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Gutachten zur Dissertation/
Report on the scientific value of doctoral thesis

”Modeling multiphase flow in porous media with an application to permafrost soil”

written by

Martin Heida

There is an interesting and promising recent approach in continuum thermodynamics, called *(MREP)-assumption* in the thesis, that determines the constitutive equations for *tensorial* and *vectorial* quantities such as the Cauchy stress and the heat flux from the knowledge of the constitutive equations for two *scalar* quantities: one of these scalars is a thermodynamical potential (the internal energy, Gibbs' potential, the enthalpy or Helmholtz' free energy) or more generally the specific entropy, the second scalar is the rate of the entropy production. The significant advantage of this approach is its consistency with the laws of thermodynamics. The choice of the constitutive equation for the entropy (or one of the above stated thermodynamical potentials) determines the structure of the rate of entropy production expressed as the scalar product of thermodynamical fluxes and thermodynamical affinities and consequently specifies what quantities form the pairs. Considering a convex functional either expressed in the terms of affinities or fluxes or both, one determines the constitutive equations by maximizing this functional with respect to either the affinities or the fluxes (but not with respect to both as they are not independent) keeping track of all relevant constraints. There is another idea associated with the concept of causality (or causes and effects) stating that thermodynamical fluxes such as force have primary roles as they caused of effects

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in thermodynamical affinities (such as the strains); consequently, the above maximization procedure should be taken with respect to thermodynamical fluxes. (The above described approaches were introduced, developed and applied successfully to several different fields by K.R. Rajagopal and his co-workers during last fifteen years.) The key issue in this approach consists in specifying the right constitutive equation for a thermodynamical potential (or entropy) and for the rate of the entropy production, that is, one needs to know what are the storing energy and dissipative mechanisms associated with the considered process of a given material.

It has been left opened for more than forty years (with partial unsatisfactory answers given for example by Cowin, Goodman or Dunn, Serrin) how to develop thermodynamically consistent framework for *compressible* Navier-Stokes-Korteweg fluid and how to generalize it to include thermal processes, non-Newtonian effects, etc. Carrying on the approaches roughly described above, Martin Heida not only significantly contributed to the development of such a robust thermodynamically consistent framework (see a joint paper published in IJES in 2010), but he has made further contributions relevant more closely to the topic of his thesis: modeling and analysis of transport and diffusive processes in permafrost soil.

To be more specific, Martin Heida's thesis includes the following new results inspired by the (MREP)-assumption:

(i) Starting from a simplified framework of the mixture theory (the simplifications consists in the following: while the balance of mass is considered for each constituent, the balance of linear and angular momentum as well as the balance of energy are considered for the mixture as a whole), *the development of the first thermodynamically consistent framework for heat conducting flows of multiphase and multicomponent, both compressible and incompressible fluids.* The developed framework contains as particular cases models bearing the names of Stefan, Allen and Cahn, Cahn and Hilliard, Lowengrub and Truskinovski, etc.

(ii) *An extension of the approach to provide boundary conditions constitutively.* This is a completely new approach that Martin Heida's develops for thermodynamically isolated materials. This leads him to talk about the concept as surface entropy, surface energy, surface temperature, etc. It calls for reconsidering the concept of zero flux through the boundary, impermeable boundary, entropy sitting at the boundary, surface entropy (energy, temperature) different from the trace of the bulk entropy (energy, temperature) on the boundary, etc.

(iii) *An introduction of thermodynamically consistent scalings.* This is performed by scaling the variables such as the length, time, and then the constitutive equations for the scalars that are supposed to be known for applying the (MREP)-assumption. There is still many possible scalings - and similarly as possible forms of the constitutive equations - they have to come from the physical characteristics of the considered process for a given material. Once such a form and a scaling is known, the constitutive equations and the scalings for other quantities comes naturally as a consequence of our apriori knowledge. Here, the scaling is developed in order to derive the effective equations for flow through porous media via the homogenization theory.

These results are presented in Chapters 1 and 4, and partially in Chapter 2, where the homogenization theory is presented via formal asymptotic expansion. (Chapter 1 starts with mentioning a few concepts of the mixture theory. This part could be more precise and specific in introducing key concepts and main difficulties.) One point worth of emphasizing concerns local and global versions of several statements - local is related to the pointwise (or almost everywhere) relations, while global version is relevant to weak formulations/integral identities. As shown in the thesis (see page 21), the local and global version are at many curcimstances equivalent, provided that the terms are meaningful (i.e. integrable), which are reasonable assumptions in this context. Since 2004, I believe that the models developed using the (MREP)-assumption are suitable for further mathematical and numerical analysis of the relevant initial and boundary value problems. Martin Heida provides another important step towards this program.

In Chapter 3, the author presents the current state of art in modeling of flows in permafrost soil, which is basically the state of art in modeling of flows through rigid porous media. Towards this topic, the main results of the thesis are presented in Chapters 6 and 7. After deriving a new model (both in the bulk and on the boundary) - the first one that is thermodynamical consistent, that is developed on clear physical assumptions, that is capable of describing thermal processes of multiphase flows of multicomponent fluids and that includes the derivation of boundary conditions - Martin Heida derives two-scale models for such multiphase flows using the formal asymptotic expansion method. Since the model for flowing mixture is themomechanically consistent and complete, there is a potential of two-scale models to explain various hysteresis phenomena observed in porous media in general and in the permafrost soil in particular (as discussed in Chapter 3 and 7).

To conclude, I would like to emphasize that Martin Heida thesis brings a lot of new material, approaches and ideas that confirms that Martin Heida is an inventive and hard-working researcher who is motivated by deep understanding of physical phenomena and mathematical issues of the problems. Thesis provides several nice results that may be basis for several nice fundamental research papers that, to my opinion, may have tremendous impact on the development of various fields including applications in biomechanics, geophysics and chemistry. Martin Heida should be careful in introducing various mathematical concepts, clearer in its statements (that differ at different parts of the thesis) and patient in finalizing his outputs (thesis includes very high amount of typos). These drawbacks are fixable, although it may take longer time to confirm their validity. Without any doubts, Martin Heida proved that he is capable of performing high level research on its own. With pleasure I recommend his thesis for its defense suggesting as possible evaluation *sehr gut*.

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