

Henning Struchtrup

# Macroscopic transport equations for rarefied gas flows

– Approximation methods in kinetic theory –

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## Preface

An important parameter to describe rarefied gases is the Knudsen number  $\text{Kn}$ , defined as the ratio between the mean free path of the gas, i.e. the average distance traveled by a gas particle between two subsequent collisions, and a macroscopic length describing the flow, e.g. a channel width or the diameter of an object exposed to the flow.

The well known laws of Navier-Stokes and Fourier are applicable only for flows at sufficiently small Knudsen numbers, and fail in the description of flows at Knudsen numbers  $\text{Kn} \gtrsim 0.05$ . These Knudsen numbers are easily reached nowadays, e.g. in microscopic flows or in high altitude flight, and a reliable set of equations that can be solved at low computational cost for the description of these flows is highly desirable.

The basic equation for the description of rarefied gases is the Boltzmann equation which describes the microscopic behavior of the gas from a statistical viewpoint. The Boltzmann equation is valid for all Knudsen numbers, but—due to the detailed microscopic description—its numerical solution is expensive.

This text discusses classical and newer methods to derive macroscopic transport equations for rarefied gases from the Boltzmann equation, for small and moderate Knudsen numbers, i.e. at and above the Navier-Stokes-Fourier level. The resulting equations are compared and tested for a variety of standard problems. The classical methods, due to Chapman and Enskog, and to Grad, yield unsatisfactory equations, which are unstable in case of the Chapman-Enskog expansion (Burnett and super-Burnett equations), and describe unphysical discontinuous shocks in case of the Grad method. Only recently, the author was involved in developing alternative methods, which yield the regularized 13 moment equations (R13 equations) that avoid the shortcomings of the classical equations, but retain their benefits. Naturally, the methods for deriving the R13 equations, and the discussion of the equations are central points in the text.

This book is intended to be accessible not only to experts, but also the novice in kinetic theory, and thus develops the topic starting from the basic

description of an ideal gas, and the derivation of the Boltzmann equation, followed by various methods for deriving macroscopic transport equations, and test problems, including shock waves and Couette flow. About forty end-of-chapter problems provide opportunity to deepen the understanding, and numerous references provide directions for further study.

My understanding of the topic benefitted immensely from discussions with many scientists and students, and I wish to thank in particular the following people and institutions: Marcello Anile, Jörg Au, Elvira Barbera, Maurice Bond, Wolfgang Dreyer, Gilberto Kremer, David Levermore, Luc Mieussens, Ingo Müller, Institute for Integrated Energy Systems (Victoria, BC), Institute for Mathematics and its Applications (Minneapolis), Natural Sciences and Engineering Research Council of Canada, Daniel Reitebuch, Tommaso Ruggeri, Adam Schuetze, TMR Project “Asymptotic Methods in Kinetic Theory”, Toby Thatcher, University of Victoria, Wolf Weiss, and Yingsong Zheng.

The R13 equations originate from a collaboration with my friend Manuel Torrillon, to whom I extend special thanks for the successful and exciting cooperation, and also for carefully proof-reading the manuscript.

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Victoria, BC

*Henning Struchtrup*  
March 2005

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## Introduction

### 1.1 Contents and scope

A gas at standard conditions (1bar, 25°C) contains ca.  $2.43 \times 10^{16}$  particles per cubic millimeter. Despite this huge number of individual particles, a wide variety of flow and heat transfer problems can be described by a rather low number of partial differential equations, namely the well-known equations of Navier-Stokes and Fourier. Due to the many collisions between particles which effectively distribute disturbances between the particles, the particles behave not as individuals, but as a continuum.

