Boltzmann Simulation by Particle Methods [†]

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1 Introduction

Particle methods to simulate rarefied gas flows have found an increasing interest in Computational Fluid Dynamics during the last decade, see for example [1], [2], [3] and [4]. The general goal is to develop numerical schemes which are reliable enough to substitute real windtunnel experiments, needed for example in space research, by computer experiments.
In order to achieve this goal one needs numerical methods solving the Boltzmann equation including all important physical effects. In general this means 3D computations for a chemically reacting rarefied gas. With codes of this kind at hand, Boltzmann simulation becomes a powerful tool in studying rarefied gas phenomena.
In the first section we briefly describe the mathematical idea behind particle methods together with a bit of its history. In a second part we explain how to simulate collision processes described by the Boltzmann equation.
In the last section we discuss some recent progress and questions.

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2 The Mathematical Idea behind Particle Methods

Let us start with a brief comment on the origin of particle or Monte–Carlo methods.
The particle methods which are used to simulate rarefied gas flows nowadays (see for example [1] and [3]) have a lot in common with the original work of Metropolis and Ulam [5] who are the originators of the classical Monte–Carlo Method.
Several ideas in the existing particle codes can already be found in the original papers.
'Only a few particles were studied in classical mechanics', meanwhile in statistical physics, 'one does not concentrate on the individual particle but studies the properties of sets of particles.' [5]
In the same way Ulam refers to set theory and its connection with the concept of indistinguishable particles:
'Here again is something that most mathematicians should learn about, namely the statistics of identical particles.' [6]
In reference [7] Borsuk and Ulam deal with the space $E(n)$ of nonordered systems of n points – which may be different or not – belonging to a metric space E equipped with the usual Hausdorff metric and ask for its topological structure. Using a different interpretation elements in $E(n)$ may be represented by discrete measures

$$\omega = \sum_{i=1}^{n} \delta_{P_i} \quad \text{with} \quad P_i \in E$$

By this representation one directly gets metrical concepts different from the Hausdorff metric and this led us to the name 'Finite Point Set' method (shortly 'FPM').
Ulam and Metropolis used this idea (together with statistics) to solve the equation

$$\partial_t u = a\Delta u + Vu$$

which they obtained from the time–independent Schrödinger equation

$$a\Delta\Psi + (E - V(x,y,z))\Psi = 0$$

by introducing the new time–dependent function $u = \Psi \exp^{-Et}$.

2.1 Particle Methods

The general idea of particle methods is the approximation of densities by discrete measures. Concerning the Boltzmann equation we consider the distribution function $f(t,x,v)$ which we want to approximate by a discrete measure of the form

$$\delta_{\omega_N} := \sum_{j=1}^{N} \alpha_j(t)\delta_{(x_j(t),v_j(t))}$$

The approximation is based on the

Weak* Convergence of δ_{ω_N} to f

Definition 1 The discrete measure δ_{ω_N} converges weakly to f if the following relation holds for all functions $\phi \in \mathcal{C}_b$

$$\int \phi \mathrm{d}\delta_{\omega_N} = \sum_{j=1}^{N} \alpha_j(t)\phi(x_j(t),v_j(t)) \quad \stackrel{N\to\infty}{\longrightarrow} \quad \int \phi f \mathrm{d}x\mathrm{d}v$$

Remark 1 Here we discover already one of the problems in this approach: moments of the forms

$$\int_{\Omega\times I\!R^3} v^k f \mathrm{d}x\mathrm{d}v$$

are not covered by weak* convergence. One way out is to consider the function $|v|^2 f$ instead of f and try to work with 'energy particles' (for a general description see [8]).

Distance between δ_{ω_n} and f

From number theory one may work with the so–called discrepancy defined by

$$\sup_{r,s\in I\!R^3} \Big| \int\limits_{R(r,s)} f \mathrm{d}P - \sum_{j:P_j\in R(r,s)} \alpha_j \Big| =: D(\delta_{\omega_N}, f)$$

where

$$P = (x,v) \quad P_j = (x_j, v_j)$$

and

$$R(r,s) = \{(x,v) \in I\!R^3 \times I\!R^3 : x^i \le r^i,\ v^i \le s^i,\ i = 1,2,3\}$$

The key point using the discrepancy is the Koksma–Hlawka inequality which gives an error estimate for the integration of a function with bounded variation.

$$|\int \phi f \mathrm{d}P - \sum_{j=1}^{N} \frac{1}{N} \phi(P_j)| \leq \mathrm{Var}[\phi] \cdot D(\delta_{\omega_N}, f)$$

Furthermore the following relation holds

$$\delta_{\omega_N} \stackrel{\text{weak}*}{\longrightarrow} f \quad \stackrel{N\to\infty}{\Longleftrightarrow} \quad D(\delta_{\omega_N}, f) \to 0$$

i.e. the weak* convergence of measures is equivalent to the convergence in the sense of the discrepancy as long as the limit measure is absolutely continuous with respect to the Lebesgue measure.
There are a lot of other possibilities to introduce a distance between δ_{ω_n} and f. From measure theory one may use the bounded Lipschitz distance.

Definition 2 The bounded Lipschitz distance between two measures is defined by

$$\mathrm{dist}(\mu, \nu) = \sup_{\phi \in D} |\int \phi \mathrm{d}(\mu - \nu)|$$

with

$$D = \{\phi \,:\, 0 \leq \phi \leq 1,\, |\phi(P) - \phi(Q)| \leq ||P - Q||\}$$

Remark 2 The bounded Lipschitz distance generates the weak* convergence too, even in the case when the limit is not absolutely continuous.

