A RESCALING VELOCITY METHOD FOR KINETIC EQUATIONS: THE HOMOGENEOUS CASE

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Abstract. In this paper, we propose a method for the numerical solution of several kinetic equations (Boltzmann and Fokker-Planck equations). A rescaling of the distribution function in velocity is performed in order to treat strong non homogeneity. We finally treat some examples in granular media where the solution converges to a Dirac measure, and the rescaling technique allows to describe the evolution of the distribution with a very good accuracy.

Keywords: Kinetic equations, Boltzmann equation, Granular gas dynamics.

AMS subject classifications. 65T50, 68Q25, 74S25, 76P05

Contents

1. Introduction.

Numerical methods for Boltzmann type equations play an important role in practical and theoretical analysis of the time evolution of a plasma or a rarefied gas. The widely used and best known of these methods is the direct simulation Monte-Carlo method due to Bird [1]. After Bird's algorithm, more sophisticated methods related to Boltzmann equations have been proposed [6]. These numerical simulations are often performed in engineering to study the evolution of a gas or a plasma. Because at the kinetic level the number of unknowns becomes too large, Monte-Carlo methods represent a good compromise between accuracy and cheap computational time. Indeed, engineers are not interested to get an accurate solution of the kinetic equation, but only require a good behavior of macroscopic quantities which are experimentally observable. However, when we are interested in a modeling issue or in a description of a very precise phenomenon, probabilistic methods become not practical. In this case accurate methods have to be used.

More recently, some efforts have been performed to construct deterministic methods, which give a more accurate behavior of the time evolution of the solution.

The general difficulty related to deterministic methods is that the solution is computed on a fixed grid, which becomes an inconvenient when the distribution function strongly evolves or when the equation describes strong scale variations. In this paper we present a rescaling technique allowing to deal with this change of scales using a gridded method. We construct a deterministic schemes for time dependent kinetic equations, which are based on two main properties

- Preservation of the main physical quantities as mass, mean velocity, energy and steady states allows to give the correct long time behavior. High order and conservative methods for the evolution of the collision step allow a very accurate discretization in velocity domain, at a reasonable computational cost.
- An adaptive scaling allows to treat strong variations of the density, velocity and temperature in space. This rescaling is also able to catch self-similar solutions, which can occur when we do not converge to a steady state (coagulation models). Due to rescaling, macroscopic quantities are not computed directly from the distribution function by computing its moments as it usually done, but are solution to moment equations. The distribution function is used to close these moment equations.

The outline of the paper is the following: we first present the rescaling method to treat homogeneous in space kinetic equations and propose different applications in plasma physics (Fokker-Planck operator) and ganular gas dynamics (inelastic Boltzmann equation). Finally, numerical simulations are presented to show the effectiveness of the present approach.

2. Basis of the Rescaling method

We first consider the homogeneous in space collision operator

$$\frac{\partial f}{\partial t} = Q(f), \quad v \in \mathbb{R}^d, \tag{2.1}$$

where $f = f(t,v)$ is the distribution function of particles and $Q(f)$ is a collision operator conserving mass. We classically get macroscopic quantities by computing moments of the distribution function with respect to v. We define the density $\rho \in \mathbb{R}^+$ and the mean velocity $u \in \mathbb{R}^d$ by

$$\rho = \int_{\mathbb{R}^d} f(t,v)\,dv, \quad u = \frac{1}{\rho}\int_{\mathbb{R}^d} f(t,v)\,v\,dv, \quad t \in \mathbb{R}^+ \tag{2.2}$$

and also $w \in \mathbb{R}^+$

$$w^2 = \frac{1}{d\,\rho(t)}\int_{\mathbb{R}^d} f(t,v)\,|v-u|^2\,dv, \quad t \in \mathbb{R}^+. \tag{2.3}$$

For the classical Boltzmann equation, these macroscopic quantities are conserved with time, which means that the shape of the distribution function evolves, but the scale remains

the same. However, in other applications as in granular gases, the energy is dissipated with time and the solution converges to a Dirac measure. Then, the long time behavior of such numerical solution becomes inappropriate, when we apply a gridded method. Indeed, the mesh size becomes inevitably too large to represent correctly the solution. Another example of such behavior is the Fokker-Planck equation when the temperature w and the mean velocity u are not conserved. Here again, after a long time a fixed grid is not suitable to represent the solution, we then have to adapt the grid to follow the velocity and temperature variations along time.