Under standard conditions a particle collides with the others very often, about  $10^9$  times per second, and travels only very short distances between collisions, about  $5 \times 10^{-8}$ m. Both numbers, known as collision frequency  $\nu$  and mean free path  $\lambda$ , depend on the number density of the gas. Flow problems in which the typical length scales  $L$  are much larger than the mean free path  $\lambda$ , or in which the typical frequencies  $\omega$  are much smaller than  $\nu$ , are well described through the laws of Navier-Stokes and Fourier. The Knudsen number  $\text{Kn} = \lambda/L = \omega/\nu$  is the relevant dimensionless measure to describe these conditions, and the Navier-Stokes-Fourier equations are valid as long as  $\text{Kn} \ll 1$ .

This condition fails to hold when the relevant length scale  $L$  becomes comparable to the mean free path  $\lambda$ . This can happen either when the mean free path becomes large, or when the length  $L$  becomes small. A typical example of a gas with large mean free path is high altitude flight in the outer atmosphere, where the mean free path must be measured in meters, not nanometers, and the Knudsen number becomes large for, e.g., a spacecraft. Miniaturization, on the other hand, produces smaller and smaller devices, e.g. micro-electro-mechanical systems (MEMS), where the length  $L$  approaches the mean free path.

Moreover, the Navier-Stokes-Fourier equations will fail in the description of rapidly changing processes, when the process frequency  $\omega$  approaches, or exceeds, the collision frequency  $\nu$ .

The Knudsen number is used to classify flow regimes as follows:

- $\text{Kn} \lesssim 0.01$ : The hydrodynamic regime, which is very well described by the Navier-Stokes-Fourier equations.
- $0.01 \lesssim \text{Kn} \lesssim 0.1$ : The slip flow regime, where the Navier-Stokes-Fourier equations can describe the flow well, but must be supplied with boundary conditions that describe velocity slip and temperature jumps at gas-wall interfaces.
- $0.1 \lesssim \text{Kn} \lesssim 10$ : The transition regime, where the Navier-Stokes-Fourier equations fail, and the gas must be described in greater detail, e.g. by the Boltzmann equation, or by extended macroscopic models.
- $\text{Kn} \gtrsim 10$ : Free molecular flow, where collisions between the particles do not play an important role, and the flow is dominated by wall/particle interactions.

*Rarefied gases* are gases outside the hydrodynamic regime, i.e. with  $\text{Kn} \gtrsim 0.01$ . For Knudsen numbers in  $0.01 \lesssim \text{Kn} \lesssim 1$ , the gas still behaves as a continuum, but the Navier-Stokes-Fourier equations lose their validity, and must be replaced by more refined sets of continuum equations which describe the behavior of the gas.

*Approximation methods* to derive equations that allow to describe processes in rarefied gases, and the evaluation of the resulting equations, are the main topic of this text. Particular emphasis is put on understanding the relations between the different methods, and between the various sets of equations that result from these. Most methods rely on expansions in the Knudsen number  $\text{Kn}$ , and therefore yield equations that cannot cover the full transition regime, but are restricted to  $0.01 \lesssim \text{Kn} \lesssim 1$ .

A rarefied gas is well described by the Boltzmann equation which describes the gas on the *microscopic* level by accounting for the translation and collisions of the particles. The solution of the Boltzmann equation is the phase density  $f$  which is a measure for the likelihood to find atoms at a location  $\mathbf{x}$  with microscopic velocities  $\mathbf{c}$ . The Boltzmann equation is the central equation in the *kinetic theory of gases*.

Macroscopic quantities such as mass density  $\rho$ , mean velocity  $\mathbf{v}$ , temperature  $T$ , pressure tensor<sup>1</sup>  $\mathbf{p}$ , and heat flux vector  $\mathbf{q}$  are weighted averages of the phase density, obtained by integration over the microscopic velocity. One way to compute the macroscopic quantities is to first solve the Boltzmann equation, and then integrate over its solution,  $f$ . Alternatively, rational methods can be used to deduce *macroscopic transport equations* from the Boltzmann equation, that is transport equations for the macroscopic quantities  $\rho$ ,  $\mathbf{v}$ ,  $T$ , etc. This is particularly suitable for processes at small and moderate Knudsen numbers, which, as it turns out, can be described by a small number of equations.

