Discretization and numerical schemes for stationary kinetic model equations

Hans Babovsky
Weierstraß Institute for
Applied Analysis and Stochastics
Mohrenstraße 39
D-10117 Berlin, Germany

Abstract

There are still many open questions concerning the relationship between (steady) kinetic equations, random particle games designed for these equations, and transitions, e.g. to fluid dynamics and turbulence phenomena. The paper presents some first steps into the derivation of models which on one hand may be used for the design of efficient numerical schemes for steady gas kinetics, and on the other hand allow to study the interplay between particle schemes and physical phenomena.
Key words: stationary kinetic equation, numerical schemes.

1 Introduction

Numerics for nonlinear kinetic equations is dominated by Monte Carlo simulation schemes - at least in the cases when complex realistic situations are to be evaluated [1]. This is due to the fact that the Boltzmann collision operator is an at least five-dimensional integral which in each iteration step has to be calculated at each point in a discretized six-dimensional phase space. This is a task which seems to be too time and memory consuming (even on any of the present supercomputers) to be solved by application of any of the classical numerical discretization schemes. A way out is given by stochastic integration methods. Such methods seem to be superior to classical schemes whenever a function to be integrated is either high-dimensional or irregular (or both) [2] - a situation which is typical for the Boltzmann collision integral. Such schemes are robust, allow in a natural way to model a lot of physical phenomena and are well-understood from a mathematical view point - as far as time evolution problems are concerned [3, 4].

On the other hand, Monte Carlo schemes are still not well understood for the calculation of stationary - in particular interior flows. There are many open questions ranging from systematic errors due to the nonlinearity of the collision operator [5] to the question whether certain features observed at numerical simulations are related to physical effects like turbulence or are artificial effects inherent to Monte Carlo schemes [6]. (However, such schemes have certain similarities to other random games which are designed to describe features of physical turbulence, see [7].) Further, random algorithms for gas kinetics may not be expected to yield the precision and resolution obtained nowadays for example in continuum flow calculations. Besides the fact that there are always fluctuations in the order of magnitude of the inverse square root of the (local) number of particles, the major drawback is that the use of many modern numerical techniques is prohibited. For example, features like multigrid and adaptive grid techniques are very unlikely to be applied efficiently to particle simulations.

Computer capacities have been rapidly increased during recent decades. In the field of numerics for the Navier Stokes equations, this development was accompanied by a tremendous progress. E.g., according to [8], a minimal (necessary, not sufficient) requirement for a code to be taken serious is that it properly resolves a Karman vortex street. A similar success for numerics of gas kinetics is in our opinion in the long run only possible, if alternatives (or better: supplements) to Monte Carlo schemes are found. This paper is intended to provide some impulses into this direction for stationary equations. The scope is

- Find an appropriate way for the decoupling of free flow and collision operators. A lot of calculational effort in Monte Carlo schemes corresponds to the preprocessing of data for collisions which do not take place (e.g. the sorting of particles in physical space, the choice of collision partners and the calculation of collision probabilities for all particles, although only a small fraction of particles suffer collisions). This should be avoided in an efficient scheme.

- Find a way to discretize the collision integral. Due to the definitions of collision relations this is not straightforward. We propose an ansatz yielding a compromise between strongly simplifying models like BGK models (which are mainly used for deterministic numerical schemes, see e.g. [9] and the references cited there) and the original operator. The general framework presented here contains features of two-particle interactions and gives way to the hope that a hierarchy of models can be derived which on one end of the scale are quite coarse and rigorously tractable with the chance of studying features like turbulence and the fluid-dynamic limit, and on the other end can be refined enough to serve as a basis for a realistic kinetic equation which can be solved by an efficient numerical scheme.

- Develop a basis on which it is possible to compare results from different numerical schemes and to gain more insight in particular into random games and Monte Carlo simulations.

