Tests of a Simulation Method for a System of Boltzmann Equations

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Abstract—We report on numerical tests of a convergent simulation scheme for the solutions of a class of nonlinear kinetic equations for rarefied gas mixtures. © 2000 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

In a recent paper [1], we have introduced a simulation scheme for the solutions of space homogeneous Boltzmann-like equations describing reacting gas mixtures which are studied in [2,3]. The result of [1] represents a generalization of an efficient numerical scheme consistent with the classical one-component Boltzmann equation developed in [4,5].

In the numerical simulation of Boltzmann-like equations modeling reacting systems, new difficulties are encountered as compared to the Boltzmann equation for the simple gas. These difficulties are essentially due to the fact that one has to take into account the presence of several components and reaction thresholds. As in the case of the classical Boltzmann equation, numerical tests of Boltzmann-like equations with exact solutions for reacting gases would be particularly useful. Unfortunately, the presently known kinetic reactive models with analytical solutions are not useful for such tests because the collisions terms are linear [6], or they are defined by trivial reaction (collision) laws [7].

However, it is still interesting to test the method [1] on the exact Krook and Wu solutions of the multicomponent Boltzmann equations [8], describing gas mixtures with nonreactive collisions (Maxwell’s molecules type collisions). Indeed, although restricted to a nonreactive case, the simulation of the multicomponent Krook and Wu model has to face one of the major difficulties encountered in the numerical solving of Boltzmann-like equations. Moreover, doing numerical
simulation on the nonreacting mixtures, the Krook and Wu kinetic model might be interesting on its own. Specifically, the goal of our numerical tests is to calculate the discrepancy [9] of exact and numerical solutions. The importance of the discrepancy, is that the Koksma-Hlavka inequality [9] provides estimations of the errors on macroscopic observables (calculated as averages of macroscopic observables with respect to the distribution function).

Our analysis is limited to the numerical simulation of space-homogeneous models. However, besides its intrinsic interest, the numerical solving of the (reacting) Boltzmann equation in the space homogeneous case could be also useful to the space dependent solutions: as for the classical Boltzmann equation [5], the numerical scheme for space dependent solutions can be reduced to a succession of simulations in space homogeneous cells.

2. KROOK-WU SOLUTIONS AND THE DESCRIPTION OF THE METHOD

We consider the Krook and Wu model for a two species gas mixture. According to the model [8], the gas one particle distribution functions $f_i(t, v)$ (for $i = 1, 2$) at the moment $t > 0$ depend only on the modulus $v = |v|$ of the velocity. The Boltzmann system of equations associated with this model (using conventional units) is

$$\frac{\partial f_i(t, v)}{\partial t} = \sum_{k=1}^{2} \lambda_{ki} \int_{\Omega} \int_{\Omega} [f_i(t, v') f_k(t, w') - f_i(t, v) f_k(t, w)] \sin \theta \, d\theta \, dz \, dw,$$

for $i = 1, 2$. Here, $\Omega$ is the unit sphere in $\mathbb{R}^3$. The constants $\lambda_{ki}$ are related with the cross section of $k$ molecules with $i$ molecules, and they satisfy

$$\frac{\lambda_{12}}{n_1} = \frac{\lambda_{21}}{n_2},$$

with $n_i$ the concentration of specie $i$. The post collisional velocities $v'$ and $w'$ between the particles $i$ and $k$ have the form

$$v' = \left(\frac{v^2 + 2m_{ik}S}{2m_{ik}}\right)^{1/2}, \quad w' = \left(\frac{w^2 - 2m_{ik}S}{2m_{ik}}\right)^{1/2},$$

where $m_{ik} = m_i/(m_i + m_k)$, and $m_i$ is the mass of the particle of specie $i$. In (3), $S$ has the expression

$$S = (m_{ik}v + m_{ik}w) \cdot (v - w)(\cos \theta - 1) + |m_{ik}v + m_{ik}w| \times (v - w)\sin \theta \cos \varepsilon.$$

It is known [1], that the system (1) has unique global solutions. The Krook and Wu solutions were found under certain conditions on parameters. Let

$$p_1 = \lambda_{22} - \lambda_{21}(3 - 2\mu), \quad p_2 = \lambda_{11} - \lambda_{12}(3 - 2\mu),$$

with $\mu = 4m_1m_2/(m_1 + m_2)^2$. One distinguishes the following two cases.

