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COMPUTATIONAL METHODS FOR THE BOLTZMANN EQUATION

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ABSTRACT. This paper contains the basic ideas and practical aspects for numerical methods for solving the Boltzmann Equation. The main field of application considered is the reentry of a Space Shuttle in the transition from free molecular flow to continuum flow. The method used will be called Finite Pointset Method (FPM) approximating the solution by finite sets of particles in a rigorously defined way. Convergence results are cited while practical aspects of the algorithm are emphasized. Ideas for the transition to the Navier Stokes domain are shortly discussed.

1. Introduction

The determination of the flow field around a space shuttle during its reentry is one of the most challenging tasks in computational fluid dynamics. The phase of the reentry where the shuttle moves down from altitudes over 150 km to lets say 70 km is not the most critical one but determines the "initial conditions" for the following critical phase. The paper deals with this first part of the reenty, which belongs to the rarefied gas regime; this means that the gas is not dense enough in order to use the normal continuum flow equations as Navier-Stokes or Euler. The similarity parameter deciding whether this is possible or not is the Knudsen number $Kn = \lambda/L$, where λ is the mean free path and L is the characteristic length of the problem (for example the curvature radius of the shuttle nose). $Kn \gtrsim 10$ designs the free molecular flow, $0.05 \lesssim Kn \lesssim 10$ defines the transitional regime, where Navier-Stokes may and in general will give wrong results.
The first attempt to treat this region was done by Bird [5], using a "Direct Simulation Monte Carlo method" (DSMC). This method developed from 1968 on simulates the microscopic behaviour of the gas, not refering to any equation which has to be solved. DSMC was and is extremely successful, carried by a deep understanding of the physics behind. From a mathematical point of view the situation however is not satisfying, since questions about convergence or the quality of

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approximations cannot even be posed. The equation which is governing the transition regime is the Boltzmann equation, from which the continuum flow equations can be derived in considering certain singular limits Kn → 0 (see for example [7]). This quite complicated equation resisted for a long time all attempts for a rigorous numerical treatment; several steps in this direction were done by Indian, Russian and American authors, but could by far not compete in practical respects with DSMC. Nanbu [24] in 1980 proposed a new method directly related to the Boltzmann equation but again suffering from practical weaknesses. However, starting from Nanbu's idea our group in Kaiserslautern succeeded from 1986 on in treating the following problems:

(i) To clarify the basic principle of particle methods and thereby constructing a whole class of numerical schemes consistent with the Boltzmann equation (including Nanbu's algorithm);
(ii) to give rigorous convergence proofs for these schemes;
(iii) to improve the computational efficiency of these methods such that they are able to treat all the cases handled by DSMC - and hopefully even more.

We want to state clearly that we consider DSMC still to be a practicable method from which we learn a lot especially with respect to physical extensions (as including interior energy, chemical reactions etc.); moreover we believe that minor modification of DSMC can be shown to belong to the class of convergent schemes, since the basic idea could be formulated in an appropriate way.

This paper focusses on problems (i) and (iii), since (ii) was discussed in several papers by Babovsky et al. [2], [4]. We call our method "Finite Pointset Method" FPM, expressing thereby the fact that it is based on the approximation of the solution by mathematical objects depending on finitely many data - as FEM or Finite Differences do. To describe this appoximation ideas, where no Monte Carlo gambling is involved, in a way which is understandable also to the engineer is the first intention; the second is to discuss practical aspects of our FPM and the third to present some ideas for connecting it with the continuum flow domains. Extensions to polyatomic gases and chemical reactions will be presented in another paper [18].

2. The Mathematical Formulation of the Problem

Our main mathematical object we wish to solve is the Boltzmann equation; it describes the evolution of a position-velocity space density $f(t,x,v)$ with $x \in \Omega \subset \mathbb{R}^3$, Ω denoting that part of the space surrounding the shuttle, where neither the free molecular flow description nor the Navier-Stokes equations are correct. Ω may therefore change with time during the reentry but for the time being we keep it fixed and discuss domain decomposition in chapter 6.

We consider here the Boltzmann equation for a one species monatomic gas - generalization to several species of molecules including interior

energy of different kind are available but would complicate our presentation unreasonably. Chemical reactions are very important but the research we know is not very much developed in this direction. We use the notation of Cercignani (see [7], pages 57 ff), so that the Boltzmann equation may be written as

$$\frac{\partial f}{\partial t} + v\cdot\frac{\partial f}{\partial x} = \frac{1}{\varepsilon}J(f,f) \tag{1a}$$

with

$$J(f,f)(t,x,v) := \int_{\mathbb{R}^3}\left[\int_0^{2\pi}\int_0^{\pi/2} B(\theta,\|V\|)\cdot\right. \tag{1b}$$

$$\left.[f(t,x,v')f(t,x,v_1')-f(t,x,v)f(t,x,v_1)]d\theta d\phi\right]dv_1 \ ;$$

here

- $V = v-v_1$
- $v' = v-n\langle n,V\rangle$
  $v_1' = v_1'+n\langle n,V\rangle$
  and $n = (\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$
- $B(\theta,\|V\|)$ characterizes the intermolecular forces and is $\sigma^2\|V\|\cdot\sin\theta\cos\theta$ for a gas of rigid spheres of diameter σ or $\|V\|^{\frac{n-5}{n-1}}\cdot\beta(\theta)$ for an inverse power potential of type $k\|x\|^{1-n}$.
- ε is proportional to the mean free path and therefore also to the Knudsen number.

By integrating with respect to n over the hemisphere $S_+^2 = \{n/\|n\| = 1 \text{ and } \langle n,V\rangle > 0\}$ instead of $d\theta d\phi$ and by using the differential scattering cross section s one may write the inner integration as

$$\int_{S_+^2} \|V\|s(\theta,\|V\|)[...]d\omega(n)$$

with

$$s(\theta,\|V\|) = \frac{1}{\|V\|\sin\theta}\,B(\theta,\|V\|) \ .$$

Equation (1) must be supplemented by initial and boundary conditions. Concerning the initial condition the following remark seems to be necessary. There are two time scales:
Time scale 1 refers to the arrival of the shuttle at a certain part of the space, when the unperturbed atmosphere is changed suddenly to the flow field around the shuttle; time scale 2 refers to the change of the unperturbed atmosphere depending on the altitude the shuttle is just

passing. Travelling with the object we may therefore consider stationary solutions of equation (1) with slowly changing boundary conditions of the far field. However, the stationary Boltzmann equation presents a tougher problem both from a theoretical (see for a survey [22] and the papers of Ukai & Asano cited there) as well as from a numerical point of view. What one does is to solve the instationary problem with the unperturbed atmosphere as initial condition, i.e. one operates on time scale 1. During the reentry one has to adapt the initial condition to the altitude the shuttle has arrived. But one should keep in mind that one is interested in different stationary solutions, i.e. in $\lim_{t\to\infty} f(t,x,v)$ but not in the dependence of f on time. t has more the character of an iteration index and may therefore be changed in order to speed up the procedure; to do this in an optimal way is a research problem for its own.

We assume furthermore that the shuttle is at rest, but the gas around moves and we consider (1) together with $f(0,x,v) = f(x,v)$ given (including the speed of the flight, because the shuttle is at rest) and with boundary onditions.

The choice of boundary conditions is very crucial; there are many indications (see for example [27]) that the solution is much more sensitive with respect to the boundary condition than to a correct model $B(\theta,\|V\|)$ for the intermolecular forces. The boundary $\partial\Omega$ of our computational domain consists of three different parts:

(a) The boundary $\partial\Omega_1$ against the shuttle surface; here we have to model the gas-surface interaction, which creates finally the drag, lift, heat transfer, pressure on the shuttle (see again [7], chapter 3). The general shape of the condition at the surface is

$$|\langle v\cdot n\rangle f(t,x,v) = \int_{\{v':\langle v'\cdot n\rangle<0\}} R(v' \to v;x) f(t,x,v')\cdot |\langle v',n\rangle| dv' \quad \text{for } v\cdot n > 0\ , \tag{2}$$

where n is the normal to the surface at x, which points into Ω and R is the scattering kernel representing the information about the surface. It is extremely difficult to find reliable scattering kernels for two reasons:

(i) It is a very complex task to describe what happens to a particle entering the surface and interacting with the molecules in the rigid body.

(ii) There are very few experimental data available.

Mathematically simple but unrealistic is specular reflexion with
$R_S(v' \to v;x) = \delta(v-v'+2n\langle n,v'\rangle)$;
practically used in the past is diffuse reflexion with
$R_D(v' \to v;x) = f_o(x,v)|\langle v,n\rangle|$, where

$$f_o(x,v) = \frac{1}{2\pi R^2 T_o^2(x)} \exp\left[-\frac{\|v-u_o(x)\|^2}{2RT_o(x)}\right]\ ,$$

$T_o(x), u_o(x)$ denoting the temperature and the velocity of the wall at x.

Maxwell proposed a combination of these kernels, namely

$$R = \alpha R_D + (1-\alpha) R_S$$

and α is called accomodation coefficient. The solution depends very sensitively on α as one can see in figure 1 presenting the lift coefficient of a solution computed numerically with different α.

