Numerical Analysis of Levermore's Moment System

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INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

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N ° 3124

THÈME 4

ISSN 0249-6399

INRIA
ROCQUENCOURT

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Thème 4 — Simulation et optimisation
de systèmes complexes
Projet M3N

Rapport de recherche n ° 3124 — Mars 1997 — 33 pages

Abstract: The simulation of transitional gas flow near rarefied regimes requires new models which can describe kinetic effects but which are less complex than the original Boltzmann equation. The strategy introduced by Levermore [1] rewrites the Boltzmann equations as a system of moment equations, with a new closure procedure. We recall here the mathematical properties of this Levermore's moment systems. Boundary conditions derived from the kinetic theory are proposed. Based on these properties, we present an original first-order kinetic scheme with explicit flux splitting and implicit source terms. A 14-moments system model is tested to simulate one-dimensional gas flows (Couette flow and normal shock wave) near the transitional regime.
Acknowledgements : This work was supported by CEA-CESTA.

Key-words: Moment's system, Boltzmann, kinetic boundary conditions, kinetic schemes, entropy, Navier-Stokes

(Résumé : tsvp)

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Analyse numérique des systèmes aux moments de Levermore.

Résumé : La simulation des écoulements dans l'atmosphère en régime transitionnel nécessite de nouveaux modèles décrivant les effets cinétiques mais moins complexes que les équations de Boltzmann. La stratégie de Levermore [1] utilise un système d'équations aux moments issus des équations de Boltzmann, fermé par un nouveau modèle exponentiel de fonction de distribution. Nous rappelons ici, les propriétés mathématiques de ce système aux moments de Levermore. Des conditions aux limites dérivées de la théorie cinétique sont proposées. Ces propriétés nous ont amenés à proposer un schéma cinétique construit à l'aide d'une décomposition de flux explicite et d'un terme source implicite. Le système aux 14 moments est testé sur différentes applications numériques d'écoulements monodimensionels (problèmes de choc, écoulements de Couette), en régime transitionnel.
Remerciements : Ce travail a été financé en grande partie par le CEA-CESTA.

Mots-clé : Systèmes aux moments, Boltzmann, conditions aux limites cinétiques, schéma cinétique, entropie, Navier-Stokes

1 Introduction

A gas may be modeled at either the macroscopic or the microscopic scale. We consider the gas at the microscopic level, as a myriad of discrete particles characterized by their velocity and position. The mathematical model at this level is the Boltzmann equation, which describes the evolution of the velocity distribution of these particles. This equation may be effectively solved numerically via Monte Carlo methods. Unfortunately, this numerical solution requires a discretisation grid whose step is at most of the order of a particle mean free path (average distance covered by a particle between two collisions). For dense gases, this length is very small compared to the macroscopic scale and the numerical solution of Boltzmann equations becomes impossible. We must abandon this kinetic model in favor of fluid dynamics. We regard then the gas as a continuous medium and the description is modeled by the fluid variables (typically the mass density, the fluid velocity, and the temperature) whose evolution will be governed either by Euler equations or by Navier-Stokes equations. In the regime that lies between molecular flow and fluid dynamics, the so-called transitional regime characterized by a Knudsen number (the ratio of the mean free path to the macroscopic scale) of order 10^{-3} to 10^{-1}, difficulties appear. Because of the computational cost in both time and storage, Monte Carlo methods are not practical but on the other hand fluid dynamics equations are not sufficiently accurate in boundary layers or across shock fronts. The first strategy used to describe such regimes, splits the gas flow in two regions: low density region, in which Monte Carlo methods must be used and fluid region, in which the velocity distribution of particle approaches the local equilibrium and then fluid equations can be used. This strategy has been proposed at INRIA in [16] for coupling Boltzmann and Euler equations and in [6] and [25] for coupling Boltzmann and Navier-Stokes.
Another strategy uses equations in moments obtained by a weighted velocity integration of the Boltzmann equations and close these equations by assuming a given a-priori expansion of the unknown velocity distribution in terms of these moments. The resulting moments system is then a combination of standard conservation laws and of additional relaxation equations, function of the collision operator, and generalizing the usual constitutive laws of fluid dynamics. Such a strategy was used by H.Grad [3], with thirteen moment equations and a velocity distribution modeled by generalized Hermite polynomials. However, the resulting closed system was not always hyperbolic and velocity distribution model could be negative, which is inconsistent with the underlying physical model.
Because the closed moment system must have a certain number of mathematical and physical properties, D.Levermore [1] has proposed new models for the velocity

distribution in the form : $exp(\underline{\alpha}.\underline{m}(\underline{v}))$. This paper presents a numerical analysis of these models and illustrate then by running some numerical applications.
After a brief discussion about kinetic theories, we will recall, in a second part, Levermore's ideas and discuss the mathematical properties of the resulting system. Consistent boundary conditions are then proposed, based on the conditions satisfied by the underlying kinetic model. Based on this mathematical analysis, we propose in the third part a first-order kinetic numerical scheme in order to solve this system. Numerical simulations of shock problems and Couette flows are finally presented to validate the 14 moments model.

2 Kinetic theories

2.1 Boltzmann equation

Let us consider the case of a gas composed of identical monoatomic particles contained within a fixed spatial domain Ω. This gas is described at the kinetic level by the Boltzmann equation. This equation governs the evolution of the distribution function $f = f(\underline{x}, \underline{v}, t)$ over the particle phase space $\Omega \times I\!R^3$ by

$$\partial_t f(\underline{x}, \underline{v}, t) + v.\partial_x f(\underline{x}, \underline{v}, t) = Q(f, f)(\underline{x}, \underline{v}, t). \tag{1}$$

The nonnegative distribution function f describes the local density of particles with position $\underline{x}$ and velocity $\underline{v}$. The operator $Q(f, f)(\underline{x}, \underline{v}, t)$ which describes the collision between the particles has the following properties:
First, this operator is assumed to have mass, velocity and energy, $\phi(\underline{v}) = 1\ ,\ \underline{v}\ ,\ \frac{1}{2}||v||^2$, as conserved quantities, that is

$$\int_{\underline{v} \in R^3} Q(f)(\underline{x}, \underline{v}, t)\phi(\underline{v}) d\underline{v} = 0.$$

Second, it satisfies the local dissipation relation

$$\int_{\underline{v} \in R^3} Q(f)(\underline{x}, \underline{v}, t) \log f d\underline{v} \leq 0, \tag{2}$$

which leads to the celebrated H-Theorem.

2.2 H-Theorem

Let us introduce the local entropy function,

$$\eta = \int_{\underline{v} \in R^3} H(f)(\underline{x}, \underline{v}, t) d\underline{v} \tag{3}$$

and the local entropy flux,

$$\psi = \int_{\underline{v} \in R^3} \underline{v}.H(f)(\underline{x}, \underline{v}, t) d\underline{v}, \tag{4}$$

with $H(f) = f \log f - f$ where f is the solution to the Boltzmann equation.
The total entropy is defined by

$$\mathcal{H} = \int_\Omega \eta dx.$$

After multiplication of the Boltzmann equation by $\log f(\underline{v}, \underline{x}, t)$, integration over the particle phase space $\Omega \times IR^3$, and use of the local dissipation relation (2), we obtain the entropy inequality

$$\partial_t \mathcal{H} - \int_{\partial\Omega} \psi.n dS \leq 0,$$

satisfied for any given domain Ω.
If we suppose now that there is no incoming entropy flux, we obtain the H-theorem,

$$\partial_t \mathcal{H} \leq 0,$$

proving entropy dissipation in any admissible evolution of a closed gas system.

2.3 Local equilibrium

At the equilibrium, the distribution f is invariant in space and time, and thus from the Boltzmann equation, the collision term must satisfy $Q(f) = 0$. We then deduce that the distribution function f is a Maxwellian

$$f(\underline{v}) = \mathcal{M} = \rho(\frac{m}{2\pi kT})^{3/2} \exp(-\frac{m}{2kT}(\underline{v} - \underline{u})^2), \tag{5}$$

where k is the Boltzmann constant, m the particle mass ($r = \frac{k}{m}$), T the gas temperature, and $\underline{u}$ the gas average velocity.

2.4 BGK model

Because of the complicated form of the collision operator, Bhatnagar, Gross and Krook have proposed a simple model for $Q(f, f)$, which describes the relaxation of f to the local equilibrium $\mathcal{M}$ by

$$Q(f) = \frac{1}{\varepsilon}(\mathcal{M}(f) - f) \tag{6}$$

with a relaxation time scale ε proportional to the Knudsen number, and $\mathcal{M}(f)$ the Maxwellian which has the same density, velocity and energy as f.

3 Moment Closure and Levermore's models

3.1 Moments system

In general, the derivation of moment equations begins with the choice of a finite dimensional linear subspace $\mathcal{E}_m$ of functions of $\underline{v}$, with basis elements $m_i(\underline{v})$. Then, the moment system is obtained by integrating Boltzmann equation over the vector $m(\underline{v}) = (m_i(\underline{v}))_{i\in\mathcal{E}_m}$ yielding,

$$\partial_t < \underline{m} f > + div(< \underline{m} \otimes \underline{v} f >) =< \underline{m}.Q(f) >, \tag{7}$$

where $< g >$ denotes the integral of $g d\underline{v}$ over the velocity space. Since each equation introduces a flux $< \underline{m} \otimes \underline{v} f >$ which can only be evaluated by the next equation, the system is not closed. Moment closures must be found such that the resulting system respects physical symmetries (translation and rotation invariance), recovers the proper fluid dynamical approximations and such that the resulting moment can be realized by some non-negative distribution. These goals can be fulfilled if $\mathcal{E}_m$ satisfies the following conditions:

(I) span $\{1, v, v^2\} \in \mathcal{E}_m$.

