MODEL REDUCTION IN CONTINUUM THERMODYNAMICS: MODELING, ANALYSIS AND COMPUTATION

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1 Overview of the Field

There are several rather different interpretations of the field *model reduction* in fluid mechanics. It can be viewed from the point of view of *mathematical modeling* as elaborating models and their adequately reduced versions that would simplify the underlying theory and produce, at lower computational costs, the desired information on the fluid system in question. *Mathematical analysis* may see the model reduction processes as a purely theoretical task, where the formal passage from the primitive to target systems is rigorously justified by the tool of modern functional analysis. *Model reduction* at this level may also include the study of systems reduced to invariant manifolds or attractors as well as explicit solution formulas based on group symmetries and other physically relevant simplifications of a given problem. Probably the most specific use of the term *model reduction* occurs in numerical analysis and implementations of numerical schemes. Here *model reduction* or *model order reduction* is understood as an effective process of reducing the number of equations used for modeling a given system, without substantial changes in the accuracy of the expected output. Unlike researchers in the field of modeling and analysis, numerical analysts have usually very clear ideas concerning the specific methods and tools used in the model reduction process. This holds, in particular, in model reduction in signal and image processing, where the model reduction can often be linked with some classical tasks of analysis and approximation theory.

The main goal of the meeting was to bring together experts in mathematical and numerical analysis as well as mathematical modeling to examine the recently emerging problems and to share ideas in a well focused environment. Given the diversity of the topics and the variety of reduced systems and their applications, these researchers would have probably never met together at any other meeting. This posed a challenge for individual presentations as well as for guiding the discussions. At the same time it gave an opportunity to see many issues from new and unconventional perspectives.

2 State of the Art and Major Challenges

The principal topics discussed during the meeting were highlighted in the key note lectures delivered by leading specialists in the respective field.

2.1 Mathematical theory of (complete) fluid systems

Complete fluid systems play the role of primitive systems in the theory of model reduction. They are designed and believed to provide a complete description of the observed phenomena. Accordingly, the fluids considered must feature all relevant physical properties: they are compressible, heat conducting, viscous, chemically reacting, or enjoying other properties as the case may be. Clearly, a mathematical description of these materials becomes rather involved; the resulting system of equations reflects the basic physical principles of conservation of mass, balance of momentum and energy, among others. The apparent mathematical complexity, however, does not necessarily imply that the model is more difficult to handle by the available mathematical tools. A typical example is *viscosity*, sometimes neglected in the models of "perfect" fluids, that may provide a strong regularizing effect and give rise to mathematically tractable models.

The relevant mathematical theory can be developed either in the framework of classical description supposing that all fields are smooth functions of space and time, or using the more recent concept of "weak" solutions, where the relevant physical principles are expressed by means of integral identities. Note that the "weak" formulation is actually much closer to the original interpretation of the underlying physical principles of balance and conservation, expressed originally in terms of integral identities rather than the more common systems of partial differential equations derived under the assumption of smoothness of all physical fields. This naturally reflects the principal focus of the underlying mathematical tools. While the differential operators focus on the local behaviour of the given functions, the integrals account for the global properties of the integrands over the domain of integration.

New mathematical tools emerged quite recently to handle the problem of solvability of complete fluid systems, among which the general concept of relative entropies (energies) and its application to the study of the mutual relation between classical and "modern" weak solutions.

The state of the art of the well-posedness theory of complete fluid systems can be summarized as follows:

- Most of the physically consistent systems are well posed *locally* in time. Specifically, for a given set of (initial) data, the problem admits a classical solution existing on an undetermined and possibly very short interval of time, see Matsumura and Nishida [19], Valli [29], Valli and Zajackowski [30], among others.

- The classical solutions could exist globally, provided the initial state of the system is closed to an equilibrium. Here, the presence of viscosity or other dissipative mechanisms play a crucial role, see Matsumura and Nishida [18].

- The weak solutions exist, under a physically grounded hypotheses imposed on the constitutive relations, globally-in-time. In general, however, they are not (known to be) uniquely determined by the data, see [10].

