Prague School of Non-Equilibrium Thermodynamics

Celebrating Miroslav Grmela's 85^{th} birthday

Faculty of Mathematics and Physics, Charles University
Sokolovská 49/83, 186 00 Prague, Czech Republic
Room K1 (2^{nd} floor), Thursday&Friday, September 19-20, 2024

Sep 19		Thursday
9:00 – 9:20	Opening	
9:20 – 9:40	Miroslav Grmela	Some Trends in Multiscale Thermodynamics
9:40 – 10:00	Péter Ván	What are the first principles?
10:00 – 10:20	Josef Málek	On the interplay between thermodynamical and PDE analysis for incompressible fluids
10:20 – 11:00	Coffee break	
11:00 – 11:20	Karl Heinz Hoffmann	Endoreversible Thermodynamics: Optimizing Distillation
11:20 – 11:40	Róbert Kovács	Experimental observation of static and dynamic thermal conductivity
11:40 – 12:00	Vít Průša	Negative thoughts on negative mass
12:00 – 14:00	Lunch break	
14:00 – 14:20	Oğul Esen (online)	Contact Dynamics, and GENERIC in Hamilton-Jacobi Formalism
14:20 – 14:40	Mátyás Szücs	A reversible – irreversible vector field splitting explicit finite-difference scheme for coupled linear thermoacoustic problems
14:40 – 15:00	Christian Maes	Clausius heat theorem from Noether's theorem
15:00 – 16:00	Coffee break	
16:00 – 16:20	Christian Maes	The Third Law of Thermodynamics for steady nonequilibrium systems
16:20 – 16:40	Kateřina Mladá	Lack-of-fit reduction in non-equilibrium thermodynamics applied to the Kac-Zwanzig model
16:40 – 17:00	Alejandro Rey (online)	Rate of Entropy Production in Evolving Interfaces and Membranes under Astigmatic Kinematics: Shape Evolution in Geometric-Dissipation Landscapes
Sep 20		**Friday**
9:20 – 9:40	François Gay-Balmaz	Variational Principles in Nonequilibrium Thermodynamics and Applications
9:40 – 10:00	Markus Lohmayer	A Compositional Approach to Modeling Electromechanical and Thermodynamic Systems
10:00 – 10:20	Yuchao Hua	Maximum power & corresponding efficiency of thermoelectric generator based on fluctuation theorem
10:20 – 11:00	Coffee break	
11:00 – 11:20	Artem Ryabov	Upper bound on entropy production in traveling-wave potentials
11:20 – 11:40	Ti-wei Xue	Discussing the applicability of Onsager reciprocal relations
11:40 – 12:00	Yi-Dan Wu	Governing Equations of Thermoelectric Generators
12:00 – 14:00	Lunch break	
14:00 – 14:20	Ilya Peshkov	The geometry of flowing continua
14:20 – 14:40	Michal Pavelka	Direct Poisson Neural Networks
14:40 – 15:00	Václav Klika	Two-phase interface subjected to small constant heat flux: a case study of nonequilibrium thermodynamic description of the interface
15:00 – 16:00	Closing	

Abstracts

Miroslav Grmela: Some Trends in Multiscale Thermodynamics. Heat engines make changes on the macroscopic scale (they move locomotives) by making changes on the microscopic scale (by forcing atoms composing the water inside the locomotives to move faster). Thermodynamics (that sprang from the invention of heat engines) is a theory of relations among levels of description involving varying amount of details. Some more recent trends in its development are the following:

(1) A passage directed from an autonomous level involving more details ((S)- level) to another autonomous level involving less details ((T)-level) is found by recognizing a pattern in the space of solutions of the (S)-level governing equations (a pattern in the (S)-phase portrait) and by identifying a submanifold ((T)-manifold $\subset$ (S)-state space) and a vector field attached to it ((T)-vector field) that generates the pattern. Geometry of the (T)-submanifold provides the (T)-fundamental thermodynamic relation and the (T)-vector field is the vector field on the (T)-level. Entropy is a potential arising in the pattern recognition process.

(2) The Boltzmann kinetic equation describes the passage from the level of particle mechanics ((PM)-level to the level-of-equilibrium- thermodynamics ((ET)-level) for an ideal gas. The abstract Boltzmann equation (GENERIC equation) describes the passage (S)-level $\rightarrow$ (ET)-level for all macroscopic systems. Its particular realizations involve the Gibbs equilibrium statistical mechanics (this a particular realization of the static version of GENERIC) and the passage Fluid-Mechanics-level $\rightarrow$ (ET)-level investigated in nonequilibrium thermodynamics. The passages ((S)-level $\rightarrow$ (T)-level are made by investigating the time evolution in the (S)-level vector fields rather than the time evolution in the (S)-level state space.

