of the leaders in the field of nonequilibrium physics and quite a number of students and, most signifcantly, of young researchers who are entering the field or have recently begun their activity. The selection of talks and the personal exchanges thus allowed very fruitful osmosis among the previous generation and the coming one. This way, the experience accumulated in the study of macroscopic systems from an atomistic perspective has now been handed over to the new generation, which is mostly interested in nanoscale and anomalous nonequilbrium phenomena, thus taking the tradition of nonequilibrium physics towards new frontiers.

Program

Monday, August 29, 2011

09:00 - 09:10 **Opening**

09:10 - 09:35 **Edie Sevick** (The Australian National University, Canberra, Australia)
Interpreting force spectroscopy of soft matter using dynamic umbrella sampling

09:35 - 10:00 **Sergio Ciliberto** (Ecole Normale Supérieure de Lyon and CNRS, France)
Heat fluctuations in and out of equilibrium bath

10:00 - 10:25 **Udo Seifert** (University of Stuttgart, Germany)
Stochastic thermodynamics of nonequilibrium steady states

10:25 - 10:50 Coffee break

10:50 - 11:15 **Paddy Royall** (University of Bristol, UK)
The nature of the glass and gel transitions: structural and dynamic insights from colloids

11:15 - 11:40 **Roberto Livi** (University of Florence, Italy)
Negative temperature states in the discrete nonlinear Schrödinger equation

11:40 - 12:05 **Matthew Dobson** (Ecole des Ponts, Paris Tech, France)
A Langevin dynamics for systems immersed in a linear nonequilibrium flow

12:05 - 12:30 **Matteo Colangeli** (Politecnico di Torino, Italy)
Projection operator methods in nonequilibrium response theory

Lunch break

14:30 - 14:55 **Stephen Williams** (The Australian National University, Canberra, Australia)
Quasi-equilibrium and the emergence of solid behaviour in amorphous materials

14:55 - 15:20 **James Reid** (Griffith University, Brisbane, Australia)
An optically trapped particle and the fluctuation relations: applying two decades of developments to one simple system

15:20 - 15:45 **Ian Snook** (RMIT University, Melbourne, Australia)
The formation and annihilation of solitons and standing strainwave superstructures in a two-dimensional colloidal crystal: a new non-equilibrium state?

15:45 - 16:10 **Gary Morriss** (University of New South Wales, Sydney, Australia)
Lyapunov exponents and modes for a quasi-onedimensional system

16:10 - 16:35 Coffee break

16:35 - 17:00 **Hadrien Bosetti** (University of Vienna, Austria)
Local covariant Lyapunov exponents and vectors for particle systems

17:00 - 17:25 **Farinaz Roshani** (Alzahra University, Iran)
Directed diffusion in complex social networks

17:25 - 17:50 **Helmuth Hüffel** (University of Vienna, Austria)
Swarms with canonical active Brownian motion

Dinner

Tuesday, August 30, 2011

09:00 - 09:25 **Giancarlo Benettin** (Universitá di Padova, Italy)
The process of approach to equilibrium in the Fermi-Pasta-Ulam problem

09:25 - 09:50 **Henk van Beijeren** (Utrecht University, The Netherlands)
The anomalous dynamics of one-dimensional Hamiltonian systems

09:50 - 10:15 **Jean-Pierre Eckmann** (University of Geneva, Switzerland)
Rattling and freezing in a 1-D transport model

10:15 - 10:40 Coffee break

10:40 - 11:05 **Herbert Spohn** (TU München, Germany)
The motion of 1-D driven interfaces: exact solutions of the KPZ equation

11:05 - 11:30 **Carl Dettmann** (University of Bristol, UK)
Diffusion processes in molecular dynamics

11:30 - 11:55 **Jesper Hansen** (Roskilde University, Denmark)
Spin-coupling in nanofluidics

11:55 - 12:20 **Antonio Politi** (CNR Istituto dei Sistemi Complessi, Firenze, Italy)
Heat conduction in the hard point chain

Lunch break

15:00 - 15:25 **Jorge Kurchan** (École Supérieure de Physique et de Chimie Industrielles, Paris, France)
An infinite family of Second Law-like inequalities

15:25 - 15:50 **Michel Mareschal** (Universite Libre de Bruxelles, Belgium)
Going beyond Navier-Stokes to describe strong shock waves in fluids

15:50 - 16:15 **Hugo Touchette** (Queen Mary, University of London, UK)
Fluctuations of a Brownian particle with dry friction