- The weak and strong solutions emanating from the same initial state coincide as long as the latter exists, see [12].

The last statement is usually called *weak-strong* uniqueness principle. As shown quite recently, the principle remain valid even in a larger class of weak solutions called *dissipative solutions*. The fact that the weak solutions exist globally in time and for any physically admissible data makes them a perfect tool for studying the problems arising in the process of model reduction, i.e., here the well justified simplification of the model while preserving its approximation properties. It allows to exploit, in particular, the singular limits arising in the scale analysis of more complex fluid systems, see [10].

One can however take a different standpoint and consider complete models for more complicated, constrained or unconstrained, fluids. Non-newtonian purely viscous or viscoelastic, compressible or incompressible, fluids; Cahn-Hillard, Allen-Cahn or Korteweg type generalizations of Navier-Stokes fluids; or equations describing flows through porous (rigid or elastic) media; or complete models arising from the theory of interacting continua can serve as examples of complete systems that differ from the compressible Navier-Stokes-Fourier fluid model and where in its full generality the mathematical theory is rather in its pregnant state.

2.2 Mathematical theory of incompressible fluids

The so-called incompressible (Newtonian) fluids can already be viewed as an example of a model reduction, here we wish to mean the well justified modification, obtained by means of the low Mach number (or incompressible) limit of a complete fluid system. Classical solvability of the underlying Navier-Stokes system represents an outstanding open problem of the theory of partial differential equations, also very popular as one of the ”millenium problems”, see Fefferman [9]. Numerical experiments may to a certain extent indicate the limitations of the rigorous mathematical theory, and the newly emerging mathematical models may offer an attractive alternative to the classical systems.

On the other hand, there are many fluids or fluid-like materials that can be well modeled as incompressible, yet their behavior cannot be described by the linear relation between the Cauchy stress and the symmetric part of the velocity gradient. As there are many such non-Newtonian features there are many different systems that have been proposed for their description. To be more specific, non-Newtonian phenomena called shear-thinning/shear-thickening and pressure thickening connected with significant heat conduction can be described by a viscous heat-conducting incompressible fluid model in which the viscosity depends on the pressure, shear rate and the temperature. The large data existence of weak solution for certain class of initial and boundary value problems is established in [3], see also Diening et al. [5] and [2] for stronger results in case where the material coefficients are independent of the pressure.

2.3 Scale analysis and singular limits

As already pointed out, singular limits give rise to reduced models after performing a scale analysis and letting some characteristic numbers go to zero or become infinite. The incompressible Navier-Stokes system, the Euler equations of gas dynamics, the Oberbeck-Boussinesq and anelastic approximation may be viewed as singular limits of complete fluid systems. Singular limits are often performed formally by means of asymptotic expansion of all quantities with respect to a singular parameter, see for example the survey paper by Klein et al. [16]. Their rigorous justification is, however, usually considerably more difficult. Recent development of the mathematical theory of complete fluid systems enables to perform rigorously certain singular limits, even in the case of the so-called ill-prepared data, where the primitive system is in a state that is ”far away” from the target stay, see [10]. Here, the new tools based on the concept of relative entropies applied to the primitive (full) system proved to be rather efficient, [11].

In non-Newtonian fluid mechanics or in the theory of mixtures, higher complexity of the models as well as the need to solve computationally given problems, the model reduction is frequently the only possible method of choice, see [27]. Reduction of the complete models can be due to constraints (such as incompressibility, rigid body dynamics, restriction to isothermal processes or no-slip boundary conditions) or due to geometrical setting in which the considered class of processes with given fluid model takes place (if one direction in the setting is significantly small it then leads for example to thin film, shallow water or shallow ice approximations) or due to other geometrical restrictions (to small deformation gradients, for example).

Clearly, a proper scaling cannot be decided by the theory but rather by experiments performed in the real world situation or by collecting and comparing numerous observations of practical experiments, numerical experiments included. On the other hand, the process of *filtering*, meaning omitting certain features of the complete system that are not “observed” in the experiments, should be rigorously justified by careful mathematical analysis in order to avoid, or at least understand, spurious solutions and unexpected oscillations in the numerical computations. Clearly, a concerted action of the specialists in the field of modeling, analysis, and numerics is needed.

