10th International Workshop on Non-Equilibrium Thermodynamics

(IWNET 2025)

Syros, Greece, June 08-11, 2025

Workshop Booklet

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Participants

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Organizing committee

Vlasis Mavrantzas	*University of Patras (Greece) & ETH Zürich (Switzerland)*
Antony Beris	*University of Delaware (USA)*
Kostas Housiadas	*University of the Aegean (Greece)*

Scientific Committee

Gian Paolo Beretta	*Università di Brescia (Italy)*
Antony Beris	*University of Delaware (USA)*
Brian J. Edwards	*University of Tennessee (USA)*
Markus Hütter	*Eindhoven University of Technology (The Netherlands)*
Vlasis Mavrantzas	*University of Patras (Greece) & ETH Zürich (Switzerland)*
Michal Pavelka	*Charles University (Czech Republic)*
Pep Español	*University Institute of Distance Education (Spain)*

Web site *https://mathweb.aegean.gr/iwnet2025*

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Welcome to:

The 10th International Workshop on Non-Equilibrium Thermodynamics

(IWNET 2025)

Non-equilibrium thermodynamics aims at understanding and describing the dynamics of out-of-equilibrium systems, particularly in connection to relaxation towards equilibrium. Non-equilibrium thermodynamics has seen over the past few decades significant new developments and still remains a vibrant field of research, contrary to equilibrium thermodynamics, with substantial challenges regarding open issues that await to be resolved.

To foster a profound comparison between different approaches to non-equilibrium thermodynamics, to unify existing ones, and to identify challenges and possibly concert research efforts, a series of workshops, called International Workshops on Non-Equilibrium Thermodynamics (IWNET), has been held in a regular fashion continuously since almost thirty years ago. A short overview of the history of these workshops is shown below.

Workshop	***Organized by***
1st IWNET, 1996 (Montréal, Canada)	Miroslav Grmela
2nd IWNET, 2000 (Oxford, United Kingdom)	Hans Christian Öttinger
3rd IWNET, 2003 (Princeton, USA)	Antony N. Beris and Brian J. Edwards
4th IWNET, 2006 (Rhodes, Greece)	Vlasis G. Mavrantzas
5th IWNET, 2009 (Cuernavaca, Mexico)	Mariano López de Haro and Federico Vásquez Hurtado
6th IWNET, 2012 (Røros, Norway)	Dick Bedeaux and Signe Kjelstrup
7th IWNET, 2015 (Hilvarenbeek, The Netherlands)	Markus Hütter and Ger Koper
8th IWNET, 2018 (Sint-Michielsgestel, The Netherlands)	Markus Hütter and Leonard Sagis
9th IWNET, 2022 (Victoria, Canada)	Henning Struchtrup

In this 10th IWNET workshop, particular emphasis is given (in addition to traditional topics) to areas or problems that open up new challenges and perspectives. In particular, IWNET 2025 highlights contributions in topics such as:

- fundamentals of non-equilibrium thermodynamics and new mathematical developments
- non-equilibrium thermodynamics applied to complex fluids (e.g., polymers), chemical systems (e.g., chemical waves), biological systems (e.g., blood, active matter), interfacial systems and solids
- kinetic theory of non-equilibrium systems
- multi-scale dynamics and thermodynamics
- fluctuations, stability and large system control beyond equilibrium
- input-driven networks and deep learning from non-equilibrium thermodynamics
- quantum systems and quantum dissipation
- relativistic hydrodynamics.

Honored Scientist: Professor Miroslav Grmela

A unique aspect of IWNET 2025 is that it features as honored scientist Professor Miroslav Grmela (https://www.polymtl.ca/expertises/en/grmela-miroslav), organizer of the 1st IWNET, whose pioneering contributions have revolutionized and shaped the field of Non-Equilibrium Thermodynamics.

Photo: Professor Miroslav Grmela

The 10th International Workshop on Non-Equilibrium Thermodynamics (IWNET 2025)

Venue:

The IWNET 2025 workshop takes place in:

Dolphin Bay Family Beach Resort
Galissas Beach
Syros Island, Cyclades 84100
Greece

Phone: +30 22810 42924
Email: info@dolphin-bay.gr
Web: https://www.dolphin-bay.gr

Photo: The Dolphin Bay Family Beach Resort

All scientific sessions and the luncheons will be held in the Dolphin Bay Resort. The format of the Workshop is as follows. After arrival in the afternoon/evening on Sunday (June 8), the scientific program starts on Monday morning (June 9) and ends on Wednesday (June 11) early afternoon. It consists of presentations (oral and poster) and discussion rounds. The program is rounded off by an afternoon-excursion and a workshop dinner on Tuesday (June 10).

The registration fee of the Workshop covers:

- the welcome reception (it includes drinks and a light dinner)
- coffee breaks and light lunches for all three days of the workshop
- a guided tour of the ancient city of Syros, and
- the official workshop dinner immediately after the tour.

Talks:

15 min for presentation + 5 min for discussion (honored speaker Prof. Miroslav Grmela: 40 min, invited speaker Prof. Zi-Kui Liu: 40 min).

Instructions for Authors:

Please upload your talk well before your session on the laptop in the lecture hall (use lunch and coffee breaks, test the presentation).

If you prefer to use your own laptop, please use an earlier break to check in advance that the connection works.

Some Other Important Information:

Emergency Phone numbers:

- Doctor: on call at the reception, or dial 112
- Bus station in Ermoupolis (the capital city of Syros): ask at the reception or visit: https://ktelsyrou.gr/

Local Transport

- Taxis: +30 22810 86222
- Public Busses: +30 22810 82575
- Port (in the capital city of Ermoupolis): Vasilikos Agent: +30 22810 84444 or visit: www.ferryhopper.com (to buy tickets online)

Internet codes at the Workshop Venue

- SSID: DolphinBayGuest
- Pass: welcome1

Short CV of Prof. Miroslav Grmela

Prof. Miroslav Grmela was born in Trnava (now Slovakia) on May 30, 1939. He is married to Viera and they have two daughters and four grandsons. Now he lives in Montréal, Canada.

He entered the Faculty of Nuclear Science and Physical Engineering of the Czech Technical University in Prague, Czechia, in 1956. In 1961, he received his MSc in Physics, and in 1966 his PhD in Theoretical Physics (neutron transport theory) from the Czechoslovak Academy of Sciences (under the supervision of Prof. L. Trlifaj), in Prague, Czechia.

His main interests include:

a) *Neutron transport theory* (Nuclear Research Institute of the Czechoslovak Academy of Sciences, Rez, Prague, Czechia, 1962-1969)

   Selected publications:
   - M. Grmela, Neutron Thermalization Based on Thermodynamics, J. of Nuclear Energy, Parts A, B 19, 81-89 (1965)
   - M. Grmela, J. Cermak and I. Marek, Calculation of Heterogeneity Effects in Fast Critical Assemblies, Publ. Joint Inst. for Nuclear Research, Dubna USSR 2415 (1965)
   - M. Grmela, Thermodynamical Aspects of Neutron Thermalization Theory, Kernenergie 11, 33-39 (1968)

b) Biophysics, Formation of fibrils in collagen solutions

   Selected publications:
   - M. Grmela, Z. Trnavska, S. Sitaj, and J. Malinsky, Certain Intermediate Metabolites and the Formation of Fibrils from Collagen Solution, Biochimica et Biophysica Acta 26, (1966)

c) *Kinetic theory of the van der Waals gas* (Physics Department, University of British Columbia, Vancouver, Canada, 1969-1973)

   Selected publications:
   - M. Grmela, Kinetic Approach to Phase Transition, J. Stat. Phys. 3, 347- 364 (1971)
   - M. Grmela, On the Approach to Equilibrium in Kinetic Theory, J. Math. Phys. 15, 35-40 (1974)
   - M. Grmela and L.S. Garcia-Colin, Compatibility of the Enskog-like Kinetic Theory with Thermodynamics. Part I, Phys. Rev. A 22, 1295-1304 (1980)
   - M. Grmela and L.S. Garcia-Colin, Compatibility of the Enskog-like Kinetic Theory with Thermodynamics. Part II, Chemically Reacting Fluids, Phys. Rev. A 22, 1304-1314 (1980)
   - M. Grmela, R. Rosen and L.S. Garcia-Colin, Compatibility of the Enskog Kinetic Theory with Hydrodynamics, J. Chem. Phys. 75, 5474 (1981)

d) *Rheology and thermodynamics* (Université de Montréal, École Polytechnique Montréal, 1973 –), in collaboration with P. Carreau, G. Lebon, J. Casas-Vazquez, D. Jou, and F. Chinesta

   i. *Static versus dynamic stability*
   ii. *Polymer processing*
   iii. *Hamiltonian and gradient dynamics in kinetic theory and fluid mechanics*

Selected publications:

- M. Grmela, On the Relationship between Dynamic and Thermodynamic Stability, Physica A 59, 657-671 (1972)
- M. Grmela, Common Structure, Compatibility and Complementarity of Mathematical Models of Injection Molding, Polym. Eng. Sci. 24, 673-685 (1984)
- M. Grmela, Particle and Bracket Formulations of Kinetic Equations, Contemporary Math. 28, 125-132 (1984)
- M. Grmela, Bracket Formulation of Dissipative Fluid Mechanics Equations, Phys. Letters A 102 A, 355-358 (1984)

Prof. Miroslav Grmela has been visiting Professor in the following Schools:

- Institut de méecanique, Université de Grenoble, France
- Université de Pau at des Pays de l' Adour, France
- École nationale supérieure des mines de Sophia Antipolis, France
- L' Institut Jean-Le-Rond-d' Alambert, Université Pierre-et-Marie-Curie, Paris, France
- Université de Liège, Belgium
- UAM Barcelona, Spain
- Eidgenössische Technische Hochshule, Zürich, Switzerland
- Zhou Pei-Yuan Center for Applied Mathematics, Tsinghua University, Beijing, China
- Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Department of Engineering Mechanics, Tsinghua University, Beijing, China
- Physics Department, UNICAMP, Brazil, ENSAM Paris, France
- École Centrale de Nantes, France
- University of Messina, Italy

Prof. Miroslav Grmela:

- has graduated 17 PhD students (among them Michal Pavelka)
- has written more than 200 publications
- is author / co-author of the following books:
  - ➢ H. Eslami, M. Grmela, "Polymer Nanocomposites: Non-equilibrium Thermodynamics and Rheology", Lambert Academic Publishing, Berlin (2010)
  - ➢ M. Pavelka, V. Klika, M. Grmela, "Multiscale Thermo-Dynamics", De Gruyter (2018)
- has written 4 books Chapters
- has received the 2018 S.G. Mason Award of the Canadian Society of Rheology

IWNET 2025: Program Overview

Syros, Greece, June 08-11, 2025

	Sunday	**Monday**	**Tuesday**	**Wednesday**
08:00		Opening Remarks		
08:20		M. Grmela		
08:40			Zi-Kui Liu	A. Skarlatos
09:00		M. Doi		F. Tietjen
09:20		R.E. Gonzalez-Narvaez	H.C. Öttinger	K. Ritos
09:40		R.V. Chamberlin	M. Pavelka	P.S. Stephanou
10:00		*Coffee Break*	*Discussion*	*Coffee Break*
10:20		G.D. Verros	*Coffee Break*	A.Winters
10:40		A. R. Méndez	A.L. García-Perciante	S.G. Yiantsios
11:00		X. Shang	V.G. Mavrantzas	G. Floudas
11:20		M. Sciacca	P. Ván	V. Harmandaris
11:40		*Discussion*	*Discussion*	*Discussion*
12:00		*Lunch Break*	*Lunch Break*	*Lunch Break*
14:00		F. Herrera-Castro	A. Maslechko	A. Kazakidi
14:20		J. Engler	H. Struchtrup	J. Badur
14:40		G. Chacón-Acosta	M. Colangeli	*General Discussion*
15:00		V. Votruba	B. Nadler	
15:20		*Coffee Break*	*Discussion*	
15:40		A.N. Beris	*Coffee Break*	
16:00		C. Reina	Poster Session	
16:20		B.J. Edwards		*End of the Workshop*
16:40		*Discussion*		
17:00		*Free time*		
17:20			*Break*	
17:40				
18:00	*Welcome & Registration*		*Excursion & Workshop Dinner*	
21:00				
22:30				

IWNET 2025: Detailed Program

Syros, Greece, June 08-11, 2025

Sunday, June 08, 2025

18:00-21:00 Welcome Reception & Meeting Registration

Monday, June 09, 2025

08:00 Welcome Remarks
V.G. Mavrantzas

08:10 Presentation of Honored Speaker, Professor Miroslav Grmela
A.N. Beris

Session 1: FUNDAMENTALS

08:20 Role of geometry in multiscale thermodynamics [1]
M. Grmela

09:00 Onsager principle in soft matter physics [2]
M. Doi

09:20 Diffusion process and the Prigogine's principle of minimum entropy production [3]
R.E. Gonzalez-Narvaez, M. López de Haro, F. Vázquez

