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Journal of Non-Newtonian Fluid Mechanics

Workshop Report

Report on the workshop on rheology and thermodynamics École Polytechnique of Montreal August 14–16, 1996

1. Introduction

Substantial interest has been developed over the past few years on the influence of thermodynamics on rheology as documented by several articles (e.g. A.I. Leonov, Rheol. Acta 15, 85 (1976), 21, 683 (1982); M. Grmela, Physica D, 21, 179 (1986), Phys. Letters A, 130, 81 (1988) Phys. Rev. E, 47, 351 (1993); G.A. Maugin and R. Drouot, Int. J. Eng. Sci. 21, 705 (1983)), review articles (e.g. M. Grmela in 'Rheological Modelling: Thermodynamical and Statistical Approaches', Lecture Notes in Physics edited by J. Casas-Vazquez and D. Jou, Vol. 381, 99 (1991); R.J.J. Jongschaap, Rep. Progr. Phys. 53, 1 (1990)) and books (e.g. A.N. Beris and B.J. Edwards, 'Thermodynamics of Flowing Systems', Oxford (1994); D. Jou, J. Casas-Vazquez and G. Lebon, 'Extended Irreversible Thermodynamics', Springer (1993), I. Müller and T. Ruggeri, 'Extended Thermodynamics', Springer (1993); B.C. Eu, Kinetic Theory and Irreversible Thermodynamics', Wiley (1992); S. Sieniutycz, 'Conservation Laws in Variational Thermodynamics', Kluwer (1994)) that have appeared on this and closely related subjects. This influence becomes more important when multiple transport phenomena need to be considered together, especially in the presence of temperature variations. However, so far, no significant effort has been developed to reconcile the various approaches that have, more or less independently, been developed to obtain the governing equations. With the opportunity of the recent international congress of rheology which attracted several of the key investigators into the Quebec region, I undertook the initiative and organized an informal workshop on Rheology and Thermodynamics in the École Polytechnique of Montreal which took place between August 14 and 16, 1996. Scope of the workshop has been to address the interrelationship of the various approaches, to identify recent successes in applications and outline the challenges and opportunities of the future. About 20 scientists together with graduate students from the École Polytechnique and McGill University participated (see the list of participants below).

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2. Topics of discussion

A rheological model is said to be compatible with thermodynamics if predictions based on the model agree with results of the observations constituting the basis of equilibrium thermodynamics. The question arises as to what are the features of the governing equations of the rheological models that guarantee their compatibility with thermodynamics. This question, often in a somewhat different context, has been studied, amongst others, by Clausius (Clausius inequality), Boltzmann (Boltzmann's H-theorem), Onsager and Casimir (Onsager-Casimir reciprocity relations), in linear irreversible thermodynamics, rational thermodynamics and extended irreversible thermodynamics. Recently, it has been argued that an analysis of the compatibility of rheological models with thermodynamics (in the form of the so called Poisson bracket formulations or the Matrix Model) provide a general structure that can serve as a pivotal point, about which the translation of a physical insight into the governing equations is organized.

The first day of the workshop was devoted to discussing recent advances in nonequilibrium thermodynamics (in particular, recent formulations of the Clausius inequality, extended irreversible thermodynamics, internal-state-variable thermodynamics, Lagrangian formulations). The role of the compatibility with thermodynamics in rheological modeling was the subject of discussions in the second day (in particular, the Hamiltonian—Poisson Bracket—dissipation bracket formulations and the Matrix Model). Connections with molecular simulations and numerical rheology were explored in the third day.

3. Conclusions from discussions

The compatibility of dynamics with thermodynamics is one of the fundamental problems of nonequilibrium statistical mechanics. Closely related to this problem are the problems of the emergence of irreversibility, pattern formation, and of other new features in macroscopic dynamics. At present, there still exists a wide range of views and approaches to these problems. Relations among some of them are known; in the most part, however, their relation remain unclear. The diversity of views was reflected in discussions at the Workshop. All participants agreed however that discussions at the Workshop and, in particular, discussions of the fundamental problems of nonequilibrium statistical mechanics in the context of more specific problems arising in rheology are very useful for both fundamental understanding and rheology. In particular, thermodynamic considerations become essential when non-isothermal effects are taken into account.

It has to emphasized that in rheology, a new rheological model arises as a result of expressing a new physical insight into macromolecular dynamics in mathematical form. The objective of the compatibility-with-thermodynamics analysis is to provide a general setting for expressing a given physical insight in intrinsically consistent governing equations. The compatibility-with-thermodynamics analysis does not replace the search for new physical insights but is complementary to it. It provides a guidance to the appropriate projections from microscopic to macroscopic levels of description as well as placing constraints on the type and form of dissipative processes, where most of the phenomenology is introduced. A similar situation arises in thermodynamics. In order to introduce a new thermodynamic equation of state, a physical insight into the specific nature of the system under consideration is needed. The insight has to be then expressed in an intrinsically consistent way. Here, general thermodynamics provides the setting. The compatibility-with-thermodynamics analysis plays thus the same role in dynamical theories as general thermodynamics plays in static (equilibrium) theories.