2 Stationary boundary value problems

2.1 A fixed point equation for stationary solutions

We consider the boundary value problem for $f = f(x, v)$

$$v_x \cdot \nabla_x f = J(f, f), \quad f_+(a, v) = \psi(a, v) \tag{2.1}$$

on $\Omega \times \mathbb{R}^p$, where $\Omega \subset \mathbb{R}^q$, $q \leq p$, is a bounded convex domain with smooth boundary $\partial\Omega$ (i.e. the inner normal $n(a)$ on $\partial\Omega$ exists for all $a \in \partial\Omega$). $v_x \in \mathbb{R}^q$ denotes the projection of $v \in \mathbb{R}^p$ onto the subspace spanned by Ω. With

$$\partial\Gamma_+ := \{(a, v) : a \in \partial\Omega, \langle n(a), v_x \rangle > 0\}, \tag{2.2}$$

$f_+ = f|_{\partial\Gamma_+}$ represents the flow through $\partial\Omega$ into Ω and is prescribed by the fixed function ψ. In many cases of interest, f_+ is given by some reflection law at the boundary, and thus ψ depends on the outgoing flow f_-. We do not consider this in the present paper. The collision operator $J(.,.)$ is defined as

$$J(f, f)(v) = J_+(f)(v) - \rho f(v) \tag{2.3}$$

with the density ρ defined by

$$\rho(x) = \int_{\mathrm{IR}^p} f(x,v)dv \tag{2.4}$$

and the gain term $J_+(.)$ given by

$$J_+(f)(v) = \int_{\mathrm{IR}^p} \int_B f(v')f(w')d\eta dw. \tag{2.5}$$

Here, B is the surface of the unit sphere in IR^p with the normalized surface measure $d\eta$, and (v', w') is obtained from (v, w) via a continuous transform $T : B \times \mathrm{IR}^p \times \mathrm{IR}^p \to \mathrm{IR}^p \times \mathrm{IR}^p$,

$$(v', w') = T_\eta(v, w) =: (T_\eta^{(1)}(v, w), T_\eta^{(2)}(v, w)), \tag{2.6}$$

satisfying $T_\eta^2 = \mathrm{id}$ for all $\eta \in B$. From the convexity of Ω follows the existence of unique mappings

$$\Phi(x, v) : (\Omega \times \mathrm{IR}^p) \cup \partial\Gamma_+ \longrightarrow \partial\Omega \tag{2.7}$$

and

$$\tau : \Omega \times \mathrm{IR}^p \longrightarrow \mathrm{IR}_+ \tag{2.8}$$

such that $x = \Phi(x, v) + \tau(x, v) \cdot v_x$. With this definition, mild solutions of the boundary value problem are defined as solutions of the fixed point equation

$$\begin{aligned} f(x,v) \;&=\; \psi(\Phi(x,v),v)\cdot \exp\left(-\int_0^{\tau(x,v)} \rho(x - sv_x)ds\right) + \\ &\int_0^{\tau(x,v)} J_+(f)(x - sv, v)\cdot \exp\left(-\int_0^s \rho(x - \sigma v_x)d\sigma\right) ds \end{aligned} \tag{2.9}$$

(see, e.g., [10]).

2.2 An iteration scheme

There are many ways to try to design iterative schemes for the numerical approximation of the fixed-point problem. E. g. one may attempt in the spirit of [11] to construct monotone sequences of upper and lower solutions converging to a solution. The study of convergent sequences is not the main objective of this paper. Therefore we restrict to the simplest iterative scheme which converges for the examples presented in the final section. It is given by

$$\begin{aligned} f^{(n+1)}(x,v) \;&=\; \psi(\Phi(x,v),v)\cdot \exp\left(-\int^{\tau(x,v)} \rho^{(n)}(x - sv_x)ds\right) + \\ &\int_0^{\tau(x,v)} J_+(f^{(n)})(x - sv_x, v)\cdot \exp\left(-\int_0^s \rho^{(n)}(x - \sigma v_x)d\sigma\right) ds \end{aligned} \tag{2.10}$$

with an appropriate choice for the initial guess $f^{(0)}$. It is reasonable to believe that in many situations such a scheme indeed converges to a stationary solution of the Boltzmann equation. In fact, for one-dimensional problems and with the density fixed at $\rho \equiv 1$ (which may be achieved through a transformation of the one-dimensional space variable), a Monte Carlo version of this iteration was tested in [12], with evidence of convergence.

It is useful to decouple the iteration into two problems of the following type:

- Problem 1: Given (for each x) a function $f = f(v)$, solve

$$g = A[f, f] \tag{2.11}$$

  with a given bilinear operator $A[.,.]$.

