

IWNET 2012



6th International Workshop on Nonequilibrium Thermodynamics and 3rd Lars Onsager Symposium

Book of Abstracts

Røros, Norway, 19-24 August 2012

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on
Nonequilibrium Thermodynamics
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Sponsors

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Scope

The application of thermodynamics to non-equilibrium systems is by no means obvious. Therefore, it is not surprising that there have been a number of theoretical developments following various approaches to deal with such systems: Classical nonequilibrium thermodynamics with internal variables, Lagrangian methods, bracket formulations, continuum or rational thermodynamics, variational formulations, extended irreversible thermodynamics, the matrix model, network thermodynamics, the GENERIC formalism and finite-time thermodynamics.

The aim of this series of workshops is 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 now to combine the various approaches in some kind of common generalized theory. In order to achieve this, a second, third and fourth international workshop were held in Oxford, 2000, Princeton, 2003 (Workshop report by A. Beris and B.J. Edwards, JNNFM 120 (2004) 1-2) and Rhodes, 2006 (Workshop report by V. G. Mavrantzas, A. N. Beris and Ath. Tzavaras, JNNFM 152 (2008) 1). The fifth international Workshop took place in Cuernavaca, 2009 (report by L. Garcia-Colin-Scherer, M. Lopez de Haro and F. Vazques Hurtado), and the sixth shall now take place in Norway, at Røros, close to Trondheim.

The proximity to the Norwegian University of Science and Technology (NTNU) means that workshop is also the 3rd International Lars Onsager Symposium. The 1st was held in 1993 on the issues of Phase transformation and transport. The 2nd was on Transport, dissipation and turbulence in 2003. Onsager's contribution to non-equilibrium thermodynamics is tremendous and it is of importance to NTNU to honor his name in the country where he was born.

The workshop will continue the efforts of bringing non-equilibrium thermodynamics to the same level of clarity and usefulness as equilibrium thermodynamics. The workshop is expected to highlight recent advances in the field, in particular, new theoretical developments and state-of-the-art modelling/simulation techniques founded on or guided by principles of non-equilibrium thermodynamics. Particular emphasis will be given to areas of possible applications that open up new challenges and perspectives as well as the more traditional topics. The first include

- * mesoscopic and confined systems,
- * granular matter, porous materials
- * interfacial phenomena and surfaces
- * biological systems

By the end of the workshop we hope that participants will not only have had the chance to widen their own views on the possibilities and present limitations of non-equilibrium thermodynamics but also to confirm the importance of establishing self-consistent links between the different levels of description (each level addressing phenomena over a specific window of length and time scales).

Summary

Summary program

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday
07:00	Arrival	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast
08:30		Welcome				
08:45		Sengers	Bresme	Qian	Sagis	Simon
09:00		1	11	21	31	37
09:15						
09:30		Ortiz de Zarate	Kizilova	Ge	Struchtrup	Rodriguez
09:45		2	12	22	32	38
10:00		Beris	Lervik	Grmela	Schweiser	Vazquez
10:15		3	13	23	33	39
10:30		Coffee	Coffee	Coffee	Coffee	Coffee
10:45		Kulinskii	Hoffman	Jou	Klika	Salgado-Garcia
11:00		4	14	24	34	40
11:15		Karlin	Fulop	Ottinger	Keller	Maruszewski
11:30		5	15	25	35	41
11:45		Erp	Serdyukov	Osmanov	Demin	Brechet
12:00		6	16	26	36	42
12:15		Discussion	Discussion	Discussion	Discussion	Discussion
12:30						Closing
12:45						
13:00		Lunch	Lunch	Lunch	Lunch	Lunch
13:15						
13:30						
13:45						
14:00	Poster Session	City tour	Poster Session	Canoeing	Departure	
14:15						
14:30						
14:45						
15:00						
15:15						
15:30						
15:45						
16:00						
16:15	Coffee	Coffee	Coffee			
16:30	Registration	Turkington	Conti	Rubi		
16:45		7	17	27		
17:00	Hutter	Rio	Pagonabarraga			
17:15	8	18	28			
17:30						
17:45	Coffee	Coffee	Coffee			
18:00	Reception	Koper	Måløy	Vlugt		
18:15		9	19	29		
18:30	Osorio	Hansen	Schnell			
18:45	10	20	30			
19:00	Dinner	Dinner	Dinner	Banquet	Dinner	

Summary topics

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	
07:00	Arrival	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast	
08:30		Welcome					
08:45 - 10:30		Fluctuations	Biological	Nonlinear reactions	Interfaces	Interfaces	
10:30		Coffee	Coffee	Coffee	Coffee	Coffee	
10:45 - 12:15		General	Rheology	Nano transport	Fluid flow	Thermodynamic theory	
12:15 - 13:00		Discussion	Discussion	Discussion	Discussion	Discussion	
13:00 - 14:00		Lunch	Lunch	Lunch	Lunch	Lunch	
14:00 - 16:30		Poster Session	City tour	Poster Session			
16:30 - 17:45		Registration	GENERIC	Measurements	Nonlinear reactions		
17:45			Coffee	Coffee	Coffee		
18:00 - 19:00		Reception	Self-Assembly	Porous media	Simulations		
19:00		Dinner	Dinner	Dinner	Banquet	Dinner	
							Departure

Technical Program

Schedule

<i>Sun, 19</i>			
16:30	Registration		
18:00	Welcome drink		

Mon, 20			
08:30	Signe Kjelstrup NTNU, Norway	Welcome	
Mon		Chair: Signe Kjelstrup	
08:45	Jan Sengers University of Maryland, College Park, USA	<i>Thermally induced non-equilibrium fluctuations: gravity and finite-size effects</i>	O-01
09:30	José Ortiz de Zárate Universidad Complutense de Madrid, Spain	<i>Fluctuations in laminar flow</i>	O-02
10:00	Antony Beris University of Delaware, USA	<i>Coupling reactions and molecular conformations in the modeling of shear banding in wormlike micellar systems.</i>	O-03
10:30	Coffee		
Mon		Chair: Dick Bedeaux	
10:45	Vladimir Kulinskii Odessa National University, Ukraine	<i>Liquid-gas spinodal and the interfacial properties from the lattice gas-fluid isomorphism approach</i>	O-04
11:15	Ilya Karlin ETH Zurich, Switzerland	<i>Simulation of turbulent flows with the entropic lattice Boltzmann method</i>	O-05
11:45	Titus van Erp NTNU, Norway	<i>Dynamical Rare event simulation techniques for equilibrium and non-equilibrium systems</i>	O-06
12:15	Discussion		
13:00	Lunch		
14:00	Poster session		
Mon		Chair: Hans Christian Öttinger	
16:45	Bruce Turkington University of Massachusetts, USA	<i>Derivation of the GENERIC form of nonequilibrium thermodynamics from a statistical optimization principle</i>	O-07
17:15	Markus Hütter Eindhoven University of Technology, The Netherlands	<i>Quasi-linear versus potential-based formulations of force-flux relations and the GENERIC for irreversible processes: comparisons and examples</i>	O-08
17:45	Coffee		
Mon		Chair: Jose Ortiz de Zarate	
18:00	Ger Koper TU Delft, The Netherlands	<i>Thermodynamics of Dissipative Self-Assembly</i>	O-09
18:30	Antonio Osorio University of Michigan, USA	<i>Self-assembled structures in immiscible systems of active, switchable nanocolloids</i>	O-10
19:00	Dinner		

Tue, 21			
Tue		Chair: Leonard Sagis	
08:45	Fernando Bresme Imperial College London, UK	<i>Computational studies of thermal transport in molecular fluids and biomolecules</i>	O-11
09:30	Natalya Kizilova Kharkov National University, Ukraine	<i>Non-equilibrium thermodynamics of heterogeneous growing biosystems</i>	O-12
10:00	Anders Lervik NTNU, Norway	<i>Active transport of the Calcium pump: Introduction of the temperature difference as a driving force</i>	O-13
10:30	Coffee		
Tue		Chair: Jürgen Keller	
10:45	Karl Heinz Hoffmann TU Chemnitz, Germany	<i>Optimizing thermodynamic cooling processes</i>	O-14
11:15	Tamás Fülöp Montavid Thermodynamic Research	<i>Rheology, plasticity and thermal expansion in a nonequilibrium thermodynamical framework</i>	O-15
11:45	Sergey Serdyukov Moscow State University, Russia	<i>Dual-phase-lag model for rapid solidification of undercooled melts</i>	O-16
12:15	Discussion		
13:00	Lunch		
14:00	City Tour		
Tue		Chair: Fernando Bresme	
16:45	Livia Conti INFN Sezione di Padova, Italy	<i>Experimental findings on 'thermal noise' of oscillators in non-equilibrium steady-states.</i>	O-17
17:15	Antonio del Río Universidad Nacional Autónoma de México, México	<i>Heat transfer in nanostructured dielectric mirrors</i>	O-18
17:45	Coffee		
Tue		Chair: Natalya Kizilova	
18:00	Knut Måløy University in Oslo, Norway	<i>Steady-state, simultaneous two-phase flow in porous media: An experimental study</i>	O-19
18:30	Alex Hansen NTNU, Norway	<i>Steady-State Two-Phase Flow in Porous Media: Open Questions</i>	O-20
19:00	Dinner		