The phase density and its moments—the macroscopic quantities—are introduced in **Chapter 2**.

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<sup>1</sup> The pressure tensor has a different sign than the stress tensor  $\mathbf{t}$  of fluid dynamics,  $\mathbf{p} = -\mathbf{t}$ .

The Boltzmann equation and its properties, such as its equilibrium states, the conservation of mass, momentum and energy, and the second law of thermodynamics, are presented and discussed in **Chapter 3**.

The classical method for the derivation of macroscopic equations for rarefied gases is the Chapman-Enskog (CE) method, which relies on an expansion of the phase density around equilibrium in terms of the Knudsen number,  $f = f_M + \text{Kn}f^{(1)} + \text{Kn}^2f^{(2)} + \dots$ , where  $f_M$  is the equilibrium phase density, known as Maxwellian distribution. The CE method gives the Euler equations at zeroth order, and the Navier-Stokes-Fourier equations at first order, with explicit expressions for viscosity and heat conductivity. Both sets of equations are cornerstones of gas dynamics in engineering applications.

Unfortunately, the success of the Chapman-Enskog method at zeroth and first order is not continued towards higher order expansions, which yield the Burnett and super-Burnett equations at second and third order, respectively. Both sets of equations suffer from instabilities in transient processes (at high frequencies or small wavelengths) and from unphysical oscillations in steady state processes.

The Chapman-Enskog method is discussed in **Chapter 4**, where it is applied first to the ES-BGK equation, which shares the main features with the Boltzmann equation, but allows an easier, and more transparent, application of the method. Subsequently, the application of the CE method for the full Boltzmann equation is sketched, and the resulting macroscopic equations up to third order are listed.

The Boltzmann equation can be replaced by an infinite set of coupled moment equations, which follows from averaging the Boltzmann equation over a complete set of functions in the microscopic velocity  $\mathbf{c}$ . The infinite set, presented and discussed in **Chapter 5**, is equivalent to the Boltzmann equation and can be used alternatively as a base for finding macroscopic transport equations.

A well-established approach to moment equations is Grad's method, which truncates the infinite system to a finite number of equations and then uses an approximation for the phase density—the Grad distribution  $f|_G$ —to close the system. Best-known is Grad's system of 13 equations with the variables  $\rho$ ,  $\mathbf{v}$ ,  $T$ ,  $\mathbf{p}$ ,  $\mathbf{q}$ , but the method can be applied to arbitrary sets of moments. The method is introduced and performed in **Chapter 6**. There, the relation between the Grad equations and the equations derived from the Chapman-Enskog expansion is extensively discussed. Indeed, the latter can be derived from the Grad equations by a CE expansion of the moments, which implies that the Grad method yields equations at higher orders in the Knudsen number (in a rather unspecific sense).

Other than the higher order equations from the Chapman-Enskog method, i.e. the Burnett and super-Burnett equations, Grad-type equations are stable in transient processes, and thus offer an alternative to higher order equations. However, they form hyperbolic equations, which implies finite transport velocities, and thus discontinuous shocks for velocities that exceed the maximum

characteristic velocity of the equations. **Chapter 7** presents a method to regularize Grad-type moment equations by means of a Chapman-Enskog expansion around the Grad distribution  $f_{|G}$  instead of expanding around the equilibrium distribution  $f_M$ . The method, pioneered by Grad and developed further by M. Torrilhon and the author, is performed on Grad's 13 moment set, and yields the regularized 13 moment, or R13, equations. These are stable, yield smooth shock structures at all velocities, and the Navier-Stokes, Burnett, and super-Burnett equations can be extracted by means of a Chapman-Enskog expansion.

The R13 equations have desirable properties, but a closer look shows that they have two drawbacks: (a) Their derivation takes Grad's moment method for granted, and it would be preferable to have a derivation that is independent of Grad's method, while relating the equations directly to orders in the Knudsen numbers. (b) The R13 equations are derived for a particular model for molecular collisions—interaction with an inverse fifth power potential (Maxwell molecules)—and their generalization to arbitrary collision potentials would be desirable.