(3) Maximization of the entropy (or the entropy-like potentials) subjected to constraints is from the mathematical point of view a Legendre transformation. We can say that the fundamental group of thermodynamics is the group of Legendre transformations. The contact geometry is thus a natural geometry for thermodynamics (both static and dynamic) since the contact structure is preserved under Legendre transformations.

(4) Mesoscopic levels in the AI dynamics of neurons (levels addressing feelings and consciousness) are waiting to be developed.

Péter Ván: What are the first principles? Thermodynamics, and in particular, the Second Law of Thermodynamics, is considered to be an emergent branch of physics derived from the statistical properties of the microscopic constituents of matter. However, this does not explain the ubiquity and the universality of thermodynamic concepts in many different theories of physics. We speak about temperature in black holes and in quark-gluon plasma, and the mathematical structure of thermodynamics plays a role in almost every branch of physics. I will argue, that this universality can only be explained if the Second Law of Thermodynamics is interpreted as a First Principle.

Josef Málek: On the interplay between thermodynamical and PDE analysis for incompressible fluids. Abstract: When computationally solving any initial-boundary-value problem governed by (a system of nonlinear) partial differential equations (PDEs), it is beneficial to know the precise meaning of the solution that one wishes to approximately compute and what are the properties of such solution. Particularly, one is interested in dealing with a solution that exists for any time interval and for any set of problem parameters, and in knowing if such a solution is uniquely determined by the initial state. With respect to dynamical problems in fluid mechanics, the two-dimensional internal flows governed by the Navier-Stokes equations serve as a prototype example when such questions are positively answered, using the concept of weak solution, which is from a thermodynamical point of view a natural concept of the solution for these types of problems.

Following this viewpoint, the objective of the talk is to present recently achieved results concerning the existence (and uniqueness) of weak solutions for three-dimensional unsteady flows of some incmpressible fluids, ranging from the activated Euler fluids on one side till heat-conducting Navier-Stokes-Fokker-Planck on the other side.

The talk is based on joint works with Miroslav Bulíček, Vít Průša and Endre Süli.

Karl Heinz Hoffmann: Endoreversible Thermodynamics: Optimizing Distillation. Distillation processes require large amounts of energy which is dissipated to heat. Reducing the associated entropy production is thus of great importance. One approach to achieve this is by using diabatic instead of adiabatic distillation columns. Here we present the large reduction potential using an Endoreversible Thermodynamics based investigation.

Róbert Kovács: Experimental observation of static and dynamic thermal conductivity. The effective modeling of heterogeneous materials requires heat equations beyond Fourier. The most straightforward alternatives have two time scales, which can be interpreted as the appearance of the static and dynamic heat conduction properties. From this point of view, the relevant models are the Guyer-Krumhansl and Jeffreys heat equations. Under particular conditions, these models can provide the same temperature history. The presentation discusses the experimental observations and the modeling alternatives for heterogeneous materials.

Vít Průša: Negative thoughts on negative mass. The concept of effective mass is frequently used for simplification of complex models. In the case of wave transmission analysis of some metamaterials the corresponding effective mass can be frequency dependent, negative and it may not even be a scalar quantity. These findings have even led some authors to suggest that Newton's second law needs to be modified within the context of classical continuum mechanics. While there is nothing wrong with the mathematical procedures used to reach these conclusions, the accompanying physical interpretation thereof is absurd. We show that the puzzling concept of negative mass can be easily eliminated provided that we model the corresponding metamaterials using an effective constitutive relation. The effective constitutive relation is a rate-type constitutive relation and the simple models we study give a clue how to design a non-trivial effective rate-type constitutive relation that is conservative, that is, possessing an associated conserved energy depending on the force/stress and its time derivatives. In short, the rate-type constitutive relations obtained in this study might be seen as a revival of hypoelastic materials.

Oğul Esen: Contact Dynamics, and GENERIC in Hamilton-Jacobi Formalism. This presentation is divided into two sections. The first objective is to develop Tulczyjew's triplet for contact dynamics, a structure suitable for performing the Legendre transformation between Herglotz-Lagrange Dynamics and Contact Hamiltonian Dynamics, even in degenerate cases. Using this framework, I will explore Implicit Contact Dynamics. The second part will focus on introducing a geometric framework for GENERIC (General Equation for the Nonequilibrium Reversible-Irreversible Coupling) within the context of contact Hamilton-Jacobi theory. GENERIC describes a dynamic system that integrates reversible and irreversible motions, where the reversible part is governed by a Poisson bracket, and the irreversible part requires a dissipation potential.

