Numerical Simulation of the Stationary One–Dimensional Boltzmann Equation by Particle Methods

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Abstract

The paper presents a numerical simulation technique – based on the well–known particle methods – for the stationary, one–dimensional Boltzmann equation for Maxwellian molecules.

In contrast to the standard splitting methods, where one works with the instationary equation, the current approach simulates the direct solution of the stationary problem.

The model problem investigated is the heat transfer between two parallel plates in the rarefied gas regime. An iteration process is introduced which leads to the stationary solution of the exact – space discretized – Boltzmann equation, in the sense of weak convergence.

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1 Introduction

Although most applications in rarefied gas dynamics are described by stationary problems, the standard simulation schemes for the computation of rarefied gas flows are derived from the instationary Boltzmann equation using the well–known splitting method [5], [6] to separate the free movement of the gas particles from the collisions between them.

It is clear that the solution of the stationary problem should not be sensitive against the time step Δt, being in this case an auxiliary iteration parameter. However the standard splitting scheme always introduces an error $\mathrm{O}(\Delta t)$ in the final result. Moreover, there is a correlation between the space discretization Δx and the time discretization Δt: to obtain an accurate solution, i.e. to decrease Δx, the ratio of Δx and Δt has to remain bounded which leads to small timesteps in the splitting method. Hence a large number of timesteps is necessary to reach the stationary state.

A more appropriate way will be to work directly with the stationary Boltzmann equation and to derive a direct simulation procedure for the stationary problem.

In the following we will construct a scheme for the stationary, one–dimensional Boltzmann equation with Maxwellian molecules. Our model problem is the heat transfer between two parallel plates at different temperatures together with diffusive boundary conditions. We will derive an iteration process which is similar to the standard splitting schemes, but leads to an exact solution of the space–discretized stationary equation.

The paper is organized as follows: in Section 2 we state our model problem and discuss the two limiting cases, namely the continuum and the free molecular limit. The integral equations which are used to derive our simulation scheme are presented in the next section. Furthermore, we present our iterative method and discuss the connection as well as the differences to the splitting method for the instationary problem.

In Section 4 we define a particle method for the iterative process given in the previous section that is based on the space discretized stationary equation and discuss the convergence properties. Some numerical results for our model problem of Section 2 are discussed in the final section.

2 Statement of the Model Problem

The following model problem is a "classical" testcase for numerical methods in rarefied gas dynamics, see for example [2], [4] and [7].

2.1 Heat Transfer between Two Parallel Plates

We consider the heat transfer between two parallel plates with diffusive boundary condition (see Fig. 1), i.e.

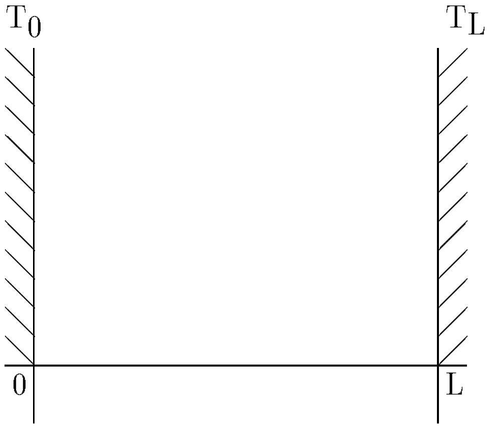

Fig. 1: Heat Transfer between Two Parallel Plates

$$\left.\begin{array}{rcl} f(0,v)|_{v>0} & = & A_0 \mathrm{e}^{-\frac{|v|^2}{2T_0}} \\ f(L,v)|_{v<0} & = & A_L \mathrm{e}^{-\frac{|v|^2}{2T_L}} \end{array}\right\} \tag{2.1}$$

where – due to mass conservation at the boundary – A_0 and A_L depend on the outgoing mass flux at $x = 0$ respectively $x = L$ and

$$\int\limits_{\mathbb{R}^3} v_x f(x,v)\,\mathrm{d}v = 0. \tag{2.2}$$

Moreover, we have one more parameter

$$M = \int\limits_0^L \int\limits_{\mathbb{R}^3} f(x,v)\,\mathrm{d}v\mathrm{d}x, \tag{2.3}$$

that defines the total mass M from the gas.