(II) $\mathcal{E}_m$ is invariant under the action of translations T_u and rotations T_o defined by $T_u F = T_u F(v) = F(v-u)$ *et* $T_o F = F(O^T v)$.

For Levermore's models, an additional property is required, using the convex cone

$$\mathcal{E}_m^c = \{\underline{m}\in\mathcal{E}_m; \int_{I\!R^d} \exp(-\underline{m}(\underline{v}))d\underline{v} < \infty\},$$

(III) $\mathcal{E}_m^c$ has an nonempty interior in $\mathcal{E}_m$.

Examples of such admissible spaces with maximal degree two are

$$\begin{aligned} \mathcal{E}_m &= span\ \{1, v, v^2\}, \\ \mathcal{E}_m &= span\ \{1, v, v\otimes v\}. \end{aligned}$$

and for maximal degree four, we can use

$$\mathcal{E}_m = span\ \{1, v, v\otimes v, v^2.v, v^4\}.$$

3.2 Levermore's models

Once an admissible $\mathcal{E}_m$ has been defined, D.Levermore [1] closes the moment system (7) by assuming that the distribution function f can be replaced by

$$F(\underline{\alpha}, \underline{v}) = \exp(\underline{\alpha}.\underline{m}(\underline{v})), \tag{8}$$

with $\underline{m}(v) \in \mathcal{E}_m$ and

$$\underline{\alpha} = \underline{\alpha}(x,t) \in I\!R_c^M = \{\alpha_i \in I\!R, 1 \leq i \leq M \ , \ \int_{v \in I\!R^d} \exp(\underline{\alpha}.\underline{m}(v))dv < +\infty\}.$$

The resulting system of moments

$$\partial_t < \underline{m} \exp(\underline{\alpha}.\underline{m}) > + div(< \underline{m} \otimes \underline{v} \exp(\underline{\alpha}.\underline{m}) >) =< \underline{m} Q(\exp(\underline{\alpha}.\underline{m})) >, \tag{9}$$

is the system proposed by Levermore. It contains m equations for m unknowns α. We discuss now its properties.

Theorem 3.1 *Model (8) is nonnegative by construction, and it corresponds to the formal solution of the entropy constrained minimization problem:*

$$J(F) = J(\exp(\underline{\alpha}.\underline{m}(v))) = \min_{f \in \mathcal{X}} \{ \int_{I\!R^d} (f \log(f) - f) d\underline{v} \ ; \ \int_{I\!R^d} \underline{m} f dv \ \textit{fixed in} \ I\!R^M \ \}$$

over the space $\mathcal{X}$ defined by

$$\mathcal{X} = \{f \in L^2(I\!R^d), f \log(f) \in L^2(I\!R^d), f \geq 0\}. \tag{10}$$

Here, the α_i are the Lagrange multipliers of the minimization constraints, fixing $\int_{I\!R^d} \underline{m} f dv$, and $J(f) = \int_{\underline{v} \in I\!R^d} (f \log(f) - f) d\underline{v}$ is the usual entropy function of the kinetic theory.

Proof

As in Levermore, let us introduce the two operators J and $\underline{\mathcal{L}}$ defined by

$$J(f) = \int_{I\!R^d} (f \log(f) - f) d\underline{v},$$

$$\underline{\mathcal{L}}(f) = \int_{I\!R^d} \underline{m} f d\underline{v},$$

and suppose the existence of a solution F in $\mathcal{X}$ of the above minimization problem. If the solution is sufficiently regular, it satisfies the first order optimality conditions

$$J'(F).g = \underline{\alpha}.\underline{\mathcal{L}}'(F).g, \forall g \in L^2(I\!R^d),$$

where $\underline{\alpha} = (\alpha_i)_{i=1}^M$ are the Lagrange multipliers associated to the constraints

$$\underline{\mathcal{L}}(f) = cte.$$

This writes

$$\int_{\underline{v}\in IR^d} g.(log(F)+F/F-1)d\underline{v} = \underline{\alpha}.\int_{v\in IR^d} g.\underline{m}(\underline{v})d\underline{v}, \forall g \in L^2(IR^d).$$

Thus, we get

$$F = \exp(\underline{\alpha}.\underline{m}(\underline{v})).$$

The solution F is unique because of the strict convexity of the functional $J(f)$ and of the convexity of the set $\mathcal{X}$.

3.3 Hyperbolicity

Let us note the moments by

$$U_\alpha(\underline{\alpha}) =< \underline{m}\exp(\underline{\alpha}.\underline{m}) >= \underline{\mathcal{L}}(F) = \frac{\partial < \exp(\underline{\alpha}.\underline{m}) >}{\partial\alpha} = \frac{\partial U}{\partial\alpha},$$

the fluxes by

$$A_\alpha(\underline{\alpha}) =< \underline{m}\otimes\underline{v}\exp(\underline{\alpha}.\underline{m}) >= \frac{\partial < \underline{v}\exp(\underline{\alpha}.\underline{m}) >}{\partial\alpha},$$

and the collision moments by

$$S(\underline{\alpha}) =< \underline{m}.Q(\exp(\underline{\alpha}.\underline{m})) > .$$

With this notation, the system (9) takes the form :
Find $\underline{\alpha}(\underline{x},t) \in IR_c^M$, such as

$$\partial_t U_\alpha(\underline{\alpha}) + divA_\alpha(\underline{\alpha}) = S(\underline{\alpha}) \ . \tag{11}$$

If the solution $\underline{\alpha}$ is locally smooth, we can develop (11) into

$$U_{,\alpha\alpha}.\partial_t\underline{\alpha} + A_{,\alpha\alpha}.\bigtriangledown_x\underline{\alpha} = S(\underline{\alpha}).$$

By construction, $U_{,\alpha\alpha}$ is symmetric positive definite as the Hessian of the strictly convex function U and $A_{,\alpha\alpha}$ is symmetric as the Hessian of $A(\underline{\alpha}) =< \underline{v}\exp(\underline{\alpha}.\underline{m}) >$. So the system (11) is symmetrisable and thus hyperbolic.
We also have the following property:

Theorem 3.2 *(I) We can find a pair of entropy functions $\eta(U_\alpha)$ and $\Phi(U_\alpha)$, with η convex, which verify the condition*

$$\nabla_{U_\alpha}\eta(U_\alpha).\,\nabla_{U_\alpha} A_\alpha = \nabla_{U_\alpha}\Phi(U_\alpha). \tag{12}$$

This pair is defined from the Legendre-Fenschel transformation of U:

$$\eta(\underline{V}) = \inf_{\alpha}(\underline{\alpha}.\underline{V} - U(\underline{\alpha})) = \underline{\alpha}(\underline{V}).\underline{V} - U(\underline{\alpha}(\underline{V})), \tag{13}$$

$$\Phi(\underline{V}) = (\underline{\alpha}.A_\alpha - A)(\underline{\alpha}(\underline{V})), \tag{14}$$

with $\underline{\alpha}(\underline{V})$ the solution of (13), that is of $U_\alpha(\underline{\alpha}(\underline{V})) = \underline{V}$.
(II) Each solution of (11) satisfies the following entropy inequality

$$\partial_t\eta(U_\alpha) + div\Phi(U_\alpha) \leq 0. \tag{15}$$

Proof (I) The Legendre-Fenschel transformation of U is convex by definition, and by construction satisfies

$$\nabla_{U_\alpha}\eta(U_\alpha) = \underline{\alpha}(U_\alpha).$$

Similarly, a direct calculation of derivatives yields

$$\nabla_{U_\alpha}\Phi(U_\alpha) = A_\alpha.\frac{\partial\underline{\alpha}}{\partial U_\alpha} + \underline{\alpha}.\frac{\partial A_\alpha}{\partial U_\alpha} - A_\alpha.\frac{\partial\underline{\alpha}}{\partial U_\alpha}.$$

Thus, we have

$$\nabla_{U_\alpha}\Phi(U_\alpha) = \frac{\partial A_\alpha(\underline{\alpha}(U_\alpha))}{\partial U_\alpha},$$

from which we easily deduce the relation (12)

$$\nabla_{U_\alpha}\eta(U_\alpha).\,\nabla_{U_\alpha} A_\alpha(U_\alpha) = \nabla_{U_\alpha}\Phi(U_\alpha).$$

(II) Let $\underline{\alpha}$ be the solution of (11) and $U_\alpha(\underline{\alpha})$ the corresponding moments. We multiply system (11) by $\underline{\alpha}$ on the left, and find

$$\partial_t(\underline{\alpha}.U_\alpha) - U_\alpha.\partial_t\underline{\alpha} + div(\underline{\alpha}.A_\alpha) - A_\alpha.\,\nabla_x\,\underline{\alpha} = \underline{\alpha}.S(\underline{\alpha}). \tag{16}$$