2.4 Analysis of multiscale problems

Asymptotic analysis plays a crucial role in the design of efficient numerical methods for flows in a singular regime. These problems are characterized by multiple space and time scales, and by the fact that the standard numerical methods may either completely fail or become expensive. As the goal is to apply numerical methods to complete fluid systems, it is important to understand the qualitative changes of solutions in the singular limit regime. A typical example are rapid oscillations of acoustic waves in the low Mach number limit that can be eliminated by the method of acoustic filtering. Clearly, applying similar techniques requires a detailed mathematical analysis of the problem.

2.5 Mathematical modeling of new materials

Mathematical modeling of a large variety of new materials represents a true challenge. Liquid crystals, polymeric fluids, geological materials, biological liquids and soft tissues, "smart" materials require a substantial modification of rheological laws as well as the underlying mathematical theory. Without an appropriate understanding the physical structure of materials it is impossible to develop a meaningful mathematical model. In addition, future material models must address complicated and interconnected thermal, mechanical and chemical processes that go far beyond the classical approaches. Growth and deformation of biological tissues, deformation of composite materials and shape memory alloys, flows of polymer or metal melts, flows of mixtures and geophysical materials, liquefaction of soil, transport processes in porous media and their interaction with the substrate form a base for important real-world applications. Theory that is developed to describe the macroscopic behaviour of complex bodies should be built on a continuum mechanics approach without incorporating ad hoc state variables that do not have a clear physical meaning. An artificial combination of microscopic and macroscopic theories should also be avoided (this by no means underestimates the role of multiscale approaches to computations).

On the other hand, mathematical properties of the rheologically more complex fluids may shed some light on the nowadays unsurmountable classical problems, the difficulty of which might be attributed to the fact that they are "incomplete", so that the information provided is not sufficient for their well-posedness in the mathematical sense. Of course, these systems are more complex than the classical models of fluid mechanics and thermodynamics. Thus, the need to find appropriate approximate models is of high importance.

2.6 Discretisation, numerical analysis and computation

Numerical computation assumes a finite dimensional approximation of the mathematical model. This is typically done using some spatial meshes over the given domain and by some form of time discretisation. The unknown functions are then approximated as linear combinations of a finite number of basis functions, which leads to of a finite dimensional representation of the original model. As the mesh refines and/or the parameter(s) characterizing the quality of the discretization (such as the time step or the size of the mesh elements) goes to zero, the state-of-the-art paradigm investigates convergence of the finite dimensional solution to the solution of the original model. Proving such convergence often requires fine mathematical techniques. Here *a-priori* error analysis indicates how the error (asymptotically) decreases as the mesh is refined. Bounds of this type do not involve *computed* approximate solution and their actual value is uncomputable because it typically involves the unknown solution of the problem. When performing computations, one needs to estimate the size of the *actual error.* This is done using the so-called *a posteriori* error analysis and it allows to stop the computations when the required accuracy is reached.

The numerical solution process represents in case of difficult problems a tremendous challenge. Despite the fact that discretisation, a-priori and a-posteriori error estimation and algebraic (matrix) computations represent well-established fields, many fundamental issues remain open. They should not be studied separately *after* the mathematical model, its possible analysis and reduction has been performed. Modeling with its mathematical analysis together with discretisation, error estimation and solving the resulting finite dimensional discrete problems should be considered interdependent and closely related tasks of a single solution process. A failure in one subtask may at the end simply mean forming of a numerically unsolvable problem and therefore failure of the whole numerical solution process.