Let us consider the stationary Boltzmann equation for (pseudo–) Maxwellian molecules written as

$$\frac{\alpha}{\rho(x)} v_x \frac{\partial f}{\partial x} + f = F(f), \tag{2.4}$$

where

$$\begin{aligned} F(f) &= \frac{1}{\rho(x)} I_+(f) \\ &= \frac{1}{\rho(x)} \int\limits_{\boldsymbol{R}^3} \int\limits_{S^2} g\left(\frac{u\cdot\omega}{|u|}\right) f(v')f(w')\mathrm{d}\omega\mathrm{d}w \qquad (2.5) \\ \rho &= \int\limits_{\boldsymbol{R}^3} f(v)\,\mathrm{d}v, \\ u &= v - w, \\ \omega &\in S^2, \\ v' &= \frac{1}{2}(v + w + |u|\omega), \\ w' &= \frac{1}{2}(v + w - |u|\omega) \end{aligned}$$

and

$$\int\limits_{-1}^{1} g(\eta)\,\mathrm{d}\eta = \frac{1}{2\pi}$$

with some constant $\alpha = \rho_*\tau$ such that the total cross section is defined by

$$\sigma_{\mathrm{tot}}(|u|) = \frac{\rho_*\tau}{|u|}$$

For our considerations it is convenient to pass to a dimensionless form – we put

$$\begin{aligned} x' &= \frac{x}{L}, \\ v' &= \frac{v}{\sqrt{T_0}}, \\ \frac{M}{LT_0^{3/2}} f(x,v) &= f'(x',v') \end{aligned}$$

and obtain from (2.4)

$$\frac{\varepsilon}{\rho(x)} v_x \frac{\partial f}{\partial x} + f = F(f), \tag{2.6}$$

where $0 < x < 1$, $\varepsilon = \frac{\alpha\sqrt{T_0}}{M}$ and we omit the sign "$'$". All notations (2.5) are valid for this equation. The boundary conditions (2.1) now read

$$\left.\begin{array}{rcl} f|^{+}_{x=0} & = & A_0 \mathrm{e}^{-\frac{|v|^2}{2}} \\ f|^{-}_{x=0} & = & A_1 \mathrm{e}^{-\frac{|v|^2}{2\theta}} \end{array}\right\} \tag{2.7}$$

with $\theta = \frac{T_L}{T_0}$. Condition (2.3) reads

$$\int_0^1 \int_{\mathbb{R}^3} f(x,v)\,\mathrm{d}v = 1 \tag{2.8}$$

Finally we simplify equation (2.6) by introducing a "mass coordinate"

$$y = \int_0^x \rho(x')\,\mathrm{d}x', \quad 0 < y < 1 \tag{2.9}$$

and obtain (changing v_x to v_y)

$$\varepsilon v_y \frac{\partial f}{\partial y} + f = F(f) \tag{2.10}$$

where

$$\left.\begin{array}{rcl} F(f) & = & \dfrac{1}{\rho(y)} I_+(f), \quad 0 < y < 1, \\ \rho(y) & = & \displaystyle\int_{\mathbb{R}^3} f(y,v)\,\mathrm{d}v, \\ f^{+}(0,v) & = & A_0 \mathrm{e}^{-\frac{|v|^2}{2}}, \\ f^{-}(1,v) & = & A_1 \mathrm{e}^{-\frac{|v|^2}{2\theta}}, \\ \theta & = & \dfrac{T_L}{T_0}, \\ \varepsilon & = & \dfrac{\alpha\sqrt{T_0}}{M} \end{array}\right\} \tag{2.11}$$

and

$$\int_{\mathbb{R}^3} v_y f(y,v)\,\mathrm{d}y = 0$$

Once the problem (2.10)–(2.11) is solved one may return to the initial variable x by equation (2.9) or

$$x = \int_0^y \frac{\mathrm{d}y'}{\rho(y')}, \quad 0 < y < 1. \tag{2.12}$$

Therefore we have also the normalization condition

$$\int_0^1 \frac{\mathrm{d}y}{\rho(y)} = 1 \tag{2.13}$$

that completes the statement of problem (2.10).

Remark 1
To understand all properties of the solution we do not need to do the trivial change of variable (2.12), so that we will consider problem (2.10) in the sections given below in the variables $0 < y < 1$ and $v \in \mathbb{R}^3$.

2.2 Two Limiting Cases

It is convenient to consider first of all the two well–known limiting cases:

a) $\varepsilon = \infty$, the so–called Knudsen gas limit and

b) $\varepsilon = 0$, the limit for continuous media.