Wed, 22			
Wed		Chair: Antony Beris	
08:45	Hong Qian University of Washington, USA	<i>Open chemical systems and their biological function</i>	O-21
09:30	Hao Ge PKU, China	<i>Heat Dissipation and Self-consistent Nonequilibrium Thermodynamics of Open Driven Systems</i>	O-22
10:00	Miroslav Grmela Ecole Polytechnique de Montreal, Canada	<i>Multiscale Guldberg-Waage-Onsager Dynamics in Small Systems</i>	O-23
10:30	Coffee		
Wed		Chair: Miroslav Grmela	
10:45	David Jou Universitat Autònoma de Barcelona, Spain	<i>Generalized transport equations for heat transfer in nanosystems: nanowires and plane sheets</i>	O-24
11:15	Hans Christian Öttinger ETH Zurich, Switzerland	<i>Nonequilibrium thermodynamics for dissipative quantum systems</i>	O-25
11:45	Maksym Osmanov ETH Zurich, Switzerland	<i>Open quantum systems coupled to classical time-evolving environments</i>	O-26
12:15	Discussion		
13:00	Lunch		
14:00	Poster session		
Wed		Chair: Jan Sengers	
16:30	Miguel Rubi University of Barcelona, Spain	<i>A mesoscopic description of reactions far from equilibrium</i>	O-27
17:15	Ignacio Pagonabarraga University of Barcelona, Spain	<i>Fluctuating hydrodynamics for chemically reacting mixtures</i>	O-28
17:45	Coffee		
Wed		Chair: Titus van Erp	
18:00	Thijs Vlugt TU Delft, The Netherlands	<i>Fick Diffusion Coefficients in Ternary Liquids from Equilibrium Molecular Dynamics</i>	O-29
18:30	Sondre Schnell TU Delft, The Netherlands	<i>Heat transfer in zeolites determined from non-equilibrium molecular dynamics simulations</i>	O-30
19:00	Banquet		

Thu, 23			
Thu		Chair: Markus Hütter	
08:45	Leonard Sagis Wageningen University, The Netherlands	<i>Dynamics of complex fluid-fluid interfaces</i>	O-31
09:30	Henning Struchtrup University of Victoria, Canada	<i>On the (im-) possibility of cold to warm distillation</i>	O-32
10:00	Marco Schweizer ETH Zurich, Switzerland	<i>Local equilibrium for interfaces and gauge transformations verified by simulations</i>	O-33
10:30	Coffee		
Thu		Chair: Karl Heinz Hoffmann	
10:45	Vaclav Klika Czech Technical University in Prague, Czech Republic	<i>Nonlinear and compatible with thermodynamics coupling of chemical kinetics with mechanics</i>	O-34
11:15	Jürgen Keller University of Siegen, Germany	<i>The Vortex Tube of Ranque and Hilsch Thermodynamic Foundations and New Applications</i>	O-35
11:45	Vitaly Demin Perm State University, Russia	<i>Macroscopic convective phenomena in non-uniformly heated liquid mixtures</i>	O-36
12:15	Discussion		
13:00	Lunch		
14:00	Canoeing		
19:00	Dinner		

Fri, 24			
Fri		Chair: Henning Struchtrup	
08:45	Jean-Marc Simon CNRS-Université de Bourgogne, France	<i>Liquid-vapour interface transfer coefficients of a two-component mixture</i>	O-37
09:30	Marcos Rodriguez University of Cape Tow, South Africa	<i>Coupled heat and mass transfer during crystallization</i>	O-38
10:00	Federico Vázquez Universidad Autónoma del Estado de Morelos, México	<i>Thermodynamic analysis of irreversibilities in thin heat conducting films</i>	O-39
10:30	Coffee		
Fri		Chair: Alex Hansen	
10:45	Raul Salgado-García Universidad Autónoma del Estado de Morelos, Mexico	<i>Resonant Response in Non-equilibrium Steady States</i>	O-40
11:15	Bordan Maruszewski Poznan University of Technology, Poland	<i>Thermodynamic model of thermoelastic interactions in media of anomalous material properties and unconcentional thermoelastic damping</i>	O-41
11:45	Sylvain Bréchet Institute of Condensed Matter Physics, EPFL, Switzerland	<i>Thermodynamics of continuous media with permanent electric polarisation and magnetisation</i>	O-42
12:15	Discussion		
13:00	Lunch		

List of Posters

	<p>Delfino Ladino-Luna Universidad Autónoma Metropolitana-Atzacapozalco</p>	<p><i>Otto and Diesel cycles modeled by considering non-instantaneous adiabats</i></p>	P-01
	<p>Miguel Olivares-Robles IPN ESIME-Culhuacan, México</p>	<p><i>Thermodynamic Optimization of Two-Stage Peltier Modules: Structure and Exergy</i></p>	P-02
	<p>Marco Barranco-Jiménez Escuela Superior de Cómputo del IPN, México</p>	<p><i>A comparative analysis of efficiency a maximum power output for some heat engines</i></p>	P-03
	<p>Francisco Sevilla Universidad Nacional Autonoma de Mexico</p>	<p><i>Equilibrium Instability from Cooperative Interactions in a System of Brownian Agents</i></p>	P-04
	<p>Jérôme Flakowski ETH Zurich, Switzerland</p>	<p><i>Simulation techniques for the nonlinear thermodynamic quantum master equation</i></p>	P-05
	<p>Vladimir Kulinskii Odessa National University, Ukraine</p>	<p><i>Self-Propelling Particles as a New Challenge for the Non-equilibrium Statistical Mechanics</i></p>	P-06
	<p>Claire Chassagne TU Delft, The Netherlands</p>	<p><i>Solving the electrokinetic equations for the polarization of a charged spheroid in an alternating electric field</i></p>	P-07
	<p>José Ortiz de Zárate Universidad Complutense de Madrid, Spain</p>	<p><i>Spatial correlation of concentration fluctuations in reaction diffusion problems by the Gillespie algorithm</i></p>	P-08
	<p>Michal Pavelka Charles University in Prague, Czech Republic</p>	<p><i>PEM fuel cells enhanced by gradient of surface energy of water in the membrane</i></p>	P-09
	<p>Marleen Kooiman Eindhoven University of Technology, The Netherlands</p>	<p><i>Coarse-Graining of Dislocation-Mediated Plasticity</i></p>	P-10
	<p>Paulina Madrigal Universidad Nacional Autónoma de México</p>	<p><i>Nonequilibrium thermodynamics in Oil distillation</i></p>	P-11
	<p>Thomas Lion The University of Edinburgh, UK</p>	<p><i>Osmosis in non-equilibrium simulations with active solute particles</i></p>	P-12
	<p>Sergey Serdyukov Moscow State University, Russia</p>	<p><i>On the Hamiltonian Structure of Extended Thermodynamics of Irreversible Processes</i></p>	P-13

Oral presentation

Thermally induced non-equilibrium fluctuations: gravity and finite-size effects

Jan V. Sengers¹, José M. Ortiz de Zárate²

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Abstract

This lecture will be concerned with fluctuations in fluids in the presence of a temperature gradient. Non-equilibrium fluctuating hydrodynamics shows that such fluctuations are always spatially long ranged due to mode-coupling effects induced by the temperature gradient. The intensity of the non-equilibrium fluctuations is greatly enhanced compared to those in equilibrium and exhibits a dramatic dependence on the wavelength at all length scales in the system. At small wavelengths the intensity of the non-equilibrium fluctuations increases with the 4th power of the wavelength. At larger wavelengths the fluctuations become affected by gravity and by finite-size effects.

We shall review how by supplementing light-scattering measurements with shadowgraph measurements experimental information covering non-equilibrium fluctuations at all relevant length scales has been obtained. Gravity effects have been beautifully demonstrated recently by comparing earth-bound experiments with experiments in a satellite [1].

References

- [1] C.J. Takacs, A. Vailati, R. Cerbino, S. Mazzoni, M. Giglio, and D.S. Cannell, Phys. Rev. Lett. 106, 244502 (2011).

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Fluctuations in laminar flow

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Abstract

One of the many physical differences between equilibrium and nonequilibrium states is the existence of mode-coupling phenomena at the linear level. Indeed, generically, dissipative fluxes have deterministic (i.e. non-random) components for systems outside equilibrium. For instance, and depending on the particular non-equilibrium mechanism, the fluid velocity or the heat flow do not average to zero. These non-vanishing averages appear in the fluctuating hydrodynamics equations, even when linearized over the fluctuations of the thermodynamic fields.

As extensively investigated in the past decades, this feature has important consequences on the theory of hydrodynamic fluctuations for systems that are not in equilibrium. In particular, equal-time field fluctuations are enhanced and become spatially long-ranged. As a corollary, and opposed to equilibrium situations, incorporation of boundary conditions is crucial for a correct description of the spatial spectrum of fluctuations, especially at large wavelengths.

In this presentation we review recent theoretical work on the intensity of thermal fluctuations in fluids under laminar flow. We identify two different mode-coupling mechanisms leading to non-equilibrium enhancement of the fluctuations: self-coupling of similar modes with different wave number and cross-coupling between wall-normal velocity and vorticity. We incorporate vanishing velocity fluctuations at the walls, and discuss the consequences for the intensity of fluctuations. For the particular case of plane Couette flow, we compare the two coupling mechanisms and conclude that cross-coupling is the most important one. The resulting enhancement is highly anisotropic, wall-normal velocity fluctuations are maximally enhanced in the streamwise direction, while wall-normal vorticity fluctuations are maximally enhanced in the spanwise direction. For the particular case of wave vector in the spanwise direction (or, alternatively, streamwise-constant fluctuations), we have obtained a compact analytical expression for the spatial spectrum of the vorticity fluctuations. These fluctuations are those maximally enhanced.

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Coupling reactions and molecular conformations in the modeling of shear banding in wormlike micellar systems

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Abstract

In the last decade considerable interest has emerged in understanding and modeling the flow behavior of concentrated wormlike micellar solutions. A significant advance was made through the two species modeling approach, explicitly considering the wormlike micelles breakdown and reconstruction, originally proposed by one of us and co-workers [1]. In the present work we revisit this model from a nonequilibrium thermodynamics point of view. We show how, employing an extension to the nonequilibrium treatment of chemical reactions that originally appeared in [2], we can develop a model based on nonequilibrium thermodynamics principles, modeling the wormlike micelles with one mode viscoelastic models, that is close to the one developed based on more ad-hoc assumptions in [1]. Using a two-fluid modeling approach we introduce shear-induced migration and allow for a systematic coupling between the number density balance equations and the rodlike micellar conformations. Thus, we not only validate that model, but we also now have a mechanism to systematically further generalize it, leading to considerable refinements. One such refinement, including a third species in the model, is explored in this work. In addition to developing model predictions in simple (homogeneous) shear and extensional flows, further applications, involving nonhomogeneous structure formation, will be discussed

References

- [1] P. A. Vasquez, G. H. McKinley, and L. P. Cook. A network scission model for wormlike micellar solutions: I. Model formulation and viscometric flow predictions. *J. Non.-Newtonian Fluid Mech.*, 144:122-139, 2007.
- [2] A. N. Beris and B. J. Edwards. *Thermodynamics of Flowing Systems*. Oxford University Press, New York, 1994.