2.2 Constructive Methods to Generate Particle Sets

Number theory provides construction methods for discrete measures δ_{ω_N} with a small distance to f. In the simplest – but at the same time 'classical' case – one considers uniformly distributed sequences in the k–dimensional unit cube, i.e. the distribution function is given by the characteristic function on the k–dimensional unit cube,

$$f(x) = \mathcal{X}_{[0,1]^k}(x) = \begin{cases} 1 & : \quad x \in [0,1]^k \\ 0 & : \quad \text{else} \end{cases}$$

These sequences are known as 'pseudo–random numbers' or 'good lattice points' and they are in detail discussed in the papers by Halton [9], Faure [10], Niederreiter [11] and Sobol [12].

Special sequences which were sucessfully applied in Quasi Monte Carlo methods are the generalized Halton sequences based on the van Neumann–Kakutani transformation:
The sequence with respect to base $p \in I\!N$ in one dimension can be written as the recurrence relation

$$x_{n+1} = T_p(x_n), \quad p \in I\!N$$

where the function T_p is defined as

$$T_p(x) = x + b_k^p$$

with

$$b_k^p = \frac{1}{p^k}(p + 1 - p^k)$$

$$k = [-\frac{\log(1-x)}{\log(p)}] + 1$$

and an arbitrary starting point $\overset{o}{x}$ in $[0, 1]$.
With the same rule one gets k–dimensional sequences by taking $p_1, ..., p_k$ relatively primes and using the above recurrence relation for every component of the quasi–random sequence (for a detailled description see [13]).
The following table shows the one dimensional discrepancy with $p = 3$ in comparison with the standard UNIX–rand subroutine. Furthermore the CPU time used to generate 10^6 random numbers is given in the table.

Tab. 2.2.1: Discrepancy and Efficiency of random numbers

	N = 29	N = 173	CPU [sec] (HP 9000/710)
Minimal Discrepancy	$1.7 \cdot 10^{-2}$	$2.9 \cdot 10^{-3}$	
UNIX–rand	$1.3 \cdot 10^{-1}$	$6.4 \cdot 10^{-2}$	2.0
v. Neumann–Kakutani	$3.5 \cdot 10^{-2}$	$9.0 \cdot 10^{-3}$	1.0

Remark 3

1) The number N in the table above is the number of points in the sequence.

2) The discrepancy is calculated using 20 independent samples. In the case of the van Neumann–Kakutani sequence this means 20 independent starting points $\overset{o}{x}$.

3) The optimal discrepancy in k dimensions is of order $\frac{\log N^{k-1}}{N}$.

For the general case one does not need uniformly distributed in the k–dimensional unit cube, but particle sets which approximate the densities of measures on the space $\mathbb{R}^k$. Hence one has to transform the point sequence from $[0,1]^k$ to a sequence which approximates a density f on $\mathbb{R}^k$.
In one dimension this can be done via the inverse of the distribution function or – if the inverse is not known explicitly – via an acceptance–rejction procedure (see for example [14]).
The situation gets more diffcult if the function f is an arbitrary not separable $\mathcal{L}_1$–integrable function on $\mathbb{R}^k$. Here one may use the Hlawka–Mück transformation [15], [16], [17].

3 The Simulation of the Collision Process

Let us consider the (monoatomic) spatially homogeneous Boltzmann equation

$$\begin{aligned} \partial_t f &= Q(f,f) \\ Q(f,f) &= \int\limits_{\mathbb{R}^3}\int\limits_{S^2} \sigma(|v-w|,\eta)\{f(t,v')f(t,w') - f(t,v)f(t,w)\}\mathrm{d}\omega(\eta)\mathrm{d}w \\ v' &= v - \eta\langle \eta, v-w\rangle \\ w' &= w + \eta\langle \eta, v-w\rangle \end{aligned}$$

together with an appropiate initial condition.
To derive a particle method we consider a time–discretized version in the form

$$f(\Delta t, v) = f(0,v) + \Delta t Q(f,f)(0,v) \tag{1}$$

As given in the last section the idea of a particle method is to approximate the function $f(t,v)$ by a discrete measure. Hence suppose that the discrete measure $\sum\limits_{i=1}^{N} \alpha_j \delta_{v_j}$ is an approximation of $f(0,\cdot)$. Now one has to to derive a particle evolution, i.e. to construct a new discrete measure $\sum\limits_{i=1}^{N} \alpha_j^* \delta_{v_j^*}$ which approximates $f(\Delta t,\cdot)$.
The key point for the particle evolution – as we will see later – is to select

collision pairs including dummy collisions:
N pairs $(v_i, v_{j(i)})_{i=1,...,N}$ have to be chosen such that

$$\sum_{i=1}^{N} \frac{1}{N} \delta_{(v_i, v_{j(i)})} \quad \text{approximates} \quad f(0,v) \cdot f(0,w)$$

if

$$\sum_{i=1}^{N} \frac{1}{N} \delta_{v_i} \quad \text{approximates} \quad f(0,v).$$