Mátyás Szücs: A reversible – irreversible vector field splitting explicit finite-difference scheme for coupled linear thermoacoustic problems. In a small vicinity of the liquid-vapor critical point, the fluid behaves strongly compressible, and in parallel, thermophysical properties perform rapid changes. All this manifests itself in the nonlinear coupling of thermal and mechanical processes, which, in linear approximation, yields thermoacoustics. Here, we present a second-order accurate, fully explicit staggered space-time grid finite difference method for such coupled linear thermoacoustic problems. Motivated by GENERIC, time integration is based on the splitting of the vector field representing the interactions affecting the dynamics into reversible and irreversible parts, which splitting procedure leads to decoupled wave and heat equations. The former is hyperbolic, while the latter is a parabolic partial differential equation, therefore, different time integration algorithms must be used to obtain a reliable, dispersion and dissipation error-free numerical solution. Finally, the thermoacoustic approximation of the supercritical Piston effect is investigated via the developed method.

Christian Maes: Clausius heat theorem from Noether's theorem. The adiabatic invariance of the thermodynamic entropy invites a connection with Noether's theorem, which has been the subject of various papers; e.g. by Wald (for black hole thermodynamics) and by Sasa et al. We revisit those results. First we show how the First Law can be obtained from Noether's theorem for mechanical systems when considering trajectories which are thermodynamically consistent. We also include macroscopic dynamics known as Gradient Flow and GENERIC for which the dynamical fluctuations show a canonical structure. We find a continuous symmetry of the corresponding path-space action when restricting to quasistatic trajectories, with the thermodynamic entropy as Noether charge. [Joint work with Aaron Beyen]

Christian Maes: The Third Law of Thermodynamics for steady nonequilibrium systems. Specific heats can be defined operationally for driven or active materials, by evaluating the (extra) released dissipated heat by the system that is entirely due to its relaxation to a new steady condition when the temperature of the environment is slightly changed. Naturally, such a nonequilibrium specific heat also discloses kinetic information about the system. Together with Karel Netocny and Faezeh Khodabandehlou, we have asked whether that heat capacity vanishes at absolute zero. It turns out that an extra (dynamical) accessibility condition is needed, compared to the equilibrium situation for the validity of the Third Law. See F.Khodabandehlou, C. Maes and K. Netočný, A Nernst heat theorem for nonequilibrium jump processes. Journal of Chemical Physics 158, 204112 (2023).

Kateřina Mladá: Lack-of-fit reduction in non-equilibrium thermodynamics applied to the Kac-Zwanzig model. Microscopic particle dynamics is purely reversible, yet when observed macroscopically, irreversible evolution occurs. How does the irreversibility emerge? On the example of Kac-Zwanzig model, we show the emergence of irreversible behavior out of a purely reversible Hamiltonian dynamics, caused only by the reduction of observed degrees of freedom. Furthermore, the irreversible evolution is found as a sum of Hamiltonian and gradient dynamics. This is done using the so-called lack-of-fit reduction.

Alejandro Rey: Rate of Entropy Production in Evolving Interfaces and Membranes under Astigmatic Kinematics: Shape Evolution in Geometric-Dissipation Landscapes. This paper presents theory and simulation of viscous dissipation in evolving interfaces and membranes under kinematic conditions, known as astigmatic flow, ubiquitous during growth processes in nature. The essential aim is to characterize and explain the underlying connections between curvedness and shape evolution and the rate of entropy production using membrane dissipation due to bending and torsion rates. The membrane dissipation model used here is known as the Boussinesq-Scriven fluid model. Since the standard approaches in morphological evolution are based on the average, Gaussian and deviatoric curvatures, which comingle shape with curvedness, this paper introduces a decoupled approach whereby shape is independent of curvedness. In this curvedness-shape landscape, the entropy production surface under constant homogeneous normal velocity decays with growth but oscillates with shape changes. Saddles and spheres are minima while cylindrical patches are maxima. The astigmatic flow trajectories on the entropy production surface, show that only cylinders and spheres grow under the constant shape. Small deviations from cylindrical shapes evolve towards spheres or saddles, where dissipation rates decrease. Taken together the results and analysis provide novel and significant relations between shape evolution and viscous dissipation in membrane and surfaces.