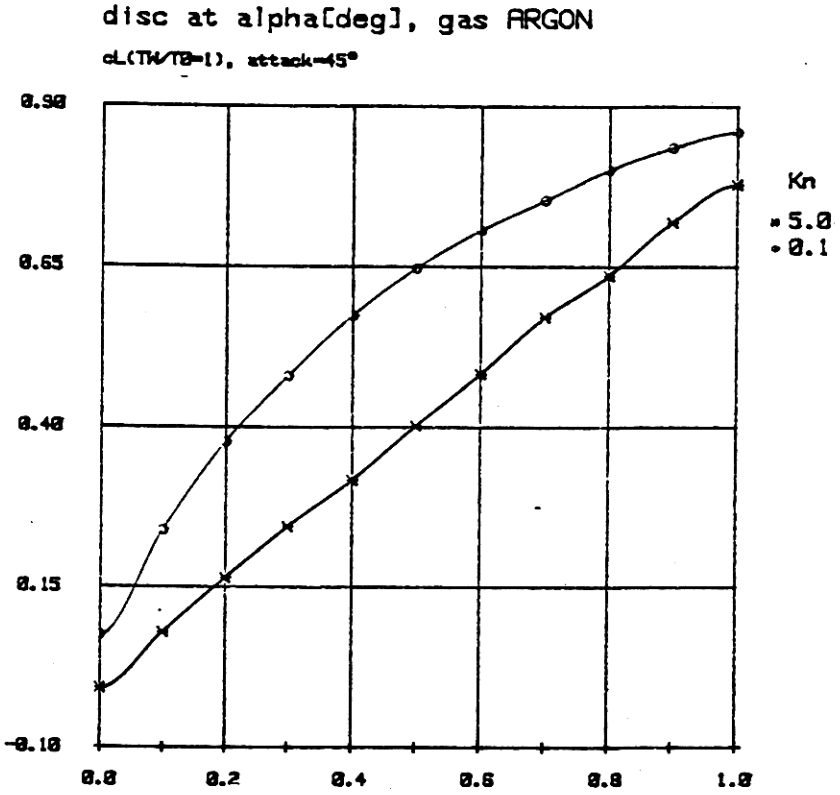

Figure 1

We have no experimental information about the best accomodation coefficient for a given surface. This fact reduces also the practical value of more elaborate models as for example that by Cercignani & Lampis (see [7']), when even two accomodation coefficients are present. However, good benchmark experiments would allow to fit the coefficients and then it is quite likely that the two coefficients in the model mentioned above could be chosen such that there is a good agreement between computation and experiment of lift, drag, heat transfer etc. (Our numerical experiments with all the boundary conditions mentioned above and with different accomodation coefficients point in this direction.)

(b) Our computational domain has to be bounded - we have to introduce an outer boundary $\partial\Omega_\infty$; its distance to the vehicle should be large enough, so that the asumption of thermodynamic equilibrium and spatial homogeneity is justified. This makes no problem in front of the shuttle - $\partial\Omega_\infty^1$ is located just in front of the shock wave. Behind the shuttle - we call this part $\partial\Omega_\infty^2$ - these asumptions are never strictly fulfilled; it is however enough that the mean velocity in the direction of the outer normal n to $\partial\Omega_\infty^2$ is supersonic. This boundary is computed during the calculation and is time dependent; at $\partial\Omega_\infty^2$ the flux into the computation domain vanishes. We therefore have for $\langle v,n\rangle < 0$, where n is the outer normal on $\partial\Omega_\infty^1$

$$f(t,x,v) = \frac{1}{2\pi R^2 T^2(t)} \exp\left[-\left(\frac{\|v-u\|^2}{2RT}\right)\right] \quad \text{at } \partial\Omega_\infty^1$$

$$= 0 \quad \text{at } \partial\Omega_\infty^2 .$$

(c) But our computational domain Ω has a third kind of boundary, the boundary $\partial\Omega_2$ against the region, where the fluid dynamic equations are valid (figure 2).

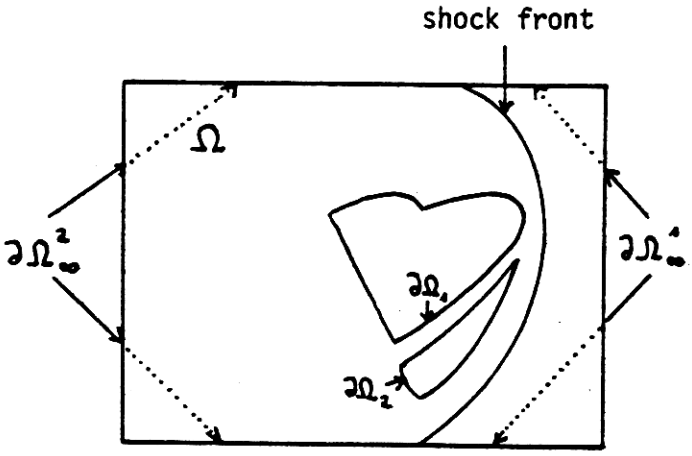

Figure 2

At this boundary the relation between the Boltzmann equation and the Euler or Navier-Stokes equations becomes important. These continuum flow equations are limits of the Boltzmann equation for small Knudsen numbers - the sense in which this limit has to be understood is crucial for our problem. In high altitudes where the Knudsen numbers are everywhere greater than 1 we are sure that the numerical solution of the Boltzmann equation is not more expensive than the solution of the Navier-Stokes or Euler equations even in regions of thermodynamic equilibrium. Further down the computational effort for the Boltzmann equation increases, but there

are still domains where the Navier-Stokes equations even with slip boundary conditions are not valid (there is still a small controversy about how "non-valid" the Navier-Stokes equations are in altitudes around 90 km, but there are experiments showing that the errors can be very significant). For Knudsen numbers smaller than 10^{-2} the Boltzmann equation becomes more expensive than Navier-Stokes and the Boltzmann regions become very small (however, the latter are never really empty - there remain kinetic boundary layers and the neighborhoods of small edges and wedges). What is really needed is a mixed flow code discovering automatically where Boltzmann, Euler and NavierStokes are valid - more precisely: Where one can get numerical simplifications from the fact that the solution is near to the Maxwell or Navier-Stokes distribution. We will discuss these questions a bit more in details in chapter 6. In our numerical treatment in chapter 3 and 4 we will neglect $\partial\Omega_2$.

We therefore shall treat the following initial boundary value problem:

$$\frac{\partial f}{\partial t} + v\cdot\frac{\partial f}{\partial x} = \frac{1}{\varepsilon}J(f,f) \tag{1}$$

$$|v\cdot n|f(t,x,v) = \int_{v'\cdot n<0} R(v'\to v;x)f(t,x,v')|v'\cdot n|dv' \text{ at } \partial\Omega_1 \tag{2}$$

$$f(t,x,v) = \frac{1}{2\pi R^2T^2(t)}\exp\left(-\frac{\|v-u\|^2}{2RT}\right) \text{ for } \langle v,n\rangle < 0 \text{ at } \partial\Omega_\infty^1$$

$$= 0 \quad \text{for } \langle v,n\rangle < 0 \text{ at } \partial\Omega_\infty^2\,, \tag{3}$$

$$f(0,x,v) = f(x,v) \tag{4}$$

(= unperturbed atmosphere depending on the altitude)

3. The basic idea of the Finite Pointset Method (FPM)

The task to solve the problem stated in section 2 numerically poses many difficult practical problems. For a 3-dimensional problem we have at least 7 variables t,x,v with a tendency to more if one includes interior energy; we have the quite complicated integral expression for J; we have finally complicated boundary conditions. Therefore there is little hope for a successful application of standard approximation methods like finite differences or finite elements. We are aware of the fact that there are nice ideas available in the direction of finite differences, ideas developed and used by several authors [29], [1], [12] - but we are also aware that they have only been applied to lower dimensional problems. Practically more successful are particle methods - particles are points with mass, position, velocity (interior energy, charge, etc.). We consider a one species monatomic gas and normalize

the total mass to 1; mass is conserved as $\int_{\mathbb{R}^3}\int_{\Omega} f(t,x,v)dxdv$ doesn't depend on t. Having N particles we may assume that each has a mass $\frac{1}{N}$, such that the i-th particle is characterized by $(x_i,v_i) \in \Omega\times\mathbb{R}^3$, i=1,...,N, i.e. by a point in $\Omega\times\mathbb{R}^3$. The collection of all N particles is therefore a finite pointset in $\Omega\times\mathbb{R}^3$

$$\omega_N := \{(x_1,v_1),\ldots,(x_N,v_N)\} .$$

We want to use finite pointsets for approximating the solution $f(t,\cdot)$ - as we use finite elements to approximate solutions of the Navier-Stokes equations. Refinement of the mesh there means enlargement of the number N here: Convergence would mean that ω_N converges to f with N tending to infinity. The only thing which has to be defined is the distance between ω_N and f - what means that ω_N is near to f?
We explain this in a simple one-dimensional situation - the extension to our situation is straightforward.

Let $\omega_N = \{x_1,\ldots,x_n\}$ be a set of points in the interval [0,1] and $f: [0,1] \to \mathbb{R}$ an integrable nonnegative function with $\int_0^1 f(x)dx = 1$. We define the discrepancy of ω_N with respect to f by

$$D(\omega_N;f) := \max_{0\le a<b\le 1} \left| \int_a^b f(x)dx - \frac{1}{N} (\text{number of points in } [a,b]) \right| \qquad (5)$$

$$= \max_{0\le a<b\le 1} \left| \int_a^b f(x)dx - \frac{1}{N} \sum_{j=1}^{N} \chi_{[a,b]}(x_j) \right|$$

where

$$\chi_M(x) = \begin{cases} 1 & \text{for } x \in M \\ 0 & \text{else .} \end{cases}$$

Discrepancy was defined by Hermann Weyl (see [28]) as a number theoretic concept and was reinvented in probability theory as Kolmogorov-Smirnov distance. It is clear that it compares the relative frequency of points in [a,b] with the "fraction of mass with distribution f in [a,b]" and considers the worst case with respect to all intervals. It is therefore the concretization of the intuitive understanding of f as a continuous particle density, but has nothing to do with any probabilistic interpretation.
The generalization to our situation is simple: If $\omega_N = \{(x_1,v_1),\ldots,(x_N,v_N)\}$ is a pointset in $\Omega\times\mathbb{R}^3$ and $f\ge 0$ integrable on $\Omega\times\mathbb{R}^3$ with integral 1, we define

$$D(\omega_N;f) = \sup_R \left| \int_R f(x,v)dxdv - \frac{1}{N} \sum_{j=1}^{N} \chi_R(x_j,v_j) \right| \qquad (5a)$$

where R denotes an arbitrary axi-parallel 6-dimensional rectangle in $\Omega\times\mathbb{R}^3$