Moreover, since we have

$$U_\alpha.\partial_t\underline{\alpha} = \partial_\alpha U.\partial_t\underline{\alpha} = \partial_t U$$

and similarly

$$A_\alpha.\,\nabla_x\,\underline{\alpha} = \nabla_\alpha A.\,\nabla_x\,\underline{\alpha} = divA,$$

equation (16) reduces to the following form

$$\partial_t(\underline{\alpha}.U_\alpha - U) + div(\underline{\alpha}.A_\alpha - A) = \underline{\alpha}.S(\underline{\alpha}) \ .$$

The local dissipation relation for the collision operator $Q(F)$

$$< Q(F).LogF > \leq 0$$

could be written with $F = \exp(\underline{\alpha}.\underline{m})$

$$\underline{\alpha}.S(\underline{\alpha}) \leq 0,$$

and implies the following conclusion

$$\partial_t \eta(U_\alpha) + div\Phi(U_\alpha) \leq 0.$$

Remark 3.3 *From Theorem 3.1, the entropy function of (11)*

$$\eta(U_\alpha) = \alpha.U_\alpha - U$$

is the minimum of all entropy functions $J(f) = \int_{\underline{v} \in I\!R^d} f\log(f) - f d\underline{v}$ *subject to the constraint that the moments* $< \underline{m}f >$ *are fixed. Indeed, the solution of the minimization problem (Th 3.1) has the form* $\exp(\underline{\alpha}.\underline{m}(\underline{v}))$.
Thus, the minimum of all entropy functions is equal to

$$J(\exp(\underline{\alpha}.\underline{m}(\underline{v}))) = \int_{\underline{v} \in I\!R^d} \underline{\alpha}.\underline{m}(\underline{v}).\exp(\underline{\alpha}.\underline{m}(\underline{v}))dv - \int_{\underline{v} \in I\!R^d} \exp(\underline{\alpha}.\underline{m}(\underline{v}))dv.$$

By definition of U *and* U_α*, this writes*

$$J(\exp(\underline{\alpha}.\underline{m}(v))) = \underline{\alpha}.U_\alpha(\underline{\alpha}) - U = \eta(U_\alpha).$$

3.4 Boundary Conditions

The weak form in space of system (11) is obtained by direct integration by part and is given by

$$\int_\Omega \phi.\partial_t U_\alpha dx - \int_\Omega \partial_x \phi.A_\alpha dx$$
$$- \int_{\partial\Omega} \phi.\{A_\alpha^+.\underline{n} + A_\alpha^-.\underline{n}\}d\gamma = \int_\Omega \phi.S_\alpha dx, \ \forall \phi \in C^1(\overline{\Omega}),$$

where $\underline{n}$ is the inward unit normal vector to $\partial\Omega$.
The incoming/outgoing half-fluxes are defined here by

$$A_\alpha^{+/-} = \int_{\underline{v}.\underline{n}\geq 0/\underline{v}.\underline{n}\leq 0} \underline{m} \otimes \underline{v} F d\underline{v}.$$

The above system is a first order system in space.
In order to have consistent boundary conditions on the boundary $\partial\Omega$ of the computational domain Ω, we have to characterize the incoming half-fluxes A^+. At inflow, this value is imposed from inflow boundary conditions specifing the incoming distribution F.
For the full Boltzmann equation, the proper wall boundary condition specifies the reflected (or incoming) "half" of the distribution function f^+ when the incident f^- (or outgoing) half is given. A classical wall boundary condition is the one in which a certain fraction $k(\underline{x})$ of the incident particles, depending on its position, is specularly reflected, and the remaining particles are absorbed by the wall and re-emitted with a Maxwellian (5) distribution associated to the temperature T_p and velocity $\underline{u}_p$ of the wall. This condition can be written

$$f^+(\underline{x},\underline{v}) = k(\underline{x}).f^-(\underline{x},\mathcal{R}\underline{v}) + (1-k(\underline{x})).M(\rho,T_p,\underline{u}_p), \tag{17}$$

where $\mathcal{R}$ is the reflection operator defined by

$$\mathcal{R}\underline{v} = \underline{v} - 2(\underline{v}.\underline{n})\underline{n}.$$

The "density of the wall" is determined by the condition that the wall does not collect particles,

$$\int_{v\in IR^d} \underline{v}.\underline{n}(f^- + f^+)(\underline{x},\underline{v})d\underline{v} = 0. \tag{18}$$

In (17), the specular reflection corresponds to $k(\underline{x}) = 1$ and total accommodation corresponds to $k(\underline{x}) = 0$.
We suppose now for simplicity that the boundary is perpendicular to the x direction. In order to evaluate the incoming half-fluxes A^+ on the wall, we suppose that the kinetic boundary conditions (17) are still valid in flux average, if we replace f, solution of the full Boltzmann equation, by the Levermore's model F. So, we find

$$\int_{IR^2}\int_{v_x\geq 0} \underline{m}(\underline{v})(F^+(\underline{x},\underline{v}) - k(\underline{x}).F^-(\underline{x},\mathcal{R}\underline{v}) - (1-k(\underline{x})).M(\rho,T_p,\underline{u}_p))v_x d\underline{v} = 0$$

with

$$\int_{v\in IR^d} (F^- + F^+)(\underline{x},\underline{v})v_x d\underline{v} = 0. \tag{19}$$

With this choice, the boundary conditions imposed to system (11) consist in imposing the incoming half flux A^+, with A^+ imposed at inflow and the incoming fluxes A^+ evaluated by

$$A^+ = \int_{IR^2} \int_{v_x \geq 0} (k(\underline{x}) F^-(\underline{x}, \mathcal{R}\underline{v}) + (1 - k(\underline{x})) M(\rho, T_p, \underline{u}_p)) \underline{m}(\underline{v}) \otimes \underline{v} d\underline{v}, \tag{20}$$

at any given wall, with density of $\mathcal{M}$ given by (19), that is $(A_\rho^+ + (A_\rho^-).\underline{n} = 0$.

4 First-order numerical scheme for the unidimensional system

We propose to take advantage of the kinetic structure of (11) to approach its exact solution by a first-order kinetic scheme with source term. This scheme is written as a time integration formula with explicit flux splitting and implicit source term. It was introduced by B.Perthame [11] for the compressible Euler equations.

4.1 Description

We build a time approximation of (11) in the following way. Let Δt be a small time step. We are given the moment U_α^n at time $t^n = n\Delta t$ and we obtain numerically the associated distribution

$$F^n(x, \underline{v}) = exp(\underline{\alpha}(x, t^n).\underline{m}(\underline{v}))$$

by solving the entropy minimization problem (Th 3.1) subject to the constraint that

$$\int_{IR^d} m(\underline{v}) F^n(x, \underline{v}) d\underline{v} = U_\alpha^n. \tag{21}$$

Then, we solve the kinetic equation

$$\begin{cases} \partial_t f + v_x.\partial_x f = Q(f) \\ f(x, t^n, \underline{v}) = F^n(x, \underline{v}) \end{cases} \tag{22}$$

with $t \in [n\Delta t, (n+1)\Delta t]$ and $\underline{v} = (v_x, v_y, v_z)$, in two steps:

(1) The linear transport equation

$$\begin{cases} \partial_t f + v_x.\partial_x f = 0 \\ f(x, t^n, \underline{v}) = F^n(x, \underline{v}) \end{cases}$$

with solution

$$\tilde{f}(x,t,\underline{v}) = F^n(x - v_x(t-t^n),\underline{v}), \tag{23}$$

is first advanced from time t^n to time t^{n+1}.

(2) The collision equation

$$\begin{cases} \partial_t f = Q(f)(x,\underline{v},t) \\ f(x,t^n,\underline{v}) = \tilde{f}(x,t^{n+1},v), \end{cases}$$

is then solved between t^n and t^{n+1} by a first order implicit scheme in time, yielding

$$f(x,t^{n+1},\underline{v}) = \tilde{f}(x,t^{n+1},\underline{v}) + \Delta t Q(f)(x,t^{n+1},\underline{v}). \tag{24}$$

By combination of the solutions (23) and (24), we obtain a consistent $O(\Delta t^2)$ approximation of the solution of (22) given by

$$f^{n+1}(x,\underline{v}) = F^n(x - v_x(t^{n+1}-t^n),\underline{v}) + \Delta t Q(f^{n+1})(x,\underline{v}). \tag{25}$$

Then, the quantities (moments of f^{n+1})

$$U_\alpha^{n+1} = \int_{IR^d} m(\underline{v}).F^n(x - v_x\Delta t,\underline{v})d\underline{v} + \Delta t \int_{IR^d} m(\underline{v}).Q(f^{n+1})(x,\underline{v})d\underline{v}, \tag{26}$$

are first-order (in Δt) approximations of the solution to (11). In order to write the numerical scheme based on this approximation, we finally replace at each time step the moments U_α^n by their cell averages

$$U_{\alpha,j}^n = \frac{1}{\Delta x}\int_{\Omega_j} U_\alpha^n dx, \tag{27}$$

over the cells Ω_j of a given mesh size $\Delta x = x_{j+1/2} - x_{j-1/2}$. We have then to compute the average of U_α^{n+1} over the same cells, which amounts to average f^{n+1} over each cell after (25).