To this aim, we propose to rescale the distribution function in velocity in order to follow the change of scales over time and choose a new unknown

$$g(t,\xi) = w^d\, f(t, u + w\,\xi), \tag{2.4}$$

which is solution to the following equation (see Proposition 2.1 below)

$$\frac{\partial g}{\partial t} - \frac{1}{w}\,\left(\, u' \cdot \nabla_\xi\, g + w'\,\mathrm{div}_\xi\,(\xi\, g)\,\right) = w^d\,\tilde{Q}(g,g), \quad \xi \in \mathbb{R}^d,$$

where $\tilde{Q}$ is such that $\tilde{Q}(g,g) = Q(f,f)$. This equation can be re-written in the conservative form

$$\frac{\partial g}{\partial t} - \mathrm{div}_\xi\left(\frac{1}{w}\,\left(u' + w'\,\xi\right) g\right) = w^d\,\tilde{Q}(g,g). \tag{2.5}$$

The density ρ is in now given by

$$\rho = \int_{\mathbb{R}^d} g(t,\xi)\, d\xi.$$

However, the mean velocity u and the temperature w^2 cannot be computed directly from g, but are solution to ordinary differential equations depending on the structure of the collision operator Q. In the general case, equations for u and w are obtained by the taking moments of Eq.(2.5), and observing that $\int g(t,\xi)\xi\, d\xi = 0$ and $\int g(t,\xi)|\xi|^2\, d\xi = d\rho$,

$$\frac{dq}{dt} \;=\; w^{d+1}\,\left(\int_{\mathbb{R}^d} \tilde{Q}(g,g)\,\xi\, d\xi\right), \quad q = \rho u, \tag{2.6}$$

$$\frac{dw}{dt} \;=\; \frac{w^d}{2\rho d}\int_{\mathbb{R}^d} \tilde{Q}(g,g)|\xi|^2\, d\xi. \tag{2.7}$$

The above results can be formalized in the following

Proposition 2.1. *Let f be a solution to the equation (2.1), where $Q(f,f)$ is a collision operator conserving at least mass*

$$\int_{\mathbb{R}^d} Q(f,f)\, dv = 0.$$

Then, the rescaled function g given by (2.4) is solution to (2.5) coupled with (2.6)-(2.7) such that

$$\frac{d}{dt}\int_{\mathbb{R}^d} g \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} d\xi = 0.$$

Proof.

It is easy to check that if f is a solution to (2.1) with a finite energy, the the rescaled function g is also a solution to (2.4). Moreover, g satisfies the following weak formulation: for any smooth function φ,

$$\frac{d}{dt}\int_{\mathbb{R}^d} g(t,\xi)\,\varphi(\xi)\,d\xi = -\frac{1}{w}\int_{\mathbb{R}^d} \left(\left(u' + w'\,\xi\right) g\right)\cdot \nabla_\xi \varphi\, d\xi + w^d \int_{\mathbb{R}^d} \tilde{Q}(g,g)\,\varphi(\xi)\,d\xi.$$

Then, taking $\varphi(\xi) = \xi$ and using the mean velocity equation (2.6), we get

$$\frac{d}{dt}\int_{\mathbb{R}^d} g(t,\xi)\,\xi\,d\xi = -\frac{1}{w}u'\rho + w^d \int_{\mathbb{R}^d} \tilde{Q}(g,g)\,\xi\,d\xi = 0.$$

Moreover, with $\varphi(\xi) = |\xi|^2$, using Eq.(2.7) for w, we obtain

$$\frac{d}{dt}\int_{\mathbb{R}^d} g(t,\xi)\,|\xi|^2\,d\xi \quad = \quad -2\frac{w'}{w} d\,\rho + w^d \int_{\mathbb{R}^d} \tilde{Q}(g,g)\,|\xi|^2\,d\xi = 0$$

□

We present some applications of this method and compute the complete system of equations for the linear Fokker-Planck equation and for the full granular Boltzmann equation.

3. Application to the Fokker-Planck equation

Consider the linear Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \mathrm{div}_v\left(\left(v - u_\infty\right) f + T_\infty\,\nabla_v f\right), \tag{3.8}$$

where u_∞ and T_∞ are given.