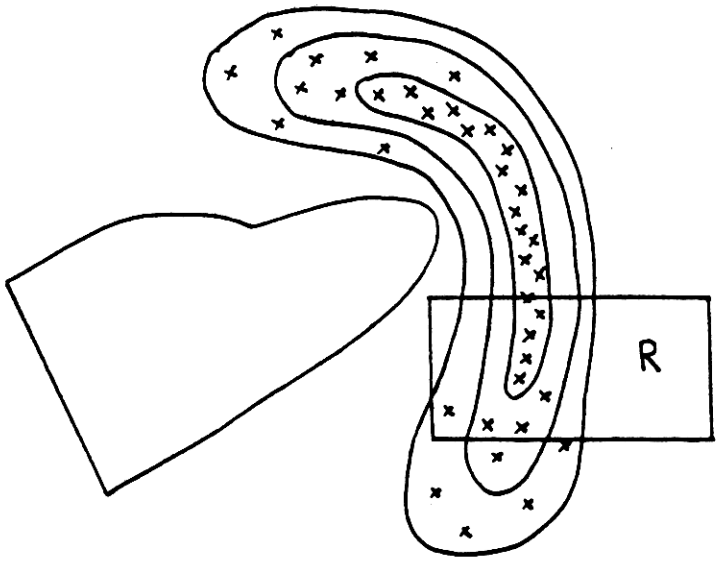

Figure 3

We mention a few consequences of the notion of discrepancy - these and a lot more useful results can be found in [19]; we used this concept for plasmaphysical computation already in 1973, see [25].

a) For every density function f there exists a sequence $(\omega_N)_{N\in\mathbb{N}}$ of finite pointsets such that $\lim_{N\to\infty} D(\omega_N,f) = 0$.

b) The possible speed of convergence is restricted by the following inequalities:

   (i) There exists a constant $A_k[f]$, depending on the dimension k (here in general k=6) and f, such that for all ω_N

$$D(\omega_N,f) \geq A_k[f] \frac{(\ln N)^{\frac{k-1}{2}}}{N} . \qquad (6a)$$

   (ii) For each f and N prime there exists a pointset ω_N and a constant $B_k[f]$, such that

$$D(\omega_N,f) \leq B_k[f] \frac{(\ln N)^k}{N} . \qquad (6b)$$

c) For k=2, $\Omega = [0,1]^2$ and f(x,v) = 1 in Ω the following construction of ω_N creates sets of "good lattice points", i.e. those, which fulfil the estimate (6b):
Let α_n be a Fibonacci-number, $\alpha_{n+2} = \alpha_n+\alpha_{n+1}$, $\alpha_1=\alpha_2=1$ and

$(x_i,v_i) = \left(\frac{(i-1)\alpha_{n-1}}{\alpha_n} \bmod 1\right)$, $1 \le i \le \alpha_n = N$; then $D(\omega_N,f) = \frac{7}{6N}\ln(6N)+\frac{1}{N}$, i.e. ω_N is a set of good lattice points.

d) Let $\phi: \Omega\times\mathbb{R}^3 \to \mathbb{R}$ be of bounded variation $V[\phi]$ ("in the sense of Hardy and Krause" - see for example [15]), then

$$\left| \int_{\Omega\times\mathbb{R}^3} \phi\cdot f \, dxdv - \frac{1}{N}\sum_{j=1}^{N} \phi(x_j,v_j) \right| \le V[\phi]D(\omega_N,f)$$

(this is the socalled Koksma-Hlavka inequality).

One may conclude from the points (a)-(d) that
- every density f can be approximated arbitrarily well by finite pointsets,
- the quality of approximation is rather slowly increasing with N, but also rather slowly increasing with the dimension k,
- the problem of constructing good approximations asks for quite tricky methods borrowed from number theory,
- the expectation values of functions ϕ with respect to the density f are approximated by the averages of ϕ over ω_N with an accuracy given by $D(\omega_N,f)$.

This explains, why FPM (or particle methods) are appropriate for problems, where the solution is a density depending on many variables (high k) and where one is mainly interested in functionals (moments, expectation values) of the solution.

We are now able to formulate the general concept of a FPM:

(1) Given the initial value $\overset{o}{f}$, find a good approximation by a finite pointset $\overset{o}{\omega}_N = \left\{(\overset{o}{x}_1,\overset{o}{v}_1),\ldots,(\overset{o}{x}_N,\overset{o}{v}_N)\right\}$.

(2) Find a time evolution of the points

$$t \to \omega_N(t) = \left\{(x_1(t),v_1(t)),\ldots,(x_N(t),v_N(t))\right\}$$

with $\omega_N(0) = \overset{o}{\omega}$ such that $\omega_N(t)$ is a good approximation of $f(t,\cdot)$, the solution of the Boltzmann equation at time t.

One may express this concept also by saying that one has to find an algorithm constructing for each N a $\overset{o}{\omega}_N$ such that $D(\overset{o}{\omega}_N,\overset{o}{f}) \to 0$ and one has to find an evolution $\omega_N(t)$ such that $D(\omega_N(t),f(t)) \to 0$ for $0 \le t \le T$.

4. The time-space discretized Boltzmann equation

As explained above we have to solve two problems, the initialization and the evolution. The first one is relatively easy, the second one quite complicated.

(1) Given $\overset{o}{f}$, construct $\overset{o}{\omega}_N$ such that $D(\overset{o}{f},\overset{o}{\omega}_N)$ is small. We would like to say: is as small as possible. This defines a min max problem: Given

f and N construct

$$\min_{\omega_N} \max_{R} \left| \int_R \overset{o}{f}\, dxdv - \frac{1}{N} \sum_{i=1}^{N} \chi_R(x_i, v_i) \right| .$$

We are aware of some attempts to attack the "inner" maximization problem, which can be reduced to a problem of combinatorial optimization - but we know until now nothing about the full problem. However we believe that a solution is crucial - we do not need algorithms which converge quickly with N tending to infinity, but give good results for given, relatively small N. What one can do practically today is the following:
One constructs first a pointset $\tilde{\omega}_N$ approximating the equidistribution with f(P) = 1 for P in the k-dimensional (k=6) unit cube. We mentioned one method in 3c for k=2. In the general case we use the following approximation procedure for the initial distribution $\overset{o}{f}$ for the initial distribution f: The spatial domain gets a rectangular grid structure at the beginning of the simulation procedure (this grid structure arises from the space discretization of the Boltzmann equation, which is explained in details later in this chapter). Now we approximate $\overset{o}{f}$ in each cell of the grid separately - one has to realize that $\overset{o}{f}$ is spatially homogeneous. The positions of the particles are simply equidistantly distributed over the whole spatial domain. This leads to a particle number N_c in each cell, which is nearly proportional to the cell size. The velocity distribution in each cell is approximated by using the modified Hammersley sequence in the 3-dimensional unit cube $[0,1]^3$, given by $(\frac{2i-1}{2N_c}, \Phi_2(i), \Phi_3(i))$, where Φ_2 and Φ_3 are the van-der-Corput sequences for the primes 2 and 3 [19]. The transformation from $[0,1]^3$ to the velocity domain $\mathbb{R}^3$ then mainly contains a transformation to spherical coordinates and the calculation of the inverse of the error function [3].

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt .$$

The modified Hammersley sequence leads - even for small particle numbers - to a good approximation of the moments of $\overset{o}{f}$, especially of the temperature.
We mention that another solution consists in just using random number generators. However, a good set of random number has to care for more than just for approximating the equidistribution. Since we consider this aspect to be important, we want to explain it shortly for the simple 1-dimensional case. What does it mean that a finite pointset $\omega_N=\{x_1,\ldots,x_N\}$ is approximately uniformly distributed in [0,1]? First we want to have the discrepancy $D(\omega_N, \chi_{[0,1]})$ to be small. In this sense the set $\left\{\frac{1}{2N}, \frac{3}{2N}, \ldots, \frac{2N-1}{2N}\right\}$ is best - its discrepancy is optimal $\frac{1}{N}$. This set would not be considered to be a

good choice for pseudorandom numbers. Why? As a sequence with this ordering these numbers are too much correlated. A simple expression for this is: Take the set $\omega_N^{(2)}$ of points in the unit square defined as pairs of subsequent members of the sequence, i.e.

$$\omega_N^{(2)} := \left\{\left(\frac{1}{2N},\frac{3}{2N}\right),\left(\frac{3}{2N},\frac{5}{2N}\right),\ldots,\left(\frac{2N-3}{N},\frac{2N-1}{N}\right)\right\} ,$$

then $D\left(\omega_N^{(2)},\chi_{[0,1]^2}\right)$ is extremely bad, always larger than $\frac{1}{4}$, since the points are all very near to the diagonal. Therefore a set created by a good pseudorandom generator should have the property that $D\left(\omega_N^{(2)},\chi_{[0,1]^2}\right)$ is small. We may continue in considering tripels, general k-tupels of subsequent numbers in ω_N to get $\omega_N^{(k)} = \left\{(x_1,\ldots,x_k),(x_2,\ldots,x_{k+1}),\ldots,(x_{N-k+1},\ldots,x_N)\right\} \subset [0,1]^k$ and compare it with the uniform distribution in the unit cube $[0,1]^k$. We say that ω_N is a k-fold approximation of $\chi_{[0,1]}$, if

$$D\left(\omega_N^{(j)},\chi_{[0,1]^j}\right) \longrightarrow 0 \quad \text{for } N \to \infty,\ 1\leq j\leq k .$$

A "real" random number generator would produce a sequence $(x_n)_{n\in\mathbb{N}}$ such that $\omega_N = \{x_1,\ldots,x_N\}$ would be a k-fold approximation for any k. A pseudorandom number generator has at least a $k\geq 2$. But what do we need for our simulation? It depends on the problem and we have to make a careful analysis to answer this question. What we want is that the final result of the simulation approximates the solution as good as possible - in the sense of discrepancy. In order to achieve this goal we have to find an approximation of some data as the initial value or the collision process - and only a convergence analysis can tell us, whether these approximations have to be simple, double or k-fold with $k\geq 3$. This convergence analysis is given in [4] and it tells us that there is no reason to approximate the initial value better than simple. This means that we would loose approximation quality in using pseudorandom generators without gaining anything. The situation is different for the simulation of collisions as we shall soon see.