The fact that the state-of-the-art results often give rather partial answers can be documented on the prevailing approach to proving convergence of the discrete approximate solution when the mesh refines using some form of *adaptation.* The proofs are based on seeing individual mesh refinement steps as contractions for some error estimators with some fixed contraction parameter independent of the mesh. This seemingly allows reaching an arbitrary prescribed accuracy in a finite number of contraction steps, which is also claimed in literature. This is, however, impossible, simply due to the fact that the discretised algebraic problem needs to be solved numerically and, apart from trivial cases, it cannot be solved exactly; see the reviews [28] and [1]. In difficult problems we even do not wish to seek a highly accurate numerical solutions of the discretised problems since that would make the whole solution process unfeasible. The principal questions which needs to be addressed is therefore what is the size of the maximal attainable accuracy of our computations, whether the prescribed required accuracy can be reached and at which price.

3 Presentation Highlights

In accordance with the general idea of the meeting, the presentations were of survey character of the state of the art in the respective fields, rather than highly specialized talks on particular technical results accessible only to the specialists in the field.

3.1 Mathematical analysis

Several presentations, including the key note lecture, were devoted to the *mathematical theory of complete fluid systems*. The existence results for both evolutionary and stationary problems in the framework of weak and dissipative solutions were discussed. The method of relative entropies was exploited both in the context of the complete fluid systems (study of singular limits, weak-strong uniqueness, long-time behavior) and in the analysis of stability of the shock waves in inviscid fluids.

The problem of *regularity or conditional regularity* plays a crucial role in the analysis of the systems of partial differential equations arising in fluid mechanics. Since the weak solutions exist globally-in-time, it is of great interest to know whether these solutions are, in fact, smooth. On the other hand, if the solutions are not (or not known to be) smooth, the regularity criteria provides a useful insight in the mechanism of a possible blow up and help to eliminate the unphysical situations. Note that regularity of solutions of the inviscid incompressible (Euler) equations still remains one of the most challenging open problems, where the alternative weak solutions exhibit a number of rather pathological properties, see DeLellis and Székehylidi [4].

Rigorous analysis of *singular limits* is an undeniable part of the model reduction process. Here, the primitive system is put in a dimensionless form, where several characteristic numbers appear as new parameters of the problem. Identifying the limit system when one or several of these parameters vanish or become infinite is a mathematical challenge. At the level of analysis, "identifying" means proving convergence of the solutions of the primitive system to those of the target system. This can be done either by compactness arguments based on uniform bounds, or by means of measuring the distance from the limit system by means of a relative entropy. This procedure, rather new in the context of heat conducting fluids, was highlighted by several speakers. Mathematical analysis of the limit system, like Oberbeck-Boussinesq system or anelastic approximation was also discussed.

3.2 Mathematical modeling

The leading topic of the modeling part of the workshop was the recent development of the *implicit constitutive theory*. A simply looking basic idea of this approach, namely writing the constitutive equation interrelating two quantities A, B in the form

$$\mathcal{F}(A, B) = 0 \text{ instead of } A = \mathcal{G}(B) \text{ or } B = \mathcal{C}(A),$$

leads to completely new complex models of materials with complicated rheology, and the use of this method in the process of model reduction is one of the revolutionary leading ideas of the workshop.

The primal advantage of the implicit constitutive theory consists in the possibility to describe much larger class of material responses. In addition, as the quantity A and B appears in the classical theories (A and B can stand for the Cauchy stress and the velocity gradient, or heat flux and the temperature gradient, or the Cauchy stress and the deformation gradient) there is no apriori need to introduce new type of boundary conditions. Even more, the implicit constitutive theory brings clarity and simplicity to the theoretical foundation of continuum mechanics: it gives transparent justification to incompressible fluids with pressure and shear-rate dependent viscosity as well as to nonlinear models within the framework of linearized elasticity (small gradients of the displacement); see Rajagopal [21] and [22].

