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Modeling and Computational Methods for Kinetic Equations

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Preface

The aim of this book is to provide a general overview of kinetic models and their applications to various contexts (gas dynamics, semiconductor modelling, granular flows, traffic flows, and so on.) Particular emphasis will be given to the derivation of the models and to the modern numerical methods available to obtain quantitative predictions from the models. The mathematical treatment, although rigorous, will be mostly maintained at a level accessible to a broad range of readers, including graduate students in applied sciences and engineers.

The relation between kinetic models and simpler, macroscopic models will be addressed in most chapters. This aspect is very important in many applications, and exposes the reader to the challenge of multiscale modelling.

The book is divided in two parts. The first is mainly devoted to the most fundamental kinetic model: the Boltzmann equation of rarefied gas dynamics. Its connections with macroscopic models through hydrodynamic limits and moments closure hierarchies are developed, as they play important roles in the more common description of gases and fluids. Then, the most widely used numerical methods for the discretization of the Boltzmann equation are reviewed: the Monte-Carlo method, spectral methods and finite-difference methods. The second part is devoted to more specific applications: plasma kinetic models with the Fokker–Planck–Landau equation and its numerical discretization, traffic flow modelling, granular media, quantum kinetic models and coagulation-fragmentation problems.

In each case, both modelling aspects and numerical methods are discussed. The originality of this book is in the consistent treatment of the models, both from the point of view of theory and modelling and from that of the numerical discretization. Most of the existing monographs focus on either one or the other of these two aspects. However, bringing these two aspects together shines light on points which are important but which are very likely to be discarded in more focused approaches. For instance, the development of spectral or multipole methods for kinetic equations was motivated by the search for efficient ways of discretizing the Boltzmann operator while preserving an accurate description of the various conservation laws as well as entropy dissipation. These properties are deeply related to the kind of system the model aims at describing. The same considerations are obviously true for traffic flow modelling, granular

media, quantum kinetic models, or coagulation-fragmentation problems, which are the four specific applications the present book intends to develop.

At the end of each chapter, a list of references will address the interested reader toward more detailed treatment of the subject, and in particular to some of the research trends in applied kinetic theory.

The first chapter of the book is an introduction to the kinetic description of particle dynamics. After an overview of available models for particle dynamics, the Boltzmann equation of rarefied gases is derived, and its main mathematical properties are recalled. Particular emphasis is given to the derivation of the hydrodynamical limits, such as Euler and Navier–Stokes equations, by the formal procedure of Hilbert and Chapman–Enskog expansion, which connect the microscopic world of molecules with the macroscopic world of gases, fluids, and thermodynamics.

The second chapter illustrates the mathematical properties of a class of hydrodynamical models that describe charge transport in semiconductors. Starting from the semiclassical Boltzmann equation for semiconductors, hydrodynamical models are deduced by applying a procedure introduced by Levermore, and based on the maximum entropy principle. It is shown that, because of the special structure of momentum space in a crystal (consequence of periodicity and band structure of the lattice), the hydrodynamical models of semiconductors possess peculiar properties, different from those of moment-based methods in gases. In particular, a local existence result and a global existence result of smooth solutions around equilibrium are presented.

The next three chapters are devoted to a presentation of the main tools available for numerical approximation of the Boltzmann equation.

Several challenges are encountered in the construction of effective numerical schemes for kinetic equations because of the dimensionality of the problem (the density function depends on seven independent scalar variables: time, physical space and velocity space); the nonlocal nature (in velocity) of the collisional kernel, which makes it hard to compute it efficiently; the nonlinearity of the problem; and the requirement to maintain the conservation properties of the equation at a discrete level. The various schemes take these requirements into account and satisfy them at different levels.

The first, and probably more widely used, tool is the Monte-Carlo method, which has several advantages over present day deterministic schemes. It is very efficient, being the method with the lowest computational cost per discrete degree of freedom, and it is extremely robust, being able to treat a wide range of regimes, including situations that are very far from thermodynamical equilibrium. Furthermore, the Monte-Carlo method can be generalized to include a large number of physical effects. This chapter is self-contained and can be read independently of the others.

Chapter 4 describes a deterministic numerical method that can be used when a highly accurate solution is required, and the system is not too far from thermodynamical equilibrium. Deterministic methods are usually more expensive than Monte-Carlo methods, but they can provide more accurate solutions, without the statistical noise typical of the Monte-Carlo approach. The method presented in the chapter is a hybrid method that combines a third-order accurate discretization in space with spectrally

accurate discretization in velocity. Effective time evolution schemes allow good efficiency even in regimes close to the hydrodynamical limit.

The next chapter illustrates the main features of finite difference discretization of the Boltzmann equation and its application to gas mixtures. Among commonly used deterministic schemes, the finite difference schemes proposed by the Japanese school are probably the most well established. Although not quite as accurate as spectral methods, they are more flexible, and allow velocity discretization, which can be more easily fitted to the problem.

The second part of the book is devoted to applications of kinetic equations. Far from being exhaustive, this part gives a broad view of the use of the kinetic approach to several different contexts.

Chapters 6 and 7 deal with the Fokker–Planck–Landau equation of plasma physics. The equation provides a kinetic description of the evolution of charged particles (electrons and ions), and arises naturally when the interactions among the particles produce many small deflections, and few large angle scatters. The chapter by Desvillettes is centered on the mathematical properties of the Fokker–Planck–Landau equation, while the chapter by Lemou describes a powerful method for the numerical solution of the equation.

Chapter 8 is a self-contained review article on traffic flow modelling. Both kinetic and hydrodynamical models are presented, and particular emphasis is given to the numerical techniques used for the approximate solution of the equations.

The next chapter is a brief review of modern kinetic models of granular material. In view of the numerous industrial applications, granular flow has attracted a lot of attention in recent years. The inelasticity of grain collisions creates new interesting mathematical problems, which are not present in the standard Boltzmann equation of gas dynamics. After the introduction of certain kinetic models of dilute granular systems, the cooling process of the system is studied and some hydrodynamical models are derived. Accurate numerical methods based on a spectral representation in velocity are also presented, and the development of fast algorithms is considered.

Chapter 10 reviews some modelling and numerical aspects in quantum kinetic theory for a gas of interacting bosons (the so-called Bose–Einstein condensation). Particular care is devoted to the development of efficient numerical schemes for the quantum Boltzmann equation that preserve the main physical features of the continuous problem, namely conservation of mass and energy, the entropy inequality, and generalized Bose–Einstein distributions as steady states. These properties are essential in order to develop numerical methods that are able to capture the challenging phenomenon of boson condensation.

The last chapter deals with the mathematical description of coagulation phenomena. The aim of the chapter is to present an overview of the mathematical analysis of coalescence equations and related models, with a focus on the statistical description at the kinetic level. Some of the main mathematical problems and results with physi-

cal interest are presented, together with mathematical tools and strategies useful to further investigate these models.

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