A warning might be necessary: In using the same deterministic set of low discrepancy again and again in a simulation procedure, one makes small errors in each step but the errors may have always the same sign and therefore may accumulate, meanwhile using a worse but always different set of pseudorandom numbers may lead to a cancellation of errors. Being aware of such systematic errors makes it easy to avoid them - we shall discuss such a problem in connection with treating the boundary condition ("numerical freezing").

(2) Our main task is to find a time evolution $\omega_N(t)$ of our pointset. We have N particles each of mass $\frac{1}{N}$ at position $x_1,\ldots,x_N$ and with velocities $v_1,\ldots,v_N$. How should we move them? The first idea may be: As nature, i.e. as billiard balls if we have a rigid sphere model. Would this fulfil our condition, would it converge? Would $\omega_N(t)$ corresponding to our billiard game converge to the solution of the Boltzmann equation f(t), if $\omega_N(0)$ tends to f? This question is not a numerical one - it is the question whether the Boltzmann equation can be derived from classical mechanics as a limit $N\to\infty$. It is therefore a very old and fundamental question - and its answer today is a weak "yes". It is the result by O.E. Landford [20], improved by Illner and Pulvirenti [16]; it is a "weak" yes, since it holds only with probability one and for a very short time (one may also look at [7], pages 40-57). Since nature cannot be imitated even by the best supercomputer (even if we consider only 10^5 particles, it would be impossible to follow the fate of each individual particle), we have to give up our first idea and must invent an artificial evolution simpler to handle but with the same effect: to remain near to the solution of the Boltzmann equation. This evolution will proceed in discrete time steps and will depend on a grid in position space; it will therefore not approximate the solution of the original Boltzmann equation but one of the time and space discretized Boltzmann equation. Babovsky and Illner showed in [4] that under certain conditions we can come as near as we like to a solution of this discretized equation - by increasing N; and we can make the difference of this solution to the "real one" as little as we like - by making the time step and the grid size smaller.

a) The time discretization of the Boltzmann equation is easy: One discretizes t by considering only $j\Delta t$, $j=0,1,2,\ldots$ and approximates (we consider only the first time step)

$$\frac{\partial f}{\partial t}+v\frac{\partial f}{\partial x}\Big/_{t=0} = \frac{\partial}{\partial t}f(t,x+vt,v)\Big/_{t=0}$$

by

$$\frac{1}{\Delta t}\Big[f(\Delta t,x+v\Delta t,v)-f(0,x,v)\Big] .$$

If $x+vt$ reaches the boundary $\partial\Omega$ during $0\le t\le\Delta t$, we have to include the boundary condition. We will not write down how this can be done exactly; $x+v\Delta t$ must be substituted by the position of a particle which hit the surface and was reflected according to a law consistent with (2). We will describe this in more details in the next chapter. The step size Δt has to be chosen such that we have in average less than one collision per particle during Δt - we shall see the mathematical reason for this also in the next chapter. We have to reach the stationary limit $t\to\infty$, which we discover by the fact that f is nowhere changing during one timestep. In practical applications it took between 100 and 150 timesteps to reach the stationary state neglecting fluctuations.

Physically the time $T = \Delta t \cdot$ number of timesteps can be interpreted as the relaxation time of an equilibrium gas suddenly perturbed by the reentry object. To obtain useful results we of course have to do some time averaging in order to avoid fluctuations of the numerical scheme. The size of these fluctuations is strongly depending on the choice of the random numbers, especially on those which we use to simulate the boundary condition at $\partial\Omega_\infty$. Low discrepancy sequences allow a quite precise approximation of the outer boundary condition with very small fluctuations. We obtain optimal condition with a time-averaging over only 20 to 30 timesteps. We have to emphasize that we do not average over several independent runs. This of course reduces the computation time drastically.

b) The space discretization means that we divide Ω into cells and approximate $x \to f(t,x,v)$ by a function $\tilde{f}(t,x,v)$, which is constant in each cell

$$\tilde{f}(t,x,v) \approx f_c(t,v) \qquad \text{for } x \in \text{Cell } c \ .$$

This is quite a rough approximation of f as a function of x by step functions; however we have not yet another idea since we need cellwise homogeneity for treating the collision term. It is crucial that the collision operator doesn't "work on the variable x", but only on v. x is involved in $\frac{\partial f}{\partial x}$ on the right hand side which we have already taken into account by the time discretization; otherwise it plays only the role of a parameter. For

$$\tilde{f}(t,x,v) = \sum_{\text{Cell } c} f_c(t,v)\chi_c(x)$$

we now construct the time-space discretized Boltzmann evolution (we again write only the first time step).
We may be tempted to write

$$\tilde{f}(\Delta t,x,v) = \tilde{f}(0,x-v\Delta t,v) + \frac{\Delta t}{\varepsilon} J(\tilde{f},\tilde{f})$$

but we have to realize that $\tilde{f}(0,x-v\Delta t,v)$ is not a step function on the cell grid and we have to decide what we really mean by $J(\tilde{f},\tilde{f})$.
In order to get a correct step function, we should do a coarse graining i.e. smear out the function $f(0,x-v\Delta t,v)$ over a cell. Precisely, we have to substitute $\tilde{f}(0,x-v\Delta t,v)$ by the step function

$$(P\tilde{f})(x,v) := \frac{\int_c \tilde{f}(0,x-v\Delta t,v)dx}{\text{volume of } c} \qquad \text{for } x \in \text{Cell } c \ .$$

The operator $P\tilde{f}$ can be interpreted as the projection of $\tilde{f}(0,x,v)$ on the space of all step functions (or even as conditional expectation of f with respect to the algebra of cells).

$J(\tilde{f},\tilde{f})$ must as well be a step function. We may choose the argument f of J to be just $\tilde{f}(0,x,v)$, which is a step function and - since J doesn't work on x - remains it after application of J. This corresponds to a simple Euler step for the integration of

$$\frac{\partial f(t,x+vt,v)}{\partial t} = J(f,f)(x,vt,v) \ .$$

It seems to be better (but there is no rigorous proof for it) to interprete $\tilde{f}$ in $J(\tilde{f},\tilde{f})$ as $P\tilde{f}$.
We get then, writing Jg instead of J(g,g)

$$\tilde{f}(\Delta t,x,v) = (1+\frac{\Delta t}{\varepsilon}J)(P\tilde{f})(x,v) \ . \qquad (7)$$

This is consistent with the convergence proof in [4] and means that we have two fractional steps, one consisting in free flow (including boundary effects) plus coarse graining, the other one treating the collisions.
We should mention that DSMC follows a different strategy in mixing free flow and collisions during a time step Δt by the socalled time counter procedure. It might give better approximations (at least, if this procedure is really consistent with the Boltzmann equation which is not clear), but it makes the algorithm less easy vectorizable - a quite important aspect for supercomputers.
We see, moreover, that this equation combines various cells, since in general $x-v\Delta t$ is not in the same cell as x. This gives rise to a computational restriction with respect to our cell grid: We will have to move particles through the grid and have to refind them after a motion very quickly, i.e. we need fast algorithms to determine in which cell a particle is. This problem is by far easier to solve for a coordinate grid, where the cells are axiparallel "rectangles". We therefore avoid a complicated shape of the cells and prefer to diminuish the cell size in regions of steep gradients. An adaptive grid structure has been developed where the adaption is done during the time evolution of $\omega_N(t)$ with respect to the flow properties. This method runs as follows: Due to the fact that the initial distribution is a global Maxwellian we can start with a rather coarse grid with cell diameters of several mean free paths. During the evolution process the grid has to be refined to cell sizes of about one mean free path in critical regions (shock, boundary layer etc.). In the cells the distribution function is supposed to be homogeneous in space. We can fulfil this requirement by observing the following inequality which arises during the proof of convergence of the algorithm [4]:

$$\sup|f(t,x+\Delta x,v)-f(t,x,v)| \exp(v^2) \leq B\cdot\Delta x$$

for some $B>0$ and all "cell sizes" Δx.
Transferring this to our finite pointset

$$\omega_N = \left\{(x_1,v_1),\ldots,(x_N,v_N)\right\} \subset \bigcup \omega_{N_c} ,$$

this requires a refinement of the grid in the following way: Choose B such that the criterion is just fulfilled for cells with a Maxwellian distribution. Then divide each cell c into parts A_i^c, $i=1,\ldots,s$, of equal size and the velocity domain filled by particles (this domain has finite volume) into equally sized subsets W_j, $j=1,\ldots,\ell$.
Then compute

$$\delta_c = \max_{\substack{i,k\in\{1,\ldots,s\}\\ j=\{1,\ldots,\ell\}}} \frac{e^{\bar{v}_j^2}}{N_c \Delta x_{i,k}} \Big| \left(\text{number of points with } x \in A_i^c, v \in W_j\right) - \left(\text{number of points with } x \in A_k^c, v \in W_j\right) \Big|$$

where $\bar{v}_j^2$ is the mean velocity square in W_j and $\Delta x_{i,k}$ is the distance of the centers of the subcells A_i^c and A_k^c.