For case a) we obtain the solution in the form

$$f(y,v) = \eta(v_y) A_0 \mathrm{e}^{-\frac{|v|^2}{2}} + \eta(-v_y) A_1 \mathrm{e}^{-\frac{|v|^2}{2\theta}} \tag{2.14}$$

where

$$\eta(z) = \begin{cases} 1 & \text{for} \quad z > 0 \\ 0 & \text{for} \quad z \le 0 \end{cases}$$

Furthermore we have the two conditions

$$\int_{\mathbb{R}^3} v_y f(y,v)\,\mathrm{d}v = 0, \qquad \int_0^1 \frac{\mathrm{d}y}{\rho(y)} = 1, \tag{2.15}$$

which read

$$\rho(y) = 1 = \frac{(2\pi)^{3/2}}{2}(A_0 + A_1\theta^{3/2}), \quad A_0 = A_1\theta^2. \tag{2.16}$$

Hence we obtain the formulae

$$\begin{aligned} A_0 &= \frac{2\sqrt{\theta}}{(2\pi)^{3/2}(1+\sqrt{\theta})}, \\ A_1 &= \frac{2}{(2\pi\theta)^{3/2}(1+\sqrt{\theta})}, \end{aligned}$$

that define completely the solution (2.14) in the limit $\varepsilon = \infty$.

For case b) the solution reads

$$f(v,y) = \rho(y)[2\pi T(y)]^{-3/2}\mathrm{e}^{-\frac{|v|^2}{2T(y)}} \tag{2.17}$$

where ρ and T satisfy the Navier–Stokes equations in the initial variable x (2.12), i.e.

$$\rho(x)T(x) = \text{const}, \quad T(0) = 1, \quad T(1) = \theta,$$
$$\frac{\mathrm{d}}{\mathrm{d}x}T(x)\frac{\mathrm{d}T}{\mathrm{d}x} = 0$$

which yields

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{\rho(x)}\frac{\mathrm{d}T}{\mathrm{d}x} = 0$$

Hence, $\rho(y)$ and $T(y)$ are defined by the equations

$$\rho(y)T(y) = \text{const}, \quad T(0) = 1, \quad T(1) = \theta \tag{2.18}$$

and

$$\frac{\mathrm{d}^2T}{\mathrm{d}y^2} = 0, \quad \int_0^1 \frac{\mathrm{d}y}{\rho(y)} = 1. \tag{2.19}$$

Finally we obtain

$$T(y) = 1 + (\theta - 1)y, \quad 0 \le y \le 1 \tag{2.20}$$

and

$$\rho(y) = \frac{1+\theta}{2[1+(\theta-1)y]}, \tag{2.21}$$

that define completely the solution (2.17) in the limit $\varepsilon = 0$.

The solutions (2.14) and (2.16) respectively (2.17),(2.20) and (2.21) may serve as test functions for any approximate solution.

3 Integral Equations and Iterative Methods

We again consider the boundary value problem (2.10) in the form

$$\varepsilon v_y \frac{\partial f}{\partial y} + f = F(f) \tag{3.1}$$

together with the boundary conditions described in Section 2.

It is not very difficult to invert explicitely the operator on the left hand side of the Boltzmann equation (3.1) and to consider the equation in integral form. However it is more convenient for our goals to use a slightly different way of inverting the operator. Following [3], we write down the problem (2.10) in the form

$$f(y,v) = (1+\varepsilon D)^{-1} F(f), \quad D = [v_y \frac{\partial}{\partial y}], \tag{3.2}$$

where the notation $[v_y \frac{\partial}{\partial y}]$ notes the operator $v_y \frac{\partial}{\partial y}$ together with the boundary conditions (2.11).

To construct the inverse operator we use the well–known operator identity

$$[1+\varepsilon D]^{-1} = \int\limits_0^\infty \mathrm{e}^{-t(1+\varepsilon D)}\,\mathrm{d}t = \frac{1}{\varepsilon}\int\limits_0^\infty \mathrm{e}^{-\frac{t}{\varepsilon}}\mathrm{e}^{-tD}\,\mathrm{d}t, \tag{3.3}$$

which reduces the inversion of $(1+\varepsilon D)$ to construct the operator exponential $\exp(-tD)$.

The following two facts are the crucial points for the rest of the considerations:

1) The operator exponential $\exp(-tD)f_0$ is simply the solution of the free motion equation

$$\begin{aligned} \frac{\partial f}{\partial t} + v_y \frac{\partial f}{\partial y} &= 0 \\ f|_{t=0} &= f_0 \end{aligned} \tag{3.4}$$

with boundary conditions (2.11).