CASE 1.

$$p_1 = p_2.$$

CASE 2.

$$2\mu^2 \left( \frac{\lambda_{21}}{p_1} - \frac{\lambda_{12}}{p_2} \right) = 1.$$
where

\[ \Phi(v; \alpha) = (2\pi \alpha)^{-3/2} \exp \left( -\frac{v^2}{2\alpha} \right), \]

\[ Q_i(t) = \frac{m_ip_iR(t)}{\xi(t)}, \]

\[ \alpha_i(t) = \frac{\xi(t)}{m_i}, \]

\[ R(t) = \frac{A \cdot \exp (A (t - t_0)) - B}{(n_1 + n_2)}, \]

\[ \xi(t) = \frac{1}{n_1 + n_2 + 2 (n_1 p_1 + n_2 p_2) R(t)}, \]

with \( A \) and \( B \) constants defined by

\[ A = \frac{\lambda_{11} \lambda_{21} \mu (3 - 2\mu p_2/p_1)}{6}, \quad B = \frac{\lambda_{11} p_1 + \lambda_{21} \mu (3 - 2\mu) p_2}{3}. \]

We recall [8], that conditions (6),(7) are of different physical nature. Given as masses and cross sections, it is possible to find a relative density \( n_1/n_2 \) such that the first condition is satisfied. The second condition does not depend on densities. Then if the second condition is fulfilled, the exact solutions can be written for all the values of \( n_1/n_2 \).

The numerical scheme developed in [1] for (space-homogeneous) Boltzmann-like equations, combines analytical methods with probabilistic techniques. The central result in [1, Theorem 10], is that almost surely, the simulated solutions converge weak (in the sense of measures), to the exact solutions of the equations. The construction of the approximative solutions needs the following steps.

(a) One provides a time discretizated version of the Boltzmann-like equations written in a weak form for measures.

(b) One approximates the initial data by sums of Dirac measures.

(c) One computes the solutions (as sums of Dirac measures), for each step of time, using the weak discretizated equations and probabilistic approximations.

In fact, because of the nonlinearity, each iteration step produces a power-like growing number of terms in the sums of point measures, approximating the exact solutions. In computations, the numerical effort would also be power-like increasing, so that the algorithm could not be effective at this level. This is the moment when the stochastic element is introduced: in order to decrease the number of terms in the sums, one proceeds by random selection.

In order to apply the numerical scheme of [1] to (1), we put equations (1) in the weak form. Then, the unknowns are measures of probability. We multiply the system (1) with a test function \( \varphi \in C_0(\mathbb{R}) \), and integrate with respect to \( dv \). By standard computations, we obtain

\[ \frac{d}{dt} \int_{\mathbb{R}^+} \varphi(v) v^2 f_i(t, v) dv = 4\pi \sum_{k=1}^{2} \lambda_{ki} \int_{\mathbb{R}_{+}^2} \int_{[0,1]^2} (\varphi(v_{ik}) - \varphi(v)) v^2 f_i(t, v) w^2 f_k(t, w) dx dy dv dw, \]

for \( i = 1, 2 \). In (11) the velocities \( v_{ik} \) are expressed, for \( v, w \in \mathbb{R}_{+} \) and \( x, y \in [0,1]^2 \), by

\[ v_{ik}(v, w, x, y) = \left\{ \begin{array}{l} \left( m_{ik}^2 + m_{ki}^2 \right) v^2 + 2m_{ki} \left( m_{ik} - m_{ki} \right) vw(2x - 1) \\ + 2m_{ik} w^2 + 2m_{ki} \left[ (v^2 + w^2) \left( m_{ik}^2 v^2 + m_{ki}^2 w^2 \right) \\ + 2 \left( m_{ki} - m_{ik} \right) \left( m_{ik} v^2 - m_{ki} w^2 \right) \\ - 2m_{ki} m_{ik} vw(2x - 1) \right] \end{array} \right\}^{1/2}. \]
Following [1], we finally obtain that the solutions of (11) on the interval [0, T] are approximated by the following convergent iteration scheme:

\[
\int_{\mathbb{R}^+} \varphi(v) F_i^{j+1}(v) dv = (1 - \Delta t \left( \lambda_{1,i} + \lambda_{2,i} \right)) \int_{\mathbb{R}^+} \varphi(v) F_i^j(v) dv + \sum_{k=1}^{2} \lambda_{ki} \int_{\mathbb{R}^+} \int_{[0,1]^2} \varphi(v_{ik}) F_k^j(v) F_j^j(w) dx dy dw,
\]

with \( i = 1, 2 \) and \( j \in \{0, \ldots, J - 1\} \).

For a sufficiently small time step \( \Delta t = T/J \), such that \((1 - \Delta t(\lambda_{1,i} + \lambda_{2,i})) > 0\), the solutions of (13) are positive and \( F_i^j(v) \) approximates \( 4 \pi v^2 f_i(j \cdot \Delta t, v) \).

We approximate the initial data \( F_i^0(v) dv \) by sums of the type \( \#_{i,N} f_i(v) = 1/N \sum_{n=1}^{N} \delta(v - v_{i,n}^0) dv \) of Dirac measures concentrated on \( N \) points \( v_{i,n}^0 \) (such that \( \#_{i,N} \) converges to \( F_i^0(v) dv \) as \( N \to \infty \) in the weak sense of measures). We approximate the Lebesgue measure on the unit square \( dx dy \) by sums of Dirac measures concentrated on \( N \) points \( 1/N \sum_{n=1}^{N} \delta(x - x_n) \delta(y - y_n) dx dy \) using the Hamersley-Van der Corput sequences. (For details, see [9].)

By direct computations, because of the product measures in the r.h.s. of (13), the next step of iteration we obtain sums of Dirac measures concentrated on \( N + 2 \cdot N^2 \) points. This will imply a power-like increasing computational effort. According to Theorem 8 of [1], we perform a succession of random selections and we keep the same number of concentration points at each step of time.

3. NUMERICAL RESULTS

In our experiments, we have taken \( n_2 = 5, \lambda_{11} = 2, \lambda_{12} = 1 \). In Case 1, \( m_1 = 1, m_2 = 3, n_1 = 10, t_0 = \ln(3p_1 + B/A)/A \). In Case 2, \( m_1 = 5, m_2 = 1, n_1 = 2, t_0 = \ln(3p_2 + B/A)/A \). The other parameters are determined by relations (2),(5)-(7).

This choice of \( t_0 \) ensures the positivity of \( f_i \) given by (8) for each \( i \geq 0 \).

In both cases, \( T = 6 \) corresponds almost to equilibrium and the “support” \([0, L]\) of initial data \( F_i^0(0,v) = 4 \pi v^2 f_i(0,v) \) is included in \([0,5]\). We approximate the measures \( F_i^0(v) dv \) with sums of Dirac measures concentrated on \( N \) the points \( \{v_{i,n}^0\}_{1 \leq n \leq N} \). The numbers \( v_{i,n}^0 \) are determined from the system of equations

\[
\int_{0}^{v_{i,n}^0} F_i^0(v) dv = \frac{nL}{N}, \quad n \in \{1, \ldots, N\}.
\]

We have used the mixed congruential method to generate sequences \( \{\omega_n\}_{n \in \mathbb{N}} \) of pseudo-random numbers. The elements \( \omega_n = z_n/b \), where \( z_n \) are given recursively by \( z_n = \lambda z_{n-1} + r \mod b \). In this relation \( b > 1 \), \( \lambda \) and \( r \) are fixed natural numbers and \( \lambda \) is relative prime with \( b \). The initialization is made with some integer \( 0 \leq z_0 < b \). Here \( b = 3 \cdot 10^{30}, r = 1987654321, \lambda = 19867917 \). Each test starts with an arbitrary positive \( z_0 < b \).

