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Report on Habitation Thesis of Michal Pavelka

Michael Pavelka's habilitation thesis concerns the multiscale geometric approach to constructing mathematical models of thermo-mechanics of continuous bodies. It summarizes six author papers written jointly with other authors in excellent journals.

In chapter 1, there is a significant declaration about the author's idea and the school of his supervisor Miroslav Grmela. Instead of constructing continuum models based as usual on balance laws and using the closure with appropriate constitutive equations, the author believes in the general structure based on a general geometric approach in which the balance laws and the constitutive relations are consequences of the geometry. The same approach based on statistical mechanics or at mesoscopic scale-like BBGKY hierarchy or moments closure in Kinetic Theory and Rational Extended Thermodynamics can be reconducted, at least in part, in a geometrical framework.

The ingredient of this approach is substantially the non-equilibrium theories based on GENERIC, which is the acronym of *General Equation for Non-Equilibrium Reversible-Irreversible Coupling*, which the principal founders were Grmela and Öttinger. The Hamiltonian part of the theory is given in two blocks, a Poisson bracket and an energy functional in a block, and the gradient part that takes into account the dissipation and in which the entropy has room.

The approach is very elegant from a mathematical point of view, and Pavelka proves to know geometry methods and the GENERIC approach very profoundly. Moreover, he gave original results on these theories listed in Chapter 4. In particular:

- 1. He was able to clarify the time-reversibility for state variables without parity like the distribution function in kinetic theory.
- 2. He gave the GENERIC version of Ehnerfest reduction via Ehnerfest regularization of Hamiltonian systems.
- 3. He considered non-convex dissipation potentials.

4. He made several contributions to theoretical electrochemistry.

The results are very interesting, and the proof is that the papers are all published in international journals.

It is an original thesis on complex and current topics. It is written clearly, and the reader can follow the author's research work well and its various generalizations from simple models to the more complex ones. Therefore, the reviewer's opinion is highly positive. The high percentage of coincidences done by Turnitin system is since dr. Pavelka's Dissertation is a collection of reprints of several published papers co-authored by Pavelka, accompanied by his commentary.

The reviewer greatly admires the elegant theories presented by the author and, particularly those that the ideas of GENERIC are conjugated with the Russian school of Godunov, where the structure of hyperbolic systems has the so-called Godunov form with the consequence that the differential systems are symmetric.

Aware that each theory has its limitations, everyone has a particular taste in choosing one approach. The reviewer want to present the following observations that are not intended to be criticisms of the excellent work presented by the author in his habilitation thesis but want to be just a stimulus for questions that the reviewer asked himself while reading the papers:

- 1. The starting point of the differential systems derives from a variational principle. In the reviewer's opinion, this is too restrictive in non-equilibrium thermodynamics. The question of a Hamiltonian part and another dissipative part is not always convincing from a physical point of view.
- 2. In Rational Thermodynamics, entropy and the entropy principle play a fundamental role. Entropy is not an observable, and the entropy law is considered a supplementary law whose compatibility itself fixes the form of the entropy, its flux, and its production as constitutive equations. Instead, the present approach considers the entropy as any other field variable, and often a simple unmotivated supplementary entropy law is postulated. Furthermore, as in all variational approaches, the equation that plays the role of the supplementary law is given by the energy equation. This, in my opinion, is very limiting from a physical point of view.
- 3. In any papers, the authors considered weak solutions or shock waves, but since the systems in consideration are non-linear and hyperbolic, it is well known that classical solutions do not always exist, and it is necessary to prolong the solutions with the weak solutions. In this circumstance, it is well known that the role of the entropy law becomes fundamental in selecting the physically acceptable solutions considering the non-uniqueness of weak solutions.
- 4. In these very general approaches, many coefficients remain undetermined. Therefore, it would be interesting to know how these arbitrary functions present

in the models, such as the relaxation times, can be determined in a particular problem.

5. Related to the previous question, the range of validity of the models themselves is not clear. For example, in the case of gases, it is known that the kinetic theory is valid for rarefied gases, i.e., when the Knudsen number is big enough, while the Navier-Stokes-Fourier theory is substantially valid for dense gas. It is shown that the kinetic theory and the Rational Extended Thermodynamics converge to the parabolic type solutions of the Navier-Stokes-Fourier equations for small Knudsen numbers.

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