2) The identity (3.3) may be written as the time–averaging

$$\begin{aligned} (1+\varepsilon D)^{-1} &= \langle \mathrm{e}^{-tD} \rangle_\varepsilon \\ \langle \Psi(t) \rangle_\varepsilon &= \int\limits_0^\infty \mathrm{e}^{-\frac{t}{\varepsilon}} \Psi(t)\,\frac{\mathrm{d}t}{\varepsilon} \end{aligned} \tag{3.5}$$

over the Poisson distribution with mean value $\langle t\rangle = \varepsilon$.

Hence, we may formulate problem (2.11) in form of an integral equation

$$f(y,v) = \langle \mathrm{e}^{-tD}F(f)\rangle_\varepsilon = \int_0^\infty \mathrm{e}^{-\frac{t}{\varepsilon}}\mathrm{e}^{-tD}F(f)\,\frac{\mathrm{d}t}{\varepsilon} \tag{3.6}$$

where

$$D = [v_y\frac{\partial}{\partial y}]$$

This equation is obviously equivalent to the standard integral form of the stationary Boltzmann equation, but the advantage is that the form of the equation directly suggests a way to solve it:

The natural iteration scheme for the Boltzmann equation defined in (2.10) is

$$\varepsilon v_y \frac{\partial f^{(n+1)}}{\partial y} + f^{(n+1)} = F[f^{(n)}] \tag{3.7}$$

with $A_{0,1}$ as defined by (2.11).

Together with equation (3.6) this scheme may be written as

$$f^{(n+1)} = \langle \mathrm{e}^{-tD}F[f^{(n)}]\rangle_\varepsilon \tag{3.8}$$

and there exists an easy way to realize the iteration by a particle method – we will return to this point in the next section.

Our final remark in this section is that the iterative scheme is very close to the usual splitting algorithm for the Boltzmann equation [5]. Let us write equation (2.10) for the instationary case

$$\frac{\partial f}{\partial t} + v_y\frac{\partial f}{\partial y} = \frac{1}{\varepsilon}[F(f) - f],$$

and put

$$\begin{aligned} f(y,v,t^{(n)}) &= f^{(n)}(y,v), \quad n \in I\!N_0 \\ t^{(n)} &= n\varepsilon \end{aligned}$$

Then we split the Boltzmann equation into two simplified equations for any time interval $t^{(n)} < t < t^{(n+1)}$.

$$\begin{aligned} f_t &= \frac{1}{\varepsilon}[F(f) - f] \\ f_t + v_y f_y &= 0. \end{aligned}$$

Moreover, let us use the explicit discretization scheme for the collision stage

$$f(t+\Delta) = \frac{\Delta}{\varepsilon} F[f(t)] + (1 - \frac{\Delta}{\varepsilon}) f(t)$$

with time step $0 < \Delta \leq \varepsilon$. If we choose the maximal time step $\Delta = \varepsilon$, then we obtain

$$f(t+\varepsilon) = F[f(t)]$$

Therefore with time step $\Delta = \varepsilon$ the splitting algorithm is equivalent to the recurrence formula

$$f^{(n+1)} = \exp(-\varepsilon D) F[f^{(n)}] \tag{3.9}$$

that corresponds to equation (3.8) of our iterative process.

Hence, we may understand that there is a systematic error included in this type of splitting algorithm. In fact, if the algorithm is convergent as $n \to \infty$, it gives a solution of

$$f(y,v) = \int_0^\infty \delta(t-\varepsilon) \mathrm{e}^{-tD} F(f) \, \mathrm{d}t, \tag{3.10}$$

and not the true stationary Boltzmannn equation (3.6). The systematic error is formally caused by using in (3.10) the "deterministic" probability density $\delta(t-\varepsilon)$ and not the Poisson distribution density $\varepsilon^{-1}\exp(-t/\varepsilon)$.

4 A Particle Method for the Stationary Equation

In the following we derive a realization for the iterative process

$$f^{(n+1)} = \langle \mathrm{e}^{-tD} F[f^{(n)}] \rangle_\varepsilon \tag{4.1}$$

by a particle method.

The measure theoretic formulation of equation (4.1) yields

$$\mu^{(n+1)} = (\kappa \otimes \nu^{(n)}) \circ T^{-1} \tag{4.2}$$

where κ denotes the Poisson measure, T^{-1} the free stream operator, i.e.

$$T^{-1}(t, f(x,v)) = f(x+tv, v)$$

and $\nu^{(n)}$ represents the gain term due to collisions of $\mu^{(n)}$, i.e.

$$\nu^{(n)} = (\mu^{(n)} \otimes \mu^{(n)} \otimes \gamma) \circ P^{-1}. \tag{4.3}$$

In (4.3) γ denotes the corresponding measure of the differential cross section and

$$P^{-1}(v, w, \omega) = \frac{1}{2}(v + w + |v - w|\omega)$$

Equation (4.2) is very similar to the standard measure theoretic formulation of particle schemes for the splitting method – see for example [5] and [8] – and it is obvious how to derive a weak–* convergent particle scheme for (4.3).