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Liquid-Gas Spinodal and the Interfacial Properties from the Lattice Gas-Fluid Isomorphism Approach

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Abstract

We use the approach [1] of the global isomorphism between lattice gas and fluid to calculate both the binodal and the spinodal curves of the molecular liquid from the corresponding characteristics of the lattice gas (Ising model) in 2D and 3D cases. This isomorphism is expressed in the relations:

$$n = n_* \frac{x}{1 + zt}, \quad T = T_* \frac{zt}{1 + zt}, \quad z = \frac{T_c}{T_* - T_c}, \quad (1)$$

between the density and temperature variables of the fluid and the lattice gas correspondingly. These relations map the equilibrium states of the lattice gas to the states of the fluid. We discuss the relations between the thermodynamic potentials of these systems and use them to calculate the liquid-gas spinodal curve surface tension and the Tolman length. The dependence of the range of the stability of the liquid phase on the relevant parameters of the potential is discussed. The results are compared with the numerical data [2].

References

- [1] V. Kulinskii, Global isomorphism between the Lennard-Jones fluids and the Ising model, *J. Chem. Phys.*, 133 (2010) 034121
- [2] A. R. Imre, G. Mayer, G. Hazi, R. Rozas, and T. Kraska, Estimation of the liquid-vapor spinodal from interfacial properties obtained from molecular dynamics and lattice Boltzmann simulations, *J. Chem. Phys.* 128, 114708 (2008); doi: 10.1063/1.2837805

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Simulation of turbulent flows with the entropic lattice Boltzmann method

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¹ *ETH Zurich, Switzerland*

Abstract

At variance with previous Lattice Boltzmann methods, the entropic version permits to describe the non-linear dynamics of short scales in a controlled and stable way. In this talk, I shall discuss the current status of the lattice Boltzmann method as an alternative for the direct numerical simulation (DNS) of high Reynolds number flow phenomena. After reviewing a recent work on 3D DNS of turbulent vortex flow with higher-order LBGK scheme [Chikatamarla et al, J. Fluid Mech. (2010)], I shall describe new boundary conditions for sub-grid simulations of wall-bounded turbulent flows. Open questions which are needed to be addressed in order to put lattice Boltzmann methods as an alternative DNS shall also be discussed.

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Dynamical Rare event simulation techniques for equilibrium and non-equilibrium systems

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Abstract

I give an overview of rare event simulation techniques to generate dynamical pathways across high free energy barriers. The methods on which I will concentrate are the reactive flux approach, transition path sampling, (replica-exchange) transition interface sampling, partial path sampling/milestoning, and forward flux sampling. These methods have in common that they aim to simulate true molecular dynamics trajectories at a much faster rate than naive brute force molecular dynamics. The advantages and disadvantages of these methods are discussed and compared for a simple one-dimensional test system. These numerical results reveal some important pitfalls of the present non-equilibrium methods that have no easy solution and show that caution is necessary when interpreting their results.

References

[1] Titus S. van Erp, *Advances in Chemical Physics*, Vol. 151, p 27 (2012).

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Derivation of the GENERIC form of nonequilibrium thermodynamics from a statistical optimization principle

Bruce Turkington¹

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Abstract

We show that the form of the governing equations for nonequilibrium thermodynamics called GENERIC by Grmela and Öttinger can be derived from a natural variational principle. Our approach employs quasi-equilibrium ensembles corresponding to a given set of macroscopic variables, as in the standard projection operator methodology of statistical mechanics. The novelty of our derivation is to consider these ensembles as trial probability densities in an optimization principle, and to characterize a macroscopic evolution as a path of these trial pdfs that is a best fit to the underlying microscopic dynamics. The lack-of-fit of such a path of pdfs is quantified by its residual with respect to the Liouville equation, and a time-integrated, ensemble-averaged, squared norm of this residual defines the cost functional in our optimization principle. Optimal paths which connect nonequilibrium initial macrostates to equilibrium determine the relaxation of the macroscopic variables. The closed reduced equations governing the macroscopic variables are deduced by the techniques of the calculus of variations, and they are found to have the GENERIC form; namely, they have a reversible term that is a Hamiltonian vector field and an irreversible term that is a gradient vector field. The potential in the irreversible term is the optimal value function associated with the cost functional, and near equilibrium it coincides with (half) the entropy production.

Our theoretical framework can be viewed as a general statistical model reduction procedure that applies to any Hamiltonian microdynamics and any set of resolved variables, and is valid far from equilibrium. Adjustable parameters enter in this statistical closure as weights assigned by the cost functional to represent the influence of unresolved fluctuations on the resolved evolution. The optimal value function is a thermodynamic potential that establishes the relation between thermodynamic forces and fluxes, and in this way our optimization framework extends the classical structure of linear irreversible thermodynamics.

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Quasi-linear versus potential-based formulations of force-flux relations and the GENERIC for irreversible processes: comparisons and examples

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Abstract

An essential part in modeling out-of-equilibrium dynamics is the formulation of irreversible dynamics. In the latter, the major task consists in specifying the relations between thermodynamic forces and fluxes. In the literature, mainly two distinct approaches are used for the specification of force-flux relations. On the one hand, quasi-linear relations are employed, which are based on the physics of transport processes and fluctuation-dissipation theorems [1,2]. On the other hand, force-flux relations are also often represented in potential form with the help of a dissipation potential [3]. We address the question of how these two approaches are related. The main result of this presentation states that the class of models formulated by quasi-linear relations is larger than what can be described in a potential-based formulation. While the relation between the two methods is shown in general terms, it is demonstrated also with the help of three examples: (i) heat conduction in rigid bodies, (ii) homogeneous chemical reactions, and (iii) slippage in complex fluids. In particular, whereas the irreversible processes (i) and (ii) are dissipative, (iii) is not. Consequently, conditions for the existence of a dissipation potential for the models of (i) and (ii) can be formulated. On the other hand, the potential for the model of (iii) is identically zero. More generally, this is the case for the model of any irreversible process which results in no dissipation. The finding that quasi-linear force-flux relations are more general than dissipation-based ones also has ramifications for the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC: e.g., [4-6]). This framework has been formulated and used in two different forms, namely a quasi-linear [5,6] and a dissipation-potential based [7-9] form, respectively, relating the irreversible evolution to the entropy gradient. It is found that also in the case of GENERIC, the quasi-linear representation encompasses a wider class of phenomena as compared to the dissipation-based formulation. Furthermore, it is found that a potential exists for the irreversible part of the GENERIC if and only if one does for the underlying force-flux relations.

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Thermodynamics of Dissipative Self-Assembly

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Abstract

Self assembled structures have frequently been discussed as model systems for biological. In contrast to most synthetic self-assembling systems the natural systems are not equilibrium processes. Attention is therefore now focusing on dissipative self-assembling systems where energy input is required to sustain the self-assembled state. These systems can adapt themselves to environmental conditions whereas their equilibrium counterparts can only assemble or disassemble. Recently, we have constructed a dissipative self-assembling system using a chemical fuel. The thermodynamic description of such non-equilibrium processes invokes some interesting questions regarding the nature of the entropy production, the relation between the driving forces and the dissipation rate, and the energy transduction pathways that will be discussed during this presentation.

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Self-assembled structures in immiscible systems of active, switchable nanocolloids

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Abstract

We consider the synthesis and fabrication of active building blocks that can dynamically switch between two or more states and assemble into novel structures. We present novel steady-state structures predicted by computer simulation to assemble in systems of switchable, immiscible building blocks. We discuss the dynamics that stabilize these structures, explore approaches to analyze the dissipative nature of the system, and provide a mapping to experimental colloidal systems where these concepts could be implemented.

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Computational studies of thermal transport in molecular fluids and biomolecules

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Abstract

Non-equilibrium phenomena play an essential role in many processes of relevance in biology, physics and materials science. One of such non-equilibrium phenomena is thermoelectricity, in which a temperature gradient applied to a circuit made from different metals induces an electric current. Temperature measuring devices, and some refrigerators rely on these thermoelectric effects. This principle is being used to manufacture materials that can efficiently convert waste heat into electricity.

Recent work indicates the possibility of generating large thermal gradients in nanoscale assemblies. Such large thermal gradients have been inferred from theoretical analyses of systems involving metal nanoparticles heated with electromagnetic radiation, a notion that is being used in cancer therapy treatments. Similarly, experimental studies of molecular motors, such as Ca²⁺-ATPase, indicate that significant thermal gradients can develop during the ion transport process. Many of these processes, particularly those in bio-molecules occur in aqueous solutions. We are currently investigating the response of aqueous solutions and interfacial water to thermal perturbations. We have recently described a novel phenomenon whereby water molecules reorient as a response to the thermal gradient, and polarize along the direction of the gradient. This polarization can result in significant electrostatic fields for thermal gradients that are achievable in biological processes and nanomaterial applications. Thermoelectric effects are well known in semiconductors, but we find that related mechanisms can arise in molecular fluids. I will also discuss how these large thermal gradients can impose a preferred orientation in non polar molecular fluids, an effect called thermo-molecular orientation.

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Non-equilibrium Thermodynamics of Heterogeneous Growing Biosystems

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Abstract

Biological bodies are formed from heterogeneous tissues which are mostly composite materials with complex mechanical, thermal, electrical, chemical properties, central and local regulation. Biomaterials have complicated internal structures adapted for external loads and exhibit optimal mechanical properties like maximal performance at total lightweight design [1]. Optimal structure of the tissues, organs and bodies is formed during their growth and development, and knowledge of principles of optimal design in nature is important for technical and biomedical applications.