- Problem 2: Given functions $g = g(x, v)$ and $\rho = \rho(x)$, solve

$$\begin{aligned} f(x,v) &= \psi(\Phi(x,v),v) \cdot \exp\left(-\int^{\tau(x,v)} \rho(x - sv_x)ds\right) + \\ &\quad \int_0^{\tau(x,v)} g(x - sv_x, v) \cdot \exp\left(-\int_0^s \rho(x - \sigma v_x)d\sigma\right) ds \end{aligned} \tag{2.12}$$

For $A[.,.]$ we choose a modification of the collision gain term J_+, as will be described in section (3.2). The second integral at the right hand side of (2.12) becomes singular for $v_x \to 0$. Therefore we continue discussing properties of $A[.,.]$ for which the function f in problem 2 is well-defined. For simplicity, we restrict to the spatially one-dimensional case: $\Omega := [0,1]$. For $v \in \mathbb{R}^p$ denote by $v_\perp$ the part of v orthogonal to v_x such that $v = (v_x, v_\perp)$. Define the space $L^{\infty,1} := L^\infty([0,1], L^1(\mathbb{R}^p))$ with corresponding norm $\|.\|_{\infty,1}$, and W as the Banach space of functions $f \in L^1$ with

$$\|f\|_W := \sup_{|v_x| \le 1} |P_{||} f(v_x)| + \|f\|_{L^1} < \infty, \tag{2.13}$$

where

$$P_{||} f(v_x) := \int f(v_x, v_\perp) dv_\perp \in L^\infty(\mathbb{R}) \tag{2.14}$$

is the projection of f into v_x-direction.

Theorem 1: *Suppose $A : L^1 \times L^1 \to W$ is a bounded bilinear operator. If $f \in L^{\infty,1}$ is nonnegative, if $g(x,v) = A[f(x,.), f(x,.)](v)$, and if*

$$\begin{aligned} h(x,v) &= \psi(\Phi(x,v),v) \cdot \exp\left(-\int_0^{\tau(x,v)} \rho[f](x - sv_x)ds\right) + \\ &\quad \int_0^{\tau(x,v)} g(x - sv_x, v) \cdot \exp\left(-\int_0^s \rho[f](x - \sigma v_x)d\sigma\right) ds \end{aligned} \tag{2.15}$$

(where $\rho[f]$ is the density related to f), then $h \in L^{\infty,1}$, h is nonnegative, and there exists a constant κ such that

$$\|h\|_{\infty,1} \leq \|\Phi\|_1 + \kappa \cdot \|f\|^2_{\infty,1}. \tag{2.16}$$

An immediate consequence is the boundedness of the recursive scheme at least for small data. Further, in the case of convergence we obtain a classical solution.

Corollary: *Define the sequence $f^{(n)}$ by equation (2.15) (with the replacements $f \to f^{(n)}$, $h \to f^{(n+1)}$).*

a) If If $\|\Phi\|_1 \leq 1/4\kappa$ and if $f^{(0)}$ is nonnegative with $f^{(0)} \leq 1/2\kappa$ then the sequence $f^{(n)}$ is also nonnegative and bounded by $1/2\kappa$.

b) If $f^{(n)}$ converges in W, then the limit is a classical solution of the fixed point problem.

P r o o f of Theorem 1: The case $\psi \equiv 0$ is trivial and is not discussed here. Because of the boundedness of $A[.,.]$ we have

$$\sup_{x\in[0,1]} \|g(x,.)\|_W \leq \|A\| \cdot \|f\|^2_{\infty,1}. \tag{2.17}$$

Suppose $v_x \neq 0$. We may assume $v_x > 0$. Then $\tau(x,v) = x/v_x$, and

$$h(x,v) \;=\; \psi(0,v)\cdot\exp\left(-\frac{1}{v_x}\int_0^x \rho[f](s)ds\right) + \frac{1}{v_x}\int_0^x g(s,v)\cdot\exp\left(-\frac{1}{v_x}\int_s^x \rho[f](\sigma)d\sigma\right)ds.$$

Define $\rho_{max} := \sup_{x\in[0,1]} \|f(x,.)\|_{L^1}$. Then

$$h(x,v) \geq h_0(x,v) := \psi(0,v)\cdot\exp\left(-\frac{x\cdot\rho_{max}}{v_x}\right) \geq \psi(0,v)\cdot\exp\left(-\frac{\rho_{max}}{v_x}\right). \tag{2.18}$$