Remark 2
It is not the aim of the current paper to describe completely the techniques to construct a particle method for the Boltzmann equation.
Hence, we only give briefly the main aspects and refer the reader to the references [5] and [8].

The main aspects in the considerations given below is to clarify the differences to standard splitting methods.

First of all, the basic idea of particle methods is to approximate the measure $\mu = \mu[x, v]$ associated to the distribution function $f(x, v)$ by discrete measures ("particles") in the form

$$\mu_N = \frac{1}{N}\sum_{i=1}^{N}\delta_{(x_i, v_i)}$$

In the limit $N \to \infty$ the discrete approximations $(\mu_N)_{N\in N}$ should converge in the weak–* sense to μ.

The second remark is that one has to introduce a cell structure on the spatial domain in order to perform the collision stage described by (4.3) when using discrete measures.

Remark 3
In the case of our model problem we divide the spatial domain – the unit interval $[0, 1]$ – into cells of length $1/M$ where M denotes the number of cells, i.e.

$$[0, 1) = \dot{\bigcup_{k=1,\dots,M}} [\frac{k-1}{M}, \frac{k}{M})$$

Then, only particles which are located in the same cell may collide. This corresponds to a space–discretized Boltzmann equation where the distribution function $f(x, v)$ is approximated by cellwise constant functions $f_k(v), k = 1, ..., M$.

Now we are able to give the first two steps of our particle method:

- choose a cell structure on the spatial domain and construct an approximation of the initial value $f^{(0)}$ of the iteration process (4.2). We refer the reader to reference [8].

- suppose that we are in the n–th iteration. Construct an approximation of the function $F(f^{(n)})$ by performing the collision stage (4.3) where all particles undergo a collision (see again [5] and [8]).

Finally we have to realize the free movement of particles described by the operator exponential $\exp(-tD)$ averaged with respect to a Poisson distribution.

Remark 4
Up to now we are close to the standard splitting methods. The next step contains the main difference of the stationary particle scheme.

Let us assume that we are in the n–th iteration and that the resulting discrete measure $\nu_N^{(n)}$ of the collision stage (4.3) is given in the form

$$\nu_N^{(n)} = \frac{1}{N}\sum_{i=1}^{N} \delta_{(x_i,v_i)}$$

and further we have

$$\nu_N^{(n)} \to \nu^{(n)}$$

if $N \to \infty$.

Then, according to equation (4.2), we have to construct a discrete approximation of the measure $(\kappa \otimes \nu^{(n)}) \circ T^{-1}$ which converges weak–* if $N \to \infty$.

To do this we take the discrete measure $\nu_N^{(n)}$ and associate to each particle $(x_i, v_i), i = 1, ..., N$ an individual time step t_i such that the set $\{t_1, ..., t_N\}$ is a set of independent Poisson distributed random numbers on $\mathbb{R}_+$.

Now we apply the free stream operator T^{-1}, i.e. we construct the discrete measure $\mu_N^{(n+1)}$ as

$$\mu_N^{(n+1)} = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i+t_iv_i,v_i}$$

Using the standard techniques as described in [1],[5] or [9], one can show that $\mu_N^{(n+1)}$ converges to $\mu^{(n+1)}$ almost surely with respect to the sets of random numbers $(\{t_1, ..., t_N\})_{N\in\mathbb{N}}$ – if $N \to \infty$ and $\nu_N^{(n)} \to \nu^{(n)}$.

Remark 5
This part together with the two steps given above completes our particle method for the iteration (4.2).

Obviously, if the exact iteration process (4.2) is convergent (which we assume without any restrictions), then the particle method described above will lead to a weak–* convergent solution of the space–discretized stationary Boltzmann equation.

Our final remark is the following: the particle method for the stationary Boltzmann equation is very similar to the standard splitting schemes for the instationary equation. The differences are as follows:

1) in the collision stage all particles undergo a collision. We refer the reader to the remarks given at the end of Section 3,

2) in the free motion of particles, in the case of the stationary eqution this is given by the operator exponential $\exp(-tD)$, each particle moves with an individual time step t which is Poisson distributed with mean value ε,

3) the space discretization Δx is completely independent of the time step in 2). Especially, if one wants to improve the space accuracy by decreasing Δx it is not necessary to reduce the time step as when using splitting methods. The convergence of the particle scheme leads – in any case – to the exact space–discretized stationary equation.