Lemma 4.1 *Under the CFL condition*

$$\Delta t \leq \frac{\Delta x}{v_x^{max}}, \tag{28}$$

the scheme (21-27) is a conservative scheme of the form

$$U_{\alpha,j}^{n+1} - U_{\alpha,j}^n = -\sigma(\mathcal{A}_{j+1/2}^n - \mathcal{A}_{j-1/2}^n) + \Delta t.S_{\alpha,j}^{n+1}, \tag{29}$$

with $\sigma = \frac{\Delta t}{\Delta x}$, $\mathcal{A}_{j+1/2} = \mathcal{A}(U_j, U_{j+1}, \sigma)$, *a specifie flux function and* v_x^{max} *a velocity to be specified later.*

Proof By definition, we have

$$U_\alpha = \int_{IR^d} m(\underline{v}).F(x,t,\underline{v})d\underline{v},$$

$$A_\alpha = \int_{IR^d} v_x.m(\underline{v}).F(x,t,\underline{v})d\underline{v},$$

$$S_\alpha = \int_{IR^d} m(\underline{v}).Q(F)(x,t,\underline{v}))d\underline{v}.$$

Averaging (26) over the cell Ω_j yields

$$U^{n+1}_{\alpha,j}\Delta x = \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{IR^d} m(\underline{v}).F^n(x - v_x\Delta t, \underline{v})d\underline{v}dx$$
$$+ \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{IR^d} m(\underline{v}).Q(f^{n+1}(x,\underline{v}))d\underline{v}dx.$$

Because $F^n(x - v_x(t-t^n), \underline{v})$ is the exact solution of (22), the first integral can be written

$$\int_{x_{j-1/2}}^{x_{j+1/2}} \int_{IR^d} m(\underline{v}).F^n(x - v_x\Delta t, \underline{v})d\underline{v}dx = \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{IR^d} m(\underline{v}).F^n(x,\underline{v})d\underline{v}dx$$
$$+ \int_{t^n}^{t^{n+1}} \{\int_{IR^d} v_x.m(\underline{v}).F^n(x_{j-1/2} - v_x(t-t^n), \underline{v})d\underline{v}$$
$$- \int_{IR^d} v_x.m(\underline{v}).F^n(x_{j+1/2} - v_x(t-t^n), \underline{v})d\underline{v}\}dt.$$

The second term, by definition, is

$$\int_{x_{j-1/2}}^{x_{j+1/2}} \int_{IR^d} m(\underline{v}).Q(f^{n+1}(x,\underline{v}))d\underline{v}dx = \Delta x S^{n+1}_{\alpha,j}.$$

In general, this term depends only on $U^{n+1}_{\alpha,j}$. For example, for the so-called BGK model (6), we have

$$S^{n+1}_{\alpha,j} = \frac{1}{\varepsilon}(\int \underline{m}\mathcal{M}(U^{n+1}_{\alpha,j}) - U^{n+1}_{\alpha,j}).$$

Altogether, we get

(30)
$$U^{n+1}_{\alpha,j}\Delta x = U^n_{\alpha,j}\Delta x + \Delta t\Delta x S^{n+1}_{\alpha,j}$$
$$- \int_{t^n}^{t^{n+1}} \int_{IR^d} v_x.m(\underline{v}).F^n(x_{j+1/2} - v_x(t-t^n), \underline{v})d\underline{v}dt$$
$$+ \int_{t^n}^{t^{n+1}} \int_{IR^d} v_x.m(\underline{v}).F^n(x_{j-1/2} - v_x(t-t^n), \underline{v})d\underline{v}dt.$$

(31)

Moreover, using the exponential decreasing of $F(\underline{\alpha}, \underline{v})$ in $\underline{v}$, we assume that

$$\exists v_x^{max} \text{ and } \epsilon \geq 0, \text{ such as } \forall v_x > v_x^{max} \ , \ F(\alpha, \underline{v}) \leq \epsilon.$$

So, the CFL condition (28) ensures that the v-integration in the integrals (of F^n) written before, is limited to v_x such as $v_x \leq v_x^{max}$, i.e.,
$v_x \Delta t \leq v_x^{max} \Delta t \leq \Delta x$.
This means that $x_{j+1/2} - v_x(t-t^n)$ (resp. $x_{j-1/2} - v_x(t-t^n)$) remains almost always in the cell neighboring $x_{j+1/2}$ (resp. $x_{j-1/2}$). If we now define for $k = j-1, j, j+1$,

$$A_k^{n,+} = \int_{v_x>0} v_x.m(v).F^n(x_k, \underline{v})d\underline{v},$$

$$A_k^{n,-} = \int_{v_x<0} v_x.m(\underline{v}).F^n(x_k, \underline{v})d\underline{v},$$

we can write

$$\int_{t^n}^{t^{n+1}} \int_{I\!R^d} v_x m(\underline{v}) F^n(x_{j+1/2} - v_x(t-t^n), \underline{v}) d\underline{v} dt = \Delta t (A_{j+1}^{n,-} + A_j^{n,+})$$

and our numerical scheme writes finally

$$U_{\alpha,j}^{n+1} = U_{\alpha,j}^n - \frac{\Delta t}{\Delta x}(A_j^{n,+} + A_{j+1}^{n,-} - A_{j-1}^{n,+} - A_j^{n,-}) + \Delta t S_{\alpha,j}^{n+1}. \tag{32}$$

4.2 Stability and entropy condition.

Theorem 4.2 *Under the assumptions and notation of Lemma 4.1, the numerical scheme (21-27) is stable, or more precisely, all the moments $U_{\alpha,j}^{n+1}$ are associated to a positive distribution function.*

Proof We will prove the conservation of the positiveness of the function $f(x, \underline{v})$ at each time step. First of all, $F^n(x, \underline{v}) = exp(\underline{\alpha}.\underline{m}(\underline{v}))$ is positive. Moreover, f^{n+1} is computed by combining the solution to the linear transport equation (23), $F^n(x - v_x(t^{n+1} - t^n), \underline{v})$, which is positive by definition, and the collision equation (24). The collision operator $Q(f)(x, \underline{v})$ in the Boltzmann equation (or BGK equation) may be expressed as a summation of a term, proportional to $f(x, t, \underline{v})$, which describes the loss due to the collision and a gain term $G(f)$ which is always positive,

$$Q(f)(x, \underline{v}) = -\lambda(f).f + G(f) \ , \ G(f) \geq 0, \ \lambda(f) \geq 0.$$

Thus, (25) takes the form

$$f^{n+1}(x,\underline{v}) = F^n(x - v_x(t^{n+1} - t^n), \underline{v}) + \Delta t(-\lambda(f^{n+1})f^{n+1} + G(f^{n+1})) \ ,$$

or more precisely

$$f^{n+1}(x,\underline{v})(1 + \Delta t\lambda(f^{n+1})) = F^n(x - v_x(t^{n+1} - t^n), \underline{v}) + G(f^{n+1}).$$

The positiveness of $f^{n+1}(x,\underline{v})$ clearly appears on this expression. Consequently, we have shown that each moment $U^{n+1}_{\alpha,j}$ is the average of a positive distribution function

$$U^{n+1}_{\alpha,j} = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}}\int_{I\!R^d} m(\underline{v})f^{n+1}(x,\underline{v})d\underline{v}dx = \int_{I\!R^d} m(\underline{v}).\frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} f^{n+1}dxd\underline{v}.$$

In particular, all moments of even degree are positive.
Let us conclude this section by the following theorem concerning the entropy in our numerical scheme.

Theorem 4.3 *Each step of our numerical scheme is entropic for the entropy function* $\eta(U_\alpha)$.

Proof As seen before, our numerical scheme could be splitted into three steps

- The construction of $F^n(x,\underline{v})$ by (21),
- The free transport step (23),
- The collision equation (24).

Let us define the entropy of (11)

$$\int_{I\!R^d} H(f)(x,t,\underline{v})d\underline{v}$$

where $H(f) = flogf - f$ for all $f \in \mathcal{X}$.
• The construction of $F^n(x,\underline{v})$ is clearly entropic because the model $exp(\alpha.m(\underline{v}))$ minimizes the entropy among all distribution functions generating the same moments (Th 3.1). Then, this minimum defined by

$$\eta(U^n_\alpha) = \alpha.U^n_\alpha - U^n$$

verifies

$$\forall x, t^n \ , \ \eta(U_\alpha^n) \leq \int_{I\!R^d} H(f^n)(x, \underline{v}) d\underline{v},$$

with f^n is the cell averaged distribution obtained at the end of step n.