09:40 Small and simple systems that favor the arrow of time [4]
R.V. Chamberlin

10:00 *Coffee Break*

Session 2: TRANSPORT PHENOMENA

10:20 On the axioms of heat transfer and multi-component diffusion in the Euclidean space [5]
K. Dubey, B. Tiwari, D. Thapliyal, R.K. Arya, G.D. Verros

10:40 On the Chapman–Enskog solution and its relation with first-order dissipative fluid theories [6]
A. R. Méndez, A. L. García-Perciante, O. Sarbach

11:00 Stochastic Norton dynamics: An alternative approach for the computation of transport coefficients in dissipative particle dynamics [7]
X. Wu, X. Shang

11:20 Nonlinearity in the heat transport models [8]
Michele Sciacca

11:40 *Discussion*

12:00 *Lunch Break*

Session 3: CHEMICAL REACTIONS - EVOLUTION

14:00 Variational approach to chemical reactions beyond local equilibrium [9]
F. Herrera-Castro, J. Antonio del Río Portilla

14:20 Chemical kinetics of Lennard-Jones cluster isomerization using the Onsager – Machlup action [10]
J. Engler, M. Pavelka

14:40 Study of the entropy production density of reversible reaction-diffusion models in narrow channels [11]
G. Chacón-Acosta, M. Núñez-López

15:00 Recognizing Generalized Gradient Dynamics by Means of Machine Learning [12]
V. Votruba, M. Pavelka

15:20 *Coffee Break*

Session 4: INTERNAL VARIABLES

15:40 A thermodynamically consistent framework for the inclusion of micro-inertia in complex materials flow models [13]
A.N. Beris, B. J. Edwards

16:00 A statistical mechanics framework for thermodynamics with internal variables and its application to phase transforming systems [14]
T. Leadbetter, P.K. Purohit, C. Reina

16:20 Methodology for incorporating constraints into Poisson and dissipation bracket theory [15]
B.J. Edwards and A.N. Beris

16:40 *Discussion*

17:00 *End of 1st day*

Tuesday, June 10, 2025

Session 5: EMERGENCE

08:40 Zentropy, free energy landscape, and non-equilibrium thermodynamics [16, INVITED]
Zi-Kui Liu

09:20 Is irreversibility emergent? Is irreversibility doomed? [17]
H.C. Öttinger

09:40 On the emergence of non-equilibrium thermodynamics from Hamiltonian mechanics [18]
K. Mladá, M. Pavelka, V. Klika

10:00 *Discussion*

10:20 *Coffee Break*

Session 6: RELATIVISTIC APPLICATIONS

10:40 Relativistic dissipative fluids in the trace-fixed particle frame: foundations and properties [19]
A.L. García-Perciante, O. Sarbach

11:00 Relativistic hydrodynamics from the generalized bracket formalism of non-equilibrium thermodynamics [20]
V.G. Mavrantzas

11:20 Thermodynamic compatibility of weakly nonlocal fluids with a scalar field [21]
P. Ván, M. Szücs

11:40 *Discussion*

12:00 *Lunch Break*

Session 7: MULTIPHASE SYSTEMS

14:00 Global isomorphism with Ising model for the properties of liquid-gas surface [22]
V. Kulinskii, A. Maslechko

14:20 Non-equilibrium processes at liquid-vapor interfaces [23]
H. Struchtrup, P. Feyzi Oskouei

14:40 Exact Response Theory and Kuramoto dynamics: dissipative effects in non-equilibrium phase transitions [24]
M. Colangeli, L. Rondoni

15:00 Thermomechanics of oriented granular gas [25]
B. Nadler, H. Struchtrup

15:20 *Discussion*

15:40 *Coffee Break*

Session 8: POSTERS AND EXCURSION

16:00 Poster Session

17:20 *Break*

18:00 *Excursion to Ancient Syros and Workshop Dinner*

22:30 *End of 2nd day*

Wednesday, June 11, 2025

Session 9: MATERIAL APPLICATIONS

08:40 Application of the Rayleighian approach to the magnetic hysteresis problem [26]
A. Skarlatos, P. Vafeas

09:00 Ultrafast entropy production in non-equilibrium magnets [27]
F. Tietjen, R.M. Geilhufe

09:20 A molecular dynamics study on hydrogen embrittlement of ferrous and non-ferrous alloys [28]
P. Syroglou, K. Ritos

09:40 A variable entanglement density constitutive model for entangled polymer melts derived using non-equilibrium thermodynamics and comparison with atomistic NEMD simulations [29]
P.S. Stephanou

10:00 *Coffee Break*

Session 10: POLYMERIC SYSTEMS

10:20 Pioneering Fluctuations in Viscoelastic Stress: A Comparison of the Temporary Network and Dumbbell models [30]
A. Winters, J. Vermant

10:40 Efforts to implement fluctuating hydrodynamics in the mesoscopic modeling of polymer solutions [31]
S.G. Yiantsios

11:00 Equilibrium and non-equilibrium dynamics of polymers confined in nanopores [32]
P. Kardasis, G. Floudas

11:20 Probing the heterogeneous non-equilibrium behavior of polymer nanocomposites via simulations across scales [33]
H. Reda, A. Chazirakis, V. Harmandaris

11:40 *Discussion*

12:00 *Lunch Break*

Session 11: DYNAMICS

14:00 A biphasic haemodynamic model in microvascular networks [34]
T. Wisitponchai, J. Wu, A. Kazakidi

14:20 Two hundred years of Sadi Carnot’s concept of heat exchange [35]
J. Badur, T. Ochrymiuk, W. Dudda

14:40 *General Discussion & Deliberations about the next IWNET Meeting*

16:00 *End of the Workshop*

Poster Presentations

P1 Stable nanothermodynamics: beyond Boltzmann’s factor for thermal equilibrium and nanoscale fluctuations
Ralph V. Chamberlin

P2 Zentropy: Integrating Quantum and Statistical Mechanics for Non-equilibrium Thermodynamics
Zi-Kui Liu

P3 Global Stability Analysis of the Dynamic Heartbeat Model

J.C. Pacheco-Páez, J.C. Chimal-Eguía, D. Ladino-Luna, J.R. Luevano-Enriquez, R.T. Páez-Hernández

P4 Behavior of the Curzon and Ahlborn cycle under the efficient power and power density criterion based on the ecological function
D. Ladino-Luna, J.C. Chimal-Eguía, J.C. Pacheco-Páez, R.T. Páez-Hernández

P5 Stability analysis of a relativistic hydrodynamics model derived from non-equilibrium thermodynamics in a Lorentz-boosted frame
Panagiotis Panagopoulos Papageorgiou, Vlasis G. Mavrantzas

P6 Modeling the Rheological Behavior of Cement Pastes
A. K. Ioannou, P. S. Stephanou

P7 Phonon hydrodynamics of short channels: solids and superfluids
L. Saluto, D. Jou

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Beris, Antony	A Thermodynamically Consistent Framework for the Inclusion of Micro-Inertia in Complex Materials Flow Models
Chacón-Acosta, Guillermo	Study of the entropy production density of reversible reaction-diffusion models in narrow channels
Chamberlin, Ralph	Small and simple systems that favor the arrow of time
Chamberlin, Ralph	Stable nanothermodynamics: beyond Boltzmann's factor for thermal equilibrium and nanoscale fluctuations (*poster*)
Colangeli, Matteo	Exact Response Theory and Kuramoto dynamics: dissipative effects in non-equilibrium phase transitions
Doi, Masao	Onsager Principle in Soft Matter Physics
Edwards, Brian	Methodology for incorporating constraints into Poisson and dissipation bracket theory
Engler, Jan	Chemical kinetics of Lennard-Jones cluster isomerization using the Onsager-Machlup action
Floudas, George	Equilibrium and non-equilibrium dynamics of polymers confined in nanopores
García-Perciante, Ana Laura	Relativistic dissipative fluids in the trace-fixed particle frame: foundations and properties
Gonzalez-Narvaez, Ruth	Diffusion process and the Prigogine's principle of minimum entropy production
Grmela, Miroslav	Role of Geometry in Multiscale Thermodynamics
Harmandaris, Vagelis	Probing the Heterogeneous Non-Equilibrium Behavior of Polymer Nanocomposites via Simulations Across Scales
Herrera-Castro, Filiberto	Variational Approach to Chemical Reactions Beyond Local Equilibrium
Kazakidi, Asimina	A biphasic haemodynamic model in microvascular networks
Liu, Zi-Kui	Zentropy, Free Energy Landscape, and Non-Equilibrium Thermodynamics
Liu, Zi-Kui	Zentropy: Integrating Quantum and Statistical Mechanics for Non-equilibrium Thermodynamics (*poster*)

Maslechko, Anastasiia	Global isomorphism with Ising model for the properties of liquid-gas surface
Mavrantzas, Vlasis	Relativistic hydrodynamics from the generalized bracket formalism of non-equilibrium thermodynamics
Méndez, Alma Rosa	On the Chapman–Enskog solution and its relation with first-order dissipative fluid theories
Nadler, Ben	Thermomechanics of Oriented Granular Gas
Öttinger, Hans Christian	Is irreversibility emergent? Is irreversibility doomed?
Pacheco-Paez, Juan Carlos	Global Stability Analysis of the Dynamic Heartbeat Model (*poster*)
Pacheco-Paez, Juan Carlos	Behavior of the Curzon and Ahlborn cycle under the efficient power and power density criterion based on the ecological function (*poster*)
Panagopoulos Papageorgiou, Panagiotis	Stability analysis of a relativistic hydrodynamics model derived from non-equilibrium thermodynamics in a Lorentz-boosted frame (*poster*)
Pavelka, Michal	On the emergence of non-equilibrium thermodynamics from Hamiltonian mechanics
Reina, Celia	A statistical mechanics framework for thermodynamics with internal variables and its application to phase transforming systems
Ritos, Konstantinos	A Molecular Dynamics Study on hydrogen embrittlement of ferrous and non-ferrous alloys
Saluto, Lidia	Phonon hydrodynamics of short channels: solids and superfluids (*poster*)
Sciacca, Michele	Nonlinearity in the heat transport models
Shang, Xiaocheng	Stochastic Norton Dynamics: An Alternative Approach for the Computation of Transport Coefficients in Dissipative Particle Dynamics
Skarlatos, Anastassios	Application of the Rayleighian approach to the magnetic hysteresis problem
Stephanou, Pavlos	A variable entanglement density constitutive model for entangled polymer melts derived using non-equilibrium thermodynamics and comparison with atomistic NEMD simulations
Stephanou, Pavlos	Modeling the Rheological Behavior of Cement Pastes (*poster*)

Struchtrup, Henning	Non-equilibrium Processes at Liquid-Vapor Interfaces
Tietjen, Finja	Ultrafast Entropy Production in Non-Equilibrium Magnets
Ván, Peter	Thermodynamic compatibility of weakly nonlocal fluids with a scalar field
Verros, George	On the axioms of heat transfer and multi-component diffusion in the Euclidean space
Votruba, Vojtěch	Recognizing Generalized Gradient Dynamics by Means of Machine Learning
Winters, Arturo	Pioneering Fluctuations in Viscoelastic Stress: A Comparison of the Temporary Network and Dumbbell models
Yiantsios, Stergios	Efforts to implement Fluctuating Hydrodynamics in the mesoscopic modeling of polymer solutions

Abstracts

(in alphabetical order of the Presenting Author)

Oral Presentations

Two hundred years of Sadi Carnot’s concept of heat exchange

Janusz Badur,(1) Tomasz Ochrymiuk,(1) Waldemar Dudda(2)

(1) Energy Conversion Department, Institute of Fluid Flow Machinery, Polish Academy of Science, Fiszera 14, 80-231 Gdańsk, Poland. Email: jb@imp.gda.pl; tomasz.ochymiuk@imp.gda.pl
(2) Faculty of Technical Sciences, University of Warmia and Mazury, Oczapowskiego 11, 10-719 Olsztyn, Poland, Email: dudda@uwm.edu.pl

Abstract:

Starting form a revalorization of Sadi Carnot’s calorness and pressureness field theory the classical principles of dissipationless heat exchange are presented within an historical perspective. Correctness of experimental data (Gay-Lussac, Desormes, Mariotte, Dulung, Petit) being the phenomenological reasons of Carnot’s concept are re-examined. Additionally, correctness of Lazar Carnot’s analogy of water fall, Alexandro Volta’s analogy of electric potential fall and Antoine Lavoisier’s analogy of flogistic potential fall is proved. Unknown relations with Aristotelian *energeja* and Euler-Bernoulli *pre-energy* are shown [2].

The principle of “re-establishment of equilibrium in the caloric”, nowadays called to be “the Carnot principle” is removed from the level of cycles into a local (3D+time) working continuum formulation, by using a proper mathematics following of the Lazare Carnot infinitesimal calculus [1]. Therefore, the mathematical picture of the isothermal process of caloric flow, which is the fundament of the Carnot cycle, can be interpreted in terms of compensating potentials of the gauge field theory.