5 Numerical Results

In the following we compare three different simulation schemes to calculate the solution of the stationary heat transfer problem at various Knudsen numbers ε:

1) the iterative particle scheme as described in the previous section where each particle has an individual Poisson distributed time step for the free motion and furthermore all particles undergo a collision in each iteration,

2) the classical splitting scheme for the instationary equation as discussed in [5] and [8],

3) the splitting scheme as given by formula (3.9) with time step $\Delta = \varepsilon$ and especially independent of the space discretization Δx.

The Knudsen number ε is varied in a range from 0.02 up to 2.0 and we compare the different schemes 1)–3) with respect to the quality of the stationary – i.e. convergent – numerical solution as well as concerning the speed of convergence of the different schemes.

For the calculations we use $M = 128$ spatial cells and start with an initial condition $f^{(0)}(x, v) = f(0, x, v)$ as a Maxwellian distribution with density 1 and temperature 1. The initial condition is approximated by 200 particles per cell, i.e. we use in total 25.600 particles to approximate the solution on the whole domain $[0, 1]$. Moreover, we use the two wall temperatures

$$T(0) = 1 \qquad T(1) = \theta = 2$$

The calculations are performed on a nCUBE 2S parallel computer using 32 nodes such that each processor computes the solution in 4 spatial cells. For the generation of uniformly distributed random numbers on the unit interval $[0, 1]$ we use the standard drand48()–subroutine implemented on the nCUBE 2S and initialize the generator according to the current processor.

In Fig. 1–7 we use the following notations

A: denotes the scheme for the stationary equation as defined in 1).

B: denotes the standard scheme for the instationary equation as defined in 2). The time step is equal to $1/M$ – M denotes the number of spatial cells.

C: denotes the scheme for the instationary equation with a fixed time step equal to ε, as defined in 3).

The first observation is that the two schemes A and B give nearly identical results: the stationary density profile for $\varepsilon = 2, \varepsilon = 0.5, \varepsilon = 0.1$ and $\varepsilon = 0.02$ are shown in figure 2, the corresponding stationary termperature profile in figure 3.

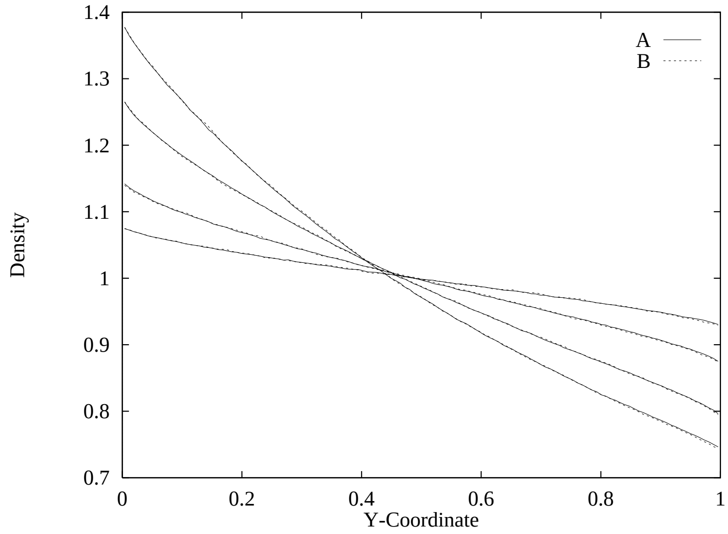

Fig. 2: Stationary Density Profile

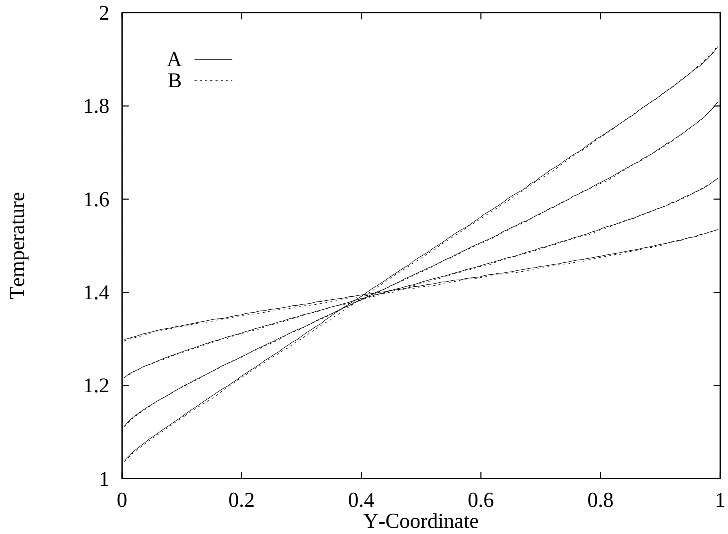

Fig. 3: Stationary Temperature Profile

In figure 2 the results for large Knudsen numbers are given by the curves which are closer to a horizontal line.