We conclude the existence of a $\rho_{min} > 0$ such that $\rho[h](x) \geq \rho_{min}$. This yields

$$h(x,v) \leq \Phi(0,v) + \frac{1}{v_x}\int_0^x g(s,v)\cdot\exp\left(-\frac{(x-s)\cdot\rho_{min}}{v_x}\right)ds. \tag{2.19}$$

A simple estimate shows that for arbitrary $\alpha,\beta > 0$

$$\frac{1}{\beta}\exp\left(-\frac{\alpha}{\beta}\right) \leq \frac{1}{\alpha+\beta}. \tag{2.20}$$

It follows

$$h(x,v) \leq \Phi(0,v) + \int_0^x g(s,v)\cdot\frac{1}{v_x + (x-s)\cdot\rho_{min}}ds \tag{2.21}$$

and

$$P_{||}h(x,v_x) \leq P_{||}\Phi(0,v_x) + \sup_{x\in[0,1]}\|g(x,.)\|_W \cdot \int_0^1 \frac{1}{|v_x| + t\cdot\rho_{min}}dt \tag{2.22}$$

if $v_x \leq 1$. The same estimate with $\Phi(0,.)$ replaced by $\Phi(1,.)$ holds for $-1 \leq v_x < 0$. Since

$$v_x \longrightarrow \int_0^1 \frac{1}{|v_x| + t \cdot \rho_{min}} dt \tag{2.23}$$

defines a function in $L^1_{loc}(\mathbb{R})$, the estimate (2.22) controlls $h(x, v)$ for $|v_x| \leq 1$. A controll for $|v_x| > 1$ is straightforward (just ignore the exponentials and $1/v_x$ in (2.19)), and the theorem is proven. $\square$

We are going to discuss numerical schemes for these problems. Certainly, problem 2 may be attacked by a classical integration scheme. Problem 1 is not straightforward if we want to work on a fixed grid in velocity space. Therefore we develop an ersatz model reflecting the correct evolution of certain moments due to two-particle interactions.

3 A model gain term

3.1 Basic ideas

There are a lot of possibilities to model gain terms for kinetic collision operators. The spectrum ranges from the Boltzmann gain term, which is the best founded one in the setting of mesoscopic descriptions, and of which a special case has been introduced in section 2.1, to descriptions like those given by BGK-like models. While the first ones are based on two-particle collisions providing physical conservation laws like momentum and energy conservation, the latter ones give merely a rough description based on local equilibria, where particles "forget" their pre-collision velocities during a collision. Such models cannot be based on two-particle mechanics.

Discrete velocity models like those surveyed in [13] are also based on two-particle mechanics; however, in general it is hard to find a "smooth" link between these models and the continuous velocity setting just by increasing the discrete-velocity domain. An exception is [14], where a discrete velocity model is derived as a finite difference scheme for the continuous setting.

In the long run, our aim is to formulate in a general setting a large class of two-particle collision models with velocities on a regular grid which serve as a bridge between theory and numerics for realistic applications. Our approach chosen here is somewhere between the original Boltzmann collision operator and BGK models. It is based on a probabilistic description of two-particle interactions which provides a correct treatment of certain physical quantities in the mean, but not for each realization.

In our opinion, such a description allows for a broad range of models starting from very crude discrete velocity models (which can be efficiently treated theoretically) to more and more refined models which come arbitrarily close to physical "reality" and which can nevertheless be treated with numerical efficiency. Our models are based on a weak formulation which is shortly introduced in the following section.

3.2 Model gain terms leaving invariant certain moments

With $A[f,f] = J_+(f)$, Problem 1 of section 2.2 reads: Given the absolutely continuous measure $f(v)dv$, calculate $g(v)dv$ as solution of the equation

$$g(v) = \int_{\mathbb{R}^p} \int_B f(v')f(w')d\eta d^2w. \tag{3.24}$$

Exploiting the symmetry properties of the collision kernel (in particular the fact that T_η is an involution), we end up with the following weak formulation (see [3]). Suppose that V is the set of continuous bounded test functions on $\mathbb{R}^2$. Multiplication of (3.1) with $\phi \in V$, integration and integral transformation (using $dv'dw' = dvdw$) leads to

$$\int_{\mathbb{R}^2} \phi(v)g(v)dv = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \int_B \phi(T_\eta^{(1)}(v,w))d\omega(\eta)f(v)d^2vf(w)d^2w \text{ for } \phi \in V. \tag{3.25}$$