• Since

$$\partial_t(flogf - f) + v.\partial_x(flogf - f) = (\partial_t f + v.\partial_x f)logf = 0 \ ,$$

we can prove that, during the free transport step between t^n et t^{n+1} , $H(\tilde{f})$ satisfies

$$(33) \qquad \begin{cases} \partial_t H(f)(x, t, \underline{v}) + v.\partial_x H(f)(x, t, \underline{v}) = 0 \\ \\ H(f)(x, t^n, \underline{v}) = H(F^n)(x, \underline{v}) \ . \end{cases}$$

Then, after integration in time and in velocity, we have

$$\int_{I\!R^d} H(\tilde{f})(x, t^{n+1}, \underline{v}) d\underline{v} = \int_{I\!R^d} H(F^n)(x, \underline{v}) d\underline{v} - \int_{t^n}^{t^{n+1}} \int_{I\!R^d} v.\partial_x H(f)(x, t, \underline{v}) d\underline{v} dt \ .$$

Now, we average over cells Ω_j (between $x_{j-1/2}$ and $x_{j+1/2}$), and setting

$$\tilde{\eta}_j^{n+1} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \tilde{\eta}^{n+1},$$

we obtain

$$\begin{aligned} \tilde{\eta}_j^{n+1} &= \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{I\!R^d} H(\tilde{f})(x, t^{n+1}, \underline{v}) d\underline{v} dx \\ &= \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{I\!R^d} H(F^n)(x, \underline{v}) d\underline{v} dx \\ &- \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \int_{I\!R^d} \int_{t^n}^{t^{n+1}} v.\partial_x H(f)(x, t, \underline{v}) dt d\underline{v} dx. \end{aligned}$$

Moreover, we have

$$\begin{aligned} &\int_{x_{j-1/2}}^{x_{j+1/2}} \int_{I\!R^d} \int_{t^n}^{t^{n+1}} v.\partial_x H(f)(x, t, \underline{v}) dt d\underline{v} dx \\ &\quad = \int_{t^n}^{t^{n+1}} \int_{I\!R^d} v.H(f)(x_{j+1/2}, t, \underline{v}) d\underline{v} dt - \int_{t^n}^{t^{n+1}} \int_{I\!R^d} v.H(f)(x_{j-1/2}, t, \underline{v}) d\underline{v} dt \ . \end{aligned}$$

And because $H(f)(x,\underline{v},t)$ is the exact solution to (33) between t^n and t^{n+1}, we find out

$$\int_{t^n}^{t^{n+1}} \int_{IR^d} v.H(f)(x_{j+1/2},t,\underline{v})d\underline{v}dt = \int_{t^n}^{t^{n+1}} \int_{IR^d} v.H(F^n)(x_{j+1/2}-v_x(t-t^n))d\underline{v}dt \ .$$

Defining the numerical entropy flux at $x_{j+1/2}$ by

$$\Phi^n_{j+1/2} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \int_{IR^d} v.H(F^n)(x_{j+1/2}-v_x(t-t^n))d\underline{v}dt \ , \tag{34}$$

and at $x_{j-1/2}$ by

$$\Phi^n_{j-1/2} = \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} \int_{IR^d} v.H(F^n)(x_{j-1/2}-v_x(t-t^n))d\underline{v}dt, \tag{35}$$

and because $F^n = exp(\alpha(x,t^n),\underline{v})$ is the minimum function of the entropy $\eta^n_j(U\alpha)$, we write

$$\eta^n_j(U\alpha) = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} \int_{IR^d} H(F^n)(x,\underline{v})d\underline{v}dx. \tag{36}$$

We can conclude that the entropy satisfies in the free transport step the numerical conservation law

$$\tilde{\eta}^{n+1}_j - \eta^n_j(U\alpha) + \sigma(\Phi^n_{j+1/2} - \Phi^n_{j-1/2}) = 0 \ . \tag{37}$$

• The solution (24) of the collision equation is

$$f^{n+1}(x,v) = \tilde{f}^{n+1}(x,\underline{v}) + \Delta t.Q^{n+1}(f)(x,\underline{v}).$$

After multiplication by $log(f^{n+1}(x,\underline{v}))$ (which is legitimate because $f^{n+1}(x,\underline{v}) \geq 0$), we get

$$\begin{aligned} f^{n+1}.log(f^{n+1})(x,\underline{v}) &= \tilde{f}^{n+1}.log(f^{n+1})(x,\underline{v}) \\ &+\Delta t.log(f^{n+1}).Q^{n+1}(f)(x,\underline{v}). \end{aligned} \tag{38}$$

Moreover, the concavity of the logarithm function implies

$$log(f) \leq log(g) + \frac{1}{g}(f-g) \ , \forall f,g \in IR^+. \tag{39}$$

Using (39) with $\tilde{f}^{n+1}$ and f^{n+1}, and after the integration of (38) over the velocity space, we obtain

$$\int_{IR^d}(f^{n+1}.log(f^{n+1}) - f^{n+1}(x,\underline{v}))d\underline{v} \leq$$
$$\int_{IR^d}(\tilde{f}^{n+1}.log(\tilde{f}^{n+1}) - \tilde{f}^{n+1})(x,\underline{v})d\underline{v} + \int_{IR^d}\Delta t.log(f^{n+1}).Q^{n+1}(f)(x,\underline{v})d\underline{v}$$

Because $Q(f)$ is assumed to satisfy the local dissipation relation

$$\int_{IR^d} Q(f).logf(x,\underline{v},t)d\underline{v} \leq 0,$$

we obtain over each cell j,

$$\eta_j^{n+1}(f^{n+1}) \leq \tilde{\eta}_j^{n+1}.$$

Finally, since $H(f)$ is a concave function, replacing f^{n+1} by its space average also decreases the entropy, which proves the decreasing of the entropy η in the third part of the scheme.

4.3 Local construction of $F(x,\underline{v},t^n) = exp(\underline{\alpha}.\underline{m}(\underline{v}))$

The first step of our numerical scheme is the evaluation of $F = \exp(\underline{\alpha}.\underline{m})$ with known moments $U_\alpha^n =< m_\alpha.F >$. As we said before, there is no explicit relation between $F(x,\underline{v},t^n)$ and U_α^n for admissible spaces $\mathcal{E}_m$ of maximal degree four or more.
To compute α, let us introduce the function

$$J(\underline{\beta}) =< \exp(\underline{\beta}.\underline{m}) > - \sum_i \beta_i.U_{\alpha_i}^n,$$

with gradient

$$\frac{\partial J}{\partial \beta_i} =< m_i \exp(\underline{\beta}.\underline{m}) > -U_{\alpha_i}^n.$$

This function is strictly convex because the Hessian matrix

$$(\frac{\partial^2 J}{\partial_{\beta_i}\partial_{\beta_j}}) = \int_{\underline{v}\in IR^d} m_i m_j exp(\underline{\beta}.\underline{m})d\underline{v}$$

is definite positive. Indeed, for every $\underline{w} \in IR^M$ we have

$$\underline{w}^T J_{\beta\beta}\underline{w} = \int_{\underline{v}\in IR^d} \underline{w}^T \underline{m}\underline{m}^T \underline{w} exp(\underline{\beta}.\underline{m})d\underline{v} = \int_{\underline{v}\in IR^d} (\underline{w}^T.\underline{m})^2 exp(\underline{\beta}.\underline{m})d\underline{v} \geq 0,$$

with equality if and only if $\underline{w} = 0$.
Therefore the equation that we have to solve

$$\frac{\partial J}{\partial \beta_i} = 0$$

has at most a solution which will then be the unique minimizer of $J(\underline{\beta})$ over IR^M. In other words, the calculation of F with known moments reduces to the α-minimization problem

$$\mathcal{P}_{\underline{\alpha}} : Find\ \underline{\alpha} \in IR^M\ such\ as\ J(\underline{\alpha}) = \min_{\underline{\beta} \in IR^M} J(\underline{\beta})$$

which we achieve numerically by a Newton algorithm.

Remark 4.4 *The positiveness of the moments U_α of even degree produced by the kinetic scheme is a necessary condition to the existence of a solution to $\mathcal{P}_{\underline{\alpha}}$.*

4.4 Discretization of the velocity space

In order to evaluate the half-fluxes

$$A_\alpha^{+/-} = \int_{v_x \geq 0 / v_x \leq 0} v_x \underline{m}(\underline{v}) F(\alpha(x,t), \underline{v}) d\underline{v},$$

in our numerical scheme and the Hessian matrix

$$J_{\alpha\alpha}(\alpha) = \int_{IR^d} \underline{m}(\underline{v}) \underline{m}(\underline{v})^T F(\alpha(x,t), \underline{v}) d\underline{v},$$

for the local construction of $F(x, \underline{v}, t^n) = \exp(\underline{\alpha}.\underline{m}(\underline{v}))$ in the minimization problem $\mathcal{P}_{\underline{\alpha}}$ by the Newton method, numerical integration rules must be used. Indeed, for most of Levermore's models (typically model constructed with exponential of polynomials of degrees greater than 4), these integrals are impossible to evaluate explicitly. The first integration rule chosen was the trapezoidal rule. Because $F(x, \underline{v}, t^n)$ decreases to zero if $\underline{v}$ goes to infinity, we can construct an interval $I_v \in IR^+$ such as

$$\int_{||\underline{v}|| > I_v} |g(\underline{v}) F(\alpha(x,t), \underline{v})| d\underline{v} < \epsilon\ ,\ \epsilon \in IR,$$

where $g(\underline{v})$ is a polynomial. Then, a trapezoidal rule can be constructed over this finite interval I_v. However, in three dimensions, because of the computational cost, we have abandoned the trapezoidal rule in favor of more efficient Gaussian formula.