The main further contributions in developing of the Carnot concept given by Holtzmann, Reech, Rankine, Gibbs, Duhem, Oettingen, Natanson, Afanasjeva are demonstrated. Finally, Carnot’s concept of an internal symmetry related to the caloric field theory is developed for the left- and right-hand Carnot cycles.

References:

[1] Ochrymiuk T., Dudda W., Badur J., On a Carnot working continuum with non-equilibrium state parameters, *Archives of Thermodynamics*, vol. 44, 4 285-316 (2023).
[2] Badur J., *Eternal Energy Conversion*, IMP Press, Gdańsk, pp 1-4.

A Thermodynamically Consistent Framework for the Inclusion of Micro-Inertia in Complex Materials Flow Models

A. N. Beris,(1) B. J. Edwards(2)

(1) Center for Research in Soft matter and Polymers (CRiSP) and Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA. Email: beris@udel.edu
(2) Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN 37996, USA. Email: bedward1@utk.edu

Abstract:

Traditionally in the development of constitutive equations governing the stress, and conformation dynamics of complex materials under flow, creeping flow assumptions are used leading to equations enforcing the microscopic balance of forces. Those originate from a consideration of the disparity between relevant microscopic and macroscopic length scales leading to macroscopic models that we call here traditional. However, as new materials are developed involving mesoscopic structures of larger sizes, and/or interest grows for the modeling of inertial microfluidic flows, it is of interest to examine the proper form of macroscopic models that go beyond the local creeping hypothesis at the microscopic level. We call here those models, where the macroscopic characteristic length approaches closer to the microscopic one, and particle momenta are important, micro-inertial models. We exploit the use of the Single Generator Bracket Formalism (SGBF) of Non-Equilibrium Thermodynamics, in properly representing the mathematical structure of these models. Starting from the description of nematic liquid crystals, an area where the first principles microinertia models have been developed in the past, we examine critically the macroscopic structure of the equations to infer rules within the framework of SGBF connecting microinertia models to their traditional equivalents. We then illustrate the application of these rules on dilute emulsions, an area where independent theoretical evidence based on both experiments and microscopic simulations as well as previous macroscopic modeling, is available. We conclude with the inference of the form that microinertia models are expected to have for viscoelastic flows.

Study of the entropy production density of reversible reaction-diffusion models in narrow channels

G. Chacón-Acosta,(1) M. Núñez-López(2)

(1) Applied Mathematics and Systems Department, Universidad Autónoma Metropolitana-Cuajimalpa, Mexico. Email: gchacon@cua.uam.mx
(2) Department of Mathematics, Instituto Tecnológico Autónomo de México,, Mexico. Email: mayra.nunez@itam.mx

Abstract:
Some biological and chemical systems exhibit spontaneously occurring ordered structures that remain stable throughout time due to mass transport processes and chemical reactions in non-equilibrium conditions. One example is the Turing mechanism, where small fluctuations in the reaction-diffusion systems can be amplified, leading to spatio-temporal patterns [1]. In this study, we examine how the geometry of the walls of a narrow channel affects the entropy production density in the reversible Gray-Scott reaction-diffusion system [2]. Some of the autocatalytic reactions observed in chemical and enzymatic reactions have been described using reversible Gray-Scott model [4,5]. Using the Fick-Jacobs effective diffusion equation, which considers modifications to the standard diffusion equation by the geometrical characteristics of the channel, we find that while the entropy density varies, its overall qualitative behavior remains unchanged [6,7]. This analysis will contribute to our understanding of the structure formation space in such systems.

References:

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Small and simple systems that favor the arrow of time

Ralph V. Chamberlin(1)

(1) Department of Physics, Arizona State University, Tempe, AZ USA 85287-1504. Email: chamberl@asu.edu

Abstract:

The second law of thermodynamics is the source of irreversibility that we experience in everyday life. One formulation of this 2nd law states that the entropy of a closed system increases irreversibly until it reaches its maximum value. Then the entropy stays at this maximum, which stabilizes the thermal equilibrium and helps to define the temperature (T) needed for Boltzmann's factor ($e^{-J/kT}$) to give the probability that a system has energy J. A common claim is that the 2nd law applies only to large and complex systems that are unlikely to return to their initial state, while small and simple systems are routinely reversible. Another claim is that the 2nd law applies only to most initial states, while entropy may decrease from some states (that are extremely unlikely for large systems). I will present evidence that such claims are false, at least for computer simulations of standard models [1-3]. In other words, we find that the 2nd law of thermodynamics is a fundamental physical law, not just a statistical rule of thumb. I will then speculate about a microscopic mechanism that may provide a basic source of irreversibility in nature.

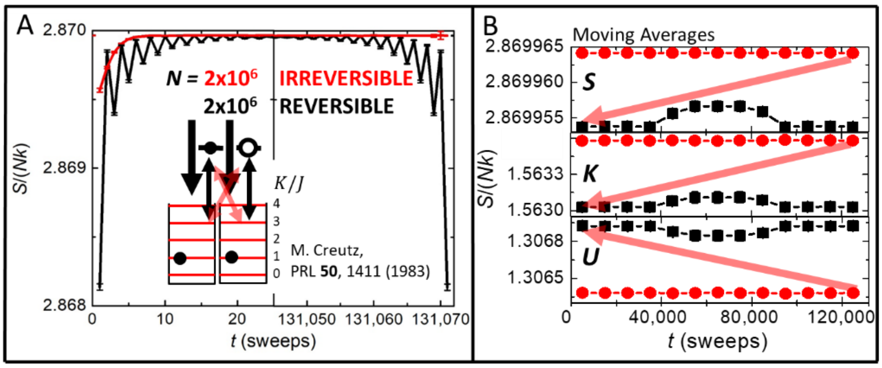

Figure 1. A) Inset: a simplified Creutz model containing two Ising spins coupled to a heat bath of two Einste
oscillators. The model allows calculation of the exact entropy of the system and its bath from their energies
step. The model is reversible if the connection between the system and its bath is methodical (black), or irre
the connection is random (red). Main figure: time-dependent entropies of two large systems, one with irreve
dynamics and one with reversible dynamics. The dynamics is reversed at the midpoint of each simulation (n
The reduction in entropy of the reversible system after this reversal demonstrates Loschmidt's paradox. B)
resolution plots of the averaged entropies of the system (U), the bath (K), and their sum (S). Arrows show t
systematic changes in each entropy upon becoming reversible.

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Exact Response Theory and Kuramoto dynamics: dissipative effects in non-equilibrium phase transitions

M. Colangeli,(1) L. Rondoni(2)

(1) Department of Information Engineering, Computer Science and Mathematics, University of L'Aquila, Via Vetoio, 67100 L'Aquila, Italy. Email: matteo.colangeli1@univaq.it
(2) Department of Mathematical Sciences, Polytechnic University of Turin, Corso Duca degli Abruzzi 24, 10129 Turin, Italy. Email: lamberto.rondoni@polito.it

Abstract:

The study of collective behaviors in systems with many degrees of freedom is part of a research endeavour which gathers a relevant fraction of the non-equilibrium thermodynamics community. The Kuramoto dynamics represents a cornerstone in this field, for it constitutes an exactly solvable model that leads to synchronization - a paradigmatic instance of a non-equilibrium phase transition [1]. In this talk we shall address the analysis of the Kuramoto dynamics through the prism of statistical mechanics, in which some known mathematical results can be cast in a new light. The behavior of Kuramoto oscillators will be investigated via an Exact Response Theory based on the Dissipation Function, which has been introduced in the field of non-equilibrium molecular dynamics [2]. We shall underline that classical linear response theory, despite being much useful even beyond its theoretical boundaries, does not generally apply to systems undergoing phase transitions [3]. The Kuramoto dynamics will thus be studied analytically as a testbed for the aforementioned Exact Response Theory. We shall derive explicit formulae for the two-time correlation functions and for the asymptotic value of the Dissipation Function. We will also highlight the non-monotonic behavior in time of the correlations, when the number of oscillators becomes large, and shall also compare our results with the predictions of Kubo's Fluctuation-Dissipation Theorem. Our analysis ultimately reveals that the exact response formalism, at variance with classical linear response formulae, can properly detect the non-equilibrium phase transition, characterized by a phase synchronization of the oscillators [4].

Acknowledgements:

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Onsager Principle in Soft Matter Physics

Masao Doi$^{(1),(2)}$

(1) School of Physics, Beihang University, Beijing 100191, China
(2) Wenzhou Institute, University of Chinese Academy of Sciences, Wenzhou 325000, China. Emails: masao.doi@buaa.edu.cn, doi.masao.y3@a.mail.nagoya-u.ac.jp

Abstract:

The Onsager principle is a variational principle proposed by Lars Onsager in 1931 in his celebrated paper on the reciprocal relation in non-equilibrium thermodynamics [1]. The principle is very important in soft matter physics [2,3]. Almost all kinetic equations which have been used to describe the dynamics of soft matter systems can be derived from this principle. Onsager principle is also very useful to derive the set of governing equations for given state variables since, like Lagrangian mechanics, it is based on energetic quantities independent of coordinate system. Furthermore, Onsager principle is giving us a convenient tool to solve these equations [4]. Since it is a principle of minimization, it can be used to get approximate solutions of the equations. Here I review the principle taking examples from the swelling dynamics of soft and glassy gels [4,5].

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Methodology for incorporating constraints into Poisson and dissipation bracket theory

Brian J. Edwards,(1) Antony N. Beris(2)

(1) Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN 37996, USA; bje@utk.edu
(2) Center for Research in Soft matter and Polymers (CRiSP) and Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716, USA; beris@udel.edu

Abstract:

The Poisson and dissipation brackets in non-equilibrium thermodynamic theory are usually derived or formulated in terms of local field density variables that are free of constraints; however, in many applications, physical constraints are imposed on these variables which must ultimately be embedded in the dynamic structure of the system represented by the Poisson and dissipation brackets. In the past thirty years, constraints have been incorporated into bracket theory a number of different ways, usually in an ad hoc fashion without any justification other than the resulting evolution equations satisfied the required constraints. Such a mathematically reckless procedure could possibly be harmful when not applied properly because key properties of the Poisson and dissipation bracket, such as the Jacobi identity, might be compromised in the process. In this presentation, we take a systematic and mathematically formalistic perspective on the incorporation of constraints into bracket theory. This methodology generally consists of two steps: 1) a mathematically proper definition of constrained functional derivatives taken with respect to Lagrange multipliers that are evaluated through the implementation of the required constraints, and 2) transformation of the unconstrained functional derivatives appearing in the Poisson and dissipation brackets to constrained functional derivatives that maintain the structure of the brackets during the transformation from unconstrained to constrained variables. The general procedure is illustrated using several common examples from fluid mechanics and transport phenomena.

Chemical kinetics of Lennard-Jones cluster isomerization using the Onsager-Machlup action

J. Engler,(1) M. Pavelka(2)

(1) Mathematical Institute, Faculty of Mathematics and Physics, Charles University, Sokolovská 83, 18675 Prague, Czech Republic. Email: engler@karlin.mff.cuni.cz
(2) Mathematical Institute, Faculty of Mathematics and Physics, Charles University, Sokolovská 83, 18675 Prague, Czech Republic. Email: pavelka@karlin.mff.cuni.cz

Abstract:

The Lennard-Jones clusters have been extensively studied as a toy model for chemical reactions. Two problems are of importance: First, to find the local minima of the LJ potential, and Second, to find the transition rates and paths between these minima [1]. We focus on the second problem. Instead of the widely used Minimum energy path (MEP) [2], we calculate the path minimizing the Onsager-Machlup action [3]

$$S[x(t)] = \frac{\Delta U}{\zeta} + \frac{1}{2}\int_0^t \left(|\dot{x}|^2 + \left(\frac{\nabla U}{\zeta}\right)^2 - \frac{2D}{\zeta}\nabla^2 U \right) d\tau$$

where $x(t)$ is the configuration of N atoms, U is the LJ potential, ζ and D are the friction and diffusion coefficients respectively. The OM action is minimized using machine learning. Our approach differs from MEP in that the OM action takes into account collisions with surrounding particles. Using this approach, we find the most probable reaction and transition rates.