Our intention is now to replace the right hand side by one that leaves the integral invariant for ϕ out of a finite dimensional space. Denote

$$V_H := \text{span}(\phi_i, i = 1, \dots N) \tag{3.26}$$

for a fixed set $H = \{\phi_i, i = 1, \dots, N\}$ of (not necessarily bounded) test functions. For a continuous mapping $S : Z \times \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}^p$ (with an appropriate set Z) and a probability measure $d\mu$ on Z we call an equation

$$\int_{\mathbb{R}^2} \phi(v)g(v)dv = \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \int_Z \phi(S(z,v,w))d\mu(z)f(v)d^2vf(w)d^2w, \quad \phi \in V \tag{3.27}$$

a "V_H-invariant" model problem for (3.1), if

$$\int_Z \phi(S(z,v,w))d\mu(z) = \int_B \phi(T_\eta^{(1)}(v,w))d\omega(\eta) \tag{3.28}$$

for all $v, w \in \mathbb{R}^p$, $\phi \in V_H$. It is this equation which is readily discretized if S is chosen appropriately. Let us point out that this formulation of a model problem preserves nonnegativity and the L^1-norm of the original collision operator.

3.3 Discretized velocity space

We discuss a discretized model problem in a two-dimensional velocity space. For $v = (v_x, v_y)^T$ denote $\phi_0 :\equiv 1$, $\phi_1(v) := v_x$, $\phi_2(v) := v_y$, $\phi_3(v) := v_x^2$, and $\phi_4(v) := v_y^2$. We develop a discretized model gain term leaving invariant these quantities. Using the explicit formula

$$T_\eta^{(1)}(v,w) = v - \langle v - w, \eta \rangle \cdot \eta, \tag{3.29}$$

straightforward integrations show that

$$\int_B \phi_0(T_\eta^{(1)}(v,w))d\omega(\eta) = 1, \tag{3.30}$$

$$\int_B \phi_1(T_\eta^{(1)}(v,w))d\omega(\eta) = \frac{v_x + w_x}{2}, \tag{3.31}$$

$$\int_B \phi_2(T_\eta^{(1)}(v,w))d\omega(\eta) = \frac{v_y + w_y}{2}, \tag{3.32}$$

$$\int_B \phi_3(T_\eta^{(1)}(v,w))d\omega(\eta) = \frac{1}{2}(v_x^2 + w_x^2) + \frac{1}{8}\left((v_y - w_y)^2 - (v_x - w_x)^2\right), \tag{3.33}$$

$$\int_B \phi_4(T_\eta^{(1)}(v,w))d\omega(\eta) = \frac{1}{2}(v_y^2 + w_y^2) + \frac{1}{8}\left((v_x - w_x)^2 - (v_y - w_y)^2\right). \tag{3.34}$$

Define the index set $G := \{(i,j), i,j = -\Gamma, \ldots, \Gamma\}$ for some $0 < \Gamma \in \mathbb{N}$ and suppose that the velocity space $\mathbb{R}^2$ is discretized to the finite regular grid $G_h := \{h \cdot (i,j), (i,j) \in G\}$. (Since it should not cause any confusion, we identify elements of G with the corresponding ones in G_h.) Suppose given two velocities v, w on the grid, $v = (i,j)$, $w = (k,l)$. According to (3.30) to (3.34) we have to define a non-negative valued function S_{ijkl} on the grid such that

$$\sum_{m,n=-\Gamma}^{\Gamma} S_{ijkl}(m,n) = 1, \tag{3.35}$$

$$\sum_{m,n=-\Gamma}^{\Gamma} m \cdot S_{ijkl}(m,n) = \frac{i+k}{2}, \tag{3.36}$$

$$\sum_{m,n=-\Gamma}^{\Gamma} n \cdot S_{ijkl}(m,n) = \frac{j+l}{2}, \tag{3.37}$$

$$\sum_{m,n=-\Gamma}^{\Gamma} m^2 S_{ijkl}(m,n) = \frac{i^2+k^2}{2} + \frac{1}{8}\left((j-l)^2 - (i-k)^2\right), \tag{3.38}$$

$$\sum_{m,n=-\Gamma}^{\Gamma} n^2 S_{ijkl}(m,n) = \frac{j^2+l^2}{2} + \frac{1}{8}\left((i-k)^2 - (j-l)^2\right). \tag{3.39}$$