**Chapter 8** presents an alternative method for deriving macroscopic transport equations that can be performed for any type of molecular interaction, and is based on accounting for the order of magnitude of moments and terms in moment equations through powers in the Knudsen number. For Maxwell molecules, the Euler and NSF equations are obtained in zeroth and first order, Grad's 13 moment equations in second order, and (a variation of) the R13 equations in third order. For non-Maxwellian molecules, the method is developed to second order, where it gives a generalization to Grad's 13 moment equations. The application to third order is discussed, but not performed.

The different sets of transport equations that are derived in Chapters 4-8 are collected in **Chapter 9**, which presents the full non-linear three-dimensional equations along with their one-dimensional form, as well as the linearized dimensionless equations in three space dimensions. Two tables are used to clarify the relations between the different models.

**Chapters 10 and 11** present the application of the various equations to standard test problems, namely stability, dispersion and damping (Chapter 10), and one-dimensional shock waves (Chapter 11). Here, the aforementioned strengths and weaknesses of the various equations are proven, e.g. the instability of the Burnett and super-Burnett equations, the occurrence of discontinuities in shock calculations for Grad's equations, and that the R13 equations are stable and yield smooth shock structures.

Boundary value problems are discussed in **Chapter 12**, which begins with the derivation of the standard jump and slip boundary conditions for the Navier-Stokes-Fourier equations. Then the ability of the various sets of macroscopic equations to describe boundary value problems in the transition regime is examined. Particular emphasis is put on linear Knudsen boundary layers, and on non-linear rarefaction effects, e.g. a heat flux not driven by a temperature gradient in Couette flow. Complete boundary conditions are

not available for equations above the Navier-Stokes-Fourier equations, and comparisons with solutions of the Boltzmann equation must rely on fitting constants of integration. These comparisons show that higher order models, in particular the R13 equations, can describe boundary value problems in the transition regime very well. The development of boundary conditions for macroscopic models is discussed, but no definitive answers are given.

The equations in the book consider only single-constituent monatomic ideal gases, the standard material in kinetic theory. Of course, kinetic theory is not restricted to monatomic gases, and is applied successfully to a host of materials such as diatomic and polyatomic gases, mixtures, electrons in semiconductors, thermal radiation, phonons, etc. The methods studied here can be used for these materials as well. However, the monatomic ideal gas, and in particular the gas of Maxwell molecules, allows to study the methods most easily. Other applications are not included due to lack of space.

The methods are nontrivial, even for a monatomic ideal gas, and require some knowledge in vector algebra and calculus. The **Appendix** provides some necessary background on tensor index notation and the formalism of trace-free tensors, and on the computation of integrals that appear frequently in the development.

The new methods and ideas presented here are still under development, and there are many presently open problems that must be addressed in the future. These include

- Reliable boundary conditions for all models above the Navier-Stokes-Fourier equations
- Equations at third order for non-Maxwellian molecules.
- Applications to mixtures, diatomic and polyatomic gases.
- Applications to non-classical gases, including photons (thermal radiation), electrons in semiconductors, and phonons.
- Hybrid models, which combine solutions of the Boltzmann equation in regions of large Knudsen numbers, to macroscopic models in regions with lower Knudsen numbers.
- Proper entropy inequalities (H-theorem) for higher order models.

The remainder of this chapter discusses monatomic ideal gases, mean free path, Knudsen number, and rarefaction effects in a rather elementary way. With the inclusion of this and the elementary chapters on phase density (Chapter 2) and Boltzmann equation (Chapter 3), the book should be accessible to the novice in kinetic theory. About forty end-of-chapter problems are intended to help the reader in deepening her understanding of the concepts. Moreover, the reader is encouraged to follow the derivations with his pencil in hand—while the main steps are described, many details had to be left out, and these should be considered as implicit problems, in addition to the explicitly stated end-of-chapter problems.