4.4.1 Weights and integration points for the 3D Gaussian rule

We can assume that in most interesting transitional regimes the distribution function $F(x, \underline{v}, t^n)$ is close to the Maxwellian equilibrium function $\mathcal{M}(x, t, \underline{v})$ (5). Therefore, we may choose a numerical integration rule which will be exact for the moments relative to a Maxwellian. In other words, we choose weights P_i and nodes $\underline{v_i}$ such that

$$\int_{I\!R^d} m(\underline{v}).\mathcal{M}(x,t,\underline{v})d\underline{v} = \sum_{i=1}^{n} P_i m(\underline{v_i})\mathcal{M}(x,t,\underline{v_i}).$$

In order to calculate these weights and integration points, we use the following strategy: First, using the symmetry of the Maxwellian and the symmetry of the domain of integration, we change Cartesian components into spherical components,

$$v_x = \sqrt{2RT}r\cos\theta\cos\phi + u_x,$$

$$v_y = \sqrt{2RT}r\sin\theta\cos\phi + u_z,$$

$$v_z = \sqrt{2RT}r\sin\phi + u_z.$$

Then, the 3-dimensional integrals split into produts of the following one-dimensional integrals,

$$\int_{-\infty}^{+\infty} r^{n+2}e^{-r^2}dr, \qquad \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \cos^{k1}\theta\sin^{k2}\theta d\theta, \qquad \int_{-\frac{\pi}{2}}^{+\frac{\pi}{2}} \cos^{k1+k2+1}\phi\sin^{k3}\phi d\phi.$$

The h-points integration formula is given by A.H.Stroud et Don Secrest [13] for the first integral. This rule is exact for polynomials that are of degree smaller than 2h-1. After change of variable $s2 = \sin\theta$ and $s3 = \sin\phi$, the second and the third integral are reduced to weighted polynomial integration over the integral [-1,+1] to be computed by Tschebyscheff and Legendre quadrature rules respectively. Altogether, the integration rule is for all function $F(\alpha(x,t), \underline{v})$,

$$\int_{I\!R^d} m(\underline{v})F(\alpha(x,t),\underline{v})d\underline{v} \approx \sum_{i=1}^{h}\sum_{j=1}^{h_1}\sum_{l=1}^{h_2} P_{ijl}m(\underline{v}_{ijl})F(\alpha(x,t),\underline{v}_{ijl}). \tag{40}$$

Here, the weights and integration points are deduced from the weights P_k and nodes r_i,$\sin\theta_j$,$\sin\phi_l$ corresponding to the 3 quadrature formulas, by

$$P_{ijl} = P_i.e^{+r_i^2}P_jP_l(2RT)^{3/2},$$

$$v_{x,ijl} = \sqrt{2RT} r_i \cos\theta_j \cos\phi_l + u_x,$$
$$v_{y,ijl} = \sqrt{2RT} r_i \sin\theta_j \cos\phi_l + u_z,$$
$$v_{z,ijl} = \sqrt{2RT} r_i \sin\phi_l + u_z.$$

5 The 14-moments closure

The linear space $\mathcal{E}_m^{14} = \{1, \underline{v}, \underline{v}\otimes\underline{v}, v^2\underline{v}, v^4\}$ is the smallest admissible space generating a closure system which recovers formally the correct Navier-Stokes approximation by asymptotic expansion. The dimension of $\mathcal{E}_m^{14}$ is (d+1)(d+4)/2 in general, that is fourteen when d=3. The model takes the form

$$F^{14} = F^{14}(\underline{\alpha}) = exp(\alpha^{(0)} + \alpha_i^{(1)} v_i + \alpha_{ij}^{(2)} v_i v_j + \alpha_i^{(3)} v^2 v_i + \alpha^{(4)} v^4) \tag{41}$$

where $i, j = 1, .., 3$ and where (k) denotes the degree of function $m(\underline{v})$. The resulting system is then given by

$$\begin{cases} \partial_t < F^{14} > + \nabla_x . < \underline{v} F^{14} > & = 0, \\ \partial_t < \underline{v} F^{14} > + \nabla_x . < \underline{v} \otimes \underline{v} F^{14} > & = 0, \\ \partial_t < \underline{v} \otimes \underline{v} F^{14} > + \nabla_x . < \underline{v} \otimes \underline{v} \otimes \underline{v} F^{14} > & =< \underline{v} \otimes \underline{v}\ Q(F^{14}) >, \\ \partial_t < v^2 \underline{v} F^{14} > + \nabla_x . < v^2 \underline{v} \otimes \underline{v} F^{14} > & =< v^2 \underline{v}\ Q(F^{14}) >, \\ \partial_t < v^4 F^{14} > + \nabla_x . < v^4 \underline{v} F^{14} > & =< v^4\ Q(F^{14}) > . \end{cases}$$

In order to write each equation in term of macroscopic quantities, we recall some definitions. As well known, the zeroth moment is the density

$$\rho(\underline{x}, t) =< F^{14} > .$$

The velocity can be defined by

$$\underline{u}(\underline{x}, t) = \frac{1}{\rho} < \underline{v} F^{14} > .$$

Let us introduce now the intrinsic velocity $\underline{c}(\underline{x}, \underline{v}, t) = \underline{v} - \underline{u}(\underline{x}, t)$. Clearly,

$$< \underline{c} F^{14} >= 0. \tag{42}$$

Second, third, and fourth c-moments are respectively

$$< \underline{c} \otimes \underline{c} F^{14} >= -\underline{\underline{\sigma}}, \tag{43}$$

which defines the Cauchy stress tensor $\underline{\underline{\sigma}}$,

$$\underline{\underline{\underline{Q}}} =< \underline{c} \otimes \underline{c} \otimes \underline{c} F^{14} >, \tag{44}$$

and

$$\mathcal{R} =< \underline{c} \otimes \underline{c} \otimes \underline{c} \otimes \underline{c} F^{14} > . \tag{45}$$

These moments define the pressure

$$p = \frac{1}{d} < c^2 F^{14} >= -\frac{1}{d} tr(\underline{\underline{\sigma}}), \tag{46}$$

the viscous stress tensor,

$$\underline{\underline{\tau}} = p\underline{\underline{Id}} + \underline{\underline{\sigma}} = \frac{1}{d} < c^2 F^{14} > - < \underline{c} \otimes \underline{c} F^{14} > \ . \tag{47}$$

and the heat flux,

$$\underline{q} =< c^2 \underline{c} F^{14} > . \tag{48}$$

By contraction of (45), we introduce the auxiliary moments

$$\underline{\underline{R}} =< c^2 \underline{c} \otimes \underline{c} F^{14} >, \tag{49}$$

$$r =< c^4 F^{14} >, \tag{50}$$

and we define

$$s =< c^4 \underline{c} F^{14} > . \tag{51}$$

With this notation, the moments in the 14-moments closure write

$$< \underline{m} F^{14} >= U_\alpha = \begin{cases} \rho \\ \rho \underline{u} \\ \rho \underline{u} \otimes \underline{u} - \underline{\underline{\sigma}} \\ \rho u^2 \underline{u} - tr(\underline{\underline{\sigma}}) \underline{u} - 2\underline{\underline{\sigma}}.\underline{u} + \underline{q} \\ \rho u^4 - 2tr(\underline{\underline{\sigma}}) u^2 - 4(\underline{\underline{\sigma}}.\underline{u}).\underline{u} + 4\underline{q}.\underline{u} + r \end{cases}$$

$$< v \otimes \underline{m} F^{14} >= A_\alpha = \begin{cases} \rho \underline{u} \\ \rho \underline{u} \otimes \underline{u} - \underline{\underline{\sigma}} \\ (\rho \underline{u} \otimes \underline{u} \otimes \underline{u})_{sym} - 3 \underline{\underline{\sigma}} \otimes \underline{u}_{sym} + \underline{\underline{\underline{Q}}} \\ \rho u^2 \underline{u} \otimes \underline{u} - tr(\underline{\underline{\sigma}}) \underline{u} \otimes \underline{u} - 4((\underline{\underline{\sigma}}.\underline{u}) \otimes \underline{u})_{sym} - \underline{\underline{\sigma}} u^2 \\ \qquad +2 \underline{\underline{\underline{Q}}}.\underline{u} + 2(\underline{q} \otimes \underline{u})_{sym} + \underline{\underline{R}} \\ \rho u^4 \underline{u} - 2tr(\underline{\underline{\sigma}}) u^2 \underline{u} - 4\underline{u}.(\underline{\underline{\sigma}}.\underline{u}) \underline{u} - 4(\underline{\underline{\sigma}}.\underline{u}) u^2 \\ \qquad +4(\underline{q}.\underline{u}).\underline{u} + 2\underline{q} u^2 + 4(\underline{\underline{\underline{Q}}}.\underline{u}).\underline{u} + r\underline{u} + 4\underline{\underline{R}}.\underline{u} + \underline{s} \end{cases}$$

and

$$S = \begin{cases} 0 \\ 0 \\ \Xi_3(\rho, \underline{u}, \underline{\underline{\sigma}}) \\ \Xi_4(\rho, \underline{u}, \underline{\underline{\sigma}}, \underline{q}) \\ \Xi_5(\rho, \underline{u}, \underline{\underline{\sigma}}, \underline{q}, r), \end{cases}$$

where Ξ_i are the moments of the collision operator

$$\Xi_i =< m_i(\underline{v}) Q(F^{14}) > .$$

5.1 Approximation of the collision operator

The classical approximation of the collision operator in the Boltzmann equation is the BGK relaxation operator,