The simplest possible choice is to seek for a function factorizing in $x-$ and $y-$direction, i.e. $S_{ijkl}(m,n) := Q_{ijkl}(m)R_{ijkl}(n)$ with the symmetry property $R_{ijkl}(n) = Q_{jkli}(n)$. This reduces the equations (3.12) to (3.16) to the three conditions

$$\sum_{m=-\Gamma}^{\Gamma} Q_{ijkl}(m) = 1, \tag{3.40}$$

$$\sum_{m=-\Gamma}^{\Gamma} m \cdot Q_{ijkl}(m) = \frac{i+k}{2}, \tag{3.41}$$

$$\sum_{m=-\Gamma}^{\Gamma} m^2 Q_{ijkl}(m) = \frac{i^2+k^2}{2} + \frac{1}{8}\left((j-l)^2 - (i-k)^2\right). \tag{3.42}$$

E.g. for $\Gamma = 1$ (i.e. for a nine-velocity model) this leads to a well-posed linear system of equations with the solution

$$Q_{ijkl}(-1) = \frac{b-a}{2}, \tag{3.43}$$

$$Q_{ijkl}(0) = 1 - b, \tag{3.44}$$

$$Q_{ijkl}(1) = \frac{a+b}{2} \tag{3.45}$$

where a and b are the right hand sides of (3.41) and (3.42). Unfortunately, this solution may become negative for a few indices which makes slight modifications necessary (see section 5.1).

4 Discretization and a deterministic scheme

4.1 Well-posedness of the collision operator

In the course of section 3.2, problem 1 (solution of (2.11)) was changed into the modified version

- Problem 1': Suppose $S : Z \times \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}^p$ sufficiently regular, and $d\mu(z)$ a probability measure on Z. Given $f = f(v)$ in a suitable function space V, find $g \in V$ such that for all ϕ in the dual spave V^*

$$\int \phi(v)g(v)dv = \int\int\int \phi(S(z,v,w))d\mu(z)f(v)dv\, f(w)dw =: T_f\phi. \tag{4.1}$$

By changing to the space of Borel measures, we can easily prove the well-posedness of the problem.

Theorem 2: *Suppose S is Borel measurable, and $d\alpha$ is a finite Borel measure on $\mathbb{R}^p$. Then there exists a unique finite Borel measure $d\beta$ on $\mathbb{R}^p$ satisfying*

$$\int_{\mathbb{R}^p} \phi(v)d\beta(v) = \int_{\mathbb{R}^p}\int_{\mathbb{R}^p}\int_Z \phi(S(z,v,w))d\mu(z)d\alpha(v)d\alpha(w) \tag{4.2}$$

for arbitrary continuous and bounded functions ϕ.

P r o o f : Since

$$\left| \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} \int_Z \phi(S(z,v,w)) d\mu(z) d\alpha(v) d\alpha(w) \right| \leq \|\phi\|_\infty \cdot (\alpha(\mathbb{R}^p))^2 \,, \tag{4.3}$$

and since for nonnegative ϕ the integral is nonnegative, the mapping

$$T_\alpha : \phi \longrightarrow \int_{\mathbb{R}^p} \int_{\mathbb{R}^p} \int_Z \phi(S((z,v,w)) d\mu(z) d\alpha(v) d\alpha(w) \tag{4.4}$$

is a positive functional on $C_0^0(\mathbb{R}^p)$. Therefore (see, e.g. [15, Ü 4.9]) there exists a σ-finite measure $d\beta$ satisfying $T_\alpha \phi = \int \phi d\beta$. Since $T_\alpha \phi < \infty$ for $\phi \in L^\infty(\mathbb{R}^p)$, $d\beta$ is finite. From classical results follows that $d\beta$ is unique (see for example the Portmanteau theorem, [16]). □