Finally check, whether $\delta_c \leq B$. If yes, no refinement is necessary, otherwise a further subdivision is necessary. This procedure gives a good grid adaption near the boundary and within the shocks. The generation of the refined grid, however, is rather time consuming, because it is not well vectorizable. One therefore should restrict the refinement procedure to every tenth time step and keep the grid fixed in between. Experience shows that this doesn't influence the results of the computation.

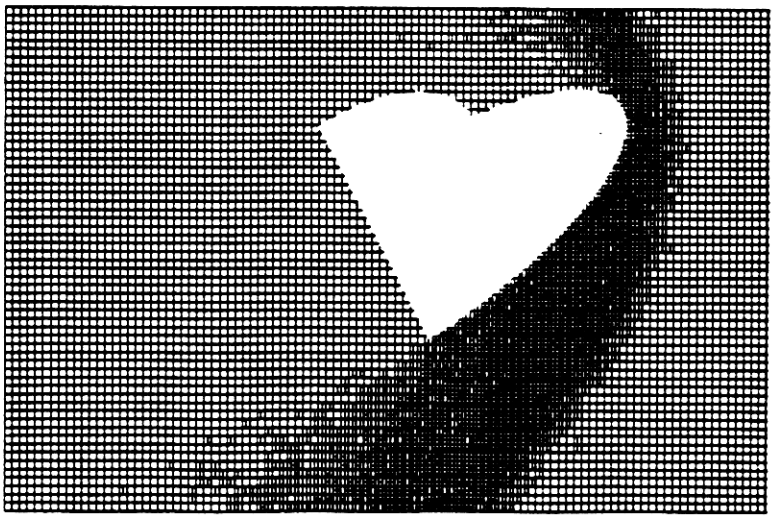

Figure 4

5. THE FINITE POINTSET METHOD FOR TIME-SPACE DISCRETIZED BOLTZMANN EQUATIONS

We know how to initialize, i.e. how to construct

$$\omega_N(0) \longrightarrow \tilde{f}(0) = f(0) = \overset{o}{f} .$$

We have to construct a one-step evolution $T_{\Delta t}$ for $\omega_N(0)$, such that $\omega_N(\Delta t) = T_{\Delta t}\omega_N(0)$ converges with $N\to\infty$ to $\tilde{f}(\Delta t)$, the solution of (7). The time evolution $\tilde{f}(0) \to \tilde{f}(\Delta t)$ given by (7) consists of two components: The free flow $x\to x-v\Delta t$ including boundary conditions and the coarse graining P - and $1+\frac{\Delta t}{\varepsilon}\cdot J$. We do the same for $T_{\Delta t}$: It consists first of free flow and then of collisions.

a) The free flow $\omega_N(0) \longrightarrow \hat{\omega}_N(\Delta t)$. Here we have to approximate $\tilde{Pf}(x,v)$ by $\hat{\omega}_N(\Delta t)$, when $\omega_N(0)$ approximates $f(0)$. $\hat{\omega}_N$ is just given by "simulating nature": We move the points of $\omega_N(0)$ freely with their velocities over Δt; if they hit the boundary we simulate again nature. That is

$$\hat{\omega}_N(\Delta t) = \left\{(x_1+v_1\Delta t, v_1), \ldots, (x_N+v_N\Delta t, v_N)\right\}$$

if no particle hits $\partial\Omega$. If particle j hits the boundary, i.e. if there is a τ with $0\le\tau\le\Delta t$, such that $x_j+v_j\tau \in \partial\Omega$, then v_j is changed according to the scattering law we discussed with boundary condition (2). If we have specular reflection, i.e. $R=R_S$, then v_j is changed into $v_j'=v_j-2n\langle n,v_j\rangle$, where n is the normal vector to $\partial\Omega$ at $x_j+v_j\tau$. With this new velocity the free flow continues until Δt is over: We get

$$x_j+v_j\tau+(\Delta t-\tau)v_j' .$$

All deterministic boundary conditions (where R has a δ-behaviour) can be treated similarly. If we have complete accomodation, we have to take a v_j' according to the distribution $f_o(v)$, the half-space Maxwellian with the temperature of the wall; in each boundary cell, quite many particles, say the subset ω_M, will hit the wall and we only have to care that $D(f_o,\omega_M)$ is small. This can be done again in a more systematic way or with help of a pseudorandom generator [3]. However, the systematic error mentioned in chapter III may become significant - we call this effect, which was studied in [23], numerical freezing". This effect arises by using uniform distributed sequences like the van der Corput-Halton or the Hammersley sequence for the generation of the outgoing velocities. It can be shown that the approximation of the energy flux from the boundary into the computational domain is always below the exact value.
This error, indeed small in a single time step, sums up during the computation and leads finally to a significant error of the energy in the whole region. This trend can be avoided by constructing sequences, which, in an oscillating way, approach the true value

from above and below; this can be easily done without changing the discrepancy.

We have also studied the Cercignani-Lampis model and construct a random number generator for the corresponding distribution:
The scattering kernel $R(v' \to v)$ of the Cercignani-Lampis model is given by

$$R(v' \to v) = |v \cdot n| f_o(v) H(v,v').$$

Here $f_o(v) = \frac{1}{2\pi R^2 T_o^2} \exp\left(-\frac{\|v\|^2}{2RT_o}\right)$ with wall temperature T_o,

$$H(v,v') = \frac{1}{\alpha_n \alpha_t (2-\alpha_t)} I_o\left(\frac{2\sqrt{1-\alpha_n}}{\alpha_n} v_n v_n'\right) \cdot$$

$$\cdot \exp\left\{-\frac{1-\alpha_n}{\alpha_n}(v_n^2+v_n'^2) - \frac{(1-\alpha_t)^2}{\alpha_t(2-\alpha_t)}(v_t^2+v_t'^2) + \right.$$

$$\left. + \frac{2(1-\alpha_t)}{\alpha_t(2-\alpha_t)} v_t' \cdot v_t\right\},$$

where $\begin{cases} v_n = (v \cdot n) \cdot n \\ v_t = (v \cdot t) \cdot t \end{cases}$ (c normal vector, t tangential vector with respect to the wall) and I_o denotes the modified Bessel function of first kind and zeroth order.
This scattering kernel can be separated into the normal and tangential components of v

$$R(v' \to v) = R_1(v_n' \to v_n) R_2(v_t' \to v_t),$$

with the corresponding accomodation coefficients α_n and α_t. The outgoing velocity v_t can be calculated by the simple formula

$$v_t^{(1)} = (1-\alpha_t) v_t'^{(1)} - \left\{-\alpha_t(2-\alpha_t)\ln(1-v_1)\right\}^{1/2} \cos(2\pi v_2)$$

$$v_t^{(2)} = (1-\alpha_t) v_t'^{(2)} - \left\{-\alpha_t(2-\alpha_t)\ln(1-v_1)\right\}^{1/2} \sin(2\pi v_2)$$

where (v_1, v_2) is a random point in the square $[0,1]^2$.

The calculation of v_n is much more complicated: The distribution of v_n is given by a socalled Polya-Aeppli-distribution. The algorithm for the generation of v_n we use can be found in [19].

After having moved all particles with their velocities we have to "refind" them, precisely: We have to know the particles contained in each cell after the motion; this is a simple task for a coordinate grid but costs much computing time for a usual finite volume grid - a

little problem if we want to connect our code with a usual Navier-Stokes code.

b) The collisions.
We were left with N_c particles in cell c - for each cell. This is an approximation for $Pf(x,v)$, a step function constant in each cell. It remains to approximate $(1+\frac{\Delta t}{\varepsilon}J)\tilde{Pf}$. Again, x is only a parameter for J, i.e. the cells can be treated independently. Take an arbitrary cell c, Pf restricted to c is a function f_c of v alone - approximated by the pointset $\{v_1,\dots,v_{N_c}\}$ of the velocities of the N_c particles in c. The positions of these particles may be forgotten until a new time step with a new free flow. (7) is now

$$f_c(\Delta t,v) = (1+\tfrac{\Delta t}{\varepsilon})J(f_c,f_c)(0,v)$$

i.e. nothing else but the time discretized <u>spatially homogeneous</u> Boltzmann equation.
Since particles are now only "velocity particles" without any position, a "natural game" simulating collisions is not possible. But still there must be some interaction between the particles - the quadratic term J makes it necessary. A collision is an interaction of two particles, which results in new velocities of both collision partners. But which pair of particles will interact?
The solution can be found in considering matchmaking procedures in some societies: Meanwhile in our society everybody finds his partner for a marriage by really meeting him/her somewhere (i.e. by moving around and "colliding" with him/her), there are some other societies with organized matchmaking - a marriage brooker selects the couples (there are no local effects, at least if our cells are not too big).

The two methods are completely different on a microscopic level but may give the same result from an economical or demographical point of view. This is what we need: A matchmaker which gives (with much less particles) the same macroscopic results as nature. In order to understand this matchmaker condition we rewrite the spatially homogeneous Boltzmann equation in a way, which was found by H. Babovsky [2]. For theoretical reasons we have to assume that

$$\int_{S^2_+} \|v\| s(\theta,\|v\|)d\omega(n) := \alpha(\|v\|) \le A \ . \qquad (8)$$

Without this assumption things could go wrong since it would be possible that $f_c(\Delta t,v)$ becomes negative - remind that (7) is with $V=v-v_1$

$$f_c(\Delta t,v) = \Big(1 - \frac{\Delta t}{\varepsilon}\int_{\mathbb{R}^3}\alpha(\|V\|)f_c(v_1)dv_1\Big)f_c(v)$$

$$+ \frac{\Delta t}{\varepsilon}\int_{\mathbb{R}^3}\int_{S^2_+}\|V\|s(\theta,\|V\|)f_c(v')f_c(v_1')d\omega(n)dv_1$$

so that (8) guarantees posivitity of $f_c(\Delta t)$ i f $\Delta t < \frac{\varepsilon}{A}$ (coming down during the reenty forces Δt has to become smaller). This condition (8) is not a trivial one - for rigid spheres, $\alpha(\|V\|)$ is proportional to $\|V\|$ and therefore not at all bounded. Practically the situation is not as bad: A is proportional to $\|V\|$ and if there is a bound for the relative velocity of two colliding particles, A remains bounded. But one has to be careful even practically: If the relative speed of many pairs of particles is rather high, Δt must be very small.