Then, the mean velocity u and the temperature $T = w^2$ computed from f using (2.2)-(2.3) are solution to a linear system of ODE's, which is obtained by multiplying (3.8) by v and $|v|^2$

$$u' = -\left(u - u_\infty\right), \quad T' = -2\left(T - T_\infty\right).$$

This system can be explicitly solved

$$u(t) = u_\infty + \left(u(0) - u_\infty\right) e^{-t}, \quad T(t) = T_\infty + \left(T(0) - T_\infty\right) e^{-2\,t}. \tag{3.9}$$

Thus, $g(t,\xi)$ is solution to the following rescaled equation

$$\frac{\partial g}{\partial t} - \mathrm{div}_\xi\left(\frac{1}{w}\left(u'(t) + w'(t)\,\xi\right) g\right) = \mathrm{div}_\xi\left(\left(\xi - \frac{u_\infty - u(t)}{w(t)}\right) g + \frac{T_\infty}{w^2}\nabla_\xi\, g\right), \quad \xi \in \mathbb{R}^d.$$

Using the equation (3.9) for u and T, we get

$$\frac{\partial g}{\partial t} - \mathrm{div}_\xi\left(\xi\, g\right) = \mathrm{div}_\xi\left(\nabla_\xi\, g\right),$$

which means that g is solution to a rescaled Fokker-Planck equation with a zero mean velocity and a temperature equal to one

$$\frac{\partial g}{\partial t} = \mathrm{div}_\xi \left(\xi\, g + \nabla_\xi\, g \right). \tag{3.10}$$

Let $(\xi_i)_i$ be a velocity grid and $g_i(t)$ an approximation of $g(t, \xi_i)$ the solution to (3.10) at time t on the grid. To get a conservative and entropic approximation, we consider the classical Chang & Cooper method [4]

$$\frac{dg_i}{dt} = \frac{1}{\Delta v} \sum_{\alpha=1}^{d} (F^\alpha_{i+1/2} - F^\alpha_{i-1/2}) =: DF_{i-1/2}, \tag{3.11}$$

with

$$F^\alpha_{i+1/2} = \tilde{\mathcal{M}}_{i+e_\alpha/2} \frac{1}{\Delta v} \left(\frac{g_{i+e_\alpha}}{\mathcal{M}_{i+e_\alpha}} - \frac{g_i}{\mathcal{M}_i} \right) = \tilde{\mathcal{M}}_{i+e_\alpha/2} D \left(\frac{g}{\mathcal{M}} \right)_{i+e_\alpha/2},$$

where e_α is the α-*th* canonical vector of $\mathbb{R}^d$, $\mathcal{M}_i$ is the projection of the normalized Maxwellian on the mesh,

$$\mathcal{M}_i = \frac{1}{(2\pi)^{d/2}} \exp\left(-|\xi|^2/2\right),$$

and

$$\tilde{\mathcal{M}}_{i+e_\alpha/2} = \frac{\mathcal{M}_i\, \mathcal{M}_{i+e_\alpha}}{\mathcal{M}_{i+e_\alpha} - \mathcal{M}_i} \left(\log(\mathcal{M}_{i+e_\alpha}) - \log(\mathcal{M}_i) \right).$$

Here D denotes the discrete divergence. The approximation $f_{\Delta v}$ of the distribution function f is then obtained by

$$f_i(t) = f_{\Delta v}(t, u(t) + w(t)\, \xi_i) = g_i(t),$$

where u and $w = \sqrt{T}$ are given by (3.9).

The properties of the above numerical method can be formalized as follows

Proposition 3.1. *Let us consider the Fokker-Planck equation (3.8) and apply the numerical method (3.11) to the rescaled distribution function g. Then,*

1. *$g_i(t)$ is a mass, momentum and energy conservative and entropic approximation to (3.10);*
2. *steady states $\mathcal{M}_{\rho, u_\infty, T_\infty}$ are exactly preserved;*
3. *if the initial data is a Maxwellian, the evolution of $f_{\Delta v}$ is then exactly computed from (3.11).*

Proof. It is easy to check that this approximation corresponds to the discretization of the weak formulation of the Fokker-Planck equation

$$\sum_i \frac{dg_i}{dt}\, \varphi_i = -\sum_i D\varphi_{i+1/2} \cdot \tilde{\mathcal{M}}_{i+1/2} D \left(\frac{g}{\mathcal{M}} \right)_{i+1/2},$$