The situation changes if we use scheme C which is

a) identical to scheme A except that the time step is for every iteration equal to ε and not Poisson distributed with mean value ε and

b) identical to scheme B except that for the scheme B the time step is equal to $1/M$.

If the Knudsen number is of the order 1 the stationary density and temperature profiles are quite different from the "true" solution – given by scheme A respectively scheme B (see figure 4 and 5). The difference vanishes in the two limits $\varepsilon = \infty$ and $\varepsilon = 0$.

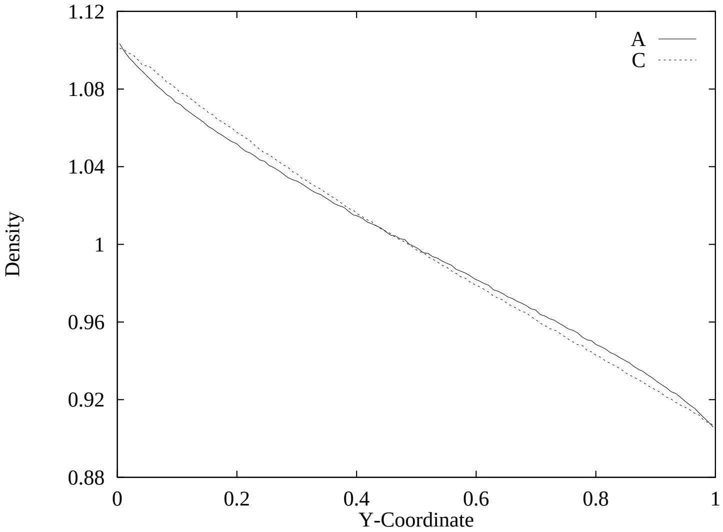

Fig. 4: Stationary Density Profile at $\varepsilon = 1.0$

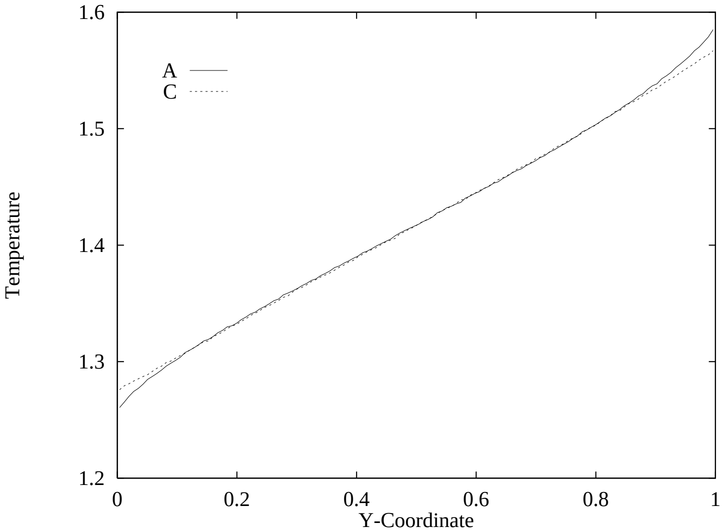

Fig. 5: Stationary Temperature Profile at $\varepsilon = 1.0$

Differences between scheme A and B, which produce – as shown above – nearly identical stationary solutions, are found in the speed of convergence. This is indicated in the figure 6 and 7: the first one shows the convergence history for the temperature in the left boundary cell at Knudsen numbers $2.0, 0.5, 0.1$ and 0.02, the second one the convergence at the right boundary cell. The quantity illustrated in both figures is the averaged temperature over the number of iterations for scheme A respectively the number of time steps for scheme B.