$$Q(F^{14}) = \frac{\rho RT}{\mu}(\mathcal{M}(F^{14})(x,v,t) - F^{14}(\alpha, v)) \tag{52}$$

which gives the correct Navier-Stokes viscosity μ when $\mathcal{M}(F^{14})$ and F^{14} have the same first moments. The associated heat conduction is given by $\kappa = \frac{d+2}{2} R\mu$ which corresponds to a gas with Prandtl number

$$Pr = \frac{d+2}{2} \frac{R\mu}{\kappa} = 1.$$

For most gases, we have $Pr \leq 1$. Thus, this approximation will generally not give the correct Navier-Stokes heat conduction. To obtain the right conduction, Levermore has introduced a generalized BGK collision operator of the form

$$Q(f) = \frac{\rho RT}{\mu}(\mathcal{M}(x,v,t) - F^{14}(\alpha, v))$$

$$+\left(\frac{(d+2)}{2}\frac{\rho R^2 T}{\kappa}-\frac{\rho RT}{\mu}\right)(\mathcal{G}(\alpha',v)-F^{14}(\alpha,v))$$

$$=\frac{\rho RT}{\mu}(\mathcal{M}(x,v,t)-\mathcal{G}(\alpha',v))+\frac{d+2}{2}\frac{\rho R^2 T}{\kappa}(\mathcal{G}(\alpha',v)-F^{14}(\alpha,v)) \tag{53}$$

where

$$\mathcal{G}(\alpha',v)=exp(\alpha'_0+\alpha'_i.v_i+\alpha'_{ij}.v_iv_j)$$

is the quadratic Gaussian closure [1] obtained from the 10 first moments of F^{14}. In this case, the collision operator can be calculated easily after computing the fourteen moments of the Maxwellian $\mathcal{M}$ and the Gaussian $\mathcal{G}$, and we find

$$\Xi=\left\{\begin{array}{l}0\\0\\\frac{\rho RT}{\mu}(p\underline{\underline{Id}}+\underline{\underline{\sigma}})\\\frac{\rho RT}{\mu}2(p\underline{\underline{Id}}+\underline{\underline{\sigma}}).\underline{u}-P_r\frac{\rho RT}{\mu}\underline{q}\\\frac{\rho RT}{\mu}(4p||u||^2+4\underline{u}.\underline{\underline{\sigma}}\underline{u}-\frac{2}{\rho}\underline{\underline{\sigma}}:\underline{\underline{\sigma}}+6\frac{p^2}{\rho})-P_r\frac{\rho RT}{\mu}(4\underline{q}.\underline{u}+r-\frac{2}{\rho}\underline{\underline{\sigma}}:\underline{\underline{\sigma}}-9\frac{p^2}{\rho})\end{array}\right\}.$$

6 Numerical tests

We test below the 14-moments model in a physical configuration close to the transition regime, and our results are compared with those of a Monte Carlo simulation performed by G.A.Bird [20].

6.1 The shock wave

The first simulation considers a one-dimensional steady shock wave. This shock wave involves the transition from a upstream supersonic flow (subscripts (l)) to a downstream subsonic flow (subscripts (d)). The shock Mach number ($Mach$) is defined by the ratio of the speed of the upstream gas to the speed of sound in this gas, $Mach=U_g/c$,where $c^2=\gamma RT_g$ with $\gamma=5/3$.
The gas is Argon with Prandtl number equal to 2/3. This gas is initialized in the two regions with the following Rankine-Hugoniot conservation relations

$$T_g=\frac{u_{xg}^2}{\gamma Mach^2}\frac{1}{R}$$

$$\rho_d = \frac{4Mach^2}{Mach^2+3}\rho_g \qquad ux_d = \frac{Mach^2+3}{4Mach^2}ux_g$$

$$T_d = \frac{(Mach^2+3)(5Mach^2-1)}{16Mach^2}T_g.$$

Then, the gas, at equilibrium has the following distribution function:

$$F_{g/d}(x,\underline{v},0) = \mathcal{M}(x,\underline{v},0) = \frac{\rho_{g/d}(x)}{(2\pi RT_{g/d}(x))^{3/2}}\exp(-\frac{(\underline{v}-\underline{u}_{g/d}(x))^2}{2RT_{g/d}(x)}).$$

The one-dimensional domain Ω is discretized with 100 identical cells whose length is equal to $0.01m$. The shock wave is made stationary in the middle of the domain Ω, by imposing the values of the moments in the extreme cells of the domain Ω.

Results

The CFL number is equal to 1. The results at convergence are obtained as soon as

$$||U_\alpha^{n+1} - U_\alpha^n||_{L^2} \leq 10^{-14}.$$

A wave with a shock Mach number of 1.2 in Argon at $273.K$ has been chosen as first case. The results are obtained after 500 iterations. The results for the density and temperature profiles are compared in Fig 1,2 with the predictions of a DSMC simulation or of a Navier-Stokes solver. The normalized value is defined by

$$h^N = \frac{h-h_g}{h_d-h_g}.$$

As expected, the three sets of results are in good agreement for this very weak wave. The corresponding results for a shock Mach number of two are shown in fig 3,4. In this case, 1293 iterations have been used to obtain convergence. The local Knudsen number is in this case greater than 0.1, and then there should be clear errors in the Navier-Stokes profiles, as confirmed by DSMC. The 14-moments model results are closed here to the Boltzmann simulation.

14-MOMENTS MODEL D.S.M.C. and Navier-stokes

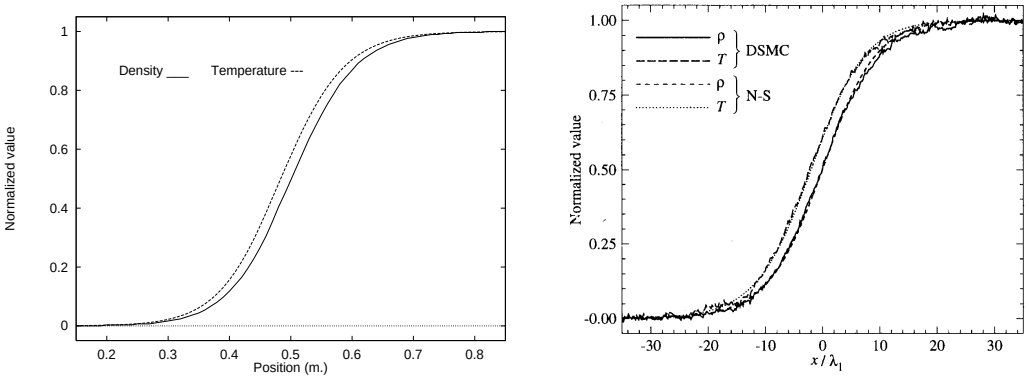

Figure 1, 2 : Temperature and density profiles in argon with $Mach = 1.2$

14-MOMENTS MODEL D.S.M.C. and Navier-stokes

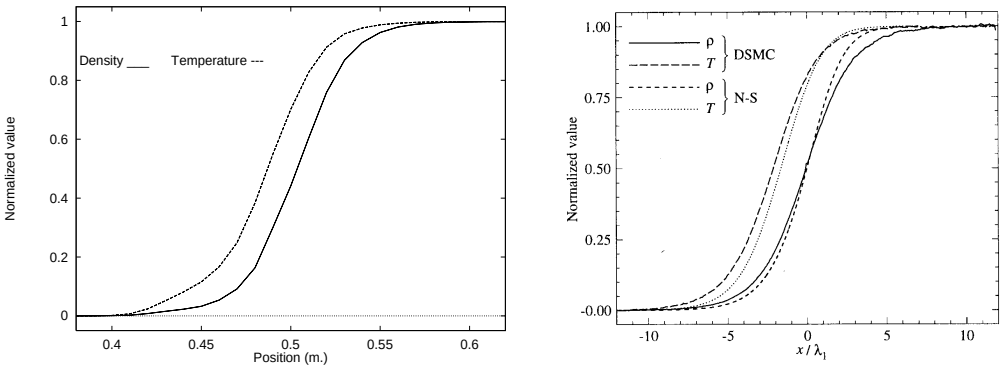

Figure 3, 4 : Temperature and density profiles in argon with $Mach = 2$.

6.2 Plan Couette flow

This second application is a one-dimensional steady flow. Plan Couette flow is the flow between two plane parallel surfaces, one of which is at rest and the other is moving. The surfaces, distant of 1 m., define a domain which we divide in 100 cells. Both boundary conditions are derived from the total accommodation kinetic conditions. This is performed by setting $k(x) = 0.$ and, temperature and velocity values to wall values in the Maxwellian in (20). The gas (Argon) is initially at equilibrium with the same temperature as the wall, equal to $273.K$. Initial density is equal to $9.27e^{-6}Kg.m^{-3}$ and the mean free path is 0.00925 m. The VHS molecular model is employed in order to evaluate th coefficient of viscosity. Prandtl number is 2/3. In the first case, the velocity of the moving surface is equal to $300m.s^{-1}$ which correspond to a small velocity gradient.

Results

The CFl number is also equal to 1. We use the same convergence criterion as in the shock problem, which is obtained after 15661 iterations. Velocity, density and temperature profiles are shown in fig 5,7,9 and are compared to Monte Carlo simulations in fig 6,8,10. Shear stress profiles are also compared too in fig 11 and 12. DSMC results are noisy, where the 14 moments results are free of noise. Steady state value of the pressure is $0.5497N.m^2$ is closed to the $0.549N.m^2$ found by G.A.Bird. Velocity and temperature slips at each surface are compared with Bird's results in the following table.

