Conference Report IV

# International Workshop on Nonequilibrium Thermodynamics (IWNET 2012) and 3rd Lars Onsager Symposium

Røros, Norway
August 19 – 24 , 2012

The Sixth International Workshop on Nonequilibrium Thermodynamics (IWNET 2012) took place together with the Third Lars Onsager Symposium (held approximately every 10 years since 1993) in Røros, Norway, from August 19th to 24th. The meeting was jointly organized by Signe Kjelstrup (Chairperson), Dick Bedeaux, Kirill Glavatskiy of the Non-equilibrium Thermodynamics Group in the Chemistry Department at the Norwegian University of Science and Technology (NTNU) in Trondheim (Norway), Alex Hansen of the Physics Department at NTNU, and by Martin Kröger from the Polymer Physics Group of the Materials Department at the Swiss Federal Institute of Technology, ETH Zurich (Switzerland). It was sponsored by the European Science Foundation (ESF-EPDS), the Gas-Technology Centre of NTNU/SINTEF and by the Norwegian Research Council (NFR). The workshop was addressed to both young and experienced researchers working in the general field of Nonequilibrium Thermodynamics, and organized into the following 12 sessions: nonequilibrium fluctuations, general theory, GENERIC framework, self-assembly, biological systems, measurements, porous media, nonlinear reactions, nanotransport, molecular simulations, interfaces and fluid flow.

The aim of the workshop was indeed to bring together and unify a variety of disparate approaches to Nonequilibrium Thermodynamics,

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ranging from classical nonequilibrium thermodynamics with internal variables and Lagrangian methods, to bracket, variational and GENERIC formulations, with the goal of achieving a common framework that can be disseminated to a broader audience, and suited for different applications in a variety of contexts, including mesoscopic and confined systems, granular matter, porous materials, interfacial phenomena and surfaces, and biological systems.

Around 60 participants attended the five days of workshops, which were held in the Røros Hotel. On Sunday 18th (arrival and registration day), a welcome party opened the meeting so that introductory discussions could take place in a casual atmosphere. On the next day, after some welcoming remarks, Signe Kjelstrup introduced series of talks devoted to the study of out of equilibrium fluctuations: the lecture by Jan Sengers presented fluctuations in fluids in the presence of a temperature gradient, and was followed by a study of hydrodynamic fluctuations for the laminar flow by José Ortiz de Zárate and a talk on wormlike micellar systems by Antony Beris. The next session, chaired by Dick Bedeaux, was more general in character, going from theoretical achievements through lattice gas-fluid isomorphism (Vladimir Kulinskii) to advanced simulation techniques for turbulent flows (Ilya Karlin) and rare events (Titus van Erp). A discussion session was then led by Signe Kjelstrup on various organization issues and the possible publication of the workshop proceedings. The afternoon session was then initially dedicated to a first poster session (the second would come the day after), and further talks. In particular, Hans Christian Öttinger chaired a talk by Bruce Turkington that rigorously justified the GENERIC formalism under a variational perspective, and a subsequent one by Markus Hütter concerning the relationship between different formulations of the force-flux relationships. José Ortiz de Zárate chaired the final talks of the day on self-assembly (a thermodynamical perspective by Ger Koper and a control-theoretical approach by Antonio Osorio).

On Tuesday Leonard Sagis chaired a session on biological systems, where transport in molecular fluids (Fernando Bresme) and temperature affinities of Calcium pumps (Anders Lervik and Signe Kjelstrup) were addressed, together with a model for the thermodynamics of biosystems' growth (Natalya Kizilova). Jürgen Keller then chaired a session for a general audience, concerning fundamental issues such as the third law of thermodynamics (Karl Heinz Hoffmann), and more applied issues like rapid solidification of undercooled melts (Sergey Serdyukov) and electrokinetic response of particles (Claire Chassagne). A tour of the city was then planned in the early afternoon, and lasted for a couple of hours. This was enough time to thoroughly inspect all the landmarks that Røros has to offer: the Church, the old mines (UNESCO World Heritage Site) museum and the only pub, which may offer the best opportunity to meet the city inhabitants (although you'll most likely end up meeting other conference participants). Back to the conference, Fernando Bresme chaired two talks about measurements in nonequilibrium situations with a wide range applications, from nanostructures (Antonio del Río) to gravitational waves detection (Livia Conti). To end the day, Natalia Kizilova chaired a session on steady-state flows in porous media, from both an experimental (Knut Måløy) and theoretical (Alex Hansen) perspective.