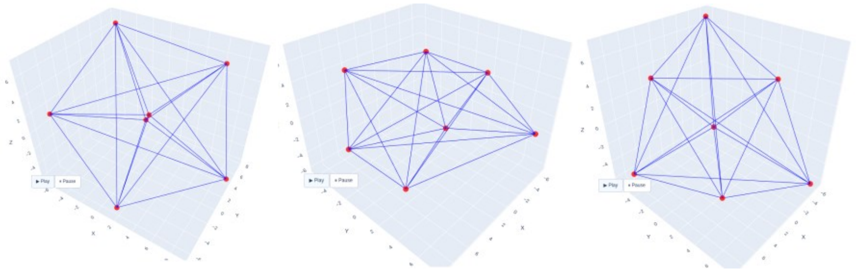

Figure: Path of LJ7 from global minimum (left) to the third lowest minimum

Acknowledgements:

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Equilibrium and non-equilibrium dynamics of polymers confined in nanopores

Panagiotis Kardasis,(1) George Floudas(1),(2)

(1) Max Planck Institute for Polymer Research, Mainz, Germany
(2) University of Ioannina, Dept. of Physics, Ioannina, Greece

Abstract:
Polymer imbibition in nanopores is a slow process that involves chain adsorption at the pore walls. The latter is associated with several non-equilibrium polymer configurations and has very long time-scales only encountered in the vicinity of the liquid-to-glass temperature [1]. However, imbibition normally takes place at a temperature located some 100 K above T_g. Herein we expored the non-equilibrium dynamics of *linear* and *star*-shaped *cis*-1,4 polyisoprenes confined within nanoporous alumina as a function of pore size, d, molar mass and functionality ($f = 2, 6, 64$) [2-4]. Two thermal protocols were tested; one resembling a *quasi-static* process (I), and another involving fast cooling followed by annealing (II). Although both protocols give identical equilibrium times, it is through protocol I that it is easier to extract the equilibrium times [3]. Both thermal protocols establish the existence of a critical temperature below which non-equilibrium effects set-in. The critical temperature depends on the degree of confinement, $2R_g/d$, and on molecular architecture. Strikingly, establishing equilibrium dynamics at all temperatures above the bulk T_g requires $2R_g/d \sim 0.02$, i.e., pore diameters that are much larger than the chain dimensions. The non-equilibrium phenomena in pores reflects the non-equilibrium configurations of the *adsorbed layer* that extent away from the pore walls [3]. The equilibrium times depend strongly on temperature, pore size and functionality. In general, star-shaped polymers require longer times to reach equilibrium because of the higher tendency for adsorption. We discuss a possible correlation of the long equilibration dynamics found near T_g with the long adsorption times found at much higher temperatures.

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Relativistic dissipative fluids in the trace-fixed particle frame: foundations and properties

A. L. García-Perciante,(1) O. Sarbach(2)

(1) Departamento de Matemáticas Aplicadas y Sistemas, Universidad Autónoma Metropolitana-Cuajimalpa, México. Email: algarcia@cua.uam.mx.
(2) Instituto de Física y Matemáticas, Universidad Michoacana de San Nicolás de Hidalgo, México. Email: olivier.sarbach@umich.mx

Abstract:

The establishment of a well-posed and causal system of equations that properly describes a relativistic dissipative fluid has been a prevalent and elusive challenge in physics for decades. Moreover, linear relativistic theories were mostly discarded since the 80's for not meeting these requirements and, in particular, for exhibiting generic instabilities [1]. However, the emergence of the so-called general first order theories [2,3] (or BDNK theories), for which hyperbolicity and causality can be obtained, subject to strong restrictions on the set of parameters involved in the formalism, is currently shifting the focus of relativistic non-equilibrium thermodynamics back to the linear regime.

In this work, it will be shown that, in the case of a particular frame and representation within the context of the aforementioned theories, causality, hyperbolicity, and stability are obtained with simple conditions that are verified for an ideal gas of hard spheres [4]. This representation of dissipative hydrodynamics is obtained from relativistic kinetic theory by applying a new version of the relativistic Chapman-Enskog method to derive the constitutive relations. The novelty of the approach consists in applying a suitable projection method to solve the linearized Boltzmann equation and to use the so-called trace-fixed particle frame, which determines the state variables by fixing the trace of the stress-energy tensor in addition to the particle current density. As we show, this leads to a linear dissipative fluid theory which, in contrast to the traditional first order theories (Eckart and Landau), is hyperbolic, causal and stable at global equilibrium states. Moreover, we prove that the full nonlinear system of equations can be cast into a first-order quasilinear system which is strongly hyperbolic, leading to a well-posed Cauchy problem [5].

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Diffusion process and the Prigogine's principle of minimum entropy production

R.E. Gonzalez-Narvaez,(1) M. López de Haro,(1) F. Vázquez(2)

(1) Centro de Investigación en Ciencias (CInC), Universidad Autónoma del Estado de Morelos (UAEM). Email: ruth.gonzalez@uaem.mx
(2) Email: vazquez@uaem.mx

Abstract:

The Prigogine's Principle of minimum entropy production (PMEP) [1,2], has been questioned. Many doubts came from the hypothesis of constant phenomenological coefficients in the linear law of classical irreversible thermodynamics (CIT) about heat flux and temperature gradient [3,4]. However, it has been proved the extended validity when the phenomenological coefficients are position dependent, for the heat transport [5] and for the thermoelectric effect [6,7]. Therefore, in this work, we show that the PMEP goes for diffusion phenomena too. It means that the diffusion process is developed with a minimum entropy production.

Acknowledgements:

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Role of Geometry in Multiscale Thermodynamics

Miroslav Grmela(1)

(1) École Polytechnique Montréal, C.P.6079 Montréal, H3C3A7, Québec, Canada

Abstract:

Macroscopic systems are composed of a large number of microscopic particles obeying the laws of classical mechanics. The objective of mesoscopic thermodynamics is to extract from trajectories of the microscopic particles overall features registered in macroscopic and mesoscopic observations. Geometry provides a framework for such investigation. There are three sources of motivation and inspiration: the classical equilibrium and non-equilibrium thermodynamics, statistical mechanics, and geometry. The main argument that led to the formulation [1],[2],[3] is the following. The fundamental group of transformations in equilibrium thermodynamics is the group of Legendre transformations. The natural geometrical setting for such group is the contact geometry. On the other hand, the natural geometrical setting for the Hamiltonian mechanics is the symplectic geometry. We must therefore begin by lifting the Hamiltonian mechanics to the setting of contact geometry. In such lifted setting the Hamiltonian mechanics, dissipation, external forces, the classical thermodynamics, and the rate thermodynamics that is applicable also for open systems coexist in harmony. The lifted formulation also reproduces and extends many results obtained previously in non-equilibrium thermodynamics (for instance the nonlinear chemical kinetics and the Rayleigh-Onsager-Prigogine-Gyarmati variational principle). The established connection between geometry and multiscale thermodynamics inspires new developments in geometry (e.g. unified product theory within the framework of Lie algebroids), in rheology, and in AI.

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Probing the Heterogeneous Non-Equilibrium Behavior of Polymer Nanocomposites via Simulations Across Scales

H. Reda,(1) A. Chazirakis,(2) V. Harmandaris(1),(2)

(1) Computation-Based Science and Technology Research Center, The Cyprus Institute, Nicosia, Cyprus
(2) Department of Mathematics and Applied Mathematics, Univrsity of Crete, Greece & IACM/FORTH, Heraklion GR-71110, Greece. Email: harman@uoc.gr

Abstract:

We present a hierarchical multi-scale methodology for predicting the macroscopic properties of polymer-based nanostructured systems, which involve atomistic simulations, coarse-grained models, homogenization approaches, and continuum models [1-3]. CG and continuum models are derived through a systematic data-driven 'bottom-up' strategy, using information from the atomistic scale without any adjustable parameter [1]. Moreover, deep learning algorithms are developed to reintroduce atomic detail on the CG scale and obtain atomistic configurations of long polymer chains [1].

The proposed computational methodology is applied to provide a detailed investigation of the heterogeneous mechanical and viscoelastic behavior of polymer nanocomposites, which is of paramount importance for their tailored design. As test systems we examine poly(ethylene oxide)/silica, PEO/SiO_2 nanocomposites across a range of temperatures, from the glassy regime to the liquid one. We present a detailed investigation of the coupling between the density, structure, and conformations of polymer chains with respect to their role in mechanical reinforcement [2]. Based on a computation of local stress and strain fields, we probe the distribution of the (local) mechanical properties, focusing on the polymer/nanofiller interphase and matrix regions. We found that the effective mass density and rigidity of the matrix region change with the filler volume fraction, while that of the interphase remains constant [3]. The observed differences regarding the rigidity between the interphase and the matrix region decrease as the temperature rises; at temperatures well above the glass transition temperature, the rigidity of the interphase approaches the matrix one. To describe the nonlinear viscoelastic behavior of polymer chains, the elastic modulus of the PEO/SiO_2 systems is further calculated as a function of the strain for the entire nanocomposite, as well as the interphase and matrix regions.

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Variational Approach to Chemical Reactions Beyond Local Equilibrium

F. Herrera-Castro,(1) J. Antonio del Río Portilla(2)

(1) Instituto de Energías Renovables, Xochicalco s/n, Azteca, 62588, Temixco, Mor. Email: hecafi@ier.unam.mx
(2) Instituto de Energías Renovables, Xochicalco s/n, Azteca, 62588, Temixco, Mor. Email: arp@ier.unam.mx

Abstract:

The formal description of chemical reactions far from equilibrium is an open task. Chemical reactions are central to various phenomena in life, industry, and the environment. In this work, we use a variational principle within the framework of extended irreversible thermodynamics to obtain relaxation equations for the fast variables to close the balance equations. Our approach extends traditional local equilibrium thermodynamics by incorporating formal expressions for the unknown generalized equations of state in terms of the non-equilibrium variables, which we can expand in lower and higher-order terms [1]. These formal expressions drive for a broader representation of non-linear and dissipative phenomena and capture wave-like behaviors, relevant to oscillatory chemical systems. The formalism aligns well with previous theoretical works [2-4] and provides additional insights into the influence of diffusion fluxes on reaction rates. The resulting equations may describe reaction velocities with different relaxation times. We present the application of this variational framework, where the relaxation equations describe the chemical reaction behavior beyond local equilibrium.

Acknowledgements:

We thank Prof. Mariano López de Haro for his relevant comments on this work. FHC thanks for the posdoctoral fellowship from Consejo Nacional de Humanidades, Ciencias y Tecnología (CONAHCyT).

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A biphasic haemodynamic model in microvascular networks

T. Wisitponchai,(1) J. Wu,(1) A. Kazakidi(1, *)

(1) Department of Biomedical Engineering, University of Strathclyde, Glasgow, UK.
(*) Email: asimina.kazakidi@strath.ac.uk

Abstract:

The mechanistic link between haemorheology and clinical pathogenesis, such as ischemia or cancer, is poorly understood due to the intrinsic variation of microvessels and the limitation of *in vivo* and *in vitro* techniques [1]. Several studies of the microcirculation have suggested that the formation of a cell-free layer (CFL) due to the core movement of red blood cells (RBCs) influences the hematocrit distribution, the wall shear stress (WSS) and velocity profiles locally.

In this study, we developed a biphasic numerical model utilising the Eulerian Multiphase (EMP) approach in Simcenter STAR-CCM+ (Siemens), where a particulate RBC phase was dispersed in a CFL phase, with different rheological properties for each phase. The model was first validated against experimental measurements [2] and then examined in simplified symmetric 3D bifurcations, with a parent diameter of 20 µm, to investigate the blood behaviour and the CFL recovery downstream of the junction.

The results demonstrated a symmetric annular CFL shape around the RBC core upstream of the junction, in the parent vessel. Downstream of the bifurcation, the narrower CFL on the inner wall increased the local wall shear stress (WSS), with peak velocities shifting toward the thicker CFL on the outer wall. The CFL asymmetry progressively returned to symmetry further downstream. These findings align with experimental data [2, 3]. The underlying mechanism of the RBC phase migration was explained by force analysis at the RBC-CFL interface, due to high slip velocity near the wall, and the generation of a local pressure gradient. Further studies could explore the haemodynamics and the mechanical response in realistic microvascular networks.

Acknowledgements:

Results were obtained using the ARCHIE-WeSt High Performance Computer (www.archie-west.ac.uk) based at the University of Strathclyde.

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Zentropy, Free Energy Landscape, and Non-Equilibrium Thermodynamics

Zi-Kui Liu(1)

(1) Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

Abstract:

Entropy is a fundamental concept in thermodynamics, and the entropy production in internal processes is crucial to non-equilibrium thermodynamics. Accurate prediction of entropy as a function of internal variables for stable, metastable, and unstable states is essential for the stability and evolution of any system. Over the past two decades, we have developed a multiscale entropy approach, recently termed zentropy theory, which integrates DFT-based quantum mechanics and Gibbs statistical mechanics. In this approach, the total energy of individual configurations is replaced by their respective free energies. Zentropy theory has proven its capability to accurately predict entropy and Helmholtz energy landscapes for stable, metastable, and unstable states of magnetic materials with strongly correlated physics and property anomalies, such as negative thermal expansion (https://doi.org/10.1007/s11669-022-00942-z). Recently, zentropy theory has been applied to predict the entropy of liquid phases and melting temperatures of various materials (https://doi.org/10.1103/physrevresearch.7.l012030). It is also being applied to ferroelectric materials (https://doi.org/10.1103/PhysRevB.110.184103), plasticity (https://doi.org/10.1016/j.ijplas.2025.104303), and superconductors (https://arxiv.org/abs/2404.00719). Based on zentropy theory's ability to predict Helmholtz energy barriers between local metastable/stable states on the Helmholtz energy landscape, we revisit the driving forces, flux equations, and entropy production for internal processes through the first, second, and combined laws of thermodynamics. This is done in terms of the theory of cross phenomena, rather than the phenomenological approaches presented in the literature (https://doi.org/10.1080/21663831.2022.2054668, https://doi.org/10.1088/1361-648X/ad4762). Recent improvements in the theory of cross phenomena will also be discussed.