From this formulation, we prove that mass, zero mean velocity and temperature are conserved [4]. Moreover, this scheme is constructed to be entropic decaying : let us take $\varphi = \log(g)$, we get

$$\begin{aligned}
&\sum_i \frac{d}{dt}\left(g_i \log(\frac{g_i}{\mathcal{M}_i})\right) \\
&= -\sum_i D\left(\log(\frac{g}{\mathcal{M}})\right)_{i+1/2} \tilde{\mathcal{M}}_{i+1/2} D\left(\frac{g}{\mathcal{M}}\right)_{i+1/2}, \\
&= -\frac{1}{\Delta v^2}\sum_i \left(\log(\frac{g_{i+e_\alpha}}{\mathcal{M}_{i+e_\alpha}}) - \log(\frac{g_i}{\mathcal{M}_i})\right) \tilde{\mathcal{M}}_{i+e_\alpha/2}\left(\frac{g_{i+e_\alpha}}{\mathcal{M}_{i+e_\alpha}} - \frac{g_i}{\mathcal{M}_i}\right) \\
&= -\frac{1}{\Delta v^2}\sum_i \left(\log(\frac{g_{i+e_\alpha}}{\mathcal{M}_{i+e_\alpha}}) - \log(\frac{g_i}{\mathcal{M}_i})\right) \tilde{\mathcal{M}}_{i+e_\alpha/2}\left(\frac{g_{i+e_\alpha}}{\mathcal{M}_{i+e_\alpha}} - \frac{g_i}{\mathcal{M}_i}\right).
\end{aligned}$$

Using the approximation $\tilde{\mathcal{M}}_{i+e_\alpha/2}$ and the fact that log is a nondecreasing function, we get the decay of the relative entropy. Finally, such a scheme provides the correct equilibrium state.

The assertion (3) directly follows from the rescaling equation and the steady state conservation. Indeed, if the initial data f_0 is a Maxwellian, the rescaled initial data $g(0)$ becomes a normalized Maxwellian with zero mean velocity and with a temperature equal to one. Thus, this initial data is exactly preserved by the scheme (3.11), whereas the mean velocity and temperature evolution is given by (3.9). □

3.1. **Numerical results.**

Sum of two Maxwellian distributions in 3D. The initial data is now chosen as the sum of two Maxwellian functions

$$f_0(v) = \frac{1}{2}\frac{5}{(2\,\pi\,v_{th}^2)^{3/2}}\left[\exp\left(-\frac{|v-v_1|^2}{2\,v_{th}^2}\right) + \exp\left(-\frac{|v-v_2|^2}{2\,v_{th}^2}\right)\right],$$

with $v_1 = (0,2,2)$, $v_2 = (0,-2,-2)$ and the thermal velocity is $v_{th} = 2$. The final time of the simulation is $T_{end} = 6$, which correspond to the equilibrium of the distribution. In Fig.1 we report the evolution of the moments of the distribution function with respect to v obtained with $n = 24$ points and compare them to a reference solution computed with many points. We compare the two numerical results with and without the rescaling methods. It is clear that the rescaling method allows to follow accurately the drift and the spreading of the distribution function when time goes on.

4. Application to the granular Boltzmann equation

4.1. **the granular Boltzmann equation.**

In absence of external forces the time evolution of a granular medium can be described at the kinetic level by the inelastic Boltzmann equation (Cf.[2])