	14 MOMENTS	DSMC
Temperature slip T-Tw	2^oK	1.4^oK
Velocity slip $u - u_w$	6.2 m/s	5 m/s

We can also compare qualitatively our results to the Navier-stokes predictions. The Navier-stokes equations, in the case of one dimensional, stationary flow reduce to the following equations:

$$\frac{\partial}{\partial x}(\rho u_x) = 0, \tag{54}$$

$$\frac{\partial p}{\partial x} - \frac{\partial \tau_{xx}}{\partial x} = 0, \tag{55}$$

$$\frac{\partial \tau_{xz}}{\partial x} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u_z}{\partial x}\right) = 0, \tag{56}$$

$$\frac{\partial q}{\partial x} = \frac{\partial}{\partial x}\left(\mu u_z \frac{\partial u_z}{\partial x}\right), \tag{57}$$

$$q = -K\frac{\partial T}{\partial x}. \tag{58}$$

From (54), we get first

$$\rho u_x = 0.$$

Thus,

$$\underline{u} = u(x)e_z. \tag{59}$$

Because of (55), the pressure is constant:

$$p(x) = p_0. \tag{60}$$

Thus, (56) reduces to

$$\tau_{xz} = \tau_0. \tag{61}$$

Finally, the equation (57) yields

$$\frac{\partial}{\partial x}\left(K\frac{\partial T}{\partial x}\right) + \tau_0\frac{\partial u}{\partial x} = 0. \tag{62}$$

In our simulation, because the walls have the same temperature, we can consider that μ and κ are constant. Then, (56) implies that $u_z(x)$ is affine and (62) gives that $T(x)$ is a parabola.
Let us remark that our numerical results are closed to this prediction.

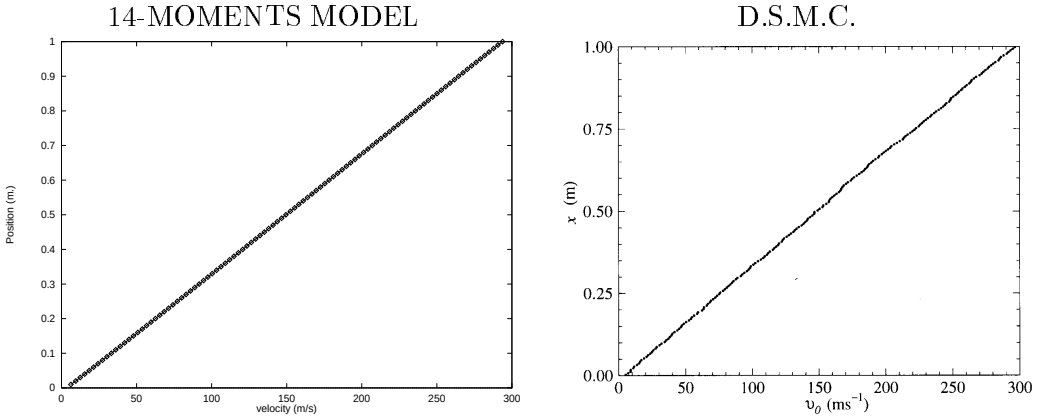

Figure 5, 6 : The velocity profile in the Couette flow at (Kn)=0.00925

14-MOMENTS MODEL D.S.M.C.

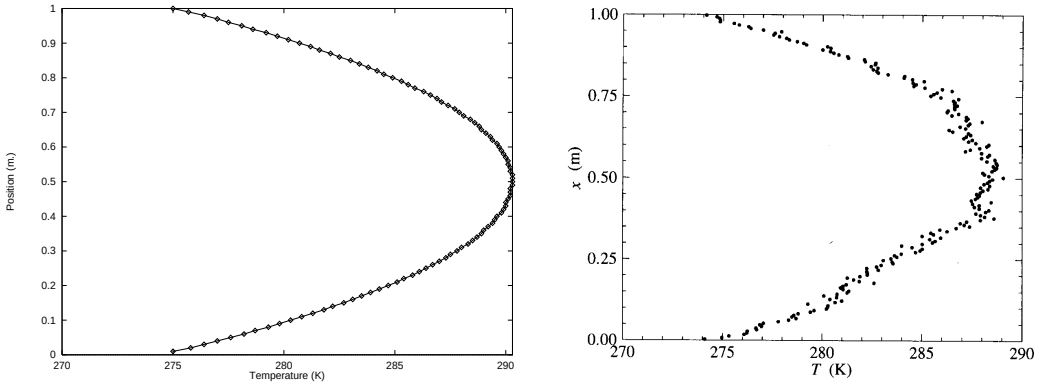

Figure 7, 8 : The temperature profile in the Couette flow at (Kn)=0.00925

14-MOMENTS MODEL D.S.M.C.

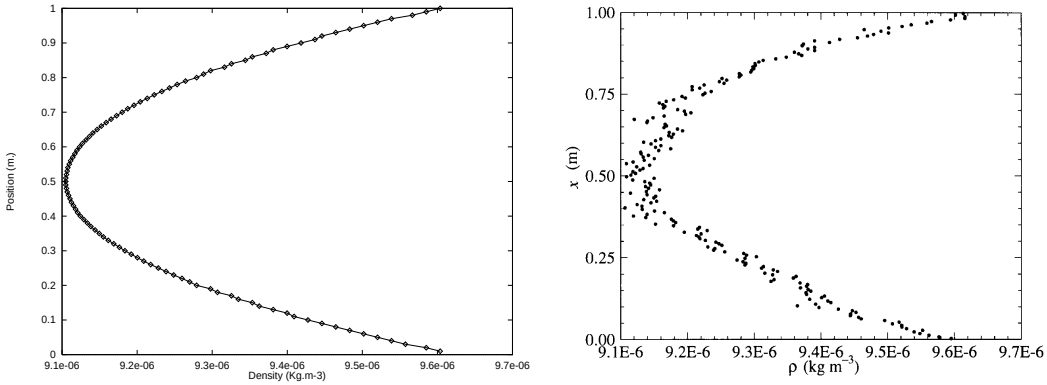

Figure 9, 10: The density profile in the Couette flow at (Kn)=0.00925

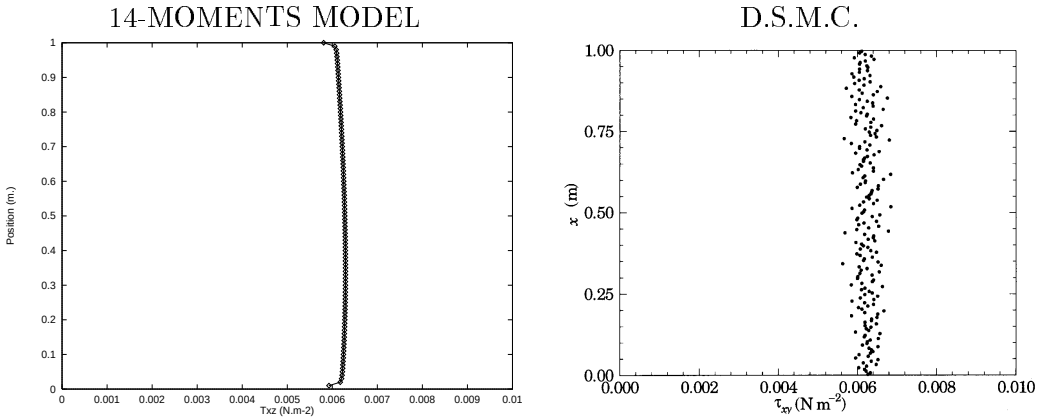

Figure 11, 12: The shear stress profile in the Couette flow at (Kn)=0.00925

The jump in the shear stress profile near the wall, which is smaller than the noise of the DSMC results, is probably due to a artificial non-zero value of the normal velocity near the wall. This small normal velocity which comes from a locally diffusion of the mass flux created by the kinetic scheme, depends only on the mesh.($u_x = .065m/s$ for $\Delta x = 0.005$ and $u_x = .121m/s$ for $\Delta x = 0.01$) A small perturbation in the term $\rho u_x \partial_x u_z$ which gives the shear stress value, appears but depends only on the mesh.

7 Conclusion

In this paper, we have recalled the mathematical properties of the moment closure hierarchies proposed by Levermore. More precisely, we have presented an entropy property of the resulting moments system and derived consistent boundary conditions. Based on these properties and because the system is deduced from the full Boltzmann equation, we have proposed a kinetic numerical scheme with implicit source term, which is stable and preserves entropy properties.
The 14-moments equations have been written and solved with this scheme in two flow configurations: a shock wave problem and a Couette flow.
These results, to our knowledge, are the first numerical results obtained with the 14-moments Levermore model with boundaries. They are compatible with the Navier-Stokes solutions with slip boundary conditions and give results with very

good agreement, and this with far less noise, with the classical DSMC solutions of the Boltzmann equations.

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Éditeur
INRIA, Domaine de Voluceau, Rocquencourt, BP 105, 78153 LE CHESNAY Cedex (France)
ISSN 0249-6399