For cases of collision kernels described by transition densities $K(.|v,w)$, we obtain again a classical model gain term. Suppose

$$\int \phi(S(z,v,w)) d\mu(z) = \int \phi(v') K(v'|v,w) dv' \tag{4.5}$$

for all test functions ϕ, and $v, w \in \mathbb{R}^p$; then $d\beta$ is absolutely continuous, and the solution of (4.1) is given by

$$g(v) = \int \int K(v|v',w') f(v') dv' f(w') dw'. \tag{4.6}$$

Since $K(.|v,w)$ is then a probability density for all v, w, we find that $g \in L^1(\mathbb{R}^p)$. In particular we conclude

Corollary: *Under the assumption (4.5), problem 1' is uniquely solvable in $V = L^1(\mathbb{R}^p)$, with the solution g given by (4.6).*

4.2 The discretized problem

Of course, the discretized case is included in Theorem 1. A formal discretization is obtained as follows. Denote the index set G and the grid G_h as in section 3.3. (We again identify elements $\alpha = (i,j) \in G$ with the corresponding elements in G_h.) Replace in equation (4.1) f by a corresponding function on G; replace $S : Z \times \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}^2$ by a discrete version $S^d : Z \times G \times G \to G$. Choose as the set of test functions the functions ψ on G. Then the right hand side of equation (4.1) turns into

$$\sum_{\alpha,\beta \in G} \int_Z \psi(S^d(z,\alpha,\beta)) d\mu(z) f_\alpha f_\beta. \tag{4.7}$$

With $\sigma_{\alpha\beta}(\gamma) := \mu(\{z \in Z : S^d(z,\alpha,\beta) = \gamma\})$, we obtain

$$\int_Z \psi(S^d(z,\alpha,\beta)) d\mu(z) = \sum_\gamma \sigma_{\alpha\beta}(\gamma). \tag{4.8}$$

Using the basis $\{\delta_\gamma, \gamma \in G\}$ of the test function space, the discretized version of problem 1' reads: Find the function g on G satisfying

$$g_\gamma = \sum_{\alpha,\beta \in G} \sigma_{\alpha\beta}(\gamma) f_\alpha f_\beta. \tag{4.9}$$

Like equation (4.6), this is an explicit formula for the solution g. Here, we do not discuss any convergence properties in the limit of the grid constant $h \to 0$. This will be studied in a future paper.

Let the one-dimensional physical space be given as the unit interval $[0,1]$. Choose $v \in \mathbb{R}^p$ fixed, and $\alpha := v_x$. Let's assume $\alpha \geq 0$. The iteration scheme of the preceding section leads to an integral equation of the form

$$f(x) = \tilde{\psi} \cdot \exp\left(-\frac{1}{\alpha}\int_0^x \rho(s)ds\right) + \int_0^{x/\alpha} g(x - s\alpha) \cdot \exp\left(-\frac{1}{\alpha}\int_s^x \rho(\sigma)d\sigma\right) ds \tag{4.10}$$

with $\tilde{\psi}$ and g given. A discretized version is given immediately as follows. Choose $N \in \mathbb{N}$ and denote $h := 1/N$ and $x_i := i \cdot h$ for $i = 0, \ldots N$. Write f_i as the approximation of $f(v)$ at x_i. Then $f_0 = \tilde{\psi}$; in a straightforward manner, a conservative first order upwind scheme is derived which leads to the recursive formula

$$f_k = \left(1 - \frac{h \cdot \rho_{k-1}}{\alpha}\right) \cdot f_{k-1} + \frac{h}{\alpha} \cdot g_{k-1}. \tag{4.11}$$

(Of course, for $\alpha < 0$, f_k is determined from the values at $k+1$ rather than at $k-1$.)

5 Numerical experiments

5.1 The setting

We consider the nine-velocity model (i.e. $\Gamma = 1$, see section 3.3) on the slab $\Omega = [0,1]$. The transition probability of a velocity (i,j) due to the influence of a "collision partner" (k,l) is given by the factorizing terms S_{ijkl} with Q_{ijkl} defined by (3.19) to (3.21). These formulas do not guarantee nonnegativity. Therefore in all cases, for which one of the terms on the right hand side of (3.19) to (3.21) is negative, we modify into

- Model 1: $Q_{ijkl}(m) := \delta_{im}$;
  this means that changes of some velocity components are simply ignored.

- Model 2: $Q_{ijkl}(m) := 1/3$ for $m = -1, 0, 1$;
  this introduces a slight smearing out in the velocity space.

