BGK and Fokker Planck Models for thermally perfect gases

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Abstract

We propose two models of the Boltzmann equation (BGK and Fokker-Planck models) for rarefied flows of thermally perfect gases. These models take into account various models of energy, which are required for high temperature flows, like for atmospheric re-entry problems as long as the pressure law for perfect gases is true. We prove that these models satisfy conservation and entropy properties (H-theorem), and we derive their corresponding compressible Navier-Stokes asymptotic.

Keywords: Fokker-Planck model, BGK model, H-theorem, Rarefied Gas Dynamics, thermally perfect gases

1 Introduction

Numerical simulation of atmospheric reentry flows requires to solve the Boltzmann equation of Rarefied Gas Dynamics. The standard method to do so is the Direct