Global isomorphism with Ising model for the properties of liquid-gas surface

V. Kulinskii,(1) A. Maslechko(2)

(1) Department of Physics and Astronomy, Odesa Mechnikov National University, Ukraine. Email: kulinskij@onu.edu.ua

(2) Department of Physics and Astronomy, Odesa Mechnikov National University, Ukraine. Email: maslechko.anastasiia@stud.onu.edu.ua, maslechko.an@gmail.com

Abstract:

Surface tension evaluation can be considered a test for adequacy of the equation of state. This communication it devoted to the attempt to determine the temperature dependence of the surface tension at the “liquid-vapor” interface in analytically simple way using the Global Isomorphism (GI) approach [1-2]. Kulinskii noticed the topological isomorphism of the phase diagrams for the isomorphic cubic lattice model and real substances, and based on empirical relations, such as the law of the rectilinear diameter and the linearity of Zeno-line, and constructed geometric affine transformations for the coexisting diagrams in the coordinates (ρ,T). These projective transformations (GI or K-transformations [3]) used for evaluation of the thermodynamic properties of the fluid from the respective ones of the lattice gas (Ising model).

The main result of this presentation states that GI can be applicable to the surface properties. For that in 2D case exact Onsager’s solution [4] is used and theory is compared with data [5, 6]. For 3D case a comparison of [7] performed with out modification to Woodbury’s equation [8] is introduced to cover right critical behavior. With this a discussion is raised about the effective thickness of the interface and a physical meaning for the latter is analyzed. In this regard, it is possible additionally to formulate a criterion for the lowest estimation of the temperature at the triple point, which had not previously been done in the application of the GI to the “bulk” properties. In general, it is shown that for such dimensionless variables, which GI relations present, similar thermodynamic behavior is observed for a fairly wide class of substances. This can be seen as an improvement on the principle of corresponding states.

Acknowledgements:

AM gratefully acknowledge VK for the global isomorphism projective transformations invention and interesting topics, and staff members from the former Department of theoretical physics for fruitful discussions.

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Relativistic hydrodynamics from the generalized bracket formalism of non-equilibrium thermodynamics

Vlasis G. Mavrantzas(1),(2)

(1) Department of Chemical Engineering, University of Patras, Patras, Greece. Email: vlasis@chemeng.upatras.gr
(2) Department of Mechanical and Process Engineering, ETH Zürich, Switzerland. Email: vlasiosm@mat.ethz.ch

Abstract:

We make use of the generalized bracket formalism of non-equilibrium thermodynamics by Beris and Edwards [1] to derive Lorentz-covariant time evolution equations for an imperfect fluid with viscosity, dilatational viscosity, and thermal conductivity. Following a similar analysis to the problem by Öttinger [2,3] through GENERIC, we include in the set of hydrodynamic variables a covariant vector playing the role of a generalized thermal force and a covariant tensor closely related to the velocity gradient tensor.

We first derive the nonrelativistic equations and then we proceed to derive the relativistic ones by elevating the thermal variable to a four-vector, the mechanical force variable to a four-by-four tensor, and by representing the Hamiltonian of the system with the time component of the energy-momentum tensor. For the Poisson and dissipation brackets we assume the same general structure as in the nonrelativistic case, but with the phenomenological coefficients in the dissipation bracket describing friction to heat and viscous effects being properly constrained so that the resulting dynamic equations be manifest Lorentz-covariant.

The final relativistic equations [4] are identical to those derived by Öttinger but the approach through the generalized bracket leaves space for alternative forms of the phenomenological coefficients describing friction that could ensure Lorentz-covariance.

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On the Chapman–Enskog solution and its relation with first-order dissipative fluid theories

A. R. Méndez,(1) A. L. García-Perciante,(2) O. Sarbach(3)

(1) Universidad Autónoma Metropolitana – Cuajimalpa, México. Email: amendez@cua.uam.mx
(2) Universidad Autónoma Metropolitana – Cuajimalpa, México. Email: algarcia@cua.uam.mx
(3) Universidad Michoacana de San Nicolás de Hidalgo, México. Email: olivier.sarbach@umich.mx

Abstract:

Most kinetic theory approaches and methods were developed in the early part of the last century to understand the transport properties of 'classical, non-relativistic' gases [1]. Therefore, it is not surprising that its relativistic counterpart contains subtle aspects that still need to be understood. Although the Chapman-Enskog procedure for solving the Boltzmann equation has proven to yield reliable results in the non-relativistic regime, the same is not as clear for gases at high temperatures. In this work, we examine the Chapman-Enskog method from two different perspectives: the well-known traditional procedure and a “more” formal approach based on the properties of the linearized collision operator [2,3]. In the non-relativistic scenario, both approaches lead to the same integral equation, but in the relativistic case the source term in the integral equation adopts two different forms. We thoroughly analyze the equivalence of this apparent discrepancy and explore some non-trivial questions that arise from this analysis.

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Thermomechanics of Oriented Granular Gas

B. Nadler,(1) H. Struchtrup(2)

(1) University of Victoria, Mechanical Engineering, Victoria, BC, Canada. Email: bnadler@uvic.ca
(2) University of Victoria, Mechanical Engineering, Victoria, BC, Canada. Email: struchtr@uvic.ca

Abstract:

In this presentation, we develop a continuum model for the thermomechanics of granular media consisting of rigid oriented particles by extending the thermodynamic state variables to account for the mesoscopic granular state. The state variables to model oriented granular gas are the mesoscopic granular temperature and the mesoscopic granular orientation in addition to the classical state variables: density, velocity and thermodynamic temperature. The granular temperature is a nonnegative scalar value that represents the energy of the agitated mesoscopic particles (energy of the particles' peculiar velocities). The mesoscopic orientation is a trace free symmetric second order tensor defined by

$$A_{ij} = \int_{S^2} f(n_k) n_i n_j da - \delta_{ij}/3$$

where n_k is the orientation and $f(n_k)$ is the probability density function of the orientation. The orientation tensor measures the deviation from isotropic orientation distribution, $f = (4\pi)^{-1}$, which is taken to be the orientational equilibrium state.

The two additional granular state variables are governed by the associated balance laws that are the mesoscopic energy and the mesoscopic orientation which are coupled with the balances of macroscopic linear momentum, microscopic energy, entropy and conservation of mass. The balance laws include constitutive laws for the fluxes and productions. The development of these constitutive laws is motivated by the second law of thermodynamics, that is, the non-negative entropy productions that drive the system toward equilibrium (maximum entropy). Taking the entropy to be quadratic with respect to the orientation tensor, the Gibbs equation is used to identify entropy fluxes and productions in term of the thermodynamic forces (deviation from equilibrium), thermodynamic fluxes (drive the system toward equilibrium) and state variables. The constitutive laws for the thermodynamic fluxes are constructed by taking these fluxes to be linear combinations of the thermodynamic forces. The phenomenological coefficient matrix is obtained using the Curie and Onsager-Casimir reciprocity principles; hence, the second law of thermodynamics requires that the phenomenological coefficient matrix is positive semi-definite.

The developed constitutive laws are compared with granular kinetic theory of spherical and oriented particles. The model is also used to study relevant boundary value problems including Couette flows and boundary agitation. It is shown that the model has good agreement with discrete simulations and experiments and can capture the observed strong dependency of the macroscopic response on the mesoscopic granular temperature and orientation.

Is irreversibility emergent? Is irreversibility doomed?

Hans Christian Öttinger(1)

(1) ETH Zürich, Quantum Center and Department of Materials, Switzerland. Email: hco@mat.ethz.ch

Abstract:

We are accustomed (or educated) to the belief that irreversibility emerges from the coarse-graining of more fundamental, reversible dynamical equations. This conception raises a number of questions and considerations, largely philosophical at their core. I argue that the most fundamental equations of Nature should be assumed to be irreversible. I seek to find arguments for the intrinsic value of emerging irreversibility. To provide concrete examples, I consider particle physics and rarefied gases as case studies.

On the emergence of non-equilibrium thermodynamics from Hamiltonian mechanics

K. Mladá,(1) M. Pavelka,(1) V. Klika(1)

(1) Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic. Email: pavelka@karlin.mff.cuni.cz

Abstract:

Consider an isolated system of many classical interacting particles. Although their dynamics can be described as purely Hamiltonian and reversible, the system can be also seen as having irreversible evolution. For instance, when the particles are initially only in one half of the available volume, eventually they will occupy the whole volume. Here, we discuss another example, the Kac-Zwanzig model, where a distinguished particle that is subject to an external quadratic potential as well as being is connected to a cloud of other small particles by springs. The distinguished particle then behaves effectively like a damped harmonic oscillator although the system of particles is purely Hamiltonian.

Here, we propose a dynamic-reduction approach based on the information theory that leads to effective irreversible equations for the distinguished particles in the form of GENERIC [1,2,3,4]. The approach does not require any fitting parameters and agrees with direct numerical simulations in a relevant range of parameters [5].

In summary, we show how non-equilibrium irreversible dynamics emerges out of purely Hamiltonian systems and the approach is illustrated on the Kac-Zwanzig model.

Acknowledgements:

All authors are grateful to Miroslav Grmela for many discussions on the research topic. The research was funded by the Czech Grant Agency.

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A statistical mechanics framework for thermodynamics with internal variables and its application to phase transforming systems

T. Leadbetter,(1) P.K. Purohit,(2) C. Reina(2)

(1) Graduate Group in Applied Mathematics and Computational Science, University of Pennsylvania. Email: tleadbe1@sas.upenn.edu

(2) Department of Mechanical Engineering and Applied Mechanics, University of Pennsylvania. Email: purohit@seas.upenn.edu, creina@seas.upenn.edu

Abstract:

We present a statistical mechanics framework for constructing predictive non-equilibrium thermodynamics models from particle systems obeying Langevin dynamics, that does not rely on fitting to experiments or lower scale simulations. The framework, called Stochastic Thermodynamics with Internal Variables (STIV) [1] only relies on the following ingredients: (i) a functional form for the microscopic probability distribution, parameterized by the state variables (these will include the classical state variables in equilibrium thermodynamics, such as strain and temperature, and internal variables needed to prescribe the non-equilibrium state), (ii) the definition of thermodynamic quantities as in stochastic thermodynamics [2], and (iii) a variational statement of the Fokker-Planck equation, proposed by Eyink [3], from which the evolution equation of the state variables can be derived.

We show how this framework can be used to construct what we believe is the first statistical mechanics derivation of a non-conservative phase field model in a one-dimensional elastic medium [4]. We remark that phase field methods are a highly popular and versatile approach for modeling interface material behavior. However, their formulation is primarily phenomenological, and the connection to lower scale physics often proceeds through parameter fitting. In contrast, the model derived via STIV is free of phenomenology, and comparisons to Langevin dynamic simulations indicate that it is highly predictive of the macroscopic response.

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A Molecular Dynamics Study on hydrogen embrittlement of ferrous and non-ferrous alloys

P. Syroglou,(1) K. Ritos(2)

(1) Department of Mechanical Engineering, University of Thessaly, Greece. Email: psyroglou@uth.gr
(2) Department of Mechanical Engineering, University of Thessaly, Greece. Email: konritos@uth.gr

Abstract:

Hydrogen storage and transportation technologies are crucial for the transition to clean and sustainable energy, as they enable the efficient use and distribution of hydrogen produced from renewable sources. The storage of hydrogen in compressed, liquid, or solid-state forms ensures a stable and reliable energy supply that can successfully substitute hydrocarbon fuels. Advancements in storage technologies improve energy density, safety, and cost-effectiveness, making hydrogen a viable alternative for transportation, industry, and grid-scale energy storage.

In this study we focus on the known problem of hydrogen embrittlement of metal alloys, examining the effects of hydrogen concentration, hydrogen location, alloy type, temperature, grain size, and other at a molecular level. To achieve this, we employ tensile simulations with the well-established Molecular Dynamics method via the LAMMPS software[1]. We primarily utilise EAM (Embedded Atom Method) type potentials, which are applicable to purely metallic materials[2] and also explore the capabilities of a novel artificial neural network (ANN) potential for pure bcc iron [3]. The main materials we will deal with are iron, aluminium and some of their alloys. Initially we determine the properties of pure and alloy metals in single crystal or polycrystalline form. Then crystalline defects and nano-cracks are introduced aiming at a more realistic material. At the last stage we introduce hydrogen in the metallic framework and examine how this affect the properties depending on its concentration, temperature and geometry of inclusions among others[4]. Our next steps will involve the study of hydrogen absorption in different metal alloys under low temperatures and/or high pressures, while exploring potential ways of counteracting the diffusion of hydrogen and preventing it through targeted changes on the structure and composition of alloys.