After the Workshop, the majority of the participants continued to discuss rheology and thermodynamics in the context of the Symposium on Thermodynamic Approaches to Rheological Modeling and Simulation that took place as a part of the XIIth International Congress on Rheology (Quebec City, August 18–23). I would like to believe that the new contacts between researches in thermodynamics and rheology that were created on the Workshop and on the Symposium will lead to the advancement of our knowledge and will give rise to Workshops on the same subject in the future.

4. Acknowledgments

I would like to express my gratitude to the Research Office, Department of Chemical Engineering and Polymer Institute (CRASP) of École Polytechnique of Montreal for providing financial support for the workshop.

5. Participants

A.N. Beris (Univ. of Delaware), P.J. Carreau (École Polytechnique de Montréal), J. Casas-Vazquez (Univ. Autonoma de Barcelona), C. Chan Man Fong (Univ. of Sherbrooke), B.Z. Dlugogorski (Univ. of Newcastle), R. Drouot (Univ. Pierre et Marie-Curie, Paris VI), B.J. Edwards (Univ. of Delaware), B.C. Eu (McGill Univ.), L.S. Garcia-Colin (Univ. Autonoma, Mexico), M. Grmela (École Polytechnique de Montréal), R.J.J. Jongschaap (Univ. of Twente, The Netherlands), D. Jou (Univ. Autonoma de Barcelona), H.C. Ottinger (ETH-Zürich), N. Phan-Thien (Univ. of Sydney), A. Rey (McGill Univ.), S. Sieniutycz (Warsaw Tech. Univ.), graduate students from École Polytechnique of Montreal and McGill Univ.

Miroslav Grmela, École Polytechnique of Montreal

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Editorial

Nonequilibrium thermodynamics and complex fluids

The application of thermodynamics to complex fluids, like polymeric liquids, dispersions, emulsions, etc. is by no means obvious. In fact, there is an overwhelming number of theories and a wide variety of approaches: classical nonequilibrium thermodynamics with internal variables, bracket formulations, continuum or rational thermodynamics, variational formulations, extended irreversible thermodynamics, the matrix model, network thermodynamics, and the general equation for the nonequilibrium reversible–irreversible coupling (GENERIC) formalism. In order to bring together and unify this variety of approaches and to achieve a common framework, suited for applications, a first international workshop was organized in 1996 in Montreal to discuss this matter (see workshop report by M. Grmela [1]). The common opinion was that it should be possible now to combine the various approaches in some kind of common generalized theory. The final goal is to bring nonequilibrium thermodynamics to the same level of clarity and usefulness as equilibrium thermodynamics. In order to achieve this, a second international workshop was organized in Oxford in August 2000.

In view of the promising recent developments in the field of nonequilibrium thermodynamics, a special issue of the *Journal of Non-Newtonian Fluid Mechanics* devoted to this subject was initiated. It is our pleasure, as guest editors of this special issue, to present the result of this initiative. Our intention was to offer a rather complete overview of the current status of the most important approaches to nonequilibrium thermodynamics and some relevant applications and special topics. We asked a number of prominent scientists to write either reviews or more specialized papers. We are glad that many of the requests were honored with valuable contributions, and our impression is that this special issue provides a well balanced introduction and overview of the current status of the various approaches to nonequilibrium thermodynamics in general and its application to complex fluids in particular.

The common root of all approaches to nonequilibrium thermodynamics (with Rational Thermodynamics as a notable exception) is classical *Equilibrium Thermodynamics*. A brief outline of the fundamentals of this subject, following the well-known textbook of Callen [2], is presented in the introductory paper by Jongschaap and Öttinger.

Classical Nonequilibrium Thermodynamics, as described, for instance, in the famous textbook by de Groot and Mazur [3] is still an important starting point for many applications to systems which are in some sense close to equilibrium. The concept of internal variables of state is often crucial in applications. In the paper by Lhuillier an application of this method to colloidal suspensions is described and a link to the two-fluid model of suspensions and the description of molecular mixtures is provided. An application

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with a diffusive internal variable of state is described in the paper by Drout and Maugin. Also based upon classical nonequilibrium thermodynamics is the paper by Rey on liquid crystal interfaces in which special variables, describing the interfacial dynamics, are discussed in some detail. The so-called *Matrix Model* for driven systems described in the paper by Jongschaap is essentially an extension of Classical Nonequilibrium Thermodynamics with a careful analysis of the role of internal and external variables. The paper gives a review of this method and its relation with other approaches, including control system theory.