Biosystems are open thermodynamic systems which are in permanent mass and energy exchange with environment. Biological growth as irreversible variations in body mass/volume/size is provided by new matter uptake from environment and its delivery and distribution to the growing cell through special conducting pathways by delivering liquids (blood, plant sap, trophic fluids and tissue fluids). Optimal performance of biosystems is connected with minimum energy loss and entropy production which can be computed for different systems, states and processes [1,2]. New matter delivered to the tissues is accumulated on the surfaces of the extracellular structures and consumed by cells. In that way growth is connected with liquid-solid phase transitions and can be described by formalism of non-equilibrium thermodynamic. Since physical and chemical reactions at the surfaces determine the growth rate and direction, the surface phenomena must be taken into account [3]. Collagen-based biotissues possess piezoelectric properties, and a wide range of electrokinetic phenomena is proper to the growing tissues. Mass, heat and charge transfer at the membranes and solid surfaces are coupled, and the relations between the forces and fluxes must be generalized for an active free energy driven medium with central and local electrical and chemical regulation.

Continual models are most relevant for mathematical modeling of growing biological bodies as multi-phase and multi-component systems [4-7]. In this paper a thermodynamic model of the heterogeneous growing material with internal variables is proposed. The material consists of several solid (extracellular matrix, connective tissues, vessel walls) and liquid phases (intracellular, extracellular and delivering liquids). The internal parameters describe the microstructure formation in solid phases. The mass, momentum and energy balance equations are formulated and the relationships between fluxes and forces are obtained from the entropy production term. The model is applied for the problem of the heterogeneous tissue growth in a rigid scaffold from a biodegradable material as slow filtration of a multicomponent liquid in a porous medium with gradually increasing porosity. The optimal regimes allowing a balance between the tissue growth and scaffold degradation are proposed for tissue engineering. Introduction of the vessel wall as separate solid phase gives an opportunity to model and control the vascularized tissue growth in scaffolds and bioreactors.

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Active transport of the Calcium pump: Introduction of the temperature difference as a driving force

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Abstract

The kinetic cycle description of ion pumping proteins does not include a temperature difference as a driving force, even though proteins such as the Ca^{2+} -ATPase ion pump is known to generate heat and participate in thermogenesis. We analyze the kinetic cycle for the operation of the Ca^{2+} -ATPase ion pump using two different frameworks: the diagram method of Hill [1] and mesoscopic non-equilibrium thermodynamics [2]. We compare these two descriptions and we discuss how a temperature difference and the corresponding heat flux can be introduced.

We then compare these descriptions with a mesoscopic non-equilibrium thermodynamic description which is not based on a kinetic cycle [3], and show that the kinetic and the mesoscopic pictures are in accordance with each other.

We also show how the mesoscopic approach can be used to identify the slow and fast steps of the model in terms of activation energies, and how this can be used to simplify the kinetic diagram.

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Optimizing Cooling Processes - A Dynamic View on the Third Law

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Abstract

The Third law is often understood to be a statement about the impossibility to reach absolute zero in a finite number of steps. The basis of this consideration is classical equilibrium thermodynamics. In this talk a dynamical view on the Third Law is presented. At the center of this approach is the question how cooling rates change as one approaches absolute zero. Especially we will study limits on the cooling rates as functions of the temperature of the cold bath. At low temperatures quantum effects become more and more important, and thus we will deal with “quantum refrigerators”. It turns out that fast adiabatic processes play a crucial role in limiting the cooling rates.

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Rheology, plasticity and thermal expansion in a nonequilibrium thermodynamical framework

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Abstract

A recent approach [1] has introduced kinematic quantities for elasticity, plasticity, and thermal expansion of solids by working on spacetime directly - rather than in a reference frame -, and utilizing the notions of the relaxed metric and the current metric of the material manifold. Namely, elastic deformedness measures the difference between the current metric and the relaxed metric, thermal expansion means a temperature dependent - typically volumetric - change of the relaxed metric, and the plastic rearrangement of the solid is described by another type of - typically volume preserving - change of the relaxed metric.

The talk reports on how these kinematic ingredients help us building a non-equilibrium thermodynamical theory for elasticity, rheology, plasticity and thermal stresses. Starting from the elastic behaviour and heat capacity, we construct the naturally emerging entropy function. Next, we find that the dynamical consequences of thermal expansion can easily be incorporated in the entropy function. In the third step, plasticity is added, and we show how the entropy production can be kept positive definite via natural constitutive prescriptions on what governs plastic changes. These prescriptions are of pseudolinear Onsagerian nature. At last, rheology is added in the form of a tensorial dynamical degree of freedom, a non-equilibrium extra term in the entropy function.

As an application, an experiment of a uniaxially loaded and plastically deformed sample is presented, and the measured results are analysed via our model.

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Dual-phase-lag model for rapid solidification of undercooled melts

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Abstract

It is well known that wide range of novel material properties can be obtained by rapid solidification of undercooled melts [1]. The evolution of solidification (nucleation and precipitation) is governed by the conditions of crystal growth. Rapid solidification leads to a significant deviation from local equilibrium within a diffuse interface and the classical transport equations of parabolic type is no longer valid. In this case a solute diffusion process in the interface and within bulk phases can be described by Maxwell-Cattaneo type constitutive equation. Thermodynamically consistent models of such processes are based on the formalism of extended irreversible thermodynamics [2-4]. In this report we consider more general model of rapid solidification based on the dual-phase-lag constitutive equation. Using dual-phase-lag diffusion equation, we generalize model for rapid solidification of undercooled melts. We show that within the framework of the proposed thermodynamic formalism the dual-phase-lag equation can be obtained [5-7].

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Experimental findings on 'thermal noise' of oscillators in non-equilibrium steady-states

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Abstract

The thermal noise is often a limit to high sensitivity experimental apparatus such as ground-based gravitational wave (GW) detectors: these are macroscopic instruments with displacement sensitivity approaching the limit set by the uncertainty principle. From the thermodynamic viewpoint, GW experiments are usually modeled as equilibrium systems, but it is doubtful that this description is justified. To assess this issue, we have conducted a systematic experimental campaign to investigate the spontaneous vibration fluctuations of low-loss mechanical oscillators in non-equilibrium steady-states. We show the experimental findings and discuss the conclusions we can infer for the gravitational wave detectors and in general for the statistical mechanics of non-equilibrium systems.

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Heat transfer in nanostructured dielectric mirrors

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Abstract

“Perfect mirrors” are usually called the dielectric mirrors because of their high reflectivity. Multilayers of alternating periodic refraction index conform the structure of these mirrors. The light that propagates in these structures interacts with its periodic refractive index, that generates wavelength gaps of forbidden transmission. If these structures are fabricated with ideal materials we obtain ideal mirrors or filters. However most of the materials present absorption but in these dielectric mirrors the absorption is almost negligible. In this work the heating of nanostructured dielectric mirrors because of absorption was measured using a thermographic technique. We present experimental results of comparing the temperature evolution after sunlight hits different metallic and dielectric mirrors. The dielectric mirrors were fabricated with multilayers of porous silicon a nanostructured material. We discuss the temperature evolution through heat transport in a multilayers system.

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Steady-state, simultaneous two-phase flow in porous media: An experimental study

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Abstract

We report on experimental studies of steady-state two-phase flow in a quasi-two-dimensional porous medium. The wetting and the nonwetting phases are injected simultaneously from alternating inlet points into a Hele-Shaw cell containing one layer of randomly distributed glass beads, initially saturated with wetting fluid. The high viscous wetting phase and the low viscous nonwetting phase give a low viscosity ratio $M = 10^{-4}$. Transient behavior of this system is observed in time and space. However, we find that at a certain distance behind the initial front a "local" steady-state develops, sharing the same properties as the later "global" steady state. In this state the nonwetting phase is fragmented into clusters, whose size distribution is shown to obey a scaling law, and the cutoff cluster size is found to be inversely proportional to the capillary number. The steady state is dominated by bubble dynamics, and we measure a power-law relationship between the pressure gradient and the capillary number. In fact, we demonstrate that there is a characteristic length scale in the system, depending on the capillary number through the pressure gradient that controls the steady-state dynamics. We have further studied the reversibility of the steady state by changing the injection rate and then returning back to the original injection rate.

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Steady-State Two-Phase Flow in Porous Media: Open Questions

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Abstract

Whereas instabilities during injection of a fluid into a porous medium already saturated with another fluid immiscible with respect to the first, have been extensively studied, the simultaneous flow of two immiscible fluids under steady-state conditions have been received surprisingly little attention.

We will in this talk present a number of phenomena and open questions - and some attempts at answering them. Among the questions we pose is what happens to the interface between two immiscible fluids flowing in parallel; is the Darcy equation (the equivalent of Ohm's law) valid when capillary and viscous forces compete – and what should replace it; can one use non-equilibrium thermodynamics to describe the macroscopic parameters characterizing the flow?

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Open chemical systems and their biological function

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Abstract

We introduce stochastic Delbruck-Gillespie process, whose Kolmogorov forward equation is known as the Chemical Master Equation and its trajectories can be sampled via the Gillespie algorithm, for nonlinear chemical reactions dynamics inside a small aqueous volume such as a biological cell. Using this formalism, we (1) illustrate the relation between nonlinear bistability with saddle-node bifurcation and first-order phase transition; (2) introduce a far-from-equilibrium thermodynamic theory for free energy, entropy and entropy production; (3) show how an analytical mechanics (i.e., Lagrangian and Hamiltonian systems) arises. We suggest the inter-attractional stochastic dynamics as a possible mechanism for isogenetic variations in cellular biology, and present a Kramers' like formula for the rate of epigenetic phenotype switching.