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Nonlinearity in the heat transport models

Michele Sciacca(1)

(1) Dipartimento di Ingegneria, Universita di Palermo, Viale delle Scienze, 90128 Palermo, Italy. E-mail: michele.sciacca@unipa.it

Abstract:

The growing possibilities of heat transfer control in solids, and in particular in nanosystems, has stimulated the research of thermal transfer modeling. In those systems where the relaxation time of the heat flux is not neglegible, the Fourier law has been generalized by the so-called Maxwell-Cattaneo (MC) equation. Additionally, in those systems with size comparable to the mean free path of heat carriers, nonlocal contributions are required to be considered, and the heat flux satisfies the so-called Guyer–Krumhansl (GK) equation (also related to phonon hydrodynamics) [1].

These models are linear differential equations for the heat flux field, and they have led to some interesting results in the propagation of thermal waves and in the hydrodynamics of heat transport. There is a recent interest to investigate the nonlinear contribution to these models, in order to analyzed similarities and differences with other well-known physical systems.

In this talk I will introduce some recent results we have found by considering the nonlinear contributions to the MC equation [2] and to the GK equation [3, 4]. In the former we have shown a parallelism with optical communications which has led to solitons. The other two papers instead are related to phonon hydrodynamics and they take into account a possible non-Newtonian generalization of the GK and the contribution (linear or nonlinear) of the walls.

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Stochastic Norton Dynamics: An Alternative Approach for the Computation of Transport Coefficients in Dissipative Particle Dynamics

X. Wu,(1) X. Shang(2)

(1) University of Birmingham, School of Mathematics, United Kingdom. Email: xxw142@student.bham.ac.uk
(2) University of Birmingham, School of Mathematics, United Kingdom. Email: x.shang.1@ bham.ac.uk

Abstract:

We study a novel alternative approach for the computation of transport coefficients at mesoscales. While standard non-equilibrium molecular dynamics (NEMD) approaches fix the forcing and measure the average induced flux in the system driven out of equilibrium, the so-called "stochastic Norton dynamics" instead fixes the value of the flux and measures the average magnitude of the forcing needed to induce it. We extend recent results obtained in Langevin dynamics [1] to consider the generalisation of the stochastic Norton dynamics in the popular dissipative particle dynamics (DPD) at mesoscales, important for a wide range of complex fluids and soft matter applications. We demonstrate that the responses profiles for both the NEMD and stochastic Norton dynamics approaches coincide in both linear and nonlinear regimes, indicating that the stochastic Norton dynamics can indeed act as an alternative approach for the computation of transport coefficients, focusing on mobility and shear viscosity. Moreover, our numerical experiments demonstrate that the stochastic Norton dynamics approach clearly outperforms the NEMD in controlling the asymptotic variance, a key metric to measure the associated computational costs.

Acknowledgements:

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Application of the Rayleighian approach to the magnetic hysteresis problem

A. Skarlatos,(1) P. Vafeas(2)

(1) Université Paris-Saclay, CEA, List, F-91120, Palaiseau, France. Email: anastasios.skarlatos@cea.fr
(2) Department of Chemical Engineering, University of Patras, 26504 Patras, Greece. Email: vafeas@chemeng.upatras.gr

Abstract:

The magnetization procedure in bulk ferromagnetic materials is a typical case of a dynamical, out of equilibrium, phenomenon. The resulting magnetization curve, as function of the external magnetic field, involves hysteresis and shares many common features with the stress-strain curve of non-linear elasticity. Specific aspects of the magnetic hysteresis can be reproduced on the basis of microscopic approaches, such as the Ising model or in some other cases via mesoscopic models focused on wall dynamics [1-4]. Despite their relative success in describing phase-transitions or 2D spin configurations, the applicability of these approaches in real materials is rather limited. Phenomenological models on the other hand, stand for a more realistic, coarse-grained approach to the problem, where the material behavior is controlled by a small number of parameters. For these reasons, such models are predominately used for engineering purposes. Several phenomenological models have been proposed in the last decades with the oldest among them rooting back to the end of 19th century. One of the most popular models, often used with numerical electromagnetic solvers, is the so-called Jiles-Atherton (JA) model, which recognises the magnetic wall pinning (the basic mechanism behind hysteresis) as a form of magnetic friction [5].

With this postulate in mind, the JA model can be recast in the theoretical framework of non-equilibrium thermodynamics. Despite the obvious theoretical interest of the task, there is hope that a more fundamental formulation of the hysteresis problem would lead to a generalization beyond the capabilities of the present phenomenological models.

In the present work, the JA model is reformulated, using the Rayleighian approach, where the classical JA differential equation of motion of the magnetization is obtained by minimization of the appropriate Rayleigh functional. This approach has been previously applied with success by Beris and Edwards in the context of viscous hydrodynamics [6]. The theoretical study is complemented by numerical results, based on data of real ferromagnetic materials.

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A variable entanglement density constitutive model for entangled polymer melts derived using non-equilibrium thermodynamics and comparison with atomistic NEMD simulations

P. S. Stephanou(1)

(1) Department of Chemical Engineering, Cyprus University of Technology, Limassol, Cyprus. Email: pavlos.stefanou@cut.ac.cy

Abstract:

Detailed non-equilibrium molecular dynamics (NEMD) simulations have shown that under flow, there is a strong reduction in the average number of entanglements per chain, a mechanism known as convective constraint release (CCR) [1]. Initially Ianniruberto and Marrucci [2], and more recently Dolata and Olmsted [3] proposed new theoretical models that account explicitly for flow-induced disentanglement. In this work, we employ the single-generator bracket formalism of non-equilibrium thermodynamics by Beris-Edwards [4] to derive a similar constitutive model [5]. In the new approach, entanglement destruction is obtained by coupling the entanglement density directly with the velocity gradient and not with the orientation tensor. Direct comparison with NEMD simulation data shows that the model can accurately describe the loss of entanglements due to the applied flow for three molecular weights by using the same value for the CCR parameter and the viscometric functions, although some discrepancies are observed in the description of the second normal stress coefficient. Overall, the model proposed here carefully derives via NET, and builds upon, the work of Ianniruberto-Marrucci and Dolata-Olmsted when stretching is not considered.

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Non-equilibrium Processes at Liquid-Vapor Interfaces

H. Struchtrup,(1) P. Feyzi Oskouei(1)

(1) Dept. of Mechanical Engineering, University of Victoria, Victoria, BC, Canada, Email: struchtr@uvic.ca

Abstract:

While evaporation of liquids and condensation of vapors are processes of daily experience, as well as commonly employed in technical systems, some finer details of these processes are still surprisingly little understood. Theoretical evaluation as well as experiments yield finite temperature jumps between liquid and vapor on both sides of the interface, and deviations of pressure from equilibrium saturation pressure. As interface effects, these jumps are mostly visible in smaller, i.e., microscopic, systems, where interface resistances contribute relatively more to overall system resistance than in macroscopic systems. Nevertheless, significant temperature jumps were reported for systems on the centimeter scale [1, 2].

In this presentation, we discuss and compare various approaches to observe and model non-equilibrium interfaces, based on molecular methods [3, 4], kinetic theory of gases [5, 6], and non-equilibrium thermodynamics [7, 8]. It will be shown that the often-used assumption of local thermodynamic equilibrium of the interface loses validity for the steep gradients encountered in molecular simulations. Accordingly, interface resistivities not only depend on the local temperature, but as well on process quantities such as heat and mass flux across the interface [8].

Acknowledgements:

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Ultrafast Entropy Production in Non-Equilibrium Magnets

F. Tietjen,(1) R. M. Geilhufe(2)

(1) Chalmers University of Technology, Department of Physics, Sweden. Email: finja.tietjen@chalmers.se
(2) Chalmers University of Technology, Department of Physics, Sweden. Email: matthias.geilhufe@chalmers.se

Abstract:

Material excitations studied far from equilibrium motivate the emergent field of ultrafast thermodynamics, which translates well-understood concepts, such as entropy and heat into characteristic time and length scales. By combining the rapid progress in ultrafast material science and non-equilibrium statistical physics, this research direction promises to build an efficient framework for the thermal control of materials, and the characterization of collective orders and phase transitions.

We present an ultrafast thermodynamics framework to model heat generation and entropy production in laser-driven ferromagnetic systems [1]. By establishing a connection between the magnetic field strength of the laser pulse and magnetization dynamics we model time-dependent entropy production rates and deduce the associated heat dissipation in epitaxial and polycrystalline FeNi and CoFeB thin films. Our theoretical predictions are validated by comparison to experimental magnetization dynamics data, shedding light on thermodynamic processes on picosecond timescales. Crucially, we incorporate recently observed inertial spin dynamics, to describe their impact on heat generation in pump-probe experiments. As such, this formalism provides novel insights into controlling heat production in magnetic systems, and contributes to advancing the understanding of non-equilibrium thermodynamics in magnetic systems, with implications for future experimental protocols in spintronics and nanotechnology.

Acknowledgements:

We acknowledge support from the Swedish Research Council (VR starting Grant No. 2022-03350), the Olle Engkvist Foundation (Grant No. 229-0443), the Royal Physiographic Society in Lund (Horisont), the Knut and Alice Wallenberg Foundation (Grant No. 2023.0087), and Chalmers University of Technology, via the department of physics and the Areas of Advance Nano and Materials.

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Thermodynamic compatibility of weakly nonlocal fluids with a scalar field

P. Ván,(1) M. Szücs(2)

(1) HUN-REN Wigner Research Centre for Physics, Department of Theoretical Physics, Budapest, Hungary. Email: van.peter@wigner.hun-ren.hu
(2) BME, Department of Energy Engineering, Budapest, Hungary. Email: szucs.matyas@wigner.hun-ren.hu
(3) Montavid Thermodynamic Research Group, Budapest, Hungary.

Abstract:

A thermodynamic derivation of weakly nonlocal nonrelativistic fluids is presented with the assumption that an additional scalar field -- a so-called internal variable, which initially has no specific physical content -- also contributes to the dynamics. The most general evolution of this field and constitutive relationships between pressure tensor and energy current density is determined via Liu's procedure. Classical holography of ideal (i.e.non-dissipative) fluids are generally proven, according to, the divergence of the pressure tensor, can be given via the gradient of a corresponding scalar potential, which expresses that a volumetric force acts on a test mass can be equivalently formulated via a surface force acts on the boundary of the corresponding region, thereby leading to a lower-dimensional formulation. Identifying the scalar field with the gravitational potential a weakly nonlocal Poisson-like equation of generalized Newtonian gravity is derived, which provides a thermodynamic compatible family of theories of modified gravity. The connection between classical and quantum fluids through the Madelung transformation is presented, and opportunities for direct generalization towards self-gravitating quantum

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On the axioms of heat transfer and multi-component diffusion in the Euclidean space

Kaushiki Dubey, Bhavya Tiwari, Devyani Thapliyal, Raj Kumar Arya,(1) George D. Verros (2)

(1) Department of Chemical Engineering, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar, India. Email: aryark@nitj.ac.in
(2) Department of Chemistry, Aristotle University of Thessaloniki, Greece. Email: gdverros@yahoo.gr

Abstract:

This paper investigates the axiomatic framework in Euclidean space for multi-component diffusion and heat transfer in near-equilibrium irreversible thermodynamics and linear extended irreversible thermodynamics (LEIT). The linearity postulate of irreversible thermodynamics concerning diffusion and heat transfer has been re-evaluated. This axiom is demonstrated to be compatible with the invariance principle of entropy production concerning a reference quantity for diffusion and heat transport in Euclidean space [1].

The requirement of adding the quasi-equilibrium assumption in multi-component isothermal diffusion and its theoretical foundations are examined. The Onsager Reciprocal Relations (ORR) for the multi-component diffusion scenario aligns with the quasi-equilibrium assumption in both near-equilibrium thermodynamics and LEIT [2]. The fundamental laws of multicomponent diffusion, such as the Onsager-Fuoss model and the Maxwell-Stefan formalism, are directly obtained utilizing both the quasi-equilibrium postulate and the ORR for isothermal multicomponent diffusion [2].

Finally, the thermal conductivity resistance in anisotropic solids such as crystals using LEIT. The fulfillment of the ORR in anisotropic bodies, such as crystals, has been demonstrated. This fulfillment is achieved by incorporating Newton's heat transfer coefficients into the calculation of the entropy production rate. Furthermore, a basic principle for the transport of heat, similar to the Onsager-Fuoss formalism for the multicomponent diffusion was established and a unifying framework for both heat transfer and multicomponent diffusion was developed.