The so-called **Extended Irreversible Thermodynamics** (EIT) is an extension of classical nonequilibrium thermodynamics in which the entropy may depend on the dissipative fluxes in addition to the classical hydrodynamic variables. A review of this method is provided in the paper by Jou and Casas-Vázquez. In this paper, EIT is compared to theories with internal variables, the GENERIC approach and the Matrix Model. In the paper by Depireux and Lebon, the problem of non-Fickian thermodynamics in a two component mixture is studied in the framework of EIT.

An important branch of nonequilibrium thermodynamics are methods based upon a *Bracket Formulation* of the underlying convective and dissipative equations. After presenting the basic idea of this method at a conference in Boulder, Colorado in the summer of 1983, M. Grmela explored and developed this field in great depth in many publications, starting with the paper [4]. A review of bracket formulations of nonequilibrium thermodynamics, including also the more recent double-generator formulation, known as GENERIC is provided in the paper by Beris. An atomistic approach to GENERIC, with a statistic mechanical formulation of the basic building blocks of GENERIC, is given in the paper by de Pablo and Öttinger, while Edwards and Dressler describe an application to nonequilibrium molecular dynamics, with emphasis on closure approximations. A further nice example of an application is provided by the paper of Wagner in which the Smoluchowski equation for colloidal suspensions is developed and analyzed through the GENERIC formalism.

Two papers of a fundamental nature are the contribution by Gorban et al., with a thorough discussion of the role of quasi-equilibrium states, and the contribution by Grmela in which a unifying framework for the treatment of externally driven systems in the context of multi-level realizations is presented.

The phenomenological *field* or *continuum formulations* of thermodynamics and the so-called *Rational Thermodynamics* are purely phenomenological. A review on this subject is provided in the paper by Muschick et al., and an extensive review on the inclusion of nonequilibrium thermodynamics into the framework of the Lagrangian formalism is given in the paper of Anthony. Finally, in the paper of Sieniutycz, the optimization of work in systems with complex fluids is discussed as an attempt to relate to the non-Newtonian fluids of particular interest to the readers of this journal.

The combined Workshop and Summer School on Nonequilibrium Thermodynamics and Complex Fluids was arranged as a satellite meeting of the 13th International Congress on Rheology in Cambridge, co-ordinated with the European Society of Rheology as EURORHEO 2000-1, and held at Keble College in Oxford on 14–18 August 2000. The meeting was attended by 62 participants from 16 countries. Offprints of all the papers in the present issue were available for the participants during the meeting. In the *summer school* part of the meeting, the main topics in the field were presented in review papers. New developments were presented in the *workshop* part (several workshop contributions are not included in this special issue). In addition, there was a free forum for discussing future directions.

The recent efforts in nonequilibrium thermodynamics, as for example, presented at the workshops in Montreal and Oxford, are strongly dominated by theoretical developments. For establishing the usefulness of the thermodynamic approach to a wider audience, and for distinguishing between different formalisms, it will be crucial to have experimental results, for example, on the thermal properties and the phase behavior of complex fluids. One of the issues of discussion in the Oxford meeting was the choice of variables in the various approaches. For future success in application to complex fluids, a flexible choice of structural variables is needed. On the one hand, the bracket formulations, including GENERIC, provide a very general framework, and the selection of specific variables clearly requires physical insight into the system of interest, whereas, on the other hand, EIT uses a very restricted set of variables, which seems to be too limited for general application to complex fluids. Another important issue is the inclusion of different levels of description including the atomistic approach. The key to successful future applications, of practical relevance, lies in the inclusion of these levels. This provides a sound foundation of the theories and in addition a connection with existing molecular models of particular systems.

Our impression, at the end of the workshop and concluding the editing of this special issue, is that a significant step forward in the direction of our final goal of unification has been made: a generally accepted consistent formulation of nonequilibrium thermodynamics seems to be emerging. The active researchers in the field become familiar with the different approaches and are seeking integration and combination of their efforts. A full unification in one single framework might not be attainable, and this is probably not even needed. As for instance in classical mechanics, where besides the common Newtonian dynamics also the Hamilton and Lagrangian formulations are available and each of them has specific advantages and disadvantages in particular cases, also in thermodynamics various approaches will remain. We anticipate that there will always be more restrictive formulations for isolated systems and more tractable formulations for driven systems. Most important, however, is that the validity of each of the methods and their interrelations should be investigated thoroughly. The final set of formulations should provide a useful tool for many applications, including the exciting area of complex fluids. Although, this goal has not yet been fully reached, we are glad to see at the workshops in Montreal (1996) and Oxford (2000) that many people are working very hard to approach it, and we hope that the present issue of the *Journal of Non-Newtonian Fluid Mechanics* will also contribute to this effort.