For particle sets with identical weights as above there is a relatively easy solution as we shall see: Choose the indices $j(i)$ uniformly in the set $\{1, ..., N\}$. If one works with arbitrary weights α_i the situation gets much more complicated [8]. One realizes, that here stochastic elements appear in the simulation procedure. Now we are able to construct the evolution:
The weak formulation of equation (1) is given by

$$\int\limits_{v \in I\!R^3} \Phi(v) f(\Delta t, v) \mathrm{d}v = \int\limits_{v \in I\!R^3} \Phi(v) f(0,v) \mathrm{d}v + \Delta t \int\limits_{v \in I\!R^3} \Phi(v) Q(f,f)(0,v) \mathrm{d}v$$

Using the structure of the collision operator $Q(f,f)$ and the relation $||f||_1 = 1$ one gets

$$\int\limits_{v \in I\!R^3} \Phi(v) f(\Delta t, v) \mathrm{d}v =$$

$$\Delta t \int\limits_{v \in I\!R^3} \int\limits_{w \in I\!R^3} \int\limits_{\eta \in S^2} \Phi(v) \sigma(|v-w|, \eta) f(0,v') f(0,w') \mathrm{d}\omega(\eta) \mathrm{d}w \mathrm{d}v$$

$$+ \int\limits_{v \in I\!R^3} \int\limits_{w \in I\!R^3} \int\limits_{\eta \in S^2} \Phi(v)(1 - \Delta t \sigma(|v-w|, \eta)) f(0,v') f(0,w') \mathrm{d}\omega(\eta) \mathrm{d}w \mathrm{d}v$$

Remark 4 In order to ensure positivity of the function $f(\Delta t, v)$ we have to assume that

$$1 - \Delta t \sigma(|v-w|, \eta) \geq 0 \quad \forall\, v, w \in I\!R^3,\ \eta \in S^2$$

which restricts the choice of the differential cross section as well as the choice of the time step Δt.

Using the relations

$$\mathrm{d}v\mathrm{d}w = \mathrm{d}v'\mathrm{d}w' \quad \text{and} \quad |v-w| = |v'-w'|$$

yields

$$\int\limits_{v\in I\!R^3} \Phi(v) f(\Delta t, v)\mathrm{d}v = \tag{2}$$
$$\int\limits_{v\in I\!R^3}\int\limits_{w\in I\!R^3}\int\limits_{\eta\in S^2} K[\Phi](v,w,\eta) f(0,v) f(0,w)\mathrm{d}\omega(\eta)\mathrm{d}w\mathrm{d}v$$

with

$$K[\Phi](v,w,\eta) = (\Delta t\sigma(|v-w|,\eta)\Phi(v') + (1-\Delta t\sigma(|v-w|,\eta))\Phi(v))$$

We introduce a variable $s \in [0,1]$ and a transformation $T(v,w,\eta,s)$ defined as

$$T(v,w,\eta,s) = \begin{cases} v' & \text{for} \quad s \le \Delta t\sigma(|v-w|,\eta) \\ v & \text{for} \quad s > \Delta t\sigma(|v-w|,\eta) \end{cases}$$

Hence equation (2) can be written

$$\int\limits_{v\in I\!R^3} \Phi(v) f(\Delta t, v)\mathrm{d}v = \tag{3}$$
$$\int\limits_{v\in I\!R^3}\int\limits_{w\in I\!R^3}\int\limits_{\eta\in S^2}\int\limits_{s\in[0,1]} (\Phi\circ T)(v,w,\eta,s) f(0,v) f(0,w)\mathrm{d}s\mathrm{d}\omega(\eta)\mathrm{d}w\mathrm{d}v$$

Equation (3) is the starting point to derive the time evolution of the discrete measure due to collisions:
One recognizes that $f(0,v)f(0,w)\mathrm{d}s\mathrm{d}\omega(\eta)\mathrm{d}w\mathrm{d}v$ defines an (absolutely continuous) measure on $I\!R^3 \times I\!R^3 \times S^2 \times [0,1]$. Hence, if we construct an approximation of this product measure using the given discrete measure at time $t = 0$, we can calculate the approximation of $f(\Delta t, v)$ simply via the transformation $T(v,w,\eta,s)$.

Theorem 1 *Let the discrete product measure δ_{μ_N} given by*

$$\delta_{\mu_N} = \sum_{i=1}^{N} \alpha_i \delta_{(v_i,w_i,\eta_i,s_i)}$$

converge weakly to $f(0,v)f(0,w)\mathrm{d}s\mathrm{d}\omega(\eta)\mathrm{d}w\mathrm{d}v$.
Suppose moreover that $\sigma(|v-w|,\eta)$ *is an a.e. continuous function. Then*

$$\delta_{\omega_n(\Delta t)} := \sum_{i=1}^{N} \alpha_i \delta_{T(v_i,w_i,\eta_i,s_i)}$$

converges weakly to $f(\Delta t, v)\mathrm{d}v$.

Applying the above theorem it becomes clear that the key point for the particle evolution will be to select collision pairs:
The first step in approximating the product measure
$f(0,v)f(0,w)\mathrm{d}s\mathrm{d}\omega(\eta)\mathrm{d}w\mathrm{d}v$ is to construct a discrete measure approximating the product $f(0,v)f(0,w)\mathrm{d}w\mathrm{d}v$ – but this exactly corresponds to the generation of collision pairs, which we mentioned above.
We consider in the following the case that the approximation of $f(0,v)$ is given by a discrete measure δ_{ω_N} with identical weigths, i.e.

$$\delta_{\omega_N} = \sum_{i=1}^{N} \frac{1}{N} \delta_{v_i} \tag{4}$$

To build up an approximation of the product means to equip every particle v_i with a collision partner out of the set $\{v_1,...,v_N\}$, see also figure 3.1.
Because all particles carry identical weights, i.e. $\alpha_i = \frac{1}{N}$, it is clear that the collision partners can be chosen uniformly on the set $\{v_1,...,v_n\}$ and this corresponds to a uniform distribution on the finite set $\{1,...,N\}$ of indices.

