Macroscopic models for rarefied gas flows

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This talk presents an overview on classical and recent methods to derive macroscopic transport equations to model rarefied gas flows, and a critical examination of the resulting models.

It is well known that the Navier-Stokes-Fourier equations cannot describe rarefaction effects in gases, which appear in processes with Knudsen numbers $Kn > 0.05$ (say). A variety of extended models can be derived from the Boltzmann equation—the basic equation to accurately describe rarefied gases—which aim at describing rarefied gas flows at least approximately. The best known among these are the Burnett and super-Burnett equations, derived by means of the Chapman-Enskog method [1], and Grad's 13 moment equations, which follow from Grad's moment method [2, 3].

Burnett and super-Burnett equations suffer from instabilities in transient processes [4], and several modifications have been suggested to stabilize the equations, including the augmented Burnett equations [5], and the regularized Burnett equations [6]. Both sets of equations improve the Burnett equations only partly, and are difficult to justify from the Boltzmann equation.

Grad's moment equations [2, 3] exhibit unphysical sub-shocks in shock structures at large Mach numbers [7, 8], and so far could not be related to the rarefaction of the gas, i.e. to the Knudsen number. Since the equations can be derived for an arbitrary number of variables, a criterion that relates the number of moments to the Knudsen number was missing.

A technique for the regularization of Grad's 13 moment equations was presented recently, producing the regularized 13 moment equations (R13) which guarantee smooth shock structures [9, 10]. However, this method can be used for any number of moments, and thus leaves the question of how many moments need to be considered unanswered.

A recent approach within the framework of extended thermodynamics, termed as "consistently ordered extended thermodynamics" (COET), gave a first answer to this question [11]. However, COET yields certain sets of Grad-type equations, and thus does not remove the problem of discontinuous shocks. Moreover, the method was only applied to simple molecular interaction models—Maxwell molecules or the BGK model—and it is not clear how the method should be generalized to more realistic interaction models.

Elements of the COET method were blended with some new ideas to design a method for deriving transport equations for rarefied gases from the Boltzmann equation within higher orders of the Knudsen number [12, 13]. The method focuses on the order of magnitude of the moments of the phase density, and the order of accuracy of the transport equations, both measured in powers of the Knudsen number. This "order of magnitude method" was developed up to the third order for the special case of Maxwell molecules [12], and it yields the Euler equations at zeroth order, the Navier-Stokes-Fourier equations at second order, Grad's 13

moment equations (with omission of a non-linear term) at second order, and the regularization of these (R13) at third order.

The order of magnitude method was also used to derive a set of 13 moment equations for arbitrary molecular interaction potentials [13]. It was shown that the new set of equations is accurate to second order, while Grad's original 13 moment equations are of second order accuracy only for Maxwell molecules and BGK models.

An important feature of the order of magnitude method is that the equations of any order are stable, other than in the Chapman-Enskog method, where the second and third order approximations—Burnett and super-Burnett equations—are unstable. The latter can be extracted from the derived equations by means of the Chapman-Enskog method. It follows that the new method includes Burnett type and Grad type equations and the regularization of the latter, and thus forms a common umbrella for all known theories for macroscopic transport equations in rarefied gases.

A difficult issue in the theory of macroscopic transport equations is the problem to ascribe boundary conditions for higher moments, which are not controlled in experiments [14]. For better understanding of this issue, the Couette flow problem was split into two sub-problems, which concern the solution in the bulk and Knudsen boundary layers.

The bulk solution requires only jump and slip boundary conditions for temperature and velocity, which are well-known, and thus the bulk solution can be obtained readily.

The ability of macroscopic equations to provide Knudsen layer solutions was discussed in Refs. [9, 15], where it was also shown that additional boundary conditions are required. Alternatively, one can fit the amplitudes of the Knudsen layer solutions to accurate numerical solutions of the Boltzmann equation. Superpositions of the bulk solutions with fitted Knudsen layer solutions can then be compared to the Boltzmann solutions. The results presented here indicate that only the R13 equations can quantitatively describe Knudsen boundary layers, while the Burnett and super-Burnett equations fail.

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Riemann problem in Extended Thermodynamics

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The Riemann problem for a system of balance laws is still an often question. We study the problem with particular attention to the asymptotic behaviour. Moreover we study also the solutions when the initial data are a "perturbation" of the Riemann data proving results similar to the one of T. P. Liu obtained in the case of conservation laws. Applications are presented in the core of Extended Thermodynamics for rarefied gases and in the case of a binary mixture of Euler fluids.

Thermodynamics of Elastic Solids up to the Melting Point

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Thermodynamic quantities of linear isotropic elastic solids, that is, elastic constants, specific heats, coefficients of thermal expansion and Grüneisen parameters are estimated and discussed on the basis of the linearized macroscopic basic equations proposed recently by the author's group [1-4]. The equations were derived from a nonequilibrium statistical-mechanical model for crystalline lattices with a continuum approximation. The equations take microscopic thermal vibration of constituent atoms into account explicitly, and they are valid in a wide temperature range including the melting point as a limiting case. Some new coefficients relating thermal vibrations of constituent atoms to temperature variation and strain are also studied in detail in both isothermal and adiabatic processes. Peculiar temperature dependences of these quantities near the melting point are found. With these analytical results, Helmholtz free energy for elastic solids is formulated explicitly up to the melting point. The present model can be applied to many nonequilibrium phenomena in solids near the melting point, for an example, wave propagation phenomena [3,5].