R.J.J. Jongschaap
H.C. Öttinger

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Editorial

Nonequilibrium thermodynamics and complex fluids☆

The application of thermodynamic information to dynamical problems in physics has a history of exactly one and a half centuries, dating back to Lord Kelvin's examination of the thermo-electric effect in 1854 [1]. In the ensuing 100 years, *Equilibrium Thermodynamics* arose as one of the most successful theories of physics, and *Linear Irreversible Thermodynamics* (LIT) came to embody the idea of extending thermodynamic knowledge to nonequilibrium systems. This extension to nonequilibrium systems generated two Nobel Prizes, one to Onsager in 1968 and one to Prigogine in 1977. By 1962, it had culminated in what many believe to be the seminal text in the field, *Nonequilibrium Thermodynamics* by de Groot and Mazur [1]. Yet, this extension to nonequilibrium systems did not enjoy the success, rigor, or utility of Equilibrium Thermodynamics. The shortcomings of LIT were evident to many scientists and engineers; unfortunately, some still hold these negative (and now erroneous) views of nonequilibrium thermodynamics to this very day.

In the 50 years just passed, much effort has been devoted by a relatively small number of researchers to establish nonequilibrium thermodynamics as a rigorous, robust, viable, and indispensable physical theory, on the par with equilibrium thermodynamics. In the early days of LIT, the theory was essentially applicable only to simple fluids; hence much of the criticism mentioned in the preceding paragraph. What use was LIT when the systems that it described could be more easily described well without it? Thus it was actually during the quest to extend this theory to complex fluids that the limitations of LIT were finally overcome: for complex materials with an inherently dynamical microstructure, raw engineering empiricism was not enough. Here, one must thoroughly understand the thermodynamics, equilibrium and non, of the physical process, hence providing a necessity for the physical theory of nonequilibrium thermodynamics that was not present for simple fluids.

Over the past four decades of the 20th century, various approaches for describing the nonequilibrium thermodynamics of complex fluids have been advanced. These include rational thermodynamics, thermodynamics with internal variables, extended irreversible thermodynamics, the matrix model, generalized brackets, and GENERIC. All of these have all been scrutinized, analyzed, re-analyzed, compared, run through a wringer, and hung out to dry.

The first two workshops of this series, held at École Polytechnique de Montreal in 1996 and at Oxford University in 2000, were focused on the analyses and comparisons described in the preceding paragraph. In the first workshop [2], the leading proponents of many different approaches to nonequilibrium thermodynamics met for the first time to discuss relationships between their theories. This was a huge first step in reconciling the disparate approaches to the subject. The principal outcome of this workshop was the agreement among the investigators in attendance that concrete analysis and comparison, presented in the literature, should be undertaken to establish a uniform and consistent hierarchy of methodologies and approaches to the subject.

By the time of the second workshop at Oxford in 2000 [3], much of this goal had been accomplished already. Many papers appeared during the interval in which the various approaches to nonequilibrium thermodynamics were analyzed in great depth and compared and contrasted with each other [4–13]. What emerged from the Oxford workshop was a feeling of appreciation and understanding of the various approaches to the subject. It was no longer a question of which approach was correct, or even best, but which one was appropriate to be used under a given circumstance. For instance, a valid question when formulating a dynamical problem would be: How could mathematical convenience be balanced with physical rigor? In other words, each approach has its advantages and drawbacks, so which was the most convenient to use could vary from one application to the next.

Having stated the above paragraph, one item of particular importance that emerged from the second workshop at Oxford was the notion that nonequilibrium thermodynamics is about more than irreversible phenomena; it also involves the time evolution of conservative phenomena, and that these must be included in contemporary dynamical theories of complex fluids. Again, for simple fluids, it was easy to separate reversible and irreversible phenomena since the conservative flow effects could always be described with well-known balance laws. But assuming that these balance laws applied directly to complex fluids, as done in rational thermodynamics, could potentially lead to erroneous evolution equations [4].

☆ A collection of papers presented at the 3rd International Workshop on Nonequilibrium Thermodynamics and Complex Fluids, Princeton, NJ, 14–17 August 2003.

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The 3rd International Workshop on Nonequilibrium Thermodynamics and Complex Fluids took place in Princeton, NJ, 14–17 August 2003. In attendance were over fifty scholars, representing a dozen nations. Forty-five presentations were delivered, with well over one hundred authors. Invited plenary and keynote lectures were given by prominent researchers in the allied areas of statistical mechanics and dynamics: Kurt Wissbrun expounded on flow-induced phase separation from an industrial perspective, Joel Lebowitz discussed the relationship between statistical mechanics and nonequilibrium thermodynamics, Yannis Kevrekidis described equation-free multiscale computations, and Arup Chakraborty related nonequilibrium thermodynamics applications to biology.

The inherent overall theme of the third workshop was decidedly different than that of its two predecessors: it shifted from focusing on the fundamental basis of nonequilibrium thermodynamics formalisms to using the same for specific applications. Most of the presentations and discussions were concerned with applying the new methodologies to difficult problems involved with modeling complex fluids; some of these applications are published here in this special issue of *JNNFM*. Those of us who were involved in the first two workshops find this trend very gratifying, and, indeed, somewhat vindicating of our efforts in organizing these workshops over the years.