16:15 - 16:40 Coffee break

16:40 - 17:05 **Bill van Megen** (RMIT University, Melbourne, Australia)
Scaling of the current time correlation function of fluids of hard sphere particles: exposing the difference between thermodynamic stability and metastability

17:05 - 17:30 **Sohail Murad** (University of Illinois at Chicago, USA)
The role of external electric fields in enhancing ion mobility, drift velocity and drift-diffusion rates in aqueous electrolyte solutions

Dinner

20:30 - 21:30 **Poster session**

Wednesday, August 31, 2011

09:00 - 09:25 **Giovanni Ciccotti** (Università di Roma "La Sapienza", Italy)
Time-dependent non-equilibrium molecular dynamics

09:25 - 09:50 **Billy Todd** (Swinburne University of Technology, Hawthorn, AU)
Accurate prediction of fluid slip

09:50 - 10:15 **Sten Sarman** (Stockholm University, Sweden)
Nonequilibrium phenomena in liquid crystals

10:15 - 10:40 Coffee break

10:40 - 11:05 **Andrea Puglisi** (Università di Roma "La Sapienza", Italy)
Non-equilibrium statistical mechanics of granular fluids: from experiment to theory

11:05 - 11:30 **Maxim Belushkin** (Ecole Polytechnique Fédérale de Lausanne)
Influence of hydrodynamics on the fluctuation theorem

11:30 - 11:55 **Stefano Bernardi** (Griffith University, Brisbane, Australia)
Lyapunov exponents in highly confined fluids

11:55 - 12:20 **Nicola Pugno** (Politecnico di Torino, Italy)
Simultaneous material and structural optimization in the spider web attachment disk

Lunch break

17:30 - 18:30 **Reception at the Hohe Mut Alm**

18:30 - 22:00 **Conference Dinner hosted by ANU**

Thursday, September 1, 2011

09:00 - 09:30 **Rainer Klages** (Queen Mary, University of London, UK)
Fluctuation relations for anomalous dynamics

09:30 - 10:00 **Siegfried Hess** (TU Berlin, Germany)
Rotating molecules and polymers subjected to a shear flow, thermostats and twirler

10:00 - 10:30 **Gunter Schuetz** (Forschungszentrum Jülich, Germany)
Space-time correlations in the ASEP conditioned on carrying a large flux

10:30 - 11:00 Coffee break

11:00 - 11:30 **Antoine Gerschenfeld** (Ecole Normale Supérieure, Paris, France)
Current fluctuations at a phase transition

11:30 - 12:00 **Peter T. Cummings** (Vanderbilt Univ. and Oak Ridge National Laboratory)
Non-equilibrium and equilibrium molecular dynamics of nanoconfined fluids and nanostructured materials

12:00 - 12:30 **Owen Jepps** (Griffith University, Brisbane, Australia)
Deterministic thermostats, theories of nonequilibrium systems, and parallels with the ergodic condition

Lunch break

14:30 - 15:00 **Michael Wilkinson** (Open University, Milton Keynes, UK)
Test-tube model for rain

15:00 - 15:30 **Guenter Radons** (TU Chemnitz, Germany)
Hyperbolicity and effective degrees of freedom of extended dynamical systems

15:30 - 16:00 **Jürgen Vollmer** (MPI for Dynamics and Selforganization, Göttingen, Germany)
Notions of entropy and entropy production in non-equilibrium systems

16:00 - 16:30 Coffee break

16:30 - 17:00 **Michael Allen** (University of Warwick, UK)
Polymer folding kinetics

17:00 - 17:30 **Peter Daivis** (RMIT University, Melbourne, Australia)
Non-equilibrium molecular dynamics study of permeation through a polymer membrane

Dinner

Friday, September 2, 2011

09:00 - 09:25 **Karl Travis** (University of Sheffield, UK)
Fragmentation of liquid droplets

09:25 - 09:50 **Livia Conti** (Istituto Nationale di Fisica Nucleare, Padova, Italy)
Nonequilibrium issues in macroscopic experiments

09:50 - 10:05 **Paolo De Gregorio** (Politecnico di Torino, Italy)
Modelling nonequilibrium macroscopic oscillators of interest to experimentalists

10:05 - 10:20 **Zhanchun Tu** (Beijing Normal University, China)
Efficiency at maximum power of Feynman's ratchet as a heat engine

10:20 - 11:00 Coffee break

11:00 - 12:00 **Denis Evans** (The Australian National University, Canberra, Australia)
Dissipation and the foundations of classical statistical mechanics

12:00 - 12:15 **Concluding remarks**

Lunch and end of the conference

13:30 Bus departure to Innsbruck Airport and Main Station.