The considered models should obey the laws of thermodynamics. The development of the implicit constitutive relations is therefore combined with another recent ingredient, namely *the principle of the maximization of the rate of entropy production*, see Rajagopal and Srinivasa [23]. Such a framework allows developing thermodynamically consistent fully three-dimensional constitutive models. Here the material is characterized by the way how it stores energy and the way how it produces entropy. These storage and production mechanisms are specified by a choice of the constitutive equation for the entropy (or another suitable thermodynamic potential) and the rate of entropy production. Concepts of implicit constitutive relations allow to handle very general forms of storage and dissipation mechanisms. The entropy production is then maximized with respect to a constraint enforcing the validity of the reduced dissipation identity, and possibly also with respect to other constraints such as the incompressibility of the material. As a condition identifying the maximum one gets the required relation between the quantity A (for example the Cauchy stress) and the quantity B (for example the symmetric part of the velocity gradient).

Such approach is based on a small set of well articulated and justified fundamental (axiomatic) assumptions. So far, this approach has been successful in providing:

- appropriate thermodynamic setting for compressible heat-conducting fluids of a Korteweg type (see [14]),
- different viewpoints on Bingham and Herschel-Bulkley fluids (and other activation or deactivation criteria in general) (see [24] and [2]),
- an approach to characterize the structure of the boundary conditions (important for complex materials) as the constitutive equations on the surface (see Heida [13]).

The effective use of this new methodology was highlighted in several talks and possible applications, in particular in mathematical analysis and numerical implementations discussed.

3.3 Discretisation, numerical analysis and computation

Besides the standard numerical topics concerning the design and analysis of convergence of the new discretisation schemes applied to complex fluid systems, a substantial part of the numerical talks was devoted to *a posteriori* estimates and the problem of reliability of numerical methods. The decisive criterion is the degree of precision in which the results of computations reflect the properties of the genuine (analytical) solution of a given equation or system.

The key lectures were devoted to the topics of *adaptivity* as a form of the discretised model reduction, construction of *efficient and robust computational algorithms* and the *control of errors* of computed approximate solutions. All speakers emphasized the interplay between the infinite dimensional function representation and the reduced discrete representation of the model. In control of the discretisation and computational error, a-posteriori error analysis must consider algebraic errors and must include investigation of numerical stability; see, e.g. [15, 26, 8] an the recent survey paper by Rannacher [25] which all contain many references to other relevant works.

Construction of efficient computational algorithms requires *global communication* transferring the information obtained for different times and/or at different (and possibly distant) parts of the solution domain. It was demonstrated how this can be achieved, e.g., via incorporating *coarse space components* in domain decomposition methods; see [6]. The coarse components representation can be considered a form of the model reduction which can be used for substantial acceleration of computations. Efficient *preconditioning* represent another principal tool for achieving the same goal; see, e.g., the classical book by Elman, Silvester and Wathen [7], which is currently being revised and extended for the second edition. Preconditioning should reflect the physical nature of the problem expressed in the mathematical model. It can be motivated using a functional analytic operator description (so called "operator preconditioning"). Practical derivation of computational algorithms is, however, often much easier using a finite dimensional algebraic setting with its description via matrices. Combination of both views can lead to development of fast and robust solvers, with *Krylov subspace methods* (see the recent book [17]) as a possible basic underlying iterative scheme. Finally, construction of *fully computable a-posteriori error estimators* which allow for the *local error control* and comparison of the size of the error from different sources (discretisation, linearization, inexact algebraic computation) is a prerequisite for reliable, robust and efficient adaptive approaches [1]. This requires combination of rather diverse techniques from functional analysis through numerical analysis to analysis of iterative matrix computations including effects of rounding errors.

4 Scientific Progress Made

One of the main achievements of the meeting was dissemination of the new methods, sofar known only to specialists in their specific (sometimes even narrow) fields, to the representatives of the modeling, analysis, discretisation and computational communities. Several possibilities of applications of theoretical tools in the analysis of convergence of numerical schemes emerged, as well as new directions in the theoretical studies discovered in the framework of the implicit constitutive theory. Last but the least, the necessity of effective feedback and comparison of results and methods used in the three leading areas - modeling, analysis, numerics - appeared as necessary for the progress in the field of model reduction, where the last term may have many (interrelated) meanings.