Theorem 2 *Suppose the measure* δ_{ω_N} *given by (4) converges weakly to* $f(0,v)$. *If the collision partners* $v_{j(i)} \in \{v_1,...,v_n\}$, $i = 1,...,N$ *are chosen uniformly out of the set* $\{v_1,...,v_n\}$ *then, almost surely, the product measures defined by*

$$\delta = \sum_{i=1}^{N} \frac{1}{N} \delta_{(v_i,v_{j(i)})}$$

converges weakly to the product $f(0,v)f(0,w)$.

Remark 5 The first proof for this theorem – based on the central limit theorem – was given by Babovsky [18]. In reference [8] the reader may find a general investigation how to construct product measures with arbitrary weigths.

In the same way one may compute the discrete approximation for the full product measure, i.e.

$$\sum_{i=1}^{N} \frac{1}{N} \delta_{(v_i, v_{j(i)}, \eta_i, s_i)} \xrightarrow{w*} f(0,v) f(0,w) \mathrm{d}s \mathrm{d}\omega(\eta) \mathrm{d}w \mathrm{d}v$$

The points η_i, $i = 1, ..., N$ and s_i, $i = 1, ..., N$ play the role of collision parameters: the velocity v_i remains constant, i.e. $v_i(\Delta t) = v_i$, if $s_i > \Delta t \sigma(|v_i - v_{j(i)}|, \eta_i)$, otherwise one has $v_i(\Delta t) = T(v_i, v_{j(i)}, \eta_i, s_i) = v_i - \eta_i \langle \eta_i, v_i - v_{j(i)} \rangle$.

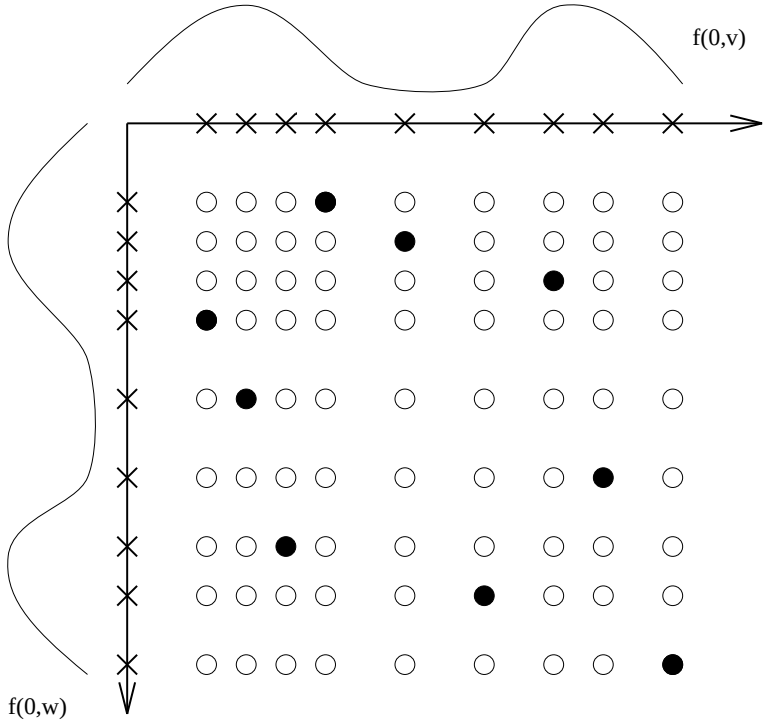

Figure 3.1: Approximation of the product $f(0,v) \cdot f(0,w)$

An important remark concerning the approximation of the product measure is the following:
Since binary collisions conserve mass, momentum and energy one has

$$\frac{\mathrm{d}}{\mathrm{d}\,\mathrm{t}} \int\limits_{v \in I\!R^3} \phi(v) f(t,v) \mathrm{d}t = 0, \quad \phi(v) = 1, v, |v|^2$$

In the case of discrete measures the conservation property means

$$\begin{aligned}
\sum_{i=1}^{N} \alpha_i &= \sum_{i=1}^{N} \alpha_i(\Delta t) \\
\sum_{i=1}^{N} \alpha_i v_i &= \sum_{i=1}^{N} \alpha_i(\Delta t) v_i(\Delta t) \\
\sum_{i=1}^{N} \alpha_i |v_i|^2 &= \sum_{i=1}^{N} \alpha_i(\Delta t) |v_i(\Delta t)|^2
\end{aligned}$$

It is easy to ensure conservation if the weights α_i are identical:
If the collision partners are chosen under the restriction

$$j(j(i)) = i \quad \forall\, i = 1, ..., N$$

and the collision parameters are chosen such that

$$\begin{aligned}
\eta_i &= -\eta_{j(i)} \\
s_i &= s_{j(i)} \quad \forall\, i = 1, ..., N
\end{aligned}$$

it is easy to verify that the conservation properties hold.
If one uses weighted particles, i.e. $\alpha_i \neq \alpha_j$, $i \neq j$, the situation is much more difficult [8]. Nevertheless it is important to control the conservation quantities in real applications [19].
Theorem 2 and its generalizations in [8] prove convergence with probability 1 since it refers to stochastic procedures: One chooses $j(i), i = 1, ..., N$ uniformly distributed on $\{1, ..., N\}$. Why do we not propose a deterministic procedure? The only goal we have in mind constructing $j(i)$ is that $(v_i, v_{j(i)})$ are appropiate integration knots, i.e.

$$\int \phi(v, w) f(0, v) f(0, w) \mathrm{d}v \mathrm{d}w \sim \frac{1}{N} \sum_{i=1}^{N} \phi(v_i, v_{j(i)})$$

for arbitrary $\phi \in \mathcal{C}^b$.
There are two reasons to use a stochastic procedure – keeping the „Monte Carlo character" of the whole algorithm.