$$Q(f,f) = Q^+(f,f) - Q^-(f,f), \tag{4.12}$$

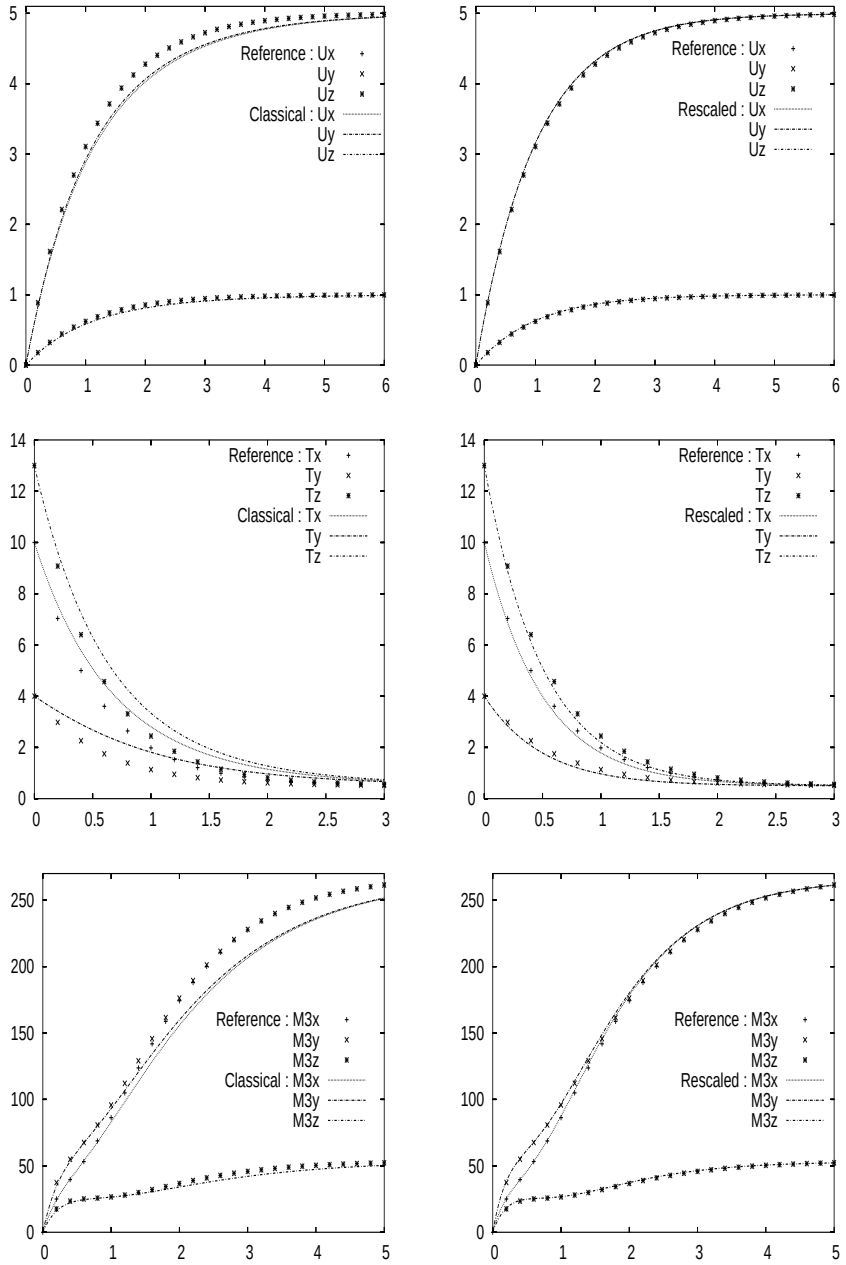

FIGURE 1. Evolution of the mean velocity, the temperature components and the third moments of f with respect to v with $n = 24$ points: classical (left) and rescaled variables (right)

where the loss term is given by

$$Q^-(f,f) = L[f]\, f, \quad \text{with } L[f] = |S^{d-1}|\, f * |v|^\lambda. \tag{4.13}$$

where the asterisk denotes the convolution, and the gain term reads

$$Q^+(f,f) = \int_{\mathbb{R}^d} \int_{S^{d-1}} {}'f\, {}'f_* J\ |v - v_*|^\lambda dn dv_*, \tag{4.14}$$

where ${}'f = f(t,{}'v)$, ${}'f_* = f(t,{}'v_*)$, and J is related to the Jacobian of the transformation from post-collisional to pre-collisional velocities, $(v, v_*) \to ({}'v, {}'v_*)$. In the general case, we only know the inverse transformation given by, but for constant restitution coefficient e, is given by

$$J = \frac{1}{e^2} \frac{|{}'v - {}'v_*|^\lambda}{|v - v_*|^\lambda}.$$

In this case an amount of energy is lost during the collision process and the solution converges to a Dirac measure, whereas mass and mean velocity are conserved with time.

To study more accurately the convergence to the equilibrium (as the behavior of the tail of the distribution function), we perform the change of variable in velocity (2.4). Here, mass and momentum are conserved with time, but the energy is dissipated. Then, g is solution to the following inelastic Boltzmann equation with a drift term

$$\frac{\partial g}{\partial t} - \frac{1-e^2}{4} \frac{\partial (\xi g)}{\partial \xi} = w^\lambda\, Q(g,g), \tag{4.15}$$

where $Q(g,g)$ is given by (4.12). Using this new formulation, we now treat the problem with the two unknowns g and $w(t)$, the latter satisfying Eq.(2.7)

$$\frac{dw}{dt} = \frac{w^{d+1}}{2\, d\, \rho} \left(\int_{\mathbb{R}^d} \tilde{Q}(g,g)\, |\xi|^2\, d\xi \right).$$