At this time, we are now more optimistic than ever that the extension of thermodynamic information to dynamical phenomena is not only practical, but extremely useful as well. Were we to venture a guess as to the theme of the 4th International Workshop on Nonequilibrium Thermodynamics and Complex Fluids, to be held in Greece during 2006, it would be that formulations of nonequilibrium thermodynamics are used to develop new computational algorithms for simulating dynamical phenomena with multiple length and time scales.

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Preface

4th International Workshop on non-equilibrium thermodynamics and complex fluids

The application of thermodynamics under non-equilibrium conditions to complex fluids, like polymeric liquids, dispersions, emulsions, etc., is by no means obvious. In fact, in the literature there exists at present an overwhelming amount of theories and a wide variety of approaches: classical non-equilibrium thermodynamics with internal variables, Lagrangian methods, bracket formulations, continuum or rational thermodynamics, variational formulations, extended irreversible thermodynamics, the matrix model, network thermodynamics, and the GENERIC formalism.

To bring together and unify this variety of approaches and to achieve a common framework, suited for applications, a first workshop was organized in 1996 in Montreal to discuss this matter (*Workshop report by M. Grmela, JNNFM 69 (1997) 105–107*). The common opinion was that it should be possible to combine the various approaches in some kind of common generalized theory. In order to achieve this, a second and a third international workshop were held in 2000 in Oxford, and in 2003 at Princeton (*workshop report by A. Beris and B.J. Edwards, JNNFM 120 (2004) 1–2*).

To help in the direction of bringing non-equilibrium thermodynamics to the same level of clarity and usefulness as equilibrium thermodynamics, *the fourth international Workshop* took place in Rhodes, in 3–7 September 2006. The workshop, which was jointly organized by FORTH-ICE/HT, the University of Patras and the Hellenic Society of Rheology, highlighted the most recent advances in the field, in particular, new theoretical developments and state-of-the-art modeling/simulation techniques founded on or guided by principles of non-equilibrium thermodynamics. Its scientific program included 3 invited lectures (by Professors C. Austen Angell, Gregoire Nicolis and Akira Onuki), 44 oral presentations and 11 posters, covering a broad range of topics: non-equilibrium thermodynamics and statistical mechanics, approaches and formalisms of non-equilibrium thermodynamics, coarse-graining and mesoscopic dynamics, multi-scale modeling and molecular simulations, non-equilibrium molecular dynamics, and theories of complex fluid deformation, followed by applications to glasses, micelles, colloids, blends and interfaces. Emphasis was given to the description of phenomena related to structure/morphology development and relaxation or dynamics in complex materials subjected to a deformation history at various length and time scales within a non-equilibrium thermodynamics framework. Adhering to a fundamental and strict non-equilibrium thermodynamics framework in order to establish self-consistent links between the different levels (each level addressing phenomena over a specific window of length and time scales) is something that became absolutely transparent by the end of the Workshop.

This Special Issue of the *Journal of Non-Newtonian Fluid Mechanics (JNNFM)* presents extended versions of nineteen (19) papers that were presented in the Workshop. They cover a variety of themes such as formulations of non-equilibrium thermodynamics for open systems and superfluids, applications to elasticity and visco-plasticity, extensions to account for wall slip, also to understand droplet deformation, thixotropic behaviour and the dynamics of vesicle suspensions, fundamental thermodynamic relationships for shearing linear viscoelastic fluids, new multi-scale modelling demonstrations, mathematical strategies for error quantification and adaptivity in the coarse-graining of extensive systems, and mathematical approaches to dynamic scaling. The Organizing and Scientific Committees of the Workshop are grateful to Professor Gareth McKinley, Editor of JNNFM, for providing this opportunity.

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Editorial

The 5th International Workshop on Non-equilibrium Thermodynamics

The notion that thermodynamics plays an important role in rheology experienced a boost when M. Grmela had the vision to organize an informal workshop on this subject in Montreal in 1996. There he gathered specialists of both branches of knowledge to discuss possible connections and common areas of opportunity. The outcome of this workshop was subsequently reported in the Journal of Non-Newtonian Fluid Mechanics (JNNFM) [1]. Grmela's belief then that the new contacts between researchers in thermodynamics and rheology would lead to an advancement of our knowledge and to more workshops devoted to this matter has fortunately materialized.

The second workshop took place in Oxford in 2000 and the aim there was to provide a complete overview of the state of development of the most important theoretical approaches to non-equilibrium thermodynamics and of some of the relevant applications. The proceedings of this workshop appeared in a special issue of JNNFM in 2001 [2] and highlighted the idea that a generally accepted consistent formulation of non-equilibrium thermodynamics seemed to be emerging and that this might proof useful for applications, including the realm of complex fluids. This led to the third workshop in Princeton in 2003 in which the main emphasis was placed on the use of non-equilibrium thermodynamics for specific applications including in particular the use of the new methodologies to address difficult problems involved with modeling complex fluids. Following the earlier experiences, the proceedings of the third workshop also appeared as a special issue of JNNFM [3].