1) Deterministic choices introduce in general smaller but more systematic errors; it may happen, that they systematically under– or overestimate a certain value, such that a cumulation of errors during several timesteps creates troubles; those effects are often avoided by using random processes, since the errors may cancel each other during the evolution (We observe these effects in handling a boundary condition). However one may try to find deterministic algorithms without those defects, which then seem to be the natural choice.

2) Our problem is a highdimensional integration test, therfore the theory of ,,information based complexity" may apply.
Typically this theory defines the complexity of algorithms approximating

$$S(F) := \int_G F \mathrm{d}x$$

for $F \in X_0, X_0$ unitball in the Sobolev space $W_p^r(G), G \subset I\!R^d$. To do so, one defines an ,,information operator" N, evaluating the elements $F \in X_0$

$$N : F \longrightarrow (\lambda_1(F), ..., \lambda_n(F)), F \in X_0$$

where λ_i are ,,evaluation functionals", feeded into the computational integration process.
An algorithm ϕ is an operator, working with the given information and $A := \phi \circ N$ is assumed to be an approximation for S.
Denoting finally by A_n the set of all approximations working with n data we get the deterministic complexity for S

$$e_n(S) := \inf_{A \in A_n} \left(\sup_{F \in X_0} \mathrm{dist}\,(S(F), A(F)) \right)$$

Since we want to use stochastic elements, ϕ and therefore A become stochastic variables on a probability field with measure μ; the same holdes for the number $\tilde{n}$ of evaluations and we consider only algorithms, for which the expectation value of this number $\tilde{n}$ is less or equal n: $E(\tilde{n}) \leq n$. Then one defines the stochastic or Monte Carlo complexity

$$e_n^{MC}(S) := \inf_{A \in A_n} \left(\sup_{F \in X_0} \int_\Omega \mathrm{dist}\,(S(F), A(\omega)(F)) \mathrm{d}\mu(\omega) \right)$$

Now the main message of the theory of information based complexity is, that – depending on the dimension d and the smoothness r of F the Monte Carlo complexity may be smaller then the deterministic e_n; there are old results by Sard [20] and Bakhvalov [21], [22] telling us that $e_n \sim N^{-r/d}$ but

$$e_n^{MC} \sim \begin{cases} n^{-r/d-1/2} & \text{if } 2 \leq p \\ n^{-r/d-1+1/p} & \text{if } 1 \leq p \leq 2 \end{cases}$$

For large d and samll r the improvement could be essential. Results of this kind seem to be transferable to our problem; they would give a theoretical foundation to an experimentally often observed fact: That for highdimensional kinetic equations Monte Carlo methods are favourable.

4 Recent Progresses and Questions

Besides the derivation of a particle method the modellization of the real gas effects is the main point in real applications. In the first part of this chapter we describe briefly the way to incorporate real gas effects in the simulation procedure. In a second part we focus on the linking of aerodynamic and kinetic descriptions.

4.1 Real Gas Effects and Chemical Reactions

In order to describe real rarefied gas flows one has to recognize that gas molecules carry internal energies of rotational and vibrational nature. This is condensed in two additional variables ε_{rot} and ε_{vib} in the Boltzmann equation, i.e.

$$f = f(t, x, v, \varepsilon_{rot}, \varepsilon_{vib})$$

Due to the fact that the rotational level spacing of 'air' molecules like nitrogen and oxygen is small ($\sim 3K$) compared to some typical equilibrium flow temperatures ($\sim 200K$) it is justified to model the rotational energy by a continuous variable ε_{rot}. The rotational energy exchange may be handled by a 'Borgnakke–Larsen' type model (see [23] and [24]) where the differential cross section is given by

$$\sigma(E; \varepsilon', \varepsilon_1' \longrightarrow \varepsilon, \varepsilon_1) =$$
$$\sigma_{\text{VHS}} \left[Z(E)\delta(\varepsilon' - \varepsilon)\delta(\varepsilon_1' - \varepsilon_1) - (1 - Z(E))C(E)(E - \varepsilon - \varepsilon_1) \right]$$

The first term represents elastic scattering, the second one completely inelastic scattering. σ_{VHS} is the differential cross section for monoatomic gases corresponding to the 'variable hard sphere' model. In reference [25] the reader may find a comparison with a very elaborate loaded sphere calculation. The results show a good agreement if the parameter of the Borgnakke–Larsen model are chosen appropiate.
Due to the vibrational level spacing ($N_2 : 3390K, O_2 : 2270K$) one has to take into account the quantum nature of vibrational energy. Hence the vibrational energy ε_{vib} takes only discrete values and may be modelled by a harmonic oscillator with finite well depth. In this case the vibrational levels are given by

$$\varepsilon_{vib}^{i} = i \cdot \Theta_{vib},\ i = 0, ..., N$$

where Θ_{vib} denotes the charateristic temperature of vibration, i the level index and N the number of harmonic oscillator levels in the potential well. The energy exchange between translational, rotational and vibrational energies may be treated by a generalized Borgnakke–Larsen model (see reference [26]). This model is a phenomenological one so it is important to fit the parameter of the model to some well–known quantities, for example the transport coefficients in equilibirum.
There exist several other approaches for the modellization of vibrational energies, see for example [27] and [28].