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Recognizing Generalized Gradient Dynamics by Means of Machine Learning

V. Votruba,(1) M. Pavelka(1)

(1) Faculty of Mathematics and Physics, Charles University. Email: vv.votruba@gmail.com

Abstract:

In recent years, many connections between thermodynamics and machine learning have emerged. While the territory of reversible evolution has been thoroughly mapped with many approaches such as Hamiltonian Neural Networks, the learning strategies for dissipative phenomena remain less explored. We propose a physics-informed neural network architecture encoding gradient dynamics that can be used to learn the dissipation potential and entropy from trajectories of a dissipative system.

Previous works, such as Variational Onsager Neural Networks, have leveraged dual formulations using the Rayleigh function, whereas our approach uses entropy and dissipation potential. The practical implementation of this design has been successfully tested on basic examples such as an overdamped particle and a simple chemical reaction, see Figure [1]. The architecture could be applied to more complex systems (e.g., fully-fledged reaction networks) or integrated with reversible networks, leading to a learning strategy that can capture the entire GENERIC formalism.

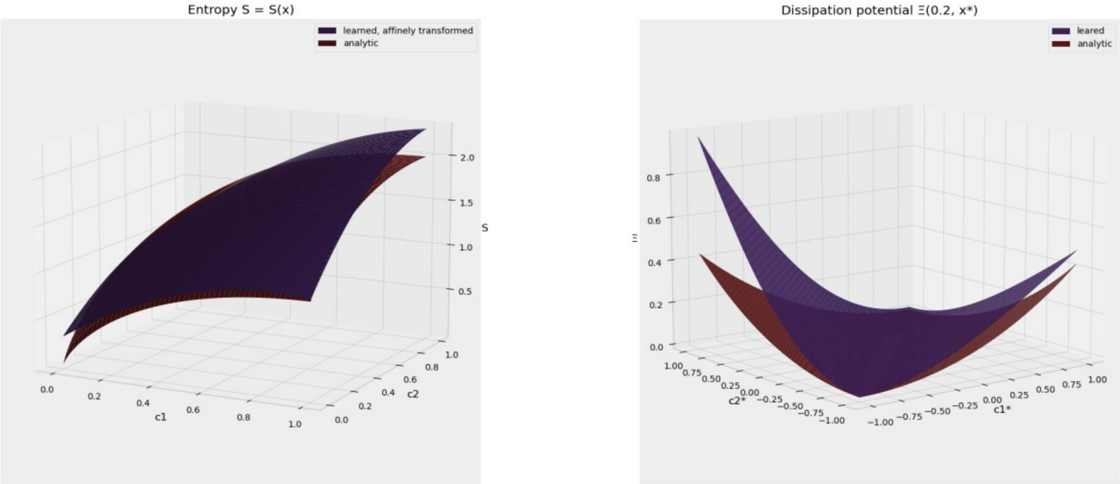

Figure 1: Learned entropy and dissipation potential for the reaction: $A \leftrightarrow B$

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Pioneering Fluctuations in Viscoelastic Stress: A Comparison of the Temporary Network and Dumbbell models

A. Winters,(1) J. Vermant(1)

(1) ETH Zürich, Soft Materials, Switzerland. Email: arturo.winters@mat.ethz.ch

Abstract:

The interpretation of scattering techniques [1] or microrheological experiments [2] is based on our knowledge of thermal fluctuations. Yet, for flows, our understanding of fluctuations is restricted to Newtonian materials, where fluctuating hydrodynamics applies fluxes uncorrelated in time and space. This corresponds to a local-equilibrium application of the Landau and Lipshitz Ansatz [3] of the fluctuation dissipation theorem (FDT). Thus, the noise is Gaussian.

In this work [4], we present novel insights into fluctuations in flowing viscoelastic materials. We illustrate the limits of the classical Gaussian approximation and show how, in the context of a local field theory, the most fundamental viscoelastic model, the Upper Convected Maxwell (UCM), exhibits different fluctuations depending on the underlying microscopic dynamics. Both the Temporary Network Model (TNM) and the Dumbbell Model (DM), which constitute model systems for two groups of microscopic models, reproduce the Maxwellian behavior. Until now, literature pointed out the equality of the two models with respect to stress evolution [5]. We now quantify differences when taking into account fluctuations and suggest techniques to measure them. Furthermore, we connect the scale of structural variables to the difference in the observed fluctuations.

With a novel formulation of the FDT, we point out that in a network system, Gaussian noise is doomed to lead to contradictions in the FDT's formulation [6]. We outline in which cases experiments, and molecular dynamics simulations should account for these findings to capture the correct microscopic dynamics of complex materials.

Acknowledgements:

We thank Prof. Öttinger for his guidance and support of the project.

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Efforts to implement Fluctuating Hydrodynamics in the mesoscopic modeling of polymer solutions

S. G. Yiantsios(1)

(1) Department of Chemical Engineering, Aristotle University of Thessaloniki, Greece. Email: yiantsio@auth.gr

Abstract:

The method of Brownian dynamics is well-known for its vast applications in the mesoscopic modeling of polymer solutions. In particular, the *bead-and-string model* has been extensively employed to study conformational, diffusional and rheological characteristics of dilute and semi-dilute polymer solutions [1-3]. A general feature of the method is that stochastic forces due to molecular thermal motion are applied to the beads, which represent the centers of hydrodynamic resistance of the polymer chains. Thus, the method results in a many-body problem for the beads exposed to thermodynamic forces and hydrodynamic interactions, the latter being expressed as pair-interactions through the Oseen or the Rotne-Prager-Yamakawa tensors. A well-known disadvantage of the numerical techniques employed to tackle such problems is that the computational operations are roughly proportional to the square of the number of beads and quickly become prohibitive if the solutions are not dilute.

In contrast, in *Fluctuating Hydrodynamics*, originally proposed by Landau and Lifshitz [4], the stochastic forces are applied to the surrounding fluid and transferred to the beads, or to any immersed bodies, through the stresses acting on them. Thus, if a numerical method is available to tackle the stochastic fluid momentum equations and it is capable of accounting for the immersed bodies in some manner [5,6], then there are two distinct advantages. First, the hydrodynamic interactions are more accurately represented, since they are inherently many-body interactions, and, second, the computational cost depends only very weakly on the number of the immersed beads. In the present discussion, some examples of application of Fluctuating Hydrodynamics to problems in polymer physics are outlined. In particular, dilute and semi-dilute solutions of linear polymer chains are considered and encouraging results are obtained on the diffusion of similar or different chains, on the diffusion of spherical nanoparticles in the solutions or in gels made of fixed inflexible chains, as well as on the viscosity of the solutions.

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Abstracts

(in alphabetical order of the Presenting Author)

Poster Presentations

Stable nanothermodynamics: beyond Boltzmann’s factor for thermal equilibrium and nanoscale fluctuations

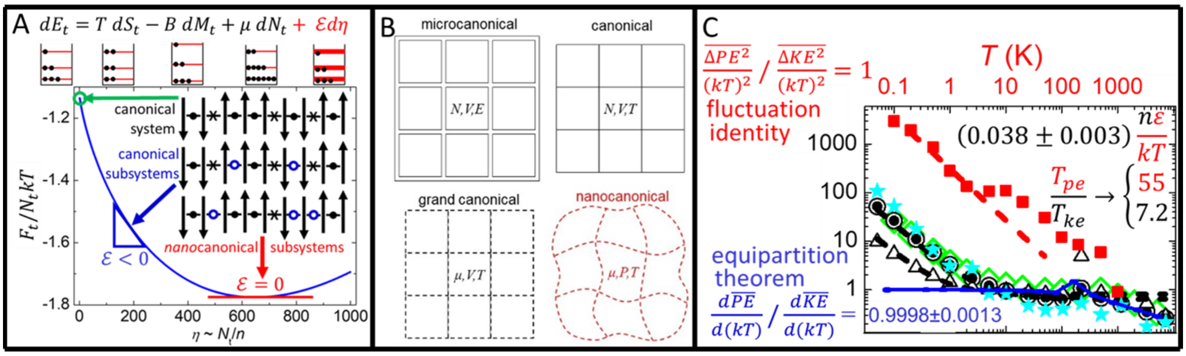
Ralph V. Chamberlin(1)

(1) Department of Physics, Arizona State University, Tempe, AZ USA 85287-1504. Email: chamberl@asu.edu

Abstract:

Hill’s theory of small system thermodynamics [1] has been called “the most extensive addition to equilibrium thermodynamics since Gibbs.” Indeed, Hill and Gibbs made mathematically similar (and comparably important!) contributions to the laws of thermodynamics. Specifically, conservation of energy during reversible processes (equation in Fig. A) requires the term introduced by Gibbs ($\mu\ dN_t$) if the total number of particles changes ($dN_t \neq 0$), plus the term introduced by Hill ($\mathcal{E}\ d\eta$) if the system contains independent internal subsystems ($d\eta \neq 0$). (Each sketch shows three energy levels, and how the net energy might be changed by each term in the equation.) Gibbs’ chemical potential is set to zero ($\mu = 0$) for the stable distribution of quantized waves, e.g. photons or phonons. Similarly, Hill’s subdivision potential is set to zero ($\mathcal{E} = 0$) to minimize the free energy (Fig. A), yielding the nanocanonical ensemble for the stable distribution of subsystems inside the system. Hill discussed this stability condition at length in section 10-3 of of his books [1], first published in 1964. To my knowledge, since 1964 only our group has applied $\mathcal{E} = 0$ to any system, providing novel insight into several “unsolved” problems in physics [2]. One example is the solution of Ising’s original (1925) model for finite chains of interacting spins (inset in Fig. A), where random breaks in the interactions (blue circles) yield $\mathcal{E} = 0$, as required for the true thermal equilibrium. Ising could not have found this solution 40 years before Hill’s work.

Two key assumptions must be met before Boltzmann’s factor ($e^{-E/kT}$) can be applied to the thermostatistics of small subsystems. 1) Each subsystem must couple to an effectively infinite heat bath that defines the temperature (T), and 2) this coupling must be very weak, but faster than the fluctuations in local energy (E). Now it is known that many measurements and computer simulations deviate significantly from these assumptions [2]. Most deviations are due to energy fluctuations that are too fast to fully couple to the heat bath. Figure C shows examples from MD simulations, where the effective temperature for equilibrium fluctuations in potential energy (T_{pe}) can be 7 to 55 times hotter than the T_{ke} for fluctuations in kinetic energy. In such cases, one must return to the fundamental laws of thermodynamics to interpret the behavior. Specifically, quantitative agreement with the fluctuations is found by using the microcanonical ensemble (Fig. B, upper left), because conservation of local energy is a more-basic law than Boltzmann’s factor.



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Zentropy: Integrating Quantum and Statistical Mechanics for Non-equilibrium Thermodynamics

Zi-Kui Liu(1)

(1) Department of Materials Science and Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

Abstract:

This poster presents zentropy theory, which is based on DFT quantum mechanics and Gibbs statistical mechanics and articulates that the total entropy of a system is composed of weighted average of quantum entropy of each configuration and information entropy across configurations. The theory's applications to the temperature-pressure phase diagram and critical phenomena in Ce and Fe_3Pt are demonstrated, showcasing both positive and negative divergences of properties at the critical point. Recently, using the entropy and Helmholtz energy of liquids derived from zentropy theory, the melting temperatures of pure elements and compounds have been accurately predicted. Additionally, zentropy theory predicts the Helmholtz energy of homogeneous systems. Considering that the stability of a system is governed by entropy production of internal processes, the entropy production and flux equations for heat conduction, mass transport, and entropy flow are discussed through the first, second, and combined laws of thermodynamics. This demonstrates an improvement over the phenomenological Onsager flux equation for cross phenomena.

Global Stability Analysis of the Dynamic Heartbeat Model

J. C. Pacheco-Paez,(1*) J. C. Chimal-Eguía,(2) D. Ladino-Luna,(3*) J. R. Luevano-Enriquez,(4) R. T. Páez-Hernández(5)

(1) Universidad Autónoma Metropolitana-A, México. Email: jcpacheco@azc.uam.mx
(2) Instituto Politécnico Nacional, CP 07738, México. Email: jchimale@ipn.mx
(3) Universidad Autónoma Metropolitana-A, México. Email: dll@correo.azc.uam.mx
(4) Universidad Autónoma Metropolitana-A, México. Email: jrle@azc.uam.mx
(5) Universidad Autónoma Metropolitana-A, México. Email: phrt@correo.azc.uam.mx
* Corresponding Authors: J. C. Pacheco-Páez, D. Ladino-Luna

Abstract:

In 1972, Zeeman [1] presented an innovative mathematical model that focused on the study of the heartbeat and nerve impulses, taking into account the most relevant dynamic characteristics of these processes. In particular, when analyzing the functioning of the heart, he focused on the dynamic properties of cardiac muscle fibers, which can be summarized in three aspects:

i. The concept of stable equilibrium, which refers to the system's ability to maintain a constant state of functioning.
ii. The threshold, which is the minimum level necessary to initiate an action, such as a heartbeat.
iii. The return to equilibrium, which describes how the system recovers after being disturbed.