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Heat Dissipation and Self-consistent Nonequilibrium Thermodynamics of Open Driven Systems

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Abstract

Nonequilibrium thermodynamics of a system in a sustained environment with influx and efflux is usually treated as a subsystem of a large closed “universe”. It is still in doubt whether there could be a satisfactory nonequilibrium thermodynamics of such an open driven system, which is solely established on its internal dynamics without involving any details of the surrounding. We show here that the perspective of a real driven nonequilibrium steady-state (NESS) sustained by ideal external regenerating systems would accomplish this object. Using the master-equation description of motor protein with and without regenerating systems as an example, we illustrate that they have identical kinetics as well as the traditional Second Law with positive entropy production rate. However, the concept of heat in the First Law is more subtle; still their difference in heat dissipation is just the minimum work that needed for the external energy regenerating system to keep the NESS (e.g., maintaining constant concentrations of ATP, ADP and Pi). This interpretation makes the heat dissipation in the NESS perspective be well defined from the equations of internal dynamics. Moreover, for systems approaching an NESS, the non-negative rate of relative entropy change gives rise to the concept of housekeeping heat, which is the ensemble averaged difference between the NESS heat dissipation and NESS entropy change within each transition. Hence this new perspective yields an extended Second Law, which emerges only from driven dynamics with external regenerating system. Our theory shows consistency and contradistinctions in thermodynamics of energy transduction and heat dissipation in the two different perspectives of nonequilibrium systems, a la Clausius and Kelvin. Furthermore, it suggests new ingredients for the thermodynamics of self-organization in driven systems.

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Multiscale Guldberg-Waage-Onsager Dynamics in Small Systems

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Abstract

Dynamics of chemical reactions, called mass-action-law dynamics, is extended to include inertia and to account for fluctuations. In the first extension the reaction fluxes or forces join mole numbers to form the set of independent state variables. Distribution functions of these variables then play the role of independent state variables in the second extension. All the time evolution equations arising in the paper are proven to be compatible among themselves and with equilibrium thermodynamics. A quantity closely related to the entropy production plays in the extended dynamics with fluxes and forces as well as in the corresponding to it fluctuating dynamics the role that entropy plays in the original massaction- law dynamics.

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Generalized Transport Equations for Heat Transfer in Nanosystems: Nanowires and Plane Sheets

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Abstract

Fourier's law for heat conduction is valid for experimental times longer than the average collision time and for length scales longer than the mean-free path. Here, we present some generalized heat transport equations incorporating non-vanishing collision time and mean-free path, and we discuss several aspects of those equations. We apply them to two physical situations: nanowires (silicon nanowires and metallic nanowires) and plane sheets (silicon layers and graphene sheets). In nanowires, those equations lead to a Fourier's equation with a size-dependent thermal conductivity: thus, in this situation Fourier's law is apparently very successful, but at the condition of suitably redefining the thermal conductivity, which is one of the main topics in heat transport in nanosystems. In contrast, in plane sheets, in radial heat transfer from a central heat source (a topic of interest for the refrigeration of nanodevices), the influence of non-local terms cannot be reduced to an effective Fourier's transport equation. Therefore, we deal also with this radial situation because it may contribute to clarify about the limits of Fourier's law. In particular, we deal with: a) influence of boundary conditions (smooth walls or rough walls) and their role on the effective thermal conductivity of nanowires; b) relative role of phonon and electron heat transfer in metallic nanowires and the conditions of validity of Wiedeman-Franz's law in metallic nanowires; c) compatibility of those equations with the second law, especially in a size domain comparable to the mean-free path; d) dynamical aspects related to thermal wave propagation.

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Nonequilibrium thermodynamics for dissipative quantum systems

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Abstract

The one and only point of this presentation is to convince the audience that, in the course of this series of workshops, we have reached an understanding of classical nonequilibrium thermodynamics in terms of geometric structures that is so deep and so powerful that its generalization to dissipative quantum systems has become almost straightforward. Some remarkable features of irreversible quantum mechanics are elaborated.

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Open quantum systems coupled to classical time-evolving environments

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Abstract

The theory of quantum systems coupled to their environments has fundamental interest (the measurement problem, the quantum-classical crossover etc.) as well as practical applications (e. g. quantum computers) [1].

We investigate quantum systems coupled to time-dependent classical environments using the nonlinear thermodynamic master equation [2]. We demonstrate how large the influence of nonlinearity is by comparing our results with linear master equations.

We show how dynamics of a classical environment affects quantum properties of a system, such as the coherence and the entanglement as well as the energy and how it can be used to control them. We also show how the feedback changes the classical evolution. We answer a highly debated question whether quantum systems coupled to non-equilibrium thermodynamic environments can be considered as non-Markovian or not.

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A mesoscopic description of reactions far from equilibrium

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Abstract

Chemical cycle kinetics is customarily analyzed by means of the law of mass action which provides a description of the rates of transformation of the substances. The connection of this description with non-equilibrium thermodynamics has traditionally been restricted to the linear domain in which reaction rates are proportional to the thermodynamic forces, the affinities. We show, by a pertinent analysis of the second law, that the connection between both approaches is deeper than thought as also holds in the nonlinear domain, for higher values of the affinities. This new perspective shows how to overcome the inherent limitation of classical non-equilibrium thermodynamics in treating cyclic reactions, providing a description of free energy transduction processes in chemical and bio-chemical closed and open cycles by means of thermodynamic principles.

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Fluctuating hydrodynamics for chemically reacting mixtures

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Abstract

The thermodynamic study of chemical reactions and activated processes can be consistently formulated in the framework of non-equilibrium thermodynamics. The non-linear character of chemical reactions requires a detailed analysis of the kinetics associated to how reactants convert into products to recover the law of mass action. To this end, one needs an enhanced variable space, which we will describe making use of Mesoscopic Non-Equilibrium Thermodynamics¹. We will show that this description allows for a proper coupling between the non-linear kinetics of activated processes and spatial diffusion and convection and how thermal fluctuations can be also consistently accounted for. We will discuss that chemical reactions affect thermal transport properties such as the thermal conductivity or the Soret coefficient², and will analyze how this approach recovers the anomalous behavior of equal time correlations³ in a chemical reacting system subject to thermal gradients.

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Fick Diffusion Coefficients in Ternary Liquids from Equilibrium Molecular Dynamics

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Abstract

An approach for computing ternary Fick diffusivities directly from equilibrium Molecular Dynamics (MD) simulations is presented and demonstrated for a liquid mixture of chloroform-acetone-methanol. In our approach, Fick diffusivities are obtained from Maxwell-Stefan (MS) diffusivities and the so-called matrix of thermodynamic factors. MS diffusivities describe the friction between different molecular species and can be directly computed from equilibrium MD simulations. The thermodynamic factor is the concentration derivative of the activity coefficient describing the deviation from ideal mixing behaviour. It is important to note that all mutual diffusion experiments measure Fick diffusion coefficients, while previous equilibrium molecular dynamics simulation did only provide MS diffusivities. The required thermodynamic factor to convert MS into Fick diffusivities and vice versa, however, has been difficult to extract from both simulations and experiments leaving a gap between theory and applications. Here, we extend an efficient computing scheme for the thermodynamic factor recently proposed by the us for ternary complex mixtures [1]. The novel computing scheme extracts the thermodynamic factor from density fluctuations in small subsystems embedded in a larger simulation box. The computed thermodynamic factor is in excellent agreement with experimental VLE data as well as calculations using the COSMO-SAC method. Our approach provides an efficient route to obtain multicomponent diffusion coefficients in liquids based on a consistent molecular picture and therefore bridges the gap between theory and experiment.

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Heat transfer in zeolites determined from non-equilibrium molecular dynamics simulations

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Abstract

The thermal conductivity of complex crystalline materials is an interesting property, though it can be difficult to determine both experimentally and computationally. Zeolites are one such material, with its wide selection of structures, and multitude of pores, channels, and cavities. In this work we have used non-equilibrium molecular dynamics (NEMD) simulations to study the heat conductivity of a wide range of zeolite systems.

The NEMD method induce a thermal gradient in the system, by simulating elastic collisions between particles in different parts of the simulation box, as described by Müller-Plathe[1]. The heat flux, J_q is determined directly from the transferred amount of heat, the heat conductivity directly follows from the temperature gradient which is calculated in the simulation:

$$\lambda = -\frac{J_q}{dT/dx} \quad (2)$$

Using simulations, we are able to determine how this conductivity depends on the loading of the zeolite, the forcefield parameters, and the orientation of the crystal. We find that the orientation of the zeolite is very important, and in some cases, the conductivity can be twice as large in one crystallographic direction.

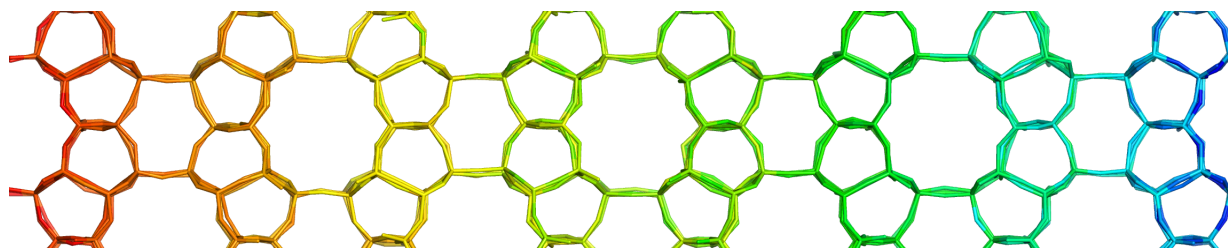


Figure 1: Temperature in FER zeolite, under a temperature gradient. The outer left- and right part of the system is perturbed, and the centre region has a linear temperature-profile.

Conclusion

Using non-equilibrium molecular dynamics, we can screen zeolites, and study the mechanisms for heat transfer in different zeolite structures. The method gives results comparable to experimental results, while the method is not very computationally intensive.