We first only consider the inelastic Boltzmann equation for Maxwellian molecules, where the solution formally converges to Dirac delta equilibrium state. We perform this test to check the accuracy of the spectral method by checking the evolution of the temperature which is analytically given by

$$T(t) = T_0\, \exp(-\gamma\, t), \tag{4.16}$$

where T_0 is the initial temperature and $\gamma = (1-e^2)/2$. In this simple case, the evolution of T is not directly coupled with the distribution function g and is computed from (4.16) (see left picture in Fig. 2). Up to a change of variable, we can always consider an initial data f_0 with a mass equal to one, a zero mean velocity and a temperature equal to one. Then, the solution g to (4.15) satisfies

$$\int_{\mathbb{R}} g(t,\xi) \begin{pmatrix} 1 \\ \xi \\ \xi^2 \end{pmatrix} d\xi = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

and the equilibrium state is given by the Lorentz function

$$g_\infty(\xi) = \frac{2}{\pi\,(1+\xi^2)^2}. \tag{4.17}$$

4.2. **Numerical results.** In this section we present several numerical results obtained by approximating (4.15). The Boltzmann operator is discretized using a spectral method [5], whereas the approximation of the drift term is realized through fourth order centered differences. The fourth order scheme has proved to be accurate enough in all the test cases here presented.

Note however that the equilibrium state is still quite difficult to approximate because of the slow zero convergence of the tails. Indeed, the third moment of g is blowing-up at $t = +\infty$. To illustrate the slow convergence of the tail we present in Fig. 2 the evolution of the third moment

$$M_3(t) = \int_{\mathbb{R}} g(t,\xi)|\xi|^3 d\xi$$

with respect to the truncation of the distribution function $V = V_{max}$ and to the number of Fourier modes N. We also present the evolution of the distribution function $g(t)$ in these new variables obtained with an uniform grid (256 points). As expected, the solution converges to (4.17) and the spectral method give the correct behavior of the tail even if it converges slowly to zero. Finally, in Fig.3, we plot the numerical solution corresponding to initial data (i) :

$$g_0(\xi) = \frac{1}{\sqrt{2\pi}}\exp(-|\xi|^2/2),$$

and (ii) :

$$g_0(\xi) \;=\; \frac{1}{2\sigma\sqrt{2\pi}}\left(\exp\left(-\frac{|\xi-3\sigma|^2}{2\sigma^2}\right)+\exp\left(-\frac{|\xi+3\sigma|^2}{2\sigma^2}\right)\right),\ \sigma^2 = 1/10.$$

We observe the very good agreement between the numerical solution and the stationary Lorentz function (4.17). In Figure 4 we present a comparison between the long time behavior of the rescaled solution (in conventional variables) and the solution obtained with the non rescaled method. It is evident how the Dirac delta is well captured by means of the scaling technique.

5. Conclusion

In this paper we present an accurate deterministic method for the numerical approximation of space homogeneous, time dependent Boltzmann equation. The method couples an accurate scheme (finite difference or spectral methods) for the treatment of the rescaled distribution function with additional equations for macroscopic quantities (mean velocity and/or energy).

It possesses a high order of accuracy for this kind of problems. The high accuracy is evident from the quality of the numerical results that can be obtained with a relatively small