Chemical Reactions
Let us consider a gas consisting of atoms A and diatomic molecules A_2 with the following chemical reactions

1) Dissociation Reaction

$$A_2 + A \quad \longrightarrow \quad A + A + A$$

2) Recombination Reaction

$$A + A + A \quad \longrightarrow \quad A_2 + A$$

This system is described by the so–called Ludwig–Heil equations (see [29] and [30]). The system represents a set of extended Boltzmann equations for the two distribution functions f_A and f_{A_2} containing terms for each process,

for example the term

$$\int W_{dis}\left((v',w',E') \longrightarrow (u,v,w)\right) \cdot \left[f'_a f'^1_A - (\frac{2h}{m})^3 f_A f^1_A f^2_A\right] \mathrm{d}u\mathrm{d}w \qquad (5)$$

describing the effect of dissociation–recombination reactions for the atomic distribution function f_A.
The main part for this set of Boltzmann equations is the correct modellization of the transition probability of the different phenomena – for example in equation (5) the modellization of $W_{dis}\left((v',w',E') \longrightarrow (u,v,w)\right)$, i.e. the probability for a dissocation–recombination reaction. Some hints may be found in [31].
The following test case shows the influence of dissociation reactions of oxygen molecules on the heat transfer coefficient of a reentry vehicle.

Tab 4.1: Influence of chemical reactions on aerodynamic characteristics

Mach	Kn	C_h^f	C_h
25	0.1	0.49	0.46
	0.5	0.67	0.66
30	0.1	0.51	0.43
	0.5	0.68	0.64

Here, C_h^f denotes the global heat transfer coefficient at the surface with frozen chemical reactions, C_h denotes the same quantity including dissociation reactions. Ma denotes the Mach number of the flow and Kn the Knudsen number.
One realizes that chemical reactions become important at high Mach and low Knudsen numbers. For a detailled description see reference [26].

4.2 The Matching with 'Macrocopic Equations'

There are two strong reasons to study the linking of kinetic and aerodynamic descriptions in the transition between equilibrium and nonequilibrium flows.

1) The continuum description using Euler or Navier Stokes equations may loose its validity in local regions near shock layers or near to the surface in the kinetic or boundary layer. Furthermore a strong rarefaction region at the lee side of a reentry vehicle is observed.

2) The Boltzmann simulation runs out of memory requirements and computation time if the mean free path of the gas particles gets near to the equilibrium limit.

Consequently the strategy will be to use an Euler scheme whenever it is possible and a Boltzmann simulation whenever it is necessary.
The following two questions arise naturally

1) Where is the macroscopic description sufficiently good?

2) If we know the boundary between the two flow region: How can we couple the two flow domains?

Some results on the first question – how to detect the different flow regions – were given by Gropengießer [32] and LeTallec et al. [33].
We will focuse in the following on question 2).
Consider the intervall $[-L, L] \subset I\!R$ divided into two overlapping regions A and B, as shown in figure 4.1.

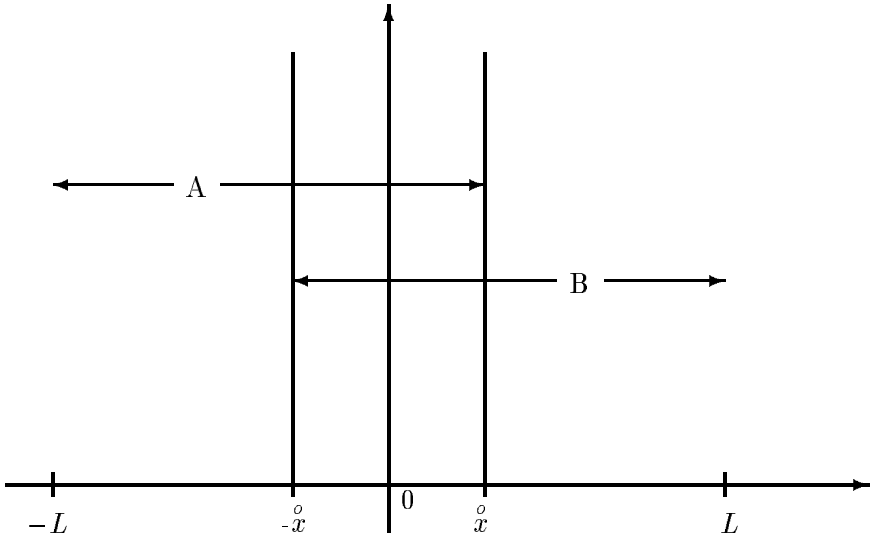

Figure 4.1: Overlapping domain for aerodynamic and kinetic equations

Suppose now that we want to compute the solution of the Euler or Navier–Stokes equations in region A (like 'Aerodynamics') and the solution of the Boltzmann equation in region B (Boltzmann region). It is obvious that we need some 'appropiate' boundary conditions at the two points $-\overset{o}{x}$ and $\overset{o}{x}$:

1) For the aerodynamic region A we have two prescribe 'some boundary values' for ρ, u and T at the point $\overset{o}{x}$. The number of boundary values depends on the situation. If we consider for example Euler equations than the number depends on the characteristics which run from $\overset{o}{x}$ into the aerodynamic region A.