Poster Session

Tuesday, August 30, 2011, at 20:30

1. **Bernhard Altaner** (MPI for Dynamics and Self-Organization, Göttingen)
   A new paradigm for (steady-state) coarse graining of stochastic dynamics

2. **Michele Bonaldi, Paolo De Gregorio, Lamberto Rondoni, Livia Conti**
   (Institute of Materials for Electronics and Magnetism,Trento, Italy)
   Thermodynamic fluctuations in actively cooled resonators

3. **Hadrien Bosetti and Harald A. Posch**
   (Faculty of Physics, University of Vienna, Austria)
   Lyapunov instability of rough hard disks

4. **James Miller** (University of Sheffield, UK)
   Modeling non-equilibrium properties in nuclear waste vitrification

5. **Daniel Truant** (The University of New South Wales, Sydney, Australia)
   The evolution of covariant Lyapunov modes

6. **Jeroen Wouters** (University of Reading, UK)
   Relevance of sampling schemes in light of Ruelle's linear response theory

Financial Report

Financial report on the conference

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1) General remarks

1. The participants payed for their rooms, which included breakfast and dinner (half pension). However, the price of the room was subsidized by the organizers to the amount of €10.00 per person per night (which amounts to a reduction of about 15 % on average). This amount was automatically subtracted from the bill, which the participants paid to the University Center. The latter was compensated by the organizing committee.

2. No travel support was given to the participants.

3. Free lunch at the University Center was provided to the participants. Furthermore, the costs for two coffee and refreshment breaks per day and the rent of the lecture facilities, as well as badges and books of abstracts were covered by the organizing committee. There was no conference fee.

4. The grant from the European Science Foundation (ESF) requires that the money should be spent predominantly for scientists from EU countries. This grant (€10.000) constituted 67 % of the conference budget. The percentage of participants from EU institutions amounted to 71 %. Since these numbers are almost identical, no difference was made between EU and non-EU participants.

5. The Australian National University provided a grant of 10,000 Australian Dollars, corresponding to €7,518.80, to cover the costs of a special dinner for all participants of the conference to celebrate the 60th birthday of Professor Denis J. Evans. Only a small amount of €347,50, by which the costs for the dinner exceeded the grant from ANU, was added to the expenses of the conference.

2) Income

1)	Grant from Griffith University, Brisbane, Australia	€	2,000.00
2)	Grant from the Poitecnico di Torino, Torino, Italy	€	1,000.00
3)	Grant from the University of Vienna, Austria (to be used for bus transfer, the book of abstracts and for badges)	€	1,449.00
4)	Grant from ESF: Total grant: €10,000. 80% of this money was transferred to the conference account at the University of Vienna. The rest is available after approval of the final report by the ESF.	€	8,000.00
5)	Grant from ANU dedicated for the Conference Dinner to celebrate the 60th birthday of Professor Denis J. Evans	€	7,518.80
	Total income at the time of the conference	€	19,967.80

3) Expenses

1)	Preparation of the conference, visit of H.A. Posch to the University Centre in Obergurgl	€	153.16
2)	Badges, Invoice from Univ. of Vienna, 10/08/2011	€	144.00
3)	Book of abstracts, costs for copying, Univ. of Vienna	€	505.00
4)	Book of abstracts, binding, Invoice by Mr. Litschauer, 11/08/2011	€	50.00
5)	Bus transfer by Fa. Tipotsch, Invoice, 15/09/2011	€	800,00
6)	University Center Obergurgl, deposit, December 2010	€	3,000.00
7)	University Center Obergurgl, rest payment, Invoice 17/09/2011	€	7,242.00
8)	Liftgesellschaft Obergurgl, Hohe Mut-Alm, deposit for Conference Dinner (fully covered by dedicated grant of ANU)	€	1,500.00
9)	Liftgesellschaft Obergurgl, Hohe Mut-Alm, Invoice # 40 and 42, 31/08/2011 Conference Dinner (fully covered by dedicated grant of ANU)	€	6.018,80
10)	Liftgesellschaft Obergurgl, Hohe Mut-Alm, Invoice # 41, 31/08/2011, Rest payment for Conference Dinner	€	347.50
	Total Expenses	€	19,760.46

Since the funds provided by the five institutions listed above exceed the total expenses for the conference by €207.34, the remaining 20 % from the grant of the European Science Foundation are not required.

It is suggested to give the surplus of €207.34 to the Faculty of Physics of the University of Vienna as a compensation for other hidden expenses in connection with the conference.