It becomes very clear that a goal of reaching a substantial progress in model reduction in continuum thermodynamics, which would open new ways of research substantially beyond the current state-of-the-art, requires utilization of specific knowledge of the physical nature of a well chosen specific problems used as case studies. There is no hope for aiming at a general approach developing a universal computational framework. The hope is rather in investigating important particular examples with utilizing similarities between mathematical description of real phenomena from different fields with cautious well-justified generalizations to possible large classes of problems whenever applicable.

5 Outcome of the Meeting

The nature of the workshop has evoked much more questions then gave answers. For various reasons, science is getting more and more specialized, which brings, together with large benefits, also a great danger of fragmentation. Researchers working in different fields of the same scientific discipline (such as mathematics) see each other more and more rarely, and they rarely communicate across the disciplines with papers which are widely read and discussed. Sometimes we can observe growing isolation instead of tightening links between communities and scientific schools. Results are developed within one field without being communicated to, considered and used within related fields. It also becomes rather difficult to challenge common well established views and approaches. The widely adopted malign overemphasizing the publish or perish policy stimulates much more the standard mainstream production over a difficult and cross-disciplinary communication. But such communication is, in our opinion, desperately needed not only for solving difficult real-world-inspired problems, but for sake of the science itself.

This workshop tried to go in the direction of building bridges between different areas of mathematics related to the main topic, with including fundamental motivations from the corresponding parts of physics. The gaps which we need to deal with are neither narrow nor shallow, and a considerable effort will be needed just to establish a regular and fruitful communication. We consider such effort immensely important. Intensive discussions between participants proved that it can work. We believe that coming months will bring materialized outcomes in the form of joint work and papers.

Among the widely discussed questions which will be further discussed or investigated we mention:

- The prevailing paradigm in numerical solving of mathematical modeling problems is based on discrete approximation of the infinite dimensional problem via the Finite Element Method (FEM). Such approximation is constructed using *locally supported* basis functions which results in algebraic problems formulated using *sparse matrices.* This is presented as a principal advantage of FEM. The common view, that the locality of FEM bases and sparsity of the resulting matrices gives a great advantage of the FEM approach over some alternative approaches in particular when solving the discretized algebraic problems, might be worth of a second thought. As mentioned above, difficult problems can not be solved without exploiting the *global transfer* of information in time and over the domain. This requirement seems to be in some controversy with the philosophy of FEM and with the sparsity of the resulting matrices. Algebraic computations then can not be efficiently done without incorporating powerful global transfers of information which is handled by computational techniques such as preconditioning in iterative methods. It seems that here algebraic computations is getting difficult partially due to form of discretisation which prefers local approximation. The difficulty may show up, e.g., in comparison (including their spatial distribution) of the errors from different sources; see [20].

- Efficient numerical computations requires reconciling of different mathematical and computational requirements which are not always in line. Parallelism and scalability do not always go along with numerical stability and a need for global communication. Computer science tools do not always serve mathematical needs. There seems to be, in general, an insufficient communication between the computer science, mathematical modeling and applied mathematics communities. The trend seems to be rather to the worse then to the better.
- An interplay of the mathematical descriptions of problems on different levels (modeling - discretisation - computation) with tools ranging from fundamental mathematical analysis to construction and analysis of methods in matrix computations (including numerical stability analysis) represents a tremendous challenge by itself. Without a genuine *will for collaboration* of experts in all these fields, no real breakthrough in the topic of the workshop can be achieved.
- In linear model reduction known in linear dynamical systems and control there is a deep underlying mathematical background such as Padé approximation, Gauss-Christoffel quadrature, continued fractions, problem of moments, minimal partial realization etc. (just give a few examples) which also links classical topics from analysis and approximation theory to modern computational tools such as Krylov subspace methods; see [17]. *Nonlinearity* makes things from this point of view extraordinary complicated. No similar unified mathematical background essentially exists and solid mathematical foundations are yet to be built.

As appeared several times in our report, no significant progress in challenges mentioned above can be achieved, in our opinion, by a group of researchers working within a narrow field. In order to bridge the gaps, a well coordinated effort of all sides is needed. This workshop has tried to make a first step in this direction.

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