We really need $\frac{\Delta t}{\varepsilon} \cdot \alpha(\|V\|) < 1$ for all particles in our cell c. Now we define a function $\Phi_{v,v_1}(y)$ on a circle κ of radius $\frac{1}{\sqrt{\pi}}$ in the plane, i.e. for $0 \leq \|y\| \leq \frac{1}{\sqrt{\pi}}$, $0 \leq \alpha \leq 2\pi$, which depends on v and v_1 and which decides whether the particles with velocities v and v_1 collide at all and if, what will be the impact parameter n of the collision. One has to realize that these impact parameter vectors n have a certain distribution (depending on $\|V\|$, if one has not the special case of rigid spheres) given by the differential cross section s; s is the density of deflection n on the unit hemisphere S^2_+ after a collision of v with v_1. Our function Φ_{v,v_1} has essentially the task to transform the uniform distribution on our circle κ into this distribution of n on S^2_+.
$\Phi_{v,v_1}(y)$ is constructed in the following way: Let us define a radius r_o by

$$\pi r_o^2 = \frac{\Delta t}{\varepsilon} \alpha(\|V\|) < 1$$

i.e. $r_o < \frac{1}{\sqrt{\pi}}$ such that the circle $r \leq r_o$ lies in κ. r_o depends on $\|V\|$. For $r_o < r < \frac{1}{\sqrt{\pi}}$, $\Phi_{v,v_1}(r \cos \alpha, r \sin \alpha)$ is defined to be that n which means no (or better a grazing) collision $\theta = \frac{\pi}{2}-$, $\phi = \alpha$. The probability that a random number generator for uniform distribution in κ produces a point in the ring $r_o < r < \frac{1}{\sqrt{\pi}}$ is equal to the probability that the two particles with velocity v and v_1 respectively do not collide at all during Δt.
For $0 \leq r \leq r_o$ a collision will happen and we have to define $\Phi_{v,v_1}(r \cos \alpha, r \sin \alpha) = n = (\theta, \phi)$. Again $\phi = \alpha$, meanwhile $\theta = \theta(r)$ (not depending on ϕ) is given as the inverse of the function $r(\theta)$ defined by

$$r^2(\theta) = \frac{2\Delta t}{\varepsilon} \int_0^{\theta} B(\phi, \|V\|) d\phi$$

(since $B \geq 0$, r is strictly monotone and the inverse exists).

One realizes that

$$r^2(\frac{\pi}{2}) = \frac{\Delta t}{\varepsilon} \int_0^{\pi/2} B(\phi, \|V\|)d\phi$$

$$= \frac{2\Delta t}{2\pi\varepsilon} \int_{S^2_+} \|V\| s(\theta, \|V\|)dn$$

$$= \frac{\Delta t}{\varepsilon\pi} \alpha(\|V\|) = r_o^2$$

It is shown in [2] that $n=\Phi_{v,v_1}(y)$ has the correct distribution given by B if y is uniformly distributed on κ. With $n=\Phi_{v,v_1}(y)$ we have immediately the result of the collision of v,v_1:

$$v' = v-n\langle n,V\rangle,\ v_1' = v_1+n\langle n,V\rangle\ .$$

One realizes that $v'=v$, $v_1'=v_1$ in case of $r>r_o$ (then $\theta=\frac{\pi}{2}$ and since θ is the polar angle against V, n is orthogonal to V). In general, v' and v' are now functions of v, v_1 and y through $n = \Phi_{v,v_1}(y)$.
Φ depends on $\|V\| = \|v-v_1\|$ and naturally on B - its values as a function of $\|V\|$ can be computed and stored for each gas at the beginning of a run.
Our equation (7) can now be written as follows:
For every set in the velocity space, for example for every "rectangle" R in $\mathbb{R}^3$ the equation

$$\int_R f_c(\Delta t,v)dv = \int_{(v,v_1,y):v'\in R} f_c(v)f_c(v_1)dvdv_1dy \qquad (7a)$$

must hold. The left hand side just gives the mass of the gas in cell c with velocity in R; the right hand side means: integrate over those v, v_1, y which guarantee that

$$v' = v-\Phi_{v,v_1}(y)\cdot\langle\Phi_{v,v_1}(y),v-v_1\rangle$$

is in R. This integration set is a subset of $\mathbb{R}^3\times\mathbb{R}^3\times\kappa$. (7a) is a weak formulation of (7), and it leads immediately to the rule for our brooker.
What he has to do is to choose out of N_c^2 possible collision pairs (we accept that our "daily life" picture goes wrong now: We allow a particle to become a partner of itself - and we don't have two classes as males and females!) precisely N_c pairs and to assign to each an impact parameter $y \in \kappa$ (if $|y| > r_o$, the collision partners do not really collide).
The crucial thing is now that in order to get convergence this assignment $v_i \to v_{j(i)}$, $y_i \in \kappa$, $i=1,\ldots,N_c$ has to be made in such a

way that the 8-dimensional finite pointset

$$\Omega_{N_c} := \left\{(v_1, v_{j(1)}, y_1), \ldots, (v_{N_c}, v_{j(N_c)}, y_{N_c})\right\}$$

is as near as possible (in the sense of discrepancy) to $f_c(v)f_c(v_1)\chi_\kappa(y)$, where $\chi_\kappa(y)$ is again the uniform distribution in κ; more precisely we have to make sure that

$$D(\Omega_{N_c}, f_c(v)f_c(v_1)\chi_\kappa(y)) \to 0 \quad \text{for} \quad N_c \to \infty.$$

One must be a bit careful here: $f_c(v)f_c(v_1)\chi_\kappa(y)$ is not normalized to 1 but has a total mass of $(\int f(v)dv)^2 \cdot 1$ - one has to use the normalized version of this function in the definition of D.
Theoretically everything is clear: Each procedure selecting Ω_{N_c} according to this condition will converge (see again [2]).

But how do we select $v_{j(i)}$ and y_i practically? y is just uniformly distributed on κ - we may therefore use a random number generator for getting a sample of N_c points in κ; we may also use a deterministic method to construct $y_1, \ldots, y_{N_c}$ such that $D\left(\left\{y_1, \ldots, y_N\right\}, \chi_{\kappa_c}(y)\right)$ is as small as possible - but should permutate this selection in every time step to avoid systematic errors. The problem of selecting $v_{j(i)}$ may become more clear by just looking at a one-dimensional case (figure 5).

Selection of N points from N^2 points
a) Monte Carlo

Selection of N points from N^2 points
b) Low Discrepancy

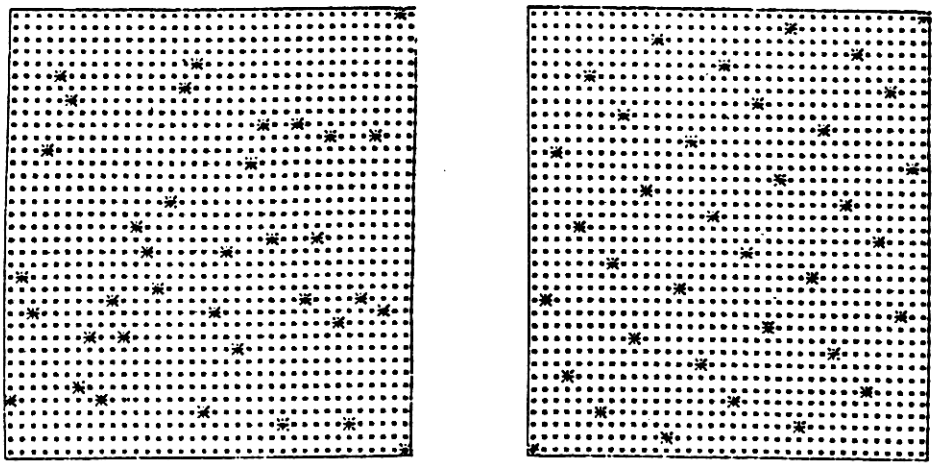

Figure 5

We consider the (v,w)-plane, have a set $\omega_N = \{v_1,\ldots,v_N\}$ on the v-axis near to f(v) and the same set on the w-axis near to f(w). The dots in the plane indicate possible collision pairs. Out of them we have to select N "crosses", such that the set of N crosses is near to the product f(v)f(w).
In the terminology of chapter 4 this means: Can we give to ω_N such an order, that $\omega_N^{(2)}$, the set of pairs is near to $f(v)\cdot f(\omega)$, i.e. that ω_N with this order is a double approximation of f. Therefore in treating the collisions, which are quadratic in nature, one needs a sampling, or better, an approximation of f by point sets, which is of second order.

The simplest method is to play with the index: Take a sample $r_1,\ldots,r_N$ for the uniform distribution in [0,1] from a random number generator and let

$$j(i) = [Nr_i] + 1 ,$$

where $[Nr_i]$ is the Gauss bracket. This fulfils our condition at least with probability one as is shown in [2]. Different i do not lead to different j(i) - the symmetry of the collision partners is lost, some particles may play the role of a collision partner several times. Clearly energy and momentum is not conserved in such a collision process, but these conservation laws are satisfied in the mean. This "Monte Carlo method" has therefore some disadvantages but is simple and therefore mostly used.
A bit more complicated is the idea to choose in every raw and column only one cross, i.e. to choose randomly a permutation π of $\{1,2,\ldots,N\}$ and put the crosses at $(v_{\pi(1)},v_{(\pi(2)}),(v_{\pi(3)},v_{\pi(4)}),\ldots,(v_{\pi(N)},v_{\pi(N)})$ - one has to consider only even numbers N, but this is not a real restriction. This methods conserves energy and momentum.