2) For the kinetic region B we have to prescribe the ingoing flux $f(t, -\overset{o}{x}, v)_{v>0}$ at the point $-\overset{o}{x}$ for all times $t > 0$.

Let us first consider the boundary condition at $-\overset{o}{x}$, i.e. the boundary conditions for the Boltzmann region B. The situation is as follows:
From the solution of the aerodynamic equation in region A we know the quantities ρ, u and T at the point $-\overset{o}{x}$.
The question now is how to construct the incoming flux $f(t, -\overset{o}{x}, v)_{v>0} = f_+(t, v)$.
The relation between the incoming and outgoing flux in the kinetic region is given by the so–called Albedo operator A, i.e.

$$f(t, -\overset{o}{x}, v)_{v<0} = f_-(t, v) = A[f_+](t, v)$$

and the Albedo operator A can be derived from the solution of the Boltzmann equation in the kinetic domain B. If we would be able to compute $A[f_+]$ and if we want continuity of moments across $-\overset{o}{x}$, we would get

$$\rho(t, -\overset{o}{x}) = \int_0^\infty f_+ \mathrm{d}v + \int_{-\infty}^0 A[f_+](t, v)\mathrm{d}v \tag{6}$$

and simila equations for u and T.
It is clear that this theoretical idea does not work practically: We are not able to construct the relation between the incoming and outgoing fluxes. This would mean that we are able to build up an explicit solution of the full Boltzmann equation. Therefore one has to restrict to some approximations of equation (6), for example to iteration procedures.
Let us investigate the boundary conditions for the aerodynamic region A. Given the distribution function $f(t, \overset{o}{x}, v)$ one has to construct the boundary values for ρ, u and T.
The best idea is to perform a layer analysis, i.e. to introduce a small transition layer, as shown in figure 4.2.

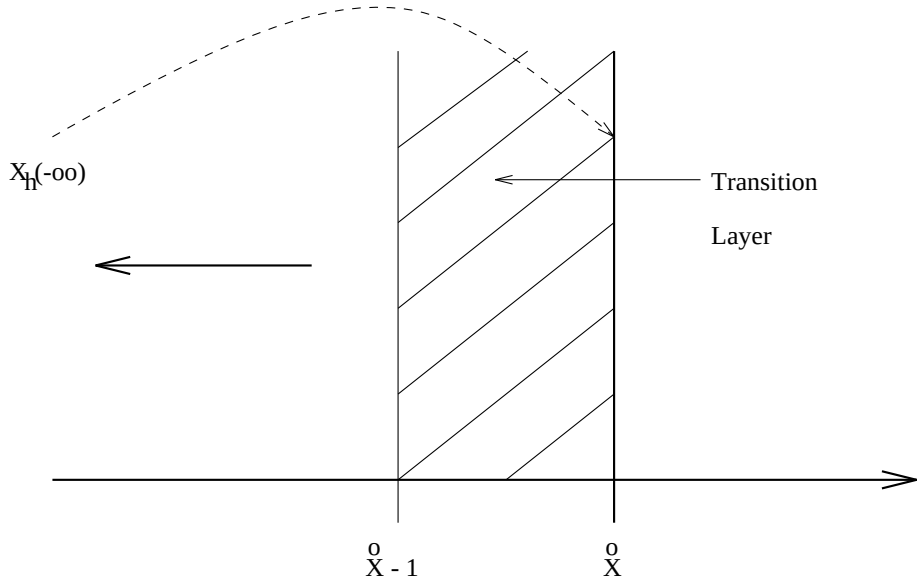

Figure 4.2: Transition layer between the two regions A and B

Using the spatial scaling

$$x \longrightarrow \frac{x - \overset{o}{x}}{\varepsilon} = \bar{x}$$

we transform the transition layer to the $\bar{x}$–intervall $(-\infty, 0]$.
Now we consider the linear kinetic equation

$$(v+u)\frac{\partial \mathcal{X}_H}{\partial x} + L\mathcal{X}_H = 0 \tag{7}$$

where the influx at $\bar{x} = 0$ is given by the flux from the kinetic region B.
We are able compute the solution $\mathcal{X}_H$ of (7) at $-\infty$ because the problem represents a linear kinetic half space problem. Hence we get the moments of $\mathcal{X}_H$ at $-\infty$. This values can be used as boundary conditions for the aerodynamic region A – simply by pulling them back to $\overset{o}{x}$.
The method gives quite good results, at least in simple testcases (see [34]).

Remark 6 The main point is to substitute the full kinetic equation inside the transition layer by a linear kinetic model. In order to use this coupling procedure it is necessary to have fast solvers for the linear half space problem defined by equation (7); this was achieved in [34] too.

Realisation of the coupling
For the description of the flow around obstacles in CFD one is typically interested only in the stationary state. Nevertheless the numerical methods work with the instationary equations and use the time parameter as an iteration index. Hence if we want to compute the coupled solution for the aerodynamic and kinetic flow region we have two possibilities to realize the coupling conditions:

1) One may use a 'Schwarz iteration', i.e. in both flow regions one calculates the stationary solution with fixed coupling conditions and iterates.