The model Zeeman developed is based on a set of nonlinear differential equations, including a second-order equation to describe the heartbeat and a third-order equation for the nerve impulse. Through this mathematical approach, Zeeman was able to demonstrate that many of the complexities observed in the heartbeat can be explained by the relatively simple behavior of muscle fibers. In 2003, researchers Jones and Sleeman [2] made a significant modification to the Zeeman model. This modification consisted of incorporating a control variable that functions as a switch, thus representing the role of the pacemaker in the heart's contraction and relaxation process. This addition was crucial to better understanding how this vital mechanism is regulated. Later, in 2014, a group of researchers led by Páez-Hernández [3] focused on studying Zeeman's dynamic equation, but with a different approach. In their research, they considered the delay times inherent to the system, which allowed them to delve deeper into its dynamics. Other studies carried out in Biology and Medicine [4-5] are, for example, the mathematical model proposed by Ross [6] in 1911, for the transmission of malaria.

Acknowledgements:

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Behavior of the Curzon and Ahlborn cycle under the efficient power and power density criterion based on the ecological function

D. Ladino-Luna,(1*) J. C. Chimal-Eguía,(2) J. C. Pacheco-Páez,(3*) R. T. Paez-Hernández(4)

(1) Universidad Autónoma Metropolitana-A, México. Email: dll@correo.azc.uam.mx
(2) Instituto Politécnico Nacional, CP 07738, México. Email: jchimale@ipn.mx
(3) Universidad Autónoma Metropolitana-A, México. Email: jcpacheco@azc.uam.mx
(4) Universidad Autónoma Metropolitana-A, México. Email: phrt@correo.azc.uam.mx
* Corresponding Author: D. Ladino-Luna, J. C. Pacheco-Páez

Abstract:

As it is known, endoreversible finite-time thermodynamics (EFTT) is considered an extension of classical equilibrium thermodynamics that includes time dependence of interaction processes with external sources, while excluding irreversible effects within the working substance in a thermal engine. The behavior of the known Curzon and Ahlborn (CA) engine [1], in which there is no thermal equilibrium between the working fluid and the reservoirs at the isothermal branches, is shown as a Carnot type cycle.

Some novelty items studied by the EFTT point of view are the stability for thermal engines [2], the thermo-economic subject [3], and various technical applications [4], among other topics. It is worth noting that Angulo-Brown [5,6] advanced an optimization criterion for the CA cycle, by the function, $E = P - T_C\sigma$ knowing as the Ecological Function; where P is the power output of the cycle and σ is the total entropy production per cycle because of the heat transfer processes between the working substance and the reservoirs. Besides, the power output and the ecological function are shown as convex functions with a single maximum, the ecological criterion has been extensively adopted for the study of various thermodynamic systems [7-9].

On the other hand, an optimization based on the alternative objective functions, besides to the maximum power output, namely maximum efficient power and maximum power density was advanced. The efficient power is defined as $P_\eta = \eta P$, where η is the efficiency of the cycle, and the power density is defined as $P_d = P / V$, where V is the maximum volume of the cycle. As a result, a brief study on the behavior of a CA engine at maximum ecological function, maximum efficient ecological, and maximum ecological density is considered in the present paper for the CA cycle. The analytical expression, its corresponding dimensionless, and normalized dimensionless expressions are shown for these objective functions.

Acknowledgements:

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Stability analysis of a relativistic hydrodynamics model derived from non-equilibrium thermodynamics in a Lorentz-boosted frame

P. Panagopoulos Papageorgiou,(1) V.G. Mavrantzas(2),(3)

(1) Department of Chemical Engineering, Massachusetts Institute of Technology, USA. Email: ppapa@mit.edu
(2) Department of Chemical Engineering, University of Patras, Greece. Email: vlasis@chemeng.upatras.gr
(3) Department of Mechanical and Process Engineering, ETH Zürich, Switzerland. Email: vlasiosm@mat.ethz.ch

Abstract:

Relativistic fluid dynamics allows for the study of physical phenomena that are of paramount importance in the fields of astrophysics and cosmology. The issue of instability [1, 2] that characterized early formulations of a generalized fluid mechanics and thermodynamics model in the relativistic limit motivated the development of new models that are compatible with the fundamental laws of thermodynamics beyond equilibrium. This was accomplished by including in the set of hydrodynamic variables a covariant vector playing the role of a generalized thermal force and a covariant tensor closely related to the velocity gradient tensor using the GENERIC [3, 4] formalism of non-equilibrium thermodynamics. In a more recent study [5], the same relativistic hydrodynamics model was derived using the single generator bracket formalism.

In this work, we have started investigating the linear stability of these relativistic hydrodynamics models as derived from non-equilibrium thermodynamics [6] in a Lorentz-boosted frame [7]. In the present contribution, we will report the linearized form of the governing equations which were obtained both analytically and computationally using a symbolic code. These linearized equations will be employed in a second step to perform a linear stability analysis under time- and space-like perturbations. The linearization covers Lorentz boosts that are both in and orthogonal to the direction of propagation of the perturbation [7]. Our work aims to extend the stability analysis of the same model equations in the rest frame carried out by Stricker and Öttinger [6] to cases where perturbations in a Lorentz-boosted frame [7] are considered.

Acknowledgements:

We would like to thank Prof. Hans Christian Öttinger for very fruitful discussions in the course of the previous [5] and current projects.

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Phonon hydrodynamics of short channels: solids and superfluids

L. Saluto,(1) D. Jou(2)

(1) Department of Engineering, University of Palermo, Italy. Email: lidia.saluto@unipa.it
(2) Department de Fisica, Universitat Autònoma de Barcelona, Institut d'Estudis Catalans, Barcelona, Spain. Email: david.jou.mirabent@gmail.com

Abstract:

Heat transport in nanosystem requires an analysis not only of thin channels, but also of short channels. Most of the efforts in the analyses of heat transport have been devoted to thin but long channels (nanowires, ribbons, nanotubes). In short channels (with length L comparable or shorter to the mean–free path l), the role of boundary walls is important [1], but sometimes the channels are short but they do not have boundary walls at their ends, they are directly open to the reservoirs, constituted of the same material as the channel, instead of a different material.

In this work we propose an expression for the effective thermal conductivity of thin and short channels in the context of phonon hydrodynamics [2,3], based on the analogy with heat transport in superfluid helium. The channels communicate two thermal reservoirs of the same material than the channel, so that there are no interfaces at the longitudinal boundaries of the channel, but only an abrupt change in the width of the system. The corresponding expression is analogous to that arising in narrow and short channels of superfluid helium between two helium reservoirs at slightly different temperatures [4], so we can compare the equations of heat transfer in solids in the phonon hydrodynamic regime with those of heat transfer in superfluid helium. The differences between both kinds of systems are also analized.

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Modeling the Rheological Behavior of Cement Pastes

A. K. Ioannou,(1) P. S. Stephanou(1)

(1) Department of Chemical Engineering, Cyprus University of Technology, Limassol, Cyprus. Email: pavlos.stefanou@cut.ac.cy

Abstract:

In the construction industry, cement is one of the most necessary building materials, alongside other materials such as gravel, sand, and lime. For the effective and appropriate use of cement as a building material, requires a necessary and extensive analysis of the dual, reversible and irreversible, rheological behavior of cement pastes. When mixing cement with water, initially a suspension is created which due to agglomeration forms a reversible structure, while as the hydration reactions between cement particles and water progress, the cement paste gradually solidifies, acquiring a new irreversible structure [1]. The paste viscosity initially decreases with time, while at long times it increases due to the creation of the irreversible structure [2]. In the present work, we introduce a mathematical model for predicting the rheological response of the cement paste. To this end, we use the Generalized Brackets formalism of non-equilibrium thermodynamics [3] so that the constitutive model is, by construction, compatible with its laws. Consequently, we adopt two scalar structural variables: a reversible one, λ_{rev}, which characterizes the completeness degree of the reversible structure (the one that is responsible for predicting the yield stress, and which is destroyed under the influence of the flow field), and an irreversible one, λ_{irr}, which characterizes the completeness degree of the irreversible structure resulting from the hydrolysis reactions [4]. We also adopt a tensorial structural variable, to characterize the deformation of the complex structure, where each part is modeled as an elastic dumbbell that can attach, either reversibly or irreversibly, to the created. The predictions of the new model compare satisfactorily with available experimental data.

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List of Participants

Badur, Janusz	Polish Academy of Science, Poland jb@imp.gda.pl
Beris, Antony	University of Delaware, USA beris@udel.edu
Chacón-Acosta, Guillermo	Universidad Autónoma Metropolitana-Cuajimalpa, México gchacon@cua.uam.mx
Chamberlin, Ralph	Arizona State University, USA ralph.chamberlin@asu.edu
Colangeli, Matteo	University of L'Aquila, Italy matteo.colangeli1@univaq.it
Doi, Masao	Beihang University, China masao.doi@buaa.edu.cn
Edwards, Brian	University of Tennessee, USA bje@utk.edu
Engler, Jan	Charles University, Czech Republic engler@karlin.mff.cuni.cz
Floudas, George	University of Ioannina, Greece & MPIP, Germany gfloudas@uoi.gr
García-Perciante, Ana Laura	Universidad Autónoma Metropolitana-Cuajimalpa, México algarcia@cua.uam.mx
Gonzalez-Narvaez, Ruth	Universidad Autónoma del Estado de Morelos, México ruth.gonzalez@uaem.mx
Grmela, Miroslav	École Polytechnique Montréal, Canada miroslav.grmela@polymtl.ca
Harmandaris, Vagelis	The Cyprus Institute, Cyprus harman@uoc.gr
Herrera-Castro, Filiberto	Instituto de Energías Renovables, México hecafi@ier.unam.mx
Hoffmann, Karl Heinz	Technische Universität Chemnitz, Germany hoffmann@physik.tu-chemnitz.de
Housiadas, Kostas	University of the Aegean, Greece housiada@aegean.gr

Kazakidi, Asimina	University of Strathclyde, UK asimina.kazakidi@strath.ac.uk
Liu, Zi-Kui	Penn State University, USA prof.zikui.liu@psu.edu
Maslechko, Anastasiia	Odesa Mechnikov National University, Ukraine maslechko.an@gmail.com
Mavrantzas, Vlasis	University of Patras, Greece vlasis@chemeng.upatras.gr
Méndez, Alma Rosa	Universidad Autónoma Metropolitana – Cuajimalpa, México amendez@cua.uam.mx
Nadler, Ben	University of Victoria, Canada bnadler@uvic.ca
Öttinger, Hans Christian	ETH Zürich, Switzerland hco@mat.ethz.ch
Pacheco-Paez, Juan Carlos	Universidad Autónoma Metropolitana-A, México jcpacheco@azc.uam.mx
Panagopoulos Papageorgiou, Panagiotis	Massachusetts Institute of Technology, USA ppapa@mit.edu
Pavelka, Michal	Charles University, Czech Republic pavelka@karlin.mff.cuni.cz
Reina, Celia	University of Pennsylvania, USA creina@seas.upenn.edu
Ritos, Konstantinos	University of Thessaly, Greece konritos@uth.gr
Saluto, Lidia	University of Palermo, Italy lidia.saluto@unipa.it
Sciacca, Michele	Universita di Palermo, Italy michele.sciacca@unipa.it
Shang, Xiaocheng	University of Birmingham, UK x.shang.1@bham.ac.uk
Skarlatos, Anastassios	Université Paris-Saclay, France anastasios.skarlatos@cea.fr
Stephanou, Pavlos	Cyprus University of Technology, Cyprus pavlos.stefanou@cut.ac.cy

Struchtrup, Henning	University of Victoria, Canada struchtr@uvic.ca
Tietjen, Finja	Chalmers University of Technology, Sweden finja.tietjen@chalmers.se
Trasarti-Battistoni, Roberto	Independent Researcher, Italy roberto.trasartibattistoni@gmail.com
Ván, Peter	HUN-REN Wigner Research Centre for Physics, Hungary van.peter@wigner.hun-ren.hu
Verros, George	Aristotle University of Thessaloniki, Greece gdverros@yahoo.gr
Votruba, Vojtěch	Charles University, Czech Republic vv.votruba@gmail.com
Winters, Arturo	ETH Zürich, Switzerland arturo.winters@mat.ethz.ch
Wu, Xinyi	University of Birmingham, UK xxw142@student.bham.ac.uk
Yiantsios, Stergios	Aristotle University of Thessaloniki, Greece yiantsio@auth.gr
Zhao, Peiyuan	University of Birmingham, UK pxz491@student.bham.ac.uk
Zhou, Jiajia	South China University of Technology, China zhouj2@scut.edu.cn

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2. *University of Patras, Greece*
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