*Figure 1 (left):*
*The participants of the workshop, in front of the conference hotel.*

*Figure 2:*
*A view of the traditional village of Røros in Norway, where the workshop took place.*





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On Wednesday Antony Beris chaired more theoretical talks on stochastic processes for open chemical systems (Hong Qian) and new approaches to study nonequilibrium steady states in open driven systems (Hao Ge), as well as a work on fluctuations with an extension of the mass-action-law dynamics by Miroslav Grmela. The latter speaker then chaired the following session on nanotransport, again from a theoretical perspective: a modification of Fourier law for non-vanishing collision times and mean-free paths (David Jou), followed by a new general perspective on nonequilibrium thermodynamics for quantum systems (Hans Christian Öttinger) with applications to open quantum systems coupled to time-evolving environements (Maksym Osmanov). Presentations on nonlinear reactions far from equilibrium (Miguel Rubi) and within transport-related issues for chemical reactions (Igniacio Paganobarraga) were chaired by Jan Sengers. Titus van Erp then introduced two studies on molecular simulations for Fick diffusion coefficients (Dick Bedeaux) and heat conductivity for zeolite systems (Sondre Schnell).

On Thursday morning, Markus Hütter introduced a session on interfaces, where Leonard Sagis compared two theoretical approaches to fluid-fluid interface and the surface stress tensor, Henning Struchtrup addressed distillation with respect to vapor layer thickness, and Marco Schweizer studied a new gauge theoretical approach to interfaces' local equilibrium. Karl Heinz Hoffmann finally chaired a session on fluid flow: coupling chemical kinetics with mechanics under thermodynamical constraints (Vaclav Klika), a vortex tube effect (Jürgen Keller) and convective phenomena for non-uniformly heated mixtures (Vitali Demin). The afternoon was dedicated to an interesting outdoor group activity: canoeing on the Glomma, the longest river of Norway (only a small portion of it was actually canoed). Although the trip was relaxing for most, it ended up being a perilous battleship game for some of the conference participants.

The last conference day was also dedicated to interfaces, where Henning Struchtrup chaired studies of liquid-vapor interface transfer coefficients (Jean-Marc Simon), heat and mass transfer in crystallization (Marcos Rodriguez), and entropy production in heat conducting thin films (Federico Vázquez). Chaired by Alex Hansen, the final session before the end of the workshop was concerned with the general theory, where Raul Salgado-García addressed the resonant response for nonequilibrium steady states, Bordan Maruszewski presented a constitutive theory in nonlinear thermoelastic isotropic solids, and Sylvain Bréchet studied the temperature and chemical potential as a function of permanent material polarization and magnetization. A final discussion was devoted to the format and the organization of the next workshop in 2015, which will most likely be held in the Netherlands.

Aside from the numerous scheduled communications, almost an hour was dedicated each day to discussions, introduced by an expert in the field, on different subjects under the common denominator of nonequilibrium thermodynamics: the aim was to establish a general state of the art of a given field, to try to critically consider the current limitations, and to outline new possible trends and directions. In this spirit, Natalia Kizilova and Ignacio Pagonabarraga led on Tuesday a discussion on biological applications and challenges for nonequilibrium thermodynamics in such complex and many variable systems; on Wednesday, Karl Heinz Hoffmann asked several questions about the role of control theory and optimization in nonequilibrium thermodynamics; Hans Christian Öttinger led a discussion on Thursday about the importance of establishing solid foundations for nonequilibrium thermodynamics, together with a common accepted language; he then addressed the concept of local equilibrium for the thermodynamics of mesoscopic and nanostructured systems.

In summary the conference spanned a wide range of subjects, and it was a very attractive occasion for researchers in the field to learn how out-of equilibrium thermodynamics is viewed, interpreted and exploited by different communities, in various contexts. However we still feel that the true goal of unifying different perspectives under a common framework has only been partially achieved, and more effort has yet to be made in such direction.

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