The fourth International Workshop on Non-equilibrium Thermodynamics and Complex Fluids was held in Rhodes in 2006. This time the importance was placed on new theoretical developments and modeling and simulation techniques based on or guided by principles of non-equilibrium thermodynamics. The description of phenomena related to the structure and morphology development and to the relaxation and dynamics in complex materials subjected to a deformation history at various length and time scales were of particular concern. Once more, the proceedings of the fourth workshop were collected in another special issue of JNNFM [4].

While the fourth workshop was taking place, we offered to organize a fifth workshop in Mexico, a proposal that was at that time well accepted. Far were we from knowing then that, when everything within the organization was more or less in place, the appearance of the A/H1N1 virus in Mexico in April, 2009 would cast serious doubts as to whether the workshop would be held at all. In spite of all the difficulties, aggravated by the rumors and the press reports, which undoubtedly prevented some people from attending, the 5th International Workshop on Non-Equilibrium Thermodynamics (IWNET 2009) took place completely safely in Cuernavaca, some 80 km south of Mexico City, from August 24 to August 28, 2009. We want to specially thank all our invited speakers and all our attendees from abroad for making the effort to overcome all the obstacles they faced before they could finally be here. In the end some 50 people from institutions in Canada, Hungary, Mexico, Norway, Russia, Spain, Switzerland and the United States of America attended the workshop. Acknowledgement is also due here for the financial support of CONACYT and for the invaluable assistance of Dr. Manuel Martínez and his team of the Consejo de Ciencia y Tecnología del Estado de Morelos (Patricia Pérez and Yair Rodríguez) in arranging the visit of the participants to the Xochicalco archeological site.

The scientific program of the workshop consisted of 9 invited lectures, 19 oral presentations and 21 posters. Compared to previous editions, in this one particular emphasis was placed on areas of possible application of non-equilibrium thermodynamics that open up new challenges and perspectives. Such areas include small and confined systems, granular matter, interfacial phenomena and biological systems. Another important innovation was the inclusion for the first time of relativistic irreversible thermodynamics as a topic of interest. Continuing with the tradition, this special issue of JNNFM gathers extended versions of some of the papers that were presented at the fifth workshop. A brief report of the activities carried out at the workshop has already appeared elsewhere [5]. We are grateful to Professors Gareth McKinley and Roland Keunings, Editors of JNNFM, for allowing us to be Guest Editors of this special issue and for their willingness to accommodate papers far beyond the usual scope of the journal. Thanks are also due to Mary Liddy, Journal Manager and Hua Luo, Content Development Coordinator for their kind assistance during the whole editorial process.

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Short Communication

The 6th international workshop on nonequilibrium thermodynamics

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The motivation for organizing a series of workshops on nonequilibrium thermodynamics (see website nonequilibrium-thermodynamics.org) has been stated very clearly in the report on the first workshop (Montreal, 1996): "Scope of the workshop has been to address the interrelationship of the various approaches, to identify recent successes in applications and outline the challenges and opportunities of the future" [1]. There was an indisputable need for a unified approach to nonequilibrium systems at that time because "so far, no significant effort has been developed to reconcile the various approaches that have, more or less independently, been developed" and, unsurprisingly, "the diversity of views was reflected in discussions at the Workshop" [1]. After the second workshop (Oxford, 2000), there was a distinct feeling "that a significant step forward in the direction of our final goal of unification has been made: a generally accepted consistent formulation of nonequilibrium thermodynamics seems to be emerging" [2]. Actually, a really gratifying situation was reached: the consistent formulation of nonequilibrium thermodynamics has been established to come in various flavors which, very much like in classical mechanics (Newton, Hamilton, Lagrange) or quantum mechanics (Schrödinger, Heisenberg), express the same physical ideas but have certain advantages in particular situations.

The first two workshops were organized as satellite meetings of the International Congresses on Rheology in Québec City (1996) and Cambridge (2000). As for the benefit brought by thermodynamics to rheology, the usefulness of thermodynamic arguments has been well established. Nonequilibrium thermodynamics provides a framework for expressing physical insight in an intrinsically coherent mathematical form. This then becomes especially important when the complexity of the system under consideration increases (as it is for example the case in dealing with biological systems). The more complex is the fluid under consideration (for example, immiscible blends with a complex structure of the interface covered with a surfactant) the more useful is the thermodynamic framework.

