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Stochastic Numerics for the Boltzmann Equation

With 98 Figures

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Preface

Stochastic numerical methods play an important role in large scale computations in the applied sciences. Such algorithms are convenient, since inherent stochastic components of complex phenomena can easily be incorporated. However, even if the real phenomenon is described by a deterministic equation, the high dimensionality often makes deterministic numerical methods intractable.

A stochastic procedure, called direct simulation Monte Carlo (DSMC) method, has been developed in the physics and engineering community since the sixties. This method turned out to be a powerful tool for numerical studies of complex rarefied gas flows. It was successfully applied to problems ranging from aerospace engineering to material processing and nanotechnology. In many situations, DSMC can be considered as a stochastic algorithm for solving some macroscopic kinetic equation. An important example is the classical Boltzmann equation, which describes the time evolution of large systems of gas molecules in the rarefied regime, when the mean free path (distance between subsequent collisions of molecules) is not negligible compared to the characteristic length scale of the problem. This means that either the mean free path is big (space-shuttle design, vacuum technology), or the characteristic length is small (micro-device engineering). As the dimensionality of this nonlinear integro-differential equation is high (time, position, velocity), its numerical treatment is a typical application field of Monte Carlo algorithms.

Intensive mathematical research on stochastic algorithms for the Boltzmann equation started in the eighties, when techniques for studying the convergence of interacting particle systems became available. Since that time much progress has been made in the justification and further development of these numerical methods.

The purpose of this book is twofold. The first goal is to give a mathematical description of various classical DSMC procedures, using the theory of Markov processes (in particular, stochastic interacting particle systems) as a unifying framework. The second goal is a systematic treatment of an extension of DSMC, called stochastic weighted particle method (SWPM). This method has been developed by the authors during the last decade. SWPM includes several new features, which are introduced for the purpose of variance reduction (rare event simulation). Rigorous results concerning the approximation of solutions to the Boltzmann equation by particle systems are given, covering both DSMC and SWPM. Thorough numerical experiments are performed, illustrating the behavior of systematic and statistical error as well as the performance of the methods.

We restricted our considerations to monoatomic gases. In this case the introduction of weights is a completely artificial approach motivated by numerical purposes. This is the point we wanted to emphasize. In other situations, like gas flows with several types of molecules of different concentrations, weighted particles occur in a natural way. SWPM contains more degrees of freedom than we have implemented and tested so far. Thus, there is some hope that there will be further applications. Both DSMC and SWPM can be applied to more general kinetic equations. Interesting examples are related to rarefied granular gases (inelastic Boltzmann equation) and to ideal quantum gases (Uehling-Uhlenbeck-Boltzmann equation). In both cases there are non-Maxwellian equilibrium distributions. Other types of molecules (internal degrees of freedom, electrical charge) and many other interactions (chemical reactions, coagulation, fragmentation) can be treated.

The structure of the book is reflected in the table of contents. Chapter 1 recalls basic facts from kinetic theory, mainly about the Boltzmann equation. Chapter 2 is concerned with Markov processes related to Boltzmann type equations. A relatively general class of piecewise-deterministic processes is described. The transition to the corresponding macroscopic equation is sketched heuristically. Chapter 3 describes the stochastic algorithms related to the Boltzmann equation. This is the largest part of the book. All components of the procedures are discussed in detail and a rigorous convergence theorem is given. Chapter 4 contains results of numerical experiments. First, the spatially homogeneous Boltzmann equation is considered. Then, a spatially one-dimensional test problem is studied. Finally, results are obtained for a specific spatially two-dimensional test configuration. Some auxiliary results are collected in two appendixes.

The chapters are relatively independent of each other. Necessary notations and formulas are usually repeated at the beginning of a chapter, instead of cross-referring to other chapters. A list of main notations is given at the end of this Preface. Symbols from that list will be used throughout the book. We mostly avoided citing literature in the main text. Instead, each of the first three chapters is completed by a section including bibliographic remarks. An extensive (but naturally not exhaustive) list of references is given at the end of the book.

The idea to write this book came up in 1999, when we had completed several papers related to DSMC and SWPM. Our naive hope was to finish it rather quickly. In May 2001 this Preface contained only one remark – “seven months left to deadline”. On the one hand, the long delay of three years was

sometimes annoying, but, on the other hand, we mostly enjoyed the intensive work on a very interesting subject. We would like to thank our colleagues from the kinetics community for many useful discussions and suggestions. We are grateful to our home institutions, the University of Saarland in Saarbrücken and the Weierstrass Institute for Applied Analysis and Stochastics in Berlin, for providing an encouraging scientific environment. Finally, we are glad to acknowledge support by the Mathematical Research Institute Oberwolfach (RiP program) during an early stage of the project, and a research grant from the German Research Foundation (DFG).

Saarbrücken and Berlin *Sergej Rjasanow*
December 2004 *Wolfgang Wagner*

List of notations

$\mathbb{R}^3$	Euclidean space
$(.,.)$	scalar product in $\mathbb{R}^3$
$\lvert . \rvert$	norm in $\mathbb{R}^3$
$\mathcal{S}^2$	unit sphere in $\mathbb{R}^3$
D	open subset of $\mathbb{R}^3$
∂D	boundary of D
$n(x)$	unit inward normal vector at $x \in \partial D$
$\sigma(dx)$	uniform surface measure (area) on ∂D
$\delta(x)$	Dirac's delta-function
I	identity matrix
$\operatorname{tr} C$	trace of a matrix C
vv^{T}	matrix with elements $v_i v_j$ for $v \in \mathbb{R}^3$
∇_x	gradient with respect to $x \in \mathbb{R}^3$
$\operatorname{div} b(x)$	divergence of a vector function b on $\mathbb{R}^3$
$\mathbb{E}\,\xi$	expectation of a random variable ξ
$\operatorname{Var}\xi$	variance of a random variable ξ
$\mathcal{B}(X)$	Borel sets of a metric space X
$\mathcal{M}(X)$	finite Borel measures on X

$$M_{V,T}(v) = \frac{1}{(2\pi T)^{3/2}} \exp\left(-\frac{|v-V|^2}{2T}\right)$$

Maxwell distribution, with $v, V \in \mathbb{R}^3$ and $T > 0$

$$\mathbb{R}^3_{in}(x) = \left\{v \in \mathbb{R}^3 \;:\; (v, n(x)) > 0\right\}$$

velocities leading a particle from $x \in \partial D$ inside D

$$\mathbb{R}^3_{out}(x) = \left\{v \in \mathbb{R}^3 \;:\; (v, n(x)) < 0\right\}$$

velocities leading a particle from $x \in \partial D$ outside D

$$\delta_{i,j} = \begin{cases} 1\,, & \text{if} \quad i = j \\ 0\,, & \text{otherwise} \end{cases}$$

Kronecker's symbol

$$\delta_x(A) = \begin{cases} 1\,, & \text{if} \quad x \in A \\ 0\,, & \text{otherwise} \end{cases}$$

Dirac measure, with $x \in X$ and $A \in \mathcal{B}(X)$

$$\chi_A(x) = \begin{cases} 1\,, & \text{if} \quad x \in A \\ 0\,, & \text{otherwise} \end{cases}$$

indicator function of a set A, with $x \in X$ and $A \subset X$

$$||\varphi||_\infty = \sup_{x \in X} |\varphi(x)|$$

for any measurable function φ on X

$$\langle \varphi, \nu \rangle = \int_X \varphi(x)\, \nu(dx)$$

for any $\nu \in \mathcal{M}(X)$ and φ such that $||\varphi||_\infty < \infty$

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