Of course this modification could be avoided by a more elaborate discrete collision model. We leave this for a future paper.

For the discretization, the step size in the position space is chosen to coincide with the parameter h in velocity space.

We compare a deterministic numerical scheme with a Monte Carlo simulation scheme. The deterministic scheme is obtained in a straightforward way by combining (4.9) (problem 1') with (4.11) (problem 2). The Monte Carlo scheme is a time evolution algorithm based on time-splitting of free flow and collisions. For the simulation of the collisions we use Nanbu's scheme with the modification of [17] which was mathematically analyzed in [3]. The stationary approximation is obtained by time-averaging.

5.2 Numerical results

We perform three numerical experiments: The calculation of an equilibrium for the homogeneous Boltzmann equation, and steady slab solutions for a zero-gradient and a non-zero gradient velocity field - both for the deterministic and for the Monte Carlo scheme.

1. Equilibrium solution: First, we calculate the homogeneous zero mean velocity equilibrium state with density 1. The deterministic iteration converges for both model 1 and 2. As expected for reasons of symmetry, the occupation densities $p(i,j)$ for the velocities (i,j) depend only on $|i|+|j|$.

$\lvert i\rvert+\lvert j\rvert$	(1)	(2)	(3)	(4)
0	0.2180	0.2136	0.2136	0.2196
1	0.1160	0.1224	0.1225	0.1215
2	0.0795	0.0742	0.0741	0.0736

Tab 1: Equilibrium $p(i,j)$

The Monte Carlo scheme exhibits a seemingly strange behaviour for model 1, since after a couple of time steps all particles are concentrated in merely one (or a few) velocity state. This state is random, but fixed once occupied by all particles. Though seemingly surprising, this effect has already been observed for Nanbu's scheme [18] and is due to the effect that because of momentum fluctuations the particle system drifts from a zero mean velocity state into a random non-zero state and freezes there. Tab. 1 shows the deterministic results for model 1 (1) and model 2 (2), and MC results for model 2 for numbers of particles per velocity state $N = 180$ (3) and $N = 18$ (4).

2. Zero gradient field: For inflow conditions at $x = 0$ and $x = 1$ given by this equilibrium state, a stationary solution is given which is constant along the interval $[0,1]$. This solution is obtained by the deterministic calculation. For the Monte Carlo scheme the situation is different. We ran test cases with up to 20 particles per velocity state (i.e. 180 particles per spatial cell). As inflow we chose a constant i.e. non-fluctuating number of particles. As a result, we observed an approximatingly constant state in the interiour, however boundary layers at the boundaries $x = 0$ and $x = 1$ (see Fig. 1 for the density profile). For model 1, the simulation result fluctuates - apart from the boundary layers - with an error of roughly 1 % (Fig.

1, solid line). The approximating 4-th order polynomial (dotted line) even lies within 0.3 % error. The error within the boundary layers increases to 2 %. For model 2, the situation is similar, however the constant state in the interior is 2 % too high. (The auxiliary lines in Fig. 1 indicate the solution $\rho \equiv 1$ and the 2.5 % error bounds.)

Fig.1: Equilibrium density profile from Monte Carlo simulation

3. Non-zero gradient field: By modifying the inflow conditions, we generate a symmetric v_y-velocity gradient. Fig. 2 shows the profile of the first moment $\overline{\rho \cdot v_y}$ obtained from deterministic computations for different Knudsen numbers. We recognize an almost constant slope for large Knudsen numbers (dotted line) and a constant (equilibrium) state in the interior with boundary layers for small Knudsen numbers (solid line). Fig. 3 reveals significant differences between the deterministic calculation (dotted line) and Monte Carlo simulations with 180 particles per cell (solid line).

5.3 Some concluding remarks

Ways to numerical high-resolution solutions are very restricted as long as one has to rely on Monte Carlo schemes. Deterministic schemes for model problems might be an alternative. Since existence and uniqueness results for steady solutions are very rare, both kinds of simulations should contribute to increase our knowledge and understanding in these cases. There is a need for high-resolution solutions, which in the future may perhaps be designed from deterministic model problems. On the other hand, a systematic investigation of random particle games may help to understand a lot more about physical phenomena connected to fluctuations.

Fig.2: Profiles of first moments for different Knudsen numbers

Fig.3: Deterministic results vs. Monte Carlo results

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