Let \( G_i(t,v) = 4 \pi \int_0^v u^2 f_i(t,u) du \), for \( i = 1, 2 \). In a first experiment, we have obtained for each \( i = 1, 2 \) ten numerical solutions for \( N = 1500 \) approximation points, at \( T = 6 \) and \( J = 16 \) iteration steps in Case 2. The numerical results are represented in Figures 1 and 2.

The errors on the solutions have been calculated in terms of discrepancies [9]. We recall that by Koksma-Hlavka inequality [9] provides estimations of the errors on macroscopic observables. In our case, the particular expression of the discrepancy between the exact and the simulated solution for each specie of particles at \( t = T \) takes the form

\[
D_i = \max_{n \in \{1, \ldots, N\}} \max \left\{ \left| \int_{0}^{v_{i,n}} F_i(T,v) dv - \int_{0}^{v_{i,n}} F_i^j(v) dv \right|, \left| \int_{0}^{v_{i,n-1}} F_i(T,v) dv - \int_{0}^{v_{i,n-1}} F_i^j(v) dv \right| \right\}, \quad i = 1, 2,
\]

(14)
where \( v_{i,0}^f = 0 \) and \( v_{i,n}^f (n \in \{1, \ldots, N\}) \), represent the concentration points of the measure \( F_i^f(v) \, dv \).

The following remark is in order. In general, the arithmetic mean of some solutions (obtained in the same conditions) is "smoother" than each solution. This is not surprising, since the convergence of the scheme is based on the law of the large numbers.

For exemplification, we considered another set of experiments where each numerical solution was the arithmetic mean of the solutions resulting from six repeated simulations. In fact, in our case, the numerical experiments have shown that more than six terms in the arithmetic mean have not improved considerably the numerical results. For similar reasons the final results on the numerical errors are expressed in terms of arithmetic means \( D_i \) of \( D_i \).
Table 1. The discrepancies $\tilde{D}_1$ and $\tilde{D}_2$ at $T = 6$ in Case 1.

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<tr>
<th>Specie 1</th>
<th>J \ N</th>
<th>16</th>
<th>32</th>
<th>64</th>
<th>128</th>
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Table 2. The discrepancies $\tilde{D}_1$ and $\tilde{D}_2$ at $T = 6$ in Case 2.

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In the following, Tables 1 and 2 present the values of $\tilde{D}_1$ and $\tilde{D}_2$ for $T = 6$ at different $J$ and $N$ for Cases 1 (6) and 2 (7), respectively.

Figure 3 represents $G_1$ at $T = 6$, and the corresponding approximative functions calculated with $J = 16$ and for different $N$ in Case 1. Figure 4 is a zoom of Figure 3.

It is known from Theorem 10 in [1] that the simulated solutions converge to the exact solutions when $\Delta t \to 0$ and $N \to \infty$, where $N$ depends on $\Delta t$. Indeed, the errors introduced by the discretized equations (13) diminish when the time step $\Delta t$ decreases. This can be seen in the next experiment.

The simulation time interval is $T = 1.5$, and $N = 3000000$ points for each specie. All the parameters are those of Case 1. Table 3 contains the arithmetic means of each discrepancy $\tilde{D}_1$ and $\tilde{D}_2$ as functions of the number of iteration step $J$.

On the other hand, the probabilistic selections introduce other errors for each iteration step. Due to this accumulation, the errors can increase when the time step diminishes, but fortunately, they are small for a small number of iteration steps.
There exist methods that enable the computation of certain macroscopic observables by avoiding the calculation of the distribution function [10]. However, the numerical solving of the Boltzmann-like equations in terms of distribution functions is important because, once the distribution function accurately calculated, the computation of any macroscopic variable can be easily performed.
Sometimes, although Boltzmann-like equations (for reactive models) cannot be exactly solved, one can obtain analytical solutions of equations for the time evolution of the macroscopic observables (density, velocity, temperature, etc.), as well as various transport coefficients (viscosity, diffusivity, etc.). Performing tests of the later equations, one can compare the exact value of some physical quantity with the same physical quantity calculated using the simulated solution (as average with respect to the distribution function). This will be the subject of a forthcoming paper.

REFERENCES