There are certainly better solutions for the selection procedure but all we found until now are too expensive. But since our condition is rather weak, there are many possibilities; it is for example not necessary that crosses and dots coincide.
With which method fulfilling the condition for Ω_{N_c} ever, we are at the end of the time step: We have collision pairs $(v_i,v_{j(i)})$ and collision parameters y_i - we determine v_i' for all $i=1,\ldots,N_c$ and end up with all particles having new positions and new velocities. This set is near to $f(\Delta t,x,v)$, the solution of the time-space discretized Boltzmann equation - and we can begin a new time step.

We have not treated interior energy, chemical reactions in the interior or at the wall and ionisation effects.

To model these effects and to evaluate the reliability of the models, is a research field in its own; there are ideas by Bird, Nanbu and others in use, but there is still no proof that they give correct results for realistic reentry problems.

6. A FEW REMARKS ON THE TRANSITION TO NAVIER-STOKES

When the shuttle comes down, the atmosphere becomes denser, the mean free path λ_∞ smaller, the computational effort for FPM (and any other Boltzmann solver) larger. Between 85 and 70 km λ_∞ drops by a factor of 10 and the number of cells in a 3-dimensional calculation has to be increased by a factor of 10^3. There is only one way out: The distriution f approaches a local Maxwellian when $\lambda_\infty \to 0$ - and one has to use this information numerically. The procedures making this approach more precise are the socalled Hilbert and Chapman-Enskog expansions of the solution f with respect to the parameter ε (proportional to λ_∞). A first order approximation is - in both expansions - given by the Euler equation, while Chapman-Enskog gives in second order Navier-Stokes. (Rigorous results on Hilbert expansion may be found for example in [6] and there are many books on the formal aspects, for example [7], [8]). In short, the distribution function

$$F_{NS}(t,x,v) = \text{Maxwell}[\rho(t,x),u(t,x),T(t,x)](v) - \varepsilon\ \text{Correction}[\rho(t,x),u(t,x),T(t,x),\eta(t,x),\lambda(t,x)](v)$$

is a solution of the Boltzmann equation with a residuum of order ε^2, if ρ, u, T are solutions of the Navier-Stokes equations with viscosity η and thermal conductivity λ depending on the differential cross section (and the temperature) and if as usual

$$\text{Maxwell}[\rho,u,T](v) = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left[-\frac{1}{2RT}|v-u|^2\right] .$$

The correction term is quite lengthy and includes some coefficients given as solutions of an integral equation involving the linearized collision operator and therefore again the differential cross section - we do not give details about it.
F_{NS} defines - for incoming molecules - the boundary conditions for the Boltzmann region coming from the Navier-Stokes domain. More complicated is the other direction: Given f in a transition layer one has to approximate it by a function of type F_{NS} in order to get good ρ, u, T as boundary conditions for the Navier-Stokes. The idea to do this is to compare the fluxes of mass, momentum and energy for f and F_{NS} across the boundary and determine ρ, u, T such that these fluxes are equal:

$$\int_{v\cdot n>0} v\cdot n\ \phi_k(v) f(t,x,v)dv = \int_{v\cdot n>0} v\cdot n\ \phi_k(v) F_{NS}[\rho,u,T](t,x,v)dv$$

with

$$\phi_k(v) = \begin{cases} 1 & \text{for } k=0 \\ v_k & \text{for } k=1,2,3 \\ |v|^2 & \text{for } k=4 \end{cases}$$

gives 5 conditions for the five unknowns ρ, u and T. We remark that one gets in this way also slip boundary conditions for the Navier-Stokes equation. There is a good survey in [9]; we refer also to

the Thèse de Doctorat de l'Université Paris Nord of F. Coron [10], where many of related equations are discussed.
We believe that theoretically the transition from Boltzmann to Navier-Stokes and vice versa may be settled - if we know, where the transition layer is. Numerically there are still many problems in the details, for example the different grid structures for Finite Volume techniques for Navier-Stokes and Finite Pointset Methods. It seems to be a tempting idea to use the socalled Boltzmann schemes for solving Euler or Navier-Stokes, since they are derived from a kinetic basis (see for example [17] or [26]), or even use the fact that f_{NS} solves the Boltzmann up to ε^2 [11]. However, these schemes are not yet enough developed to compete with the schemes normally used for planes etc.
Another problem seems to be very important with respect to the transition: Where is it allowed to pass from Boltzmann to Navier-Stokes or - where is it necessary to leave Navier-Stokes and to use Boltzmann? The answer to the first question seems to be easier: If f is sufficiently near to F_{NS}, one may use Navier-Stokes. Near with respect to which metric? Discrepancy may be a choice, relative entropy

$$\int f \ln \frac{f}{F_{NS}} \, dxdv$$

another one; all of them may create to many numerical difficulties and a simpler "solution" can be to consider the local Knudsen number Kn(x), where locality stems from the fact that the mean free path λ_n depends on x and the typical length depends on the typical length of the shuttle in vicinity (nose curvature, chord length etc.). This "solution" has some draw backs - mainly since Kn(x) is not so rigorously defined and since Kn(x) small (how small?) is certainly not sufficient. These problems are even more serious, if one is faced by the second question: Assume that we solve only Navier-Stokes, even in regions where it is physically not justified - how do we recognize this fact?
One proposal by Bird and others is to consider $\frac{\nabla\rho}{\rho}$, which should not become to large. We believe (and C. Bardos and his group are working in the same direction) that a sensitive feature is the entropy flux, which in the Boltzmann picture is defined by

$$Q_E^B[f] := -k \int_{\mathbb{R}^3} J(f,f) \ln f \, dv$$

and which for Navier-Stokes may be gained from inserting F_{NS} instead of f into Q_E^B, getting an expression depending only on ρ, u, T, λ, η, ∇T and

$$\langle \nabla u \rangle = \left(\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \operatorname{div}(u) \cdot f_{ij},\ 1 \le i,j \le 3 \right) ,$$

namely

$$Q_E^{NS}[f_{NS}] := -\frac{\lambda}{T^2} \nabla T \cdot \nabla T - \frac{2\eta}{T} \langle \nabla u \rangle : \langle \nabla u \rangle .$$

It is a consequence of the Boltzmann equation that in the interior of Ω (not at the boundary)

$$Q_E^B[f] \leq 0$$

for any exact solution f of the Boltzmann equation with equality only for f=Maxwell.
In Navier-Stokes calculations however, especially in shock r egions, Q_E^{NS} may become positive. Positivity of Q_E^{NS} is therefore a sign that F_{NS} is not near to the exact solution of the Boltzmann equation - too "much positivity" force us to leave Navier-Stokes. What means "too much" is still to be investigated, maybe by comparing Q_E^B and Q_E^{NS}, if both solutions are available.

A complete flow code, which is the final goal, should be able to discover automatically, where Euler, Navier-Stokes and Boltzmann regions are located and to shift automatically the "free boundary" between these regions during the reentry. The Boltzmann region, in high altitudes covering almost everything behind the shock will shrink and end up just to form a kinetic layer around the shuttle. But there is still some way to go.

7. SOME COMPUTATIONAL RESULTS

Let us finally demonstrate by a few examples that FPM is a successful method to compute complicated flow fields. In order to do so we will only show some pictures and refer for details to our papers [13] and [14].

Figure 6 gives an impression of the Mach field (the space dependent sound speed) around a 2-dimensional "double" ellipse (a shape considered to be near to a shuttle), figure 7 shows the corresponding grid refinement. Figure 8 presents a result from 3-dimensional computation, a section of the temperature field around a flat disc at 75° angle of attack ([13]). Far away from the disc the Knudsen number is 0.1, the gas temperature is 190 K and the speed of the gas (remember that we consider objects at rest but the gas moving) is Mach 15.6. Wall and stagnation temperature are considered to be equal. Figure 9 turns to a more realistic 3-dimensional object, a delta wing, and gives the density field around it [14]. Here we have Kn=0.01, T_∞=13.5 K, T_{wall}=620 K and V_∞=Mach 20.2. All the calculations presented here were done in the frame of the European Space Agency programme called "HERMES development programme" and were sponsored by a "contrat d'études et de recherches" between La Société Avions Marcel Dassault-Breguet Aviation and the University of Kaiserslautern. The calculations were done on a Fujitsu VP100 (in parts VP400) in Kaiserslautern (and Karlsruhe).