François Gay-Balmaz: Variational Principles in Nonequilibrium Thermodynamics and Applications. In this talk, I will present a variational formulation for nonequilibrium thermodynamics that extends the critical action principle of mechanics to include irreversible processes such as friction, heat and matter exchange, and chemical reactions. The structure of this formulation is reminiscent of the Lagrange-d'Alembert approach and accommodates both closed and open thermodynamic systems. Applications to interconnection, thermodynamically consistent modeling, and structure-preserving discretization will be provided for finite- and infinite-dimensional systems. Additionally, I will discuss the derivation of single- and double-generator (GENERIC/metriplectic) bracket formalisms from a variational perspective.

Markus Lohmayer: A Compositional Approach to Modeling Electromechanical and Thermodynamic Systems. This talk presents a formal language for multiphysics modeling, specifically designed for mechanical, electromagnetic, and thermodynamic systems with local equilibrium. The language facilitates the development of complex models by hierarchically composing simpler subsystems through a graphical syntax that clearly displays energy-based interconnections. This compositional approach reduces cognitive load and enhances communication in multidisciplinary environments. Additionally, it simplifies the encapsulation, reuse, and modification of models. The language enforces consistency with fundamental thermodynamic laws, such as conservation of energy and non-negative entropy production. To illustrate the approach, an electro-magneto hydrodynamics model is presented. This model integrates a Maxwell model of electromagnetic waves and a Navier-Stokes-Fourier fluid model, which itself has an ideal fluid model as a subsystem, demonstrating the potential to streamline model development.

Yuchao Hua: Maximum power & corresponding efficiency of thermoelectric generator based on fluctuation theorem. Thermoelectricity has long been a highly active research topic, which holds a great potential to create solid- state energy converters capable of converting heat into electricity without moving components. Furthermore, thermoelectric generator (TEG) can also serve as very crucial paradigmatic model for the researches of irreversible thermodynamics, like Onsager reciprocal relations (ORRs), and the efficiency at maximum power, etc. Here, we investigate the maximum power and efficiency of thermoelectric generators through devising a set of protocols for the isothermal and adiabatic processes of thermoelectricity to build a Carnot- like thermoelectric cycle, with the analysis based on fluctuation theorem (FT). The Carnot efficiency can be readily obtained for the quasi-static thermoelectric cycle with vanishing power. The maximum power- efficiency pair of the finite-time thermoelectric cycle is derived, which is found to have the identical form to that of Brownian motors characterized by the stochastic thermodynamics. However, it is of significant discrepancy compared to the linear-irreversible and endoreversible-thermodynamics-based formulations. The distinction with the linear-irreversible-thermodynamics case could result from the difference in the definitions of Peltier and Seebeck coefficients in the thermoelectric cycle. As for the endoreversible thermodynamics, we argue the applicability of endoreversibility could be questionable for analyzing the Carnot-like thermoelectric cycle, due to the incompatibility of the endoreversible hypothesis that attributes the irreversibility to finite heat transfer with thermal reservoirs, though the distinction in the mathematical expressions can vanish with the assumption that the ratio of thermoelectric power factors at the high and low temperatures (γ) is equal to the square root of the temperature ratio, $\gamma = \sqrt{T_L/T_H}$ (this condition could significantly deviate from the practical case). Lastly, utilizing our models as a concise tool to evaluate the maximum power-efficiency pairs of realistic thermoelectric material is presented with a case study on the n-type Silicon.

Artem Ryabov: Upper bound on entropy production in traveling-wave potentials. We propose a bound on average entropy production for overdamped Brownian motion in external time-dependent potentials having a shape of a traveling wave. Dynamics of such a system can be mapped onto a thermodynamically consistent time-homogeneous Markov process, for which so-called thermodynamic uncertainty relations are valid. While these relations represent lower bounds on average entropy production, a bound proposed here estimates the entropy production from above. This upper bound implies a restriction on the kinetic efficiency of particle transport considered in recent experiments.

Ti-wei Xue: Discussing the applicability of Onsager reciprocal relations. In 1931, Onsager [1,2] discovered a deep underlying reciprocal relation in irreversible transport coupling phenomena, for which he was awarded the Nobel Prize in chemistry in 1968. However, by reviewing his work we found that the reciprocal relation can be proved rigorously only if the flux is defined as the time derivative of an extensive state variable and the force is defined as the partial derivative of entropy with respect to the corresponding state variable. We have recently proved it again using the method of equilibrium thermodynamics [3], which suggests that the reciprocal relation for this choice of force-flux pairs is only a reflection of underlying symmetry of equilibrium thermodynamics. Callen [4] thought that this choice of force-flux pairs corresponds to a special type of transient processes near equilibrium and its expansion to irreversible steady-state processes far from equilibrium involves an approximation. We believe, however, that there might be an essential difference between the reciprocal relations of steady-state and transient processes, which needs to be further explored.