Very appropriately, to keep the field alive the theme of the third workshop (Princeton, 2003) was deliberately "shifted from focusing on the fundamental basis of nonequilibrium thermodynamics formalisms to using the same for specific applications" [3]. By inviting inspiring keynote speakers, strong emphasis was put on the industrial perspective (Kurt Wissbrun), the background of nonequilibrium statistical mechanics (Joel Lebowitz), the mathematics of multiscale computations (Yannis Kevrekidis) and serious applications to biology (Arup Chakraborty). As this series of workshops was initially linked to rheology, a focus on applications related to structure/morphology development and relaxation or dynamics in complex materials at the fourth workshop (Rhodes, 2006) provided the natural playground for the goal of bridging scales. A key conclusion of the Rhodes workshop is definitely worthwhile to be remembered, namely the importance of "adhering to a fundamental and strict nonequilibrium thermodynamics framework in order to establish self-consistent links between the different levels (each level addressing phenomena over a specific window of length and time scales)" [4]. In the fifth workshop (Cuernavaca, 2009), "particular emphasis was placed on areas of possible application of nonequilibrium thermodynamics that open up new challenges and perspectives. Such areas include small and confined systems, granular matter, interfacial phenomena and biological systems" [5].

The most recent sixth workshop, organized by Signe Kjelstrup, Dick Bedeaux and Kirill Glavatskiy from Norwegian University of

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Science and Technology in Trondheim, took place on 19–24 August 2012 in Røros, Norway. The organizers had decided to join the meeting with the third Lars Onsager Symposium. Fifty eight participants from 18 countries presented and discussed their recent results and ideas in the foundation of multiscale nonequilibrium thermodynamics and in its applications concerning meso- and nano-scale systems encountered in rheology, chemical kinetics, heterogeneous systems with interfaces, porous media, and biological systems. Lively discussions included also dissipative quantum mechanics and thermodynamics associated with fluctuations and numerical analysis. The future of nonequilibrium thermodynamics and the series of international workshops was addressed in daily discussion sessions. A detailed conference report reviewing the program can be found in [6]. In short, the Røros workshop (2012) has shown that nonequilibrium thermodynamics is a lively field with great potential. Some of the challenges for the future that have been identified at the workshop are the following:

- Mathematical formulation of the physics involved in the multiscale nonequilibrium thermodynamics plays an essential role in our understanding of the micro-macro relations and in our ability to develop interesting and important applications. The formulation should rely on geometrical concepts expressing in a coordinate free way the coarse graining and closures leading from micro- to macro-descriptions. Particularly important and revealing is then the investigation of coarse graining, called nonequilibrium statistical mechanics, that starts with the completely microscopic description. Another very important challenge is to regard discretizations needed in numerical analysis as physically meaningful (i.e. structure preserving) coarse graining processes. The mathematical setting should also include prerequisites for proving existence and uniqueness of solutions. A close collaboration with mathematics community will be crucial for addressing these challenges.
- Bulk-boundary physics, playing a very important role in applications, is intrinsically multiscale since the processes taking place on the boundary involve details that can, and usually are, ignored in the bulk. The proper thermodynamic coupling of two- and three-dimensional systems needs to be developed in the fully nonlinear regime. Any progress in this direction will also be directly applicable to heterogeneous and multiphase systems involving interfaces.
- Many nanoscale applications require quantum mechanics as the point of departure. Development of quantum mechanics that is manifestly compatible with thermodynamics and with classical mechanics will certainly continue to be intensely investigated subject in nonequilibrium thermodynamics.
- Another new feature arising in nanoscale applications is the small size of the systems under consideration. The systems are macroscopic but nevertheless small so that their behavior appears to be size dependent and the usual thermodynamic limit cannot be applied. A systematic incorporation of this new aspect into equilibrium and nonequilibrium thermodynamics, started by Terrell Hill, remains to be a challenge for the future.
- Processes taking place in biological systems involve chemical reactions coupled to mechanical processes. Development of a fully nonlinear nonequilibrium and multiscale thermodynamics suitable for biological applications represents thus another challenge that we expect to be discussed on future workshops.
- Complementary to reductions (i.e. to investigations of passages to more macroscopic levels) are extensions, in particular then extensions by introducing fluctuations. A clear mathematical formulation of the complementarity is still another invitation to make nonequilibrium thermodynamics more complete and more suitable for applications.

Since the long-term success of nonequilibrium thermodynamics depends on the high-level eduction of young scientists and engineers (and their teachers), it has been suggested at Røros that every other workshop should be combined with a *summer school in nonequilibrium thermodynamics* taught by pioneers in the field. Such a summer school was greatly appreciated as an integral part of the Oxford workshop (2000).

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Markus Hütter* and Ger Koper

Editorial

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Dear readers,

The International Workshop on Nonequilibrium Thermodynamics IWNET2015 took place July 5–10, 2015, in Hilvarenbeek (The Netherlands). It has been the 7th workshop in the IWNET-series (see www.nonequilibrium-thermodynamics.org), with 74 participants from 22 countries. Previous meetings were held in Montréal (1996), Oxford (2000), Princeton (2003), Rhodes (2006), Cuernavaca (2009), and Røros (2012).