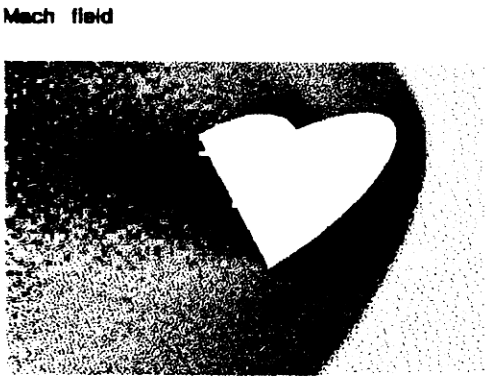

Figure 6

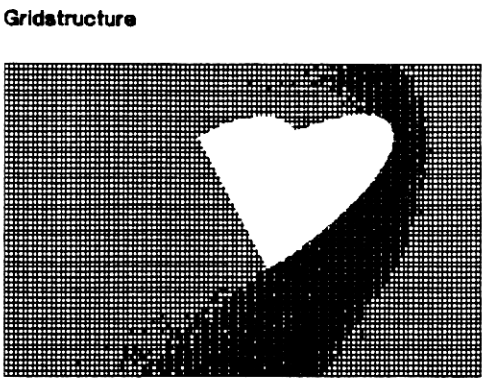

Figure 7

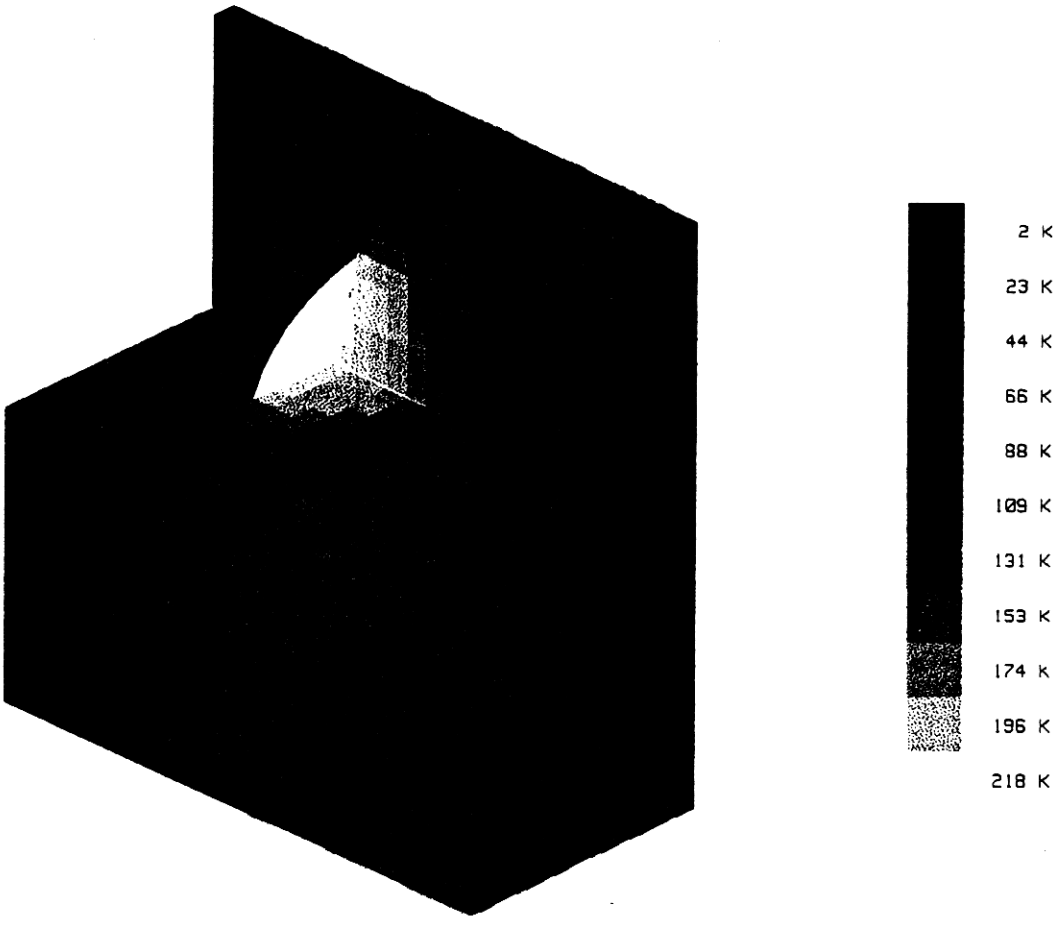

Figure 8

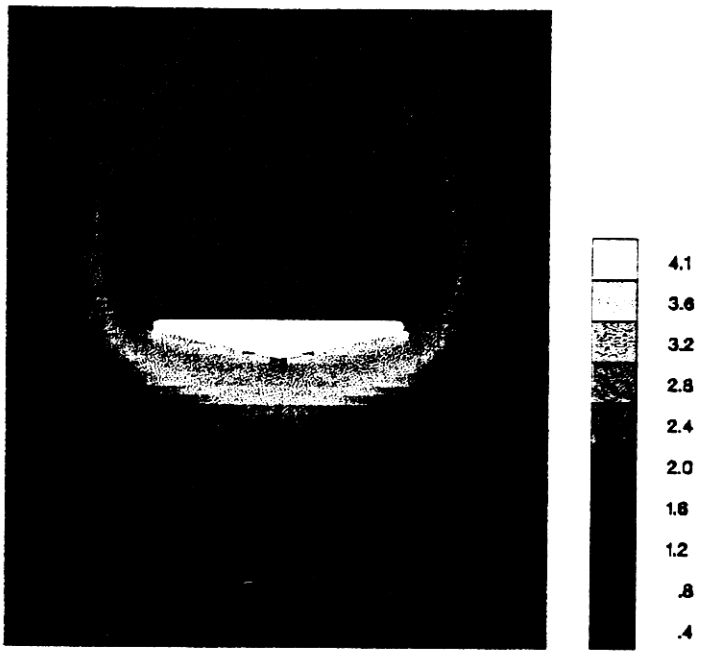

Figure 9

References

[1] **Aristov, V.V., Tscheremissine, F.G.:** The conservative splitting method for solving the Boltzmann equation, USSR Comp. Math. and Math. Phys., Vol. 20, p. 208 (1980)

[2] **Babovsky, H.:** A Convergence Proof for Nanbu's Boltzmann Simulation Scheme, European Journal of Mechanics B/Fluids, 8, no. 1 (1989)

[3] **Babovsky, H., Gropengießer, F., Neunzert, H., Struckmeier, J., Wiesen, B.:** Application of well-distributed sequences to the numerical simulation of the Boltzmann equation, to appear in Computational and Applied Mathematics

[4] **Babovsky, H., Illner, R.:** A Convergence Proof for Nanbu's Simulation Method for the full Boltzmann equation,SIAM Journal of Numerical Analysis, Vol. 26, no. 1, pp. 45-65 (1989)

[5] **Bird, G., Moss, J.:** Direct Simulation of Transitional Flow for Hypersonic Reentry Conditions, AIAA paper no. 84-0223, 1984

[6] **Caflish, R.:** The fluid dynamic limit of the nonlinear Boltzmann equation, Comm. Pure & Appl. Math., Vol. 33, pp. 651-666 (1980)

[7] **Cercignani, C.:** The Boltzmann Equation and its Applications, Springer 198

[7'] **Cercignani, C.:** Scattering Kernels for Gas-Surface Interaction, Workshop on Hypersonic Flows for Reentry Problems, Antibes Tome 1, 1990

[8] **Chapman, S., Cowlings, T.G.:** The mathematical theory of non-uniform gases, Cambridge University Press, 1970

[9] **Coron, F.:** Derivation of slip boundary conditions for the Navier Stokes System from the Boltzmann Equation, To appear in Journal of Statistical Physics

[10] **Coron, F.:** Applications de la théorie cinétique à l'aérodynamique hypersonique: une approche mathématique, Thèse de Doctorat de l'Université Paris Nord

[11] **Elizarova, T.G., Chetverushkin, B.N.:** Kinetical consistent finite difference gasdynamic schemes, to appear in: Japanese Journal of Aerospace Science

[12] **Frezzotti, A., Parani, R.:** Direct Numerical Solution of the Boltzmann Equation for a Binary Mixture of Hard Sphere Gases, to appear in Meccanica

[13] **Gropengießer, F., Neunzert, H., Struckmeier, J., Wiesen, B.:** Rarefied gas flow around a disc with different angles of attack, in preparation

[14] **Gropengießer, F., Neunzert, H., Struckmeier, J., Wiesen, B.:** Rarefied gas flow around a 3d-deltawing at low Knudsen number, in preparation

[15] **Hlavka, E.:** Funktionen von beschränkter Variation in der Theorie der Gleichverteilung, Ann. Math. pura et appl. IV, 54 (1961)

[16] **Illner, R., Pulvirenti, M.:** Global validity of the Boltzmann Equation for two- and three-dimensional rare gas in vacuum: Comm. Math. Phys. 121, 143-146 (1989)

[17] **Kaniel, S.:** A kinetic model for the compressible flow equations, Indiana University Mathematics Journal, Vol. 37, No. 3, 1988

[18] **Körber, S., Wiesen, B.:** A comparison of a Microscopic and a Phenomenological Model for a Polyatomic Gas, in preparation

[19] **Kuipers, L., Niederreiter, H.:** Uniform distribution of sequences, John Wiley & Sons (1974)

[20] **Landford, O.E.:** The evolution of large classical systems, Proceedings of the 1974 Battelle Rencontres on Dynamical Systems, J. Moser ed., Springer Lecture Notes in Physics no. 35, pp. 1-111 (1975)

[21] **Lécot, C.:** Low Discrepancy sequences for solving the Boltzmann Equation, to appear

[22] **van der Mee, C.V.M.:** Stationary Solutions of the Nonlinear Boltzmann Equation in a Bounded Spatial Domain, Math. Meth. in the Appl. Sciences, Vol. 11, pp. 471-481 (1989)

[23] **Mißmahl, G.:** Randwertprobleme bei der Boltzmann Simulation, Diplomarbeit, University of Kaiserslautern (1990)

[24] **Nanbu, K.:** Direct Simulation Schemes derived from the Boltzmann Equation, J.Phys. Japan 49, p. 2042 (1980)

[25] **Neunzert, H., Wick, J.:** Die Theorie der asymptotischen Verteilung und die numerische Lösung von Integrodifferentialgleichungen, Num. Math. 21, pp. 234-243 (1973)

[26] **Perthame, B.:** Boltzmann type schemes and the entropy property, to appear in SIAM Journal on Numerical Analysis

[27] **Platkowski, T.:** private communication

[28] **Weyl, H.:** Über die Gleichverteilung von Zahlen mod 1, Math. Ann. 77 (1916)

[29] **Yen, S.M.:** Numerical Solution of the Nonlinear Boltzmann Equation for Nonequilibrium Gas Flow Problems, Ann. Rev. Fluid Mech., Vol. 16, pp. 67-97 (1984)

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