2) One tries to work with a 'direct coupling' [35], i.e. for every local time iteration the coupling conditions are updated. The main idea here is, that for free molecular flow the Albedo is trivial and that during a time step Δt we first care for the free flow before simulating the collisions.

How crucial coupling conditions are is shown by the following

Example 1 [34]
Consider the kinetic equation

$$\partial_t \phi_\varepsilon + (v+u)\partial_x \phi_\varepsilon + \frac{1}{\varepsilon}(\phi_\varepsilon - \langle \phi_\varepsilon \rangle) = 0, \quad (t,x,v) \in I\!R_+ \times [-1,1]^2$$

with

$$\langle \phi_\varepsilon \rangle = \int_{-1}^{1} \phi_\varepsilon \, \mathrm{d}v$$

and the aerodynamic equation which holds in the limit $\varepsilon \to 0$

$$\partial_t \theta + u \partial_x \theta = 0, \quad u > 0$$

Figure 4.3 illustrates the result of several coupling strategies.

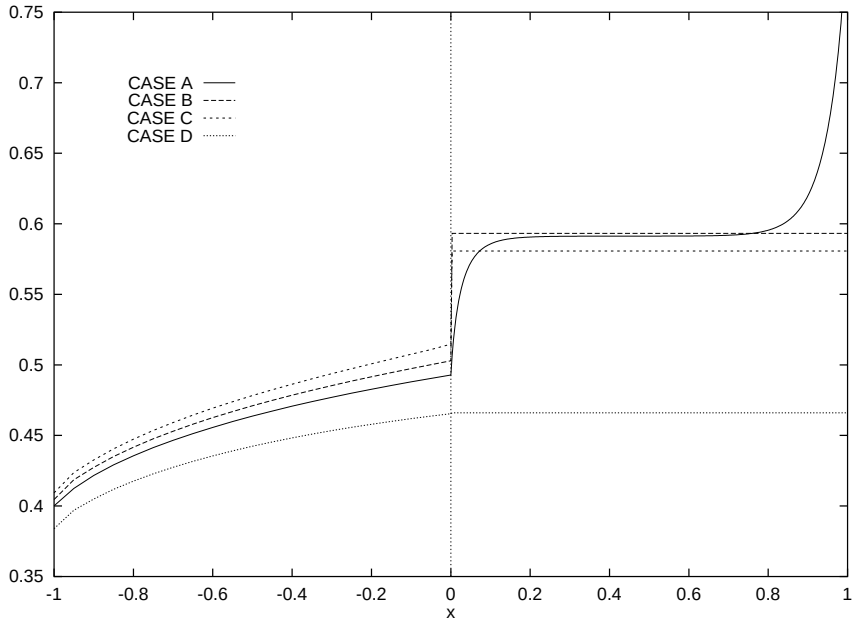

Figure 4.3: Coupling of two flow domains

Case A gives the result for the coupling of two kinetic equations with $\varepsilon = 1$ on $[-1, 0]$ and $\varepsilon = 0.01$ on $[0, 1]$. The coupling conditions at $x = 0$ are simply given by

$$\int_{-1}^{1} \phi_1 \mathrm{d}v = \int_{-1}^{1} \phi_{0.01} \mathrm{d}v$$

All other cases represent results from the coupling of the kinetic equation on $[-1, 0]$ with $\varepsilon = 1$ and the aerodynamic equation on $[0, 1]$.
Case B is the result using a layer analysis as described above. The asymptotic behaviour of $\mathcal{X}_H$ gives the boundary condition $\Theta(0, t)$ for the aerodynamic equation on the left side of the domain.
Case C presents the coupling using the fluxes at the boundary, i.e.

$$\begin{aligned} \int_{v+u>0} (v+u)\phi(t,0,v)\mathrm{d}v &= \int_{v+u>0} (v+u)\Theta(t,0)\mathrm{d}v \\ \phi|_{v+u<0} &= \Theta(t,0) \end{aligned}$$

Finally the results of case D are obtained using continuity of the zeroth moment of the coupled solution, i.e.

$$\begin{aligned} \int_{-1}^{1} \phi(t,0,v)\mathrm{d}v &= \int_{-1}^{1} \Theta(t,0)\mathrm{d}v \\ \phi|_{v+u<0} &= \Theta(t,0) \end{aligned}$$

4.3 Concluding Remark

Particle methods for solving the Boltzmann equation for real gases have become a reliable instrument to perform experiments for rarefied gases. Different approaches as DSMC or our FPM have become rather similar, but still show some differences mainly with respect to their theoretical foundation. Other new ideas as for example by Rogier and Schneider [36] or Degond [37] which differ mainly in their concept of convergence are promizing but still have to show their power in 3D real gas cases.
From a theoretical point of view there is still a gap between the best existence result for the Boltzmann equation (as presented by P.L.Lions) and our convergence results: The properties of a solution we need are not guaranteed by the existence theorem. But the fact that there is no uniqueness theorem in this context shows the difficulty which may be connected with this gap. There is much work to be done.
From a more practical point of view particle simulations are quite satisfactory. However if one wants to include more physical effects without doing to many handwaving arguments – for example ionization when very different timescales given by the collision or plasma frequency respectively become important –, one has to invent many improvements in details of the code.
Anyhow: Scientific computing has made the Boltzmann equation originally invented for the explanation of basic phenomena a tool for computer experiments which substitute without loss of reliability real experiments.

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