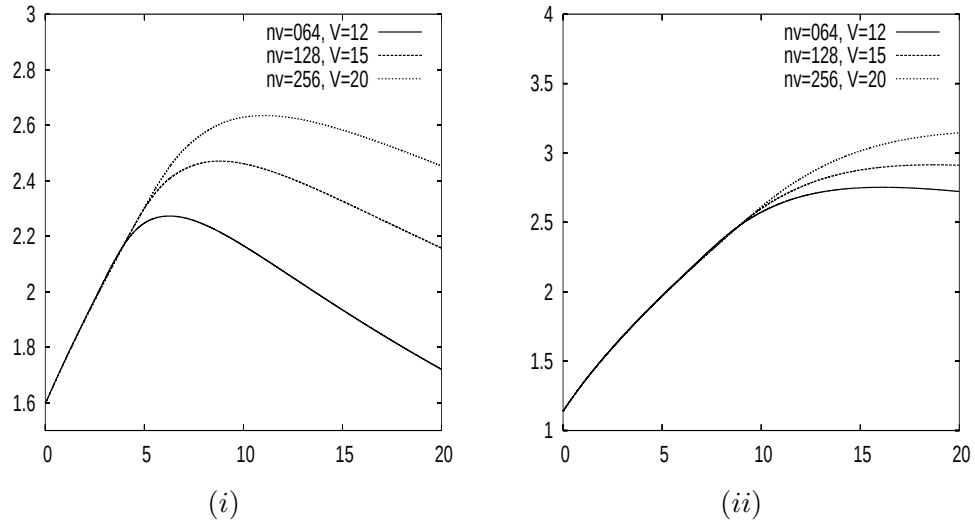

FIGURE 2. 1D Inelastic Maxwellian Molecules: blow-up of the third order moment of the rescaled distribution g corresponding to (i) and (ii).

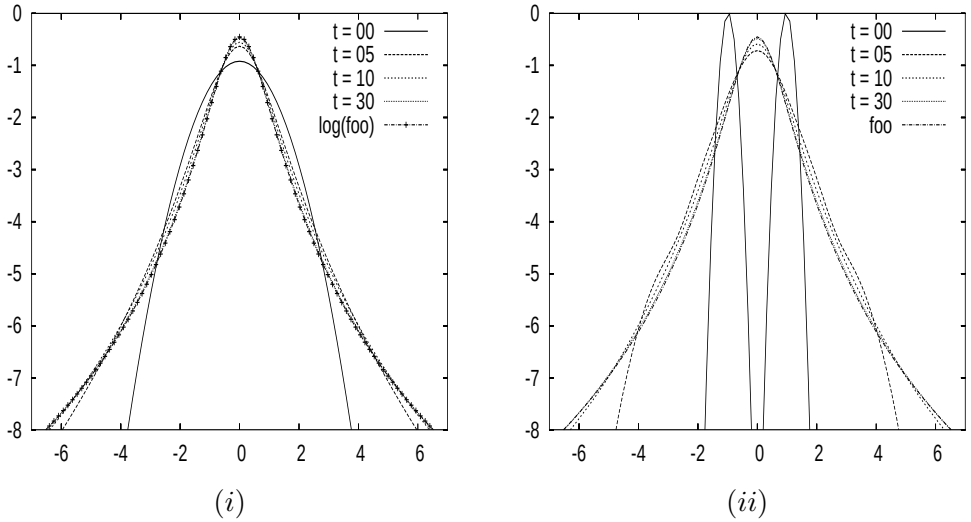

FIGURE 3. 1D Inelastic Maxwellian Molecules: time evolution of the log-solution corresponding to initial data (i) and (ii) in rescaled variables and f_∞ denotes the Lorentz function

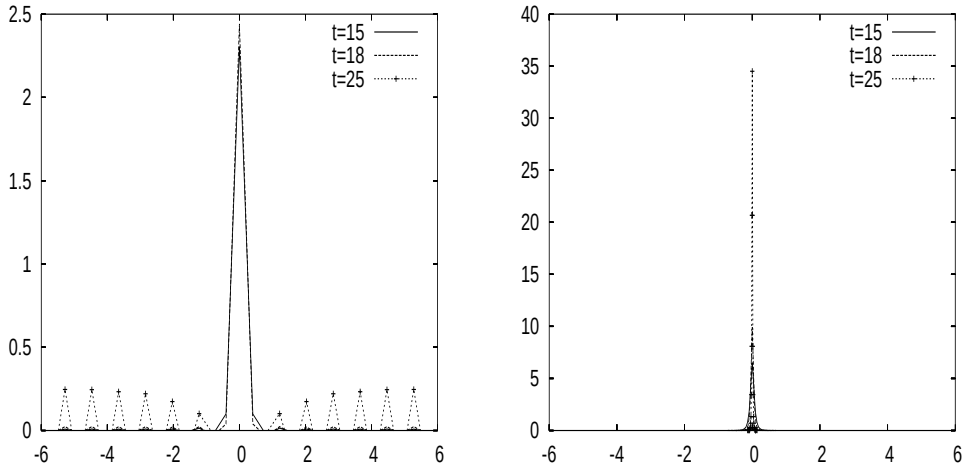

FIGURE 4. 1D Inelastic Maxwellian Molecules: comparison of the large time solution corresponding to initial data (i) obtained from computations in classical variables (a) and from rescaled variables (b).

number of grid points in velocity domain. Finally, comparison with classical techniques show the effectiveness of the present method for a wide class of problems.

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