Acknowledgement

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Dynamics of complex fluid-fluid interfaces

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Abstract

Surface rheological properties often play an important role in the stability and stress-deformation behavior of emulsions, foam, biological fluids, or immiscible blends [1]. This is particularly true when the interfaces in these systems have a complex microstructure, for example, when the surface active components stabilizing the interface form a 2d gel phase, a 2d glass phase, or 2d (liquid) crystalline phase. Applied deformations induce changes in the microstructure of the interface, and the resulting changes in the surface rheological properties (such as surface shear thinning and thixotropic behavior) affect the behavior of the multiphase system on a macroscopic scale. Most currently available constitutive models for the surface extra stress tensor either do not account for the strain (rate) dependence of surface rheological properties, or are appropriate only for infinitesimally small rates, where departures from linear behavior are very small [1]. In this paper we will discuss recent advances in the development of nonlinear constitutive equations for the stress-deformation behavior of fluid-fluid interfaces in the framework of nonequilibrium thermodynamics (NET). Using the classical irreversible thermodynamics (CIT) framework, and the general-equation-for-the-nonequilibrium-reversible-irreversible-coupling (GENERIC) framework, we construct models that describe the effect of microstructural changes on the nonlinear response of an interface to a deformation through a dependence of the surface stress tensor on a set of scalar and a tensorial structural variables. We present the time evolution equations for these structural variables, and evaluate the ability of these types of models to describe shear thinning behavior of an interface stabilized by anisotropic colloidal particles in both simple and oscillatory shear. We find that both frameworks allow us to construct nonlinear expressions for the surface extra stress tensor capable of describing the shear thinning behavior observed experimentally for this type of interface, but the CIT model gives realistic predictions only for small departures from equilibrium, whereas the GENERIC framework allows us to create models valid also far from equilibrium. These results show that microstructural models developed using NET provide a valuable tool for the analysis of the highly nonlinear dynamics of multiphase systems with complex liquid-liquid interfaces.

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On the (im-) possibility of cold to warm distillation

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Abstract

Irreversible thermodynamics provides interface conditions that yield temperature and chemical potential jumps at phase boundaries. The interfacial jumps allow unexpected transport phenomena, such as the inverted temperature profile [Pao, *Phys. Fluids* 14, 306-312 (1971)] and mass transfer from a cold to a warm liquid driven by a temperature difference across the vapor phase [Mills & Phillips, *Chem. Phys. Lett.* 372, 615–619 (2002)]. Careful evaluation of the thermodynamic laws has shown [Bedeaux, Hermans & Ytrehus, *Physica A* 169, 263-280, 1990] that the inverted temperature profile will be observed for processes with a large heat of vaporization. We show that cold to warm mass transfer through the vapor from a cold to a warm liquid is only possible when the heat of evaporation is sufficiently small, as long as the vapor layer thickness is relatively small. Investigation of the overall experimental apparatus and the non-equilibrium interface conditions allows to estimate the maximum vapor layer thickness that would permit this particular transport mode.

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Local equilibrium for interfaces and gauge transformations verified by simulations

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Abstract

The classical approach to equilibrium interfacial thermodynamics in phase coexistence describes the interface as a separate two dimensional thermodynamic system characterized by excess densities. Gibbs' original formulation relies on the uniformity of intensive variables throughout the system. Therefore, it cannot be directly applied to nonequilibrium situations such as evaporation/condensation processes or heterogeneous catalysis, where jumps in temperature and chemical potential across the interface can occur.

We present a conceptually clear formulation of local equilibrium for interfaces [1]. In particular, we gain new insights by formulating, in terms of gauge transformations, the ambiguity in locating the interface. This notably allows us to generalize the Clapeyron relationships to nonequilibrium situations. We support our theoretical predictions by performing stringent tests with extensive nonequilibrium molecular dynamics simulations.

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Nonlinear and compatible with thermodynamics coupling of chemical kinetics with mechanics

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Abstract

Motivated by biological applications (e.g. bone tissue development and regeneration) we investigate coupling between chemical kinetics and mechanics. Solutions to the coupled system of time evolution equations are required to agree with thermodynamics. Rate coefficients arising in the resulting modification of the law of mass action appear to depend in an appropriate way on the fields describing mechanics. Predictions of the extended nonlinear chemical kinetics are compared with predictions of the previously developed linear extension (valid only near chemical and mechanical equilibrium) and with results of experimental observations of certain biological systems.

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The Vortex Tube of Ranque and Hilsch Thermodynamic Foundations and New Applications

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Abstract

In the Vortex Tube by Ranque (1931) and Hilsch (1945) a pressurized flow of gas or vapor is expanded and separated in two partial flows the temperatures of which are respectively above and below the temperature of the incoming flow (vortex tube effect). Some basic physical aspects of this separation process will be discussed.

Also , a simple thermodynamic model will be described allowing to calculate the temperatures of the outgoing partial fluid flows at given conditions of the entrance flow and a characteristic parameter of the vortex tube.

The tube can be used to increase on principle the coefficient of performance (COP) of a variety of engineering cycle processes like the Clausius - Rankine-process, compression – refrigeration - and heat pump - processes. It also may be applied in air separation or gas purification processes like the Skarstrom pressure swing adsorption process to increase the yield flow or to reduce energy demands of these processes.

Several examples will be presented in brief, some of them including a (patented) Thermo – Valve which is kind of an augmented vortex tube allowing to expand compressed liquids non - isenthalpically, i.e. with simultaneous gain of heat. Preliminary calculations and experiments have shown that this non-isenthalpic liquid expansion process can be of economic interest in refrigeration cycles using carbon dioxide (CO₂) as working fluid and then may increase the COP of the process by (5-10)%

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Macroscopic convective phenomena in non-uniformly heated liquid mixtures

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Abstract

Thermal non-stationary convection of binary and multi-component liquid mixtures in thin channels of different configurations was investigated experimentally and theoretically. Connected channels and Hele-Shaw cell with boundaries of high heat conductivity were used as working cavities. Experiments were held with the following mixtures: 1) carbon tetrachloride (CCl_4) in decane ($\text{C}_{10}\text{H}_{22}$), 2) aqueous solutions of sodium sulfate (Na_2SO_4), 3) water-ethanol mixtures, 4) magnetic fluid (stable colloidal suspension of ultra-fine ferromagnetic particles in kerosene).

It was shown that over the threshold of convection specific "flop-over" oscillatory flows with very large period take place in the cases of binary molecular mixtures with normal thermodiffusion (1, 2) and magnetic fluids with different concentration of particles (4-12%). Direct numerical simulation on the base of hydrodynamics equations confirmed to results of experiments. On the other hand stationary convective flow was settled in molecular mixtures with anomalous thermodiffusion (3) that also was verified by the numerical calculations.

Physical mechanisms were suggested to explain observed phenomena. According to our point of view the complex "flop-over" oscillatory regimes in binary molecular mixtures with normal thermodiffusion are determined by division of components in horizontal plane when the liquid moves predominantly along vertical heat-conducting boundaries of a cavity [1].

Analogously to molecular mixtures periodic change of flow direction in magnetic fluid is explained by molecular thermodiffusion of kerosene components and depends on weak effect of particles sedimentation. During numerical modeling there was no reason to take into account thermodiffusion of particles to describe the experiments with magnetic colloids.

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Liquid-vapour interface transfer coefficients of a two-component mixture

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Abstract

Exchanges of mass and energy between different bulk phases occur through interfaces and surfaces. The mass and energy transfers could be well described in bulk phases using the non-equilibrium thermodynamics; its extension to interfaces was systematically investigated the last ten years using molecular dynamics simulation [1]. Evaporation / condensation processes are endothermic / exothermic phenomena, as a consequence the surface exhibits large couplings between heat and mass transfer, stronger than in the adjacent bulk phases. This effect strongly influences the dynamics of evaporation / condensation. In the presentation after a short overview of the entropy production expressions and the transport equations applied to surfaces, molecular dynamics results of a liquid-vapor system of a two-component mixture composed of Lennard-Jones atoms submitted to external heat and mass fluxes [2] will be shown. Comparing with equilibrium simulations, it was verified that the local equilibrium hypothesis was valid for the whole surface, which is an important hypothesis of non-equilibrium thermodynamics. Based on the transport equations, the transfer coefficients, i.e. the resistivities to heat and mass transfer and their coupling were then computed using direct method and the integral relations. Like for the one component systems, the results show the large thermal diffusion effects that cannot be neglected in order to model the dynamics of evaporation / condensation, adsorption / desorption processes.

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Coupled heat and mass transfer during crystallization

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Abstract

Crystallization takes place and is a key factor in a large variety of industrial and chemical processes such as pharmaceutical production, food processing, or petrochemical production. Control of crystal growth mechanisms is essential in order to obtain the desired product purity and quality. Crystallization is a pure thermodynamic process where coupled heat and mass transfer depend on the local supersaturation, i.e. the responsible driving force for crystal growth. Supersaturation depends on the local temperature and concentration. Therefore, in order for the crystal surface to develop, the surrounding liquid interface must be supersaturated. In the case of exothermal crystallization these conditions mean lower temperature and higher concentration than the equilibrium temperature and concentration values. An exothermal crystallization process occurs because the system changes to a lower energy state liberating this excess of energy to the surroundings. This heat release during crystallization creates an increase of temperature on the local front of the growing crystal affecting the local supersaturation, density and viscosity, thus crystal growth and heat diffusion. On the other hand, these variables are coupled to the mass transfer, as these changes directly affect mass diffusion and therefore the local concentration gradients. Detailed knowledge of these coupling effects and their impact on development of the interface is necessary to control growth rates, impurity uptake, morphology and crystal structure and defects.

To achieve such knowledge, in situ measurements of the developing crystal solid-liquid interface were undertaken. In order to obtain the local temperature field fluctuations surrounding a growing crystal, Liquid Crystal Thermometry was used and simultaneous image data was acquired, documenting the growth rate of the crystal in a temperature gradient. The flux-force relations were described using non-equilibrium thermodynamic theory for the heterogeneous system, and the corresponding transport coefficients were determined (diffusion coefficients and heat of transfer).