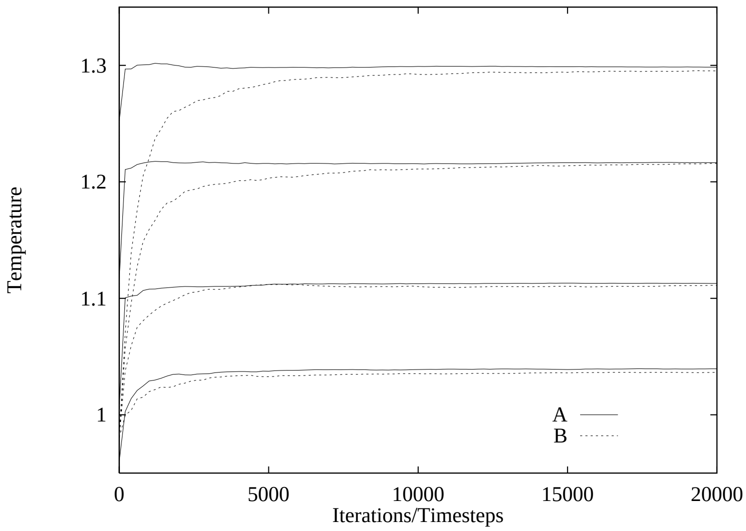

Fig. 6: Convergence History for the Left Boundary Cell

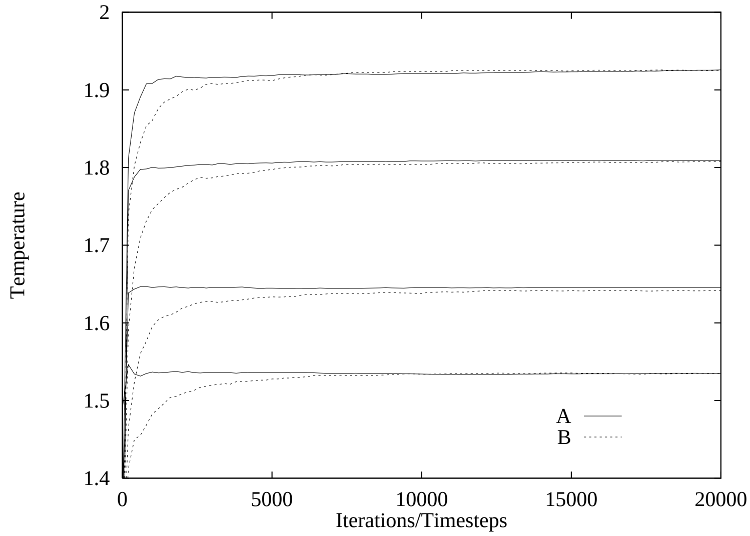

Fig. 7: Convergence History for the Right Boundary Cell

The results show that – especially for Knudsen numbers of order 1 – scheme A converges much faster then scheme B.

On the other hand scheme A is more time–consuming then scheme B, because of the collision stage where all particles undergo a collision and the large number of gas–surface–interactions which have to be computed if ε if of order 1. The corresponding CPU times for 20.000 iterations respectively time steps is given in table 1.

Tab. 1: CPU times in min:sec

Scheme	$\varepsilon = 2.0$	$\varepsilon = 0.5$	$\varepsilon = 0.1$	$\varepsilon = 0.02$
A	87:40	64:15	61:52	57:13
B	25:25	26:43	29:54	36:19

Nevertheless, if one compares the computational effort with the speed of convergence, scheme A is more efficient than scheme B, especially at Knudsen numbers of order 1, since the speedup of the convergence overcomes the increasing numerical effort.

6 Conclusion

Nearly all simulation techniques to calculate rarefied gas flows which are applied up to now are based on instationary flows together with a splitting method to separate the free motion from the collisions between the gas particles.

Nevertheless, in most applications one is interested in the steady state solution of the Boltzmann equation.

To obtain a space accurate solution it is necessary to perform an iteration scheme with small timesteps and this increases the number of iterations necessary to reach the stationary state.

Furthermore, the solution obtained using this approach is a first order in time approximation and therefore dependent on the time discretization.

In the present paper we derived a particle method directly for the – space–discretized – stationary Boltzmann equation with Maxwellian molecules. Hence, in case of convergence, the particle scheme leads to the exact solution of the stationary problem.

The numerical techniques are quite similar to the standard splitting approach except that in each iteration all particles undergo a collision – which increases the computational effort – and that each particle is equipped with an individual, Poisson distributed "artificial" time step with mean value equal to the related Knudsen number. Especially, the time steps remain unchanged if one increases the spatial accuracy.

The computational effort is reduced by the fact that the iterative process converges much faster than the time iterations of the instationary splitting approach, especially if the Knudsen number is of order 1.

Obviously, it is necessary to generalize the stationary particle method to the full Boltzmann equation, i.e. for non–Maxwellian molecules in more than one space dimensions. This will be the topic of subsequent papers.

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