At IWNET2015, five pre-selected topics have been covered, with both a summer-school and a workshop part. The topics were Fundamental issues in nonequilibrium thermodynamics; Fundamental underpinnings of and rigorous mathematical results in nonequilibrium thermodynamics; Coarse-graining techniques and truly multiscale simulations; Role of thermodynamics in modeling the dynamics of complex materials under deformation; Heterogeneous systems, interfaces, system-boundaries and small systems. These topics are typical for the IWNET-series, as they cover both the fundamental aspects of nonequilibrium thermodynamics and advanced applications. Already in the early days of the IWNET-series, such a balance between fundamental and more applied topics has proven very fruitful; indeed, traditionally, a significant fraction of IWNET-participants has a strong interest in the modeling of complex fluids. The detailed program as well as the presentations of the invited lecturers of the IWNET2015 can be found online at www.iwnet2015.org.

Although most material covered in the invited lectures for the summer school part has already been published in various forms in the past, some of it was original and hence this issue contains three contributions related to these tutorial lectures: Mielke, Peletier, and Renger deal with a generalization of Onsager's reciprocity relations to gradient flows with nonlinear mobility (pp. 141–149); with respect to bridging scales, Ilg gives a tutorial example of systematic coarse-graining toward hydrodynamics with spin angular momentum (pp. 89–97); and the modeling of mechanical behavior of complex materials is addressed in the contribution of Gladkov, Kochmann, Hütter, Reese, and Svendsen with a non-isothermal phase-field approach (pp. 131–139).

The remainder of this issue contains five contributions related to regular oral presentations at the IWNET2015. Particularly, as far as fundamental/mathematical issues are concerned, the contribution of Santamaría-Holek, Pérez-Madrid, and Rubí discusses a local quasi-equilibrium description of multiscale systems (pp. 123–130). Giona, Brasiello, and Crescitelli elaborate on generalized Poisson-Kac processes (pp. 107–114), and the effect of finite propagation velocity (pp. 115–122). Cirillo, Colangeli, and Muntean study in their paper stationary currents in particle systems with constrained hopping rates (pp. 99–106), and Semkiv and Hütter examine the effect of physical aging and mechanical rejuvenation (pp. 79–88).

The next workshop in this series, IWNET2018, will take place end of June/beginning of July 2018 again in the Netherlands, organized by Markus Hütter (Eindhoven University of Technology) and Leonard Sagis (Wageningen University).

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Markus Hütter*

Editorial

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Dear readers,

Last year, 63 participants from 18 countries gathered for the 8th edition of the International Workshop on Non-Equilibrium Thermodynamics IWNET (see http://www.nonequilibrium-thermodynamics.org for more details), which was organized by Markus Hütter (Eindhoven University of Technology) and Leonard Sagis (Wageningen University and Research) and was held in Sint-Michielsgestel, close to the city of 's Hertogenbosch in the Netherlands. Previous meetings in this series took place in Montréal (1996), Oxford (2000), Princeton (2003), Rhodes (2006), Cuernavaca (2009), Røros (2012), and Hilvarenbeek (2015).

The 5-day workshop consisted of invited lectures, regular presentations, poster sessions, and discussion sessions, on the following topics:

Topic:	*Invited speaker:*
New Conceptual Developments	Alexander Gorban (University of Leicester, UK)
Complex Fluids and Solids	Mike Cates (University of Cambridge, UK)
Large Fluctuations	Hugo Touchette (Stellenbosch University, South Africa)
Quantum Dissipation	Armen Allahverdyan (Yerevan Physics Institute, Armenia)

The topics thus ranged from the fundamentals of non-equilibrium thermodynamics in general, establishing links to other branches of physics and mathematics (large fluctuations, quantum dissipation), to the rather applied field of mechanical behavior of complex materials.

This issue of the Journal of Non-Equilibrium Thermodynamics contains four peer-reviewed publications of work that has been presented at the workshop last year. Particularly, the contributions are the following: In the field of New Conceptual Developments, Miroslav Grmela, Michal Pavelka, Vaclav Klika, Bing-Yang Cao, and Nie Bendian present "Entropy and entropy production in multiscale dynamics" (pp. 217–233); in the field of Complex Fluids and Solids, Paul M. Mwasame, Norman J. Wagner, and Antony N. Beris describe "Microinertia effects in material flow" (pp. 235–246), and Mátyás Szücs and Tamás Fülöp elaborate on "Kluitenberg-Verhás rheology of solids in the GENERIC framework" (pp. 247–259); in the field of Quantum Dissipation, Walter Aschbacher presents his results on "A rigorous scattering approach to quasifree fermionic systems out of equilibrium" (pp. 261–275).

The 9th workshop in this series, IWNET2021, will take place in 2021 in Victoria, Canada, and will be organized by Henning Struchtrup (University of Victoria).

Markus Hütter
Guest editor

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