[1] Onsager L. Reciprocal relations in irreversible processes. I. Phys. Rev., 1931, 37, 405.

[2] Onsager L. Reciprocal relations in irreversible processes. II. Phys. Rev., 1931, 38, 22265.

[3] Xue TW, Guo ZY. Thermodynamic Derivation of the Reciprocal Relation of Thermoelectricity. Entropy, 2024, 26, 202.

[4] Callen H. B. The Application of Onsager's Reciprocal Relations to Thermoelectric, Thermomagnetic, and Galvanomagnetic Effects. Phys. Rev., 1948, 73, 1349 – 1358.

Yi-Dan Wu: Governing Equations of Thermoelectric Generators. For reasons such as the fact that the electrical circuit in a thermoelectric generator consists of p-type and n-type materials in which the charge carriers are different, we conclude that the thermoelectric process in TEGs is not a thermoelectric cycle but a combination of the heat and electricity conductive processes. We have developed a comprehensive system of control equations for TEGs, providing a quantitative framework to elucidate how various parameters affect conversion efficiency. The calculations for maximum output power are consistent with experimental data. However, in contrast to the prevailing literature, which posits that thermoelectric conversion efficiency monotonically increases with the Seebeck coefficient, our findings indicate the presence of a maximum efficiency at a specific Seebeck coefficient. The position of this maximum is influenced by factors such as load resistance, external thermal resistance, internal electrical resistance, and thermal resistance.

Ilya Peshkov: The geometry of flowing continua. We discuss a differential geometry viewpoint on the modeling of irreversible deformations of continua. It is demonstrated that the intrinsic geometry of a flowing continuum is inherently non-Euclidean and can be described in terms of Cartan's moving frames.

Michal Pavelka: Direct Poisson Neural Networks. Imagine a time-series of snapshots of states of a mechanical system. How to recognize the dynamical system from that snapshots? As mechanics can be expressed in terms of Hamiltonian dynamics, the goal is to recognize the underlying Poisson bracket and energy. Direct Poisson neural networks (DPNNs) provide an automatic tool solving that task [1].

[1] M. Šípka, M. Pavelka, O. Esen, and M. Grmela, Direct Poisson neural networks: learning non-symplectic mechanical systems, Journal of Physics A: Mathematical and Theoretical 56(49), 2023.

Václav Klika: Two-phase interface subjected to small constant heat flux: a case study of nonequilibrium thermodynamic description of the interface. There are two main approaches to modelling interfaces within nonequilibrium thermodynamics, the so-called sharp and diffuse interface models. Both of them are based on the assumption of local equilibrium (LEA) in the bulk, but the latter additionally assumes the validity of this concept also within the interface itself (as the thermodynamic description is available and smoothly varying even within the interface), that is on a finer length scale, which we call super-LEA. Instead of testing the two approaches against molecular dynamic simulations, we explore the mutual compatibility of these two description of an interface in a nonequilibrium situation. Based on the level of detail in the two frameworks, one naturally cannot reconstruct a diffuse interface model from a sharp interface counterpart. One can test, however, whether diffuse interface models are indeed a more detailed description of the interface. Namely, assuming that both approaches are valid, we use the diffuse interface model (van der Waals entropy together with the Cahn-Hilliard type energy with the mass density as the order parameter) and its sharp interface counterpart (with the additional set of interfacial state variables subjected to known thermodynamic constraints) to test their mutual compatibility and indirectly verify the correctness of the additional super-LEA of the diffuse models. That is, thanks to super-LEA, we define five interfacial temperatures that should be equal. However, when we analyze diffuse interface results like experimental or simulation data in terms of sharp interfaces, we show that, contrary to molecular simulation data, they do not yield equal interfacial temperatures. We argue that the culprit is the super-LEA which is most prominently expressed in the accessibility of the entropy density profile. Nevertheless, it is observed that there is an inconsistency between diffuse and sharp interface descriptions, they cannot be both correct. The sharp interface framework has been recently tested against molecular dynamics and the obtained results suggest that that super-LEA is the potential weakness of the diffuse framework. In this sense, sharp interfaces are found to be superior to diffuse interfaces in their general ability to model physical systems with interfaces.