The experimental setup consisted of a cubic quartz cell with a Thermochromic Liquid Crystal sheet in the middle. On the squared bottom of the cell was a square, flat heat exchanger surface and on the top of the cell two orifices which allow introduction or extraction of solution and possible volume expansion. The whole cell was thermally insulated from the exterior by a double wall. The gap was under vacuum or filled by argon gas. The Thermochromic Liquid Crystal sheet was illuminated by a cold white light source and pictured with a 3 Mega pixel digital color camera. Images were post-processed to obtain temperature fields and corresponding growth rates. Experiments are reported on crystallization of ice in different aqueous solution concentrations keeping the same heat exchanger surface temperature. The results showed a direct relation between different crystal growth rates, morphology and structure of ice and development and thickness of the thermal boundary layer interface surrounding the crystal growing surface. This can be explained by coupling of mass and heat fluxes.

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Thermodynamic analysis of irreversibilities in thin heat conducting films

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Abstract

The size of dielectric and semiconductor based devices has become of the order of the phonon's mean free path or smaller with new technologies. Their performance however is affected by the high operation temperatures reached due to their reduced sizes. The sources of irreversible processes must then be studied in order to improve operation conditions to assure an optimal functioning. In this work we undertake the theoretical analysis of the entropy production in heat conducting thin films from the point of view of Linear Irreversible thermodynamics. The experimentally observed reduction of the thermal conductivity with the thickness of the film is considered in the description through the use of an expression obtained on Boltzmann equation grounds. The fluctuating nature of heat flux is described by introducing proper stochastic terms in the constitutive heat flux equation. Besides the entropy generation for different thickness of the conducting film we study the group velocity of Fourier modes, the response of the system under external temperature gradients and the spectrum of temperature fluctuations. Our findings allow us to feature a kind of dynamical phase transition when the film thickness equals the mean free path of phonons.

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Resonant Response in Non-equilibrium Steady States

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Abstract

The time-dependent probability density function of the order parameter of a system evolving towards a stationary state exhibits an oscillatory behavior if the eigenvalues of the corresponding evolution operator are complex. The frequencies ω_n , with which the system reaches its stationary state, correspond to the imaginary part of such eigenvalues. If the system (at the stationary state) is further driven by a small and oscillating perturbation with a given frequency ω , we formally prove that the linear response to the probability density function is enhanced when $\omega = \omega_n$ for $n \leq N$. We prove that the occurrence of this phenomenon is characteristic of systems that are in a non-equilibrium stationary state. In particular we obtain an explicit formula for the frequency- dependent mobility in terms of the relaxation to the stationary state of the (unperturbed) probability current. We test all these predictions by means of numerical simulations considering an ensemble of non-interacting overdamped particles on a tilted periodic potential.

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Thermodynamical Model of Thermoelastic Interaction in Media of Anomalous Material Properties and Unconventional Thermoelastic Damping

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Abstract

Dynamical irreversible processes running in the condensed matter are always accompanied by energy dissipation. The main reason of such fact comes from internal structure of material bodies. Changes of crystal symmetry, production of defects like dislocations, vacancies, evolution of grain boundaries, internal friction, phase transitions, and the like that occur in various media decide about rate, quality and quantity of that dissipation. Also a geometry of a material is responsible for the irreversibility of the dynamical processes.

From the thermodynamical point of view the above properties are described mainly by constitutive theories.

In the paper we focus on a constitutive theory in a nonlinear thermoelastic isotropic solid within the extended thermodynamical model. Stress-strain-temperature relations for materials of so-called normal and negative properties (negative Poisson's ratio and the negative heat expansion coefficient) have been considered.

That theory can be implemented to unconventional description of the thermoelastic damping phenomenon observed in thermoelastic materials of finite extent. Material nonlinearity and negative properties have been also taken into considerations. The theory concerns a situation when instead of the common thermal transfer there occurs also an additional heat flux coming from periodic deformation (different parts of the body are alternatively compressed and extended causing that sometimes a problem becomes 2D-3D). Hence an additional dissipation coming from the thermoelastic damping has been observed. Moreover, an unconventional thermoelastic hysteresis effects have been described.

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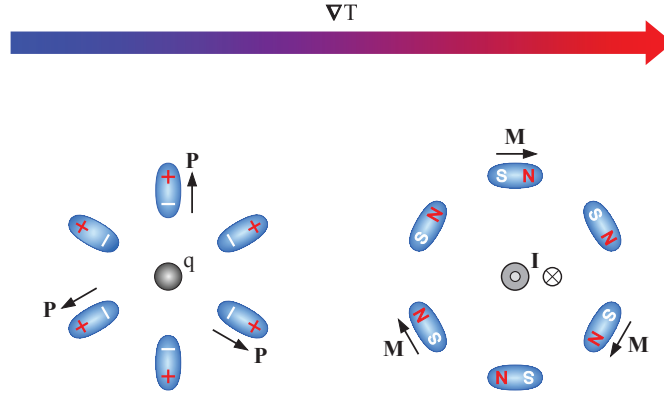
Thermodynamics of continuous media with permanent electric polarisation and permanent magnetisation

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Abstract

In order to understand the interplay between charge, spin and heat current, we decided to establish the thermodynamics of continuous media with permanent polarisation and permanent magnetisation in the presence of electromagnetic fields.



At local thermal equilibrium between the matter and the electromagnetic fields, we derived explicit expressions for the temperature and chemical potentials in terms of the electromagnetic fields, the permanent electric polarisation and the permanent magnetisation, i.e.

$$T(s, n, \vec{P}, \vec{M}, \vec{D}, \vec{E}) = T^{\text{mat}}(s, n) + \frac{1}{2} \frac{\partial \overset{\leftrightarrow}{\varepsilon}^{-1}}{\partial s} \cdot (\vec{D} - \vec{P}) \otimes (\vec{D} - \vec{P}) + \frac{1}{2} \frac{\partial \overset{\leftrightarrow}{\mu}^{-1}}{\partial s} \cdot (\vec{B} - \mu_0 \vec{M}) \otimes (\vec{B} - \mu_0 \vec{M}) ,$$

$$\mu(s, n, \vec{P}, \vec{M}, \vec{D}, \vec{E}) = \mu^{\text{mat}}(s, n) + \frac{1}{2} \frac{\partial \overset{\leftrightarrow}{\varepsilon}^{-1}}{\partial n} \cdot (\vec{D} - \vec{P}) \otimes (\vec{D} - \vec{P}) + \frac{1}{2} \frac{\partial \overset{\leftrightarrow}{\mu}^{-1}}{\partial n} \cdot (\vec{B} - \mu_0 \vec{M}) \otimes (\vec{B} - \mu_0 \vec{M}) .$$

Our thermodynamical approach leads to more general coupling terms in the linear phenomenological relations than those obtained earlier for the thermodynamics of continuous media with electromagnetic fields by de Groot and Mazur (S. R. de Groot and P. Mazur, *Non-equilibrium thermodynamics* Dover: New York, (1984)). As an example, our general formalism describes properties of electrorheological fluids: a non-uniform electric field generates a dissipative shear stress, i.e.

$$\overset{\leftrightarrow}{\sigma}^{\text{mat}} = \overset{\leftrightarrow}{\beta}_P(s, n, \vec{P}, \vec{M}, \vec{D}, \vec{E}) \cdot (\vec{\nabla} \otimes \vec{E}) .$$

Similarly, it describes properties of magnetorheological fluids: a non-uniform magnetic field generates a dissipative angular stress, i.e.

$$\overset{\leftrightarrow}{\Theta} = \overset{\leftrightarrow}{\beta}_M(s, n, \vec{P}, \vec{M}, \vec{D}, \vec{E}) \cdot (\vec{\nabla} \otimes \mu_0 \vec{H}) .$$

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Poster presentation

Otto and Diesel cycles modeled by considering non-instantaneous adiabats

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Abstract

In the context of the so-called finite time thermodynamics have been studied two ways of analyzing the performance of the thermodynamic cycles: when the cycle is considered internally reversible, endoreversible cycle, and when the cycle is considered with internal irreversibilities, non-endoreversible cycle. The total cycle time regarded is as the sum of the times of the non-adiabatic processes, where they appear, assuming these as the total cycle time of cycle, so it is assumed that the adiabatic processes are practically instantaneous. The Curzon-Ahlborn cycle¹, Otto cycle and Diesel cycle have been analyzed in this way, in the context of finite time thermodynamics²⁻⁴. However, as it is known, the adiabatic processes are idealizations of real processes, and there is not guarantee do not lose heat by radiation or working substance internally stop using some amount of heat during these processes. Thus, Otto and Diesel cycles are idealizations that describe approximately the behavior of real internal combustion, which are open systems whose working substance is a mixture of substances (air+fuel), studied in this way in texts of classical equilibrium thermodynamics^{5,6}.

In the present paper we propose a simple procedure to obtain alternative expressions for power output and thermal efficiency for the Otto and Diesel cycles, including time for adiabatic processes in the cycle, despite being very small as these, it may take into account to obtain theoretical results for more in line with reality. In case of Curzon-Ahlborn cycle, some authors have proposed a way to take into account the duration of adiabatic processes^{7,8}, so that they can obtain approximate expressions of the power function with a parameter that includes the compression ratio. The time for adiabatic processes is proposed by comparing the adiabatic and the isothermal work and assuming the same thermal engine model discussed in references 2 and 3.

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Thermodynamic Optimization of Two-Stage Peltier Modules: Structure and Exergy

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Abstract

In this work we undertake the theoretical analysis of a two-stage semiconductor thermoelectric module (TEM) which contains an arbitrary and different number of thermocouples, n_1 and n_2 , in each stage (pyramid-styled TEM). The analysis is based on a dimensionless entropy balance set of equations. We study the effects of n_1 and n_2 , the flowing electric currents through each stage, the applied temperatures and the thermoelectric properties of the semiconductor materials on the exergetic efficiency. Our main result implies that the electric currents flowing in each stage must necessarily be different with a ratio about 4.3 if the best thermal performance and the highest temperature difference possible between the cold and hot side of the device are pursued. This fact had not been pointed out before for pyramid-styled two stage TEM. The ratio n_1/n_2 should be about 8.

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A comparative analysis of efficiency a maximum power output for some heat engines

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Abstract

In this work, we present a comparative analysis of the efficiencies at maximum power out for different devices; first, we analyze the expressions of the efficiency at maximum power for two models of heat engines: a model of Curzon-Ahlborn (macroscopic) and a Novikov model, in these two cases, two kinds of heat transfer laws were considered; one, a heat transfer due to free convection described by Newton's Law of cooling and two, a phenomenologic heat transfer comes from linear irreversible thermodynamics. On the other hand, we present the efficiencies at maximum power for stochastic (mesoscopic) heat engines obtained by Schmiedl and Seifert and presented in EPL 81 20003 (2008), also we compared these efficiencies with the results presented recently by Esposito et al. published in Phys. Rev. Lett. 105, 150603 (2010). For comparing, we expanding the expressions of efficiencies up to the third-order term of η_c , were η_c is the efficiency of Carnot ($\eta_c = 1 - T_2/T_1$). We found some interesting similarities for the expressions of efficiencies between the macroscopic and mesoscopic models of heat engines.

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Equilibrium Instability from Cooperative Interactions in a System of Brownian Agents

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Abstract

We show, by building a minimal Vicsek's inspired model, that cooperative interactions among Brownian agents, as those used in modeling "flocking behavior," leads to instability of the thermodynamic branch characterized by a vanishing average direction of motion (disordered phase) of the system. At a critical value of the coupling, the system develops a global nonvanishing particle current (cooperative behavior) taking the system far from the equilibrium branch.

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Simulation techniques for the nonlinear thermodynamic quantum master equation

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Abstract

The great majority of quantum systems exposed to non-equilibrium environments are far too complex to be numerically solved at the microscopic level. To tackle this problem, various coarse-graining strategies have been developed with the central idea to reduce the degrees of freedom of the environment to few relevant variables [1]. The generally obtained linear quantum master equations suffer from multiple deficiencies such as improper relaxation behavior [2,3]. Using thermodynamic arguments, an alternative highly nonlinear equation resolving some of these issues has been proposed recently [4].

We explain here how to simulate the evolution of open quantum systems based on this recent formulation using deterministic as well as stochastic techniques [5,6]. We conclude by a numerical exploration of the thermodynamic nature of the nonlinear master equation for heat bath environments by examining the link between entropy production and loss of quantum coherence, a crucial property for nanoscale applications.

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Self-Propelling Particles as a New Challenge for the Non-equilibrium Statistical Mechanics

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Abstract

The dynamics of the systems of self-propelling particles have attracted much attention in last two decades. The minimal model which is widely used for modeling such systems is the Vicsek. In essential, these systems are represented as the mechanical systems with the nonholonomical constraints for the velocities. It has been discovered that the introduction of noise leads to the transitions between different dynamical regimes. The “microscopic“ dynamical equations for such systems are nonhamiltonian. This hinders the application of the machinery of the standard nonequilibrium theory based on the Liouville equation etc. In such situation the only way is the kinetic approach much like Boltzmann original derivation of the kinetic equation. In this contribution we represent some results on the kinetic regime of the Vicsek model the hydrodynamic limit and the relation with the Kuramoto model of the spontaneous synchronization.

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Solving the electrokinetic equations for the polarization of a charged spheroid in an alternating electric field

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Abstract

The so-called standard set of electrokinetic equations (Poisson-Boltzmann, Navier-Stokes, Conservation of mass) has been solved both analytically and numerically for spherical, cylindrical and planar geometries [1]. However most particles of interest for research are non-spherical. Most of them (ex: clays, oxides) can be modeled by either oblate or prolate spheroids. The work on the electrokinetic response of spheroidal particles is limited sofar to spheroids with very thin double layers, where analytical solutions can be obtained [2]. It is our aim to solve numerically the set of electrokinetic equations for spheroids, with no restriction on the size of the double layer. In a second step, the analytical expressions will be corrected based on the results so as to be valid for all double layer sizes, in line with the work we did for spheres [2].

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Spatial correlation of concentration fluctuations in reaction diffusion problems by the Gillespie algorithm

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Abstract

During the last decades the spectrum of thermal fluctuations in non-equilibrium thermodynamic systems has been widely studied. It has been shown that static correlations have generically long range behaviour, while the fluctuations around equilibrium states are always short ranged (except in the neighbourhood of critical points). These investigations may be helpful to elucidate whether or not there exist thermodynamic potentials out of equilibrium, and could exclude the local potentials.

Among the non-equilibrium thermodynamic states that have been studied theoretically, there are examples of binary reaction-diffusion systems in which the inverse chemical reaction and the direct chemical reaction occur through different paths, avoiding chemical equilibrium. It is hard to develop an experimental set up to verify the theoretical conclusions in this case, because it is difficult to find a two-component system whose kinetics is as simple as the ones theoretically studied. A numerical simulation could be a better way to confirm the theory for this kind of problems. More over, there are so far very few simulations that focus on non-equilibrium fluctuations. This is why a simulation of equilibrium and non-equilibrium reaction-diffusion problem is of current interest.

The Gillespie algorithm is a Montecarlo method that simulates efficiently a system of chemical reactions through the chemical master equation. Although it was developed in 1976, the interest in this algorithm has grown during the last years, particularly because of its proven utility in Biophysical problems. The Gillespie algorithm was originally conceived to describe chemical kinetics, but it can be applied to diffusion processes as well, by assuming that the diffusion of one particle from one domain of the system to other can be handled as a chemical reaction with a certain probability.

We have performed extensive simulations of one dimensional reaction diffusion problems using the Gillespie algorithm. We studied the system with an equilibrium chemical reaction (a simple association-dissociation), and as an example of a non-equilibrium reaction we studied the WOH model. We have confirmed numerically that for the equilibrium chemical reaction, spatial correlations are short ranged, while for the non-equilibrium chemical reaction spatial correlations are long ranged, as predicted by the theory.

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PEM fuel cells enhanced by gradient of surface energy of water in the membrane

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Abstract

A thermodynamic theory of mixtures [1] comparable to modern theories of mixtures [2] is developed within the framework of classical irreversible thermodynamics. Moreover, contributions of interactions between constituents of the mixture to internal energy of the mixture are extracted so that their macroscopic consequences are revealed. The theory is then applied to polymer electrolyte membranes of fuel cells. In fact, the membrane is a porous medium in which inherent gradient of surface energy of water, induced by interaction between water and the pores, could be present. Consequently, a model of the membrane [3] is developed within the presented theory of mixtures, and the effect of the gradient of surface energy in the membrane is calculated. It appears that gradient of surface energy is a very promising tool for water management in the membrane.

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Coarse-Graining of Dislocation-Mediated Plasticity

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Abstract

Many technological applications, ranging from cars to micro-electronic devices, fail due to inelastic deformation of metals. Even though there is a vast amount of knowledge on the deformation of metals, today's technological innovations towards smaller, lighter and smarter components also demand for more reliability and predictability. Therefore, new models of metal plasticity, based on microscopic descriptions, are called for. Plastic deformation in metals occurs due to the motion of dislocations, i.e. line-like defects in the crystal structure. On a discrete level, it is quite well understood what a dislocation is, how individual dislocations move under an applied stress, and how they interact. However, in engineering applications, one is interested in plastic deformation at a larger scale, and hence in the collective arrangement and motion of dislocations. We try to construct the evolution equation for the dislocation density from a microscopic description of dislocations. To that end, non-equilibrium statistical mechanics and projection-operator techniques are used for coarse graining, as also advocated in the context of the General Equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC). At present, the focus is on the calculation of the free energy.

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Nonequilibrium thermodynamics in Oil distillation

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Abstract

A nonequilibrium model for oil distillation in an adiabatic packed column is developed in this paper. The nonequilibrium model includes the calculation of the rates of mass and heat transfer between vapour and liquid phases, entropy production in a tray, entropy production by component and total entropy production rate. The necessary data of the oil mixture have been obtained at the Mexican Petroleum Institute. This oil mixture and the adiabatic column were chosen because the unit operation of oil distillation is inefficient in the industry and using a nonequilibrium model will hopefully allow us to get more information of the system than what one obtains from the conventional thermodynamics analysis. For instance, such an analysis accounts for the performance of the column quite well. In addition, to our knowledge oil distillation has not yet been analyzed from a nonequilibrium thermodynamics perspective.

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Osmosis in non-equilibrium simulations with active solute particles

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Abstract

Osmosis is a fundamental and important process, responsible for physical and biological phenomena ranging from water desalination to the flow of sap in plants. In the classic osmosis experiment, in which two solutions of differing concentration are separated by a semi-permeable membrane, an initial imbalance in the solvent chemical potentials causes solvent to flow from low to high solute concentration. This leads to the well-known osmotic pressure difference at equilibrium. We present Molecular Dynamics (MD) simulations of a non-equilibrium version of this experiment, in which the solute particles are active. This is achieved in two distinct ways: by coupling the solute particles to a separate, higher temperature thermostat or by propelling them using an external force, as a model for bacterial or colloidal swimmers. Our simulations allow us to define a new, osmotic effective temperature for the active solute particles. Furthermore, for active solutes, our simulations reveal an interesting and counter-intuitive reverse osmotic phenomenon: the active solute particles can drive solvent particles out of the more concentrated solution, in direct contrast to osmotic flow in non-active systems. Our results could have interesting implications for the likely osmotic behaviour of suspensions of active particles such as motile bacteria or colloidal "swimmers".

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On the Hamiltonian Structure of Extended Thermodynamics of Irreversible Processes

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Abstract

The conventional version of extended irreversible thermodynamics (EIT) [1-3] is based on the assumption that the generalized entropy density is a function of both usual thermodynamic variables and the corresponding dissipative fluxes. Hamiltonian structure of traditional version of EIT is considered in [1,2,4,5]. In this Note, we consider another version of extended thermodynamics [6,7], which proceeds from the postulate that entropy density is function of the usual variables and its material time derivatives. We show that Hamiltonian structure is preserved and balance laws both for usual and additional variables can be derived. Within this formalism we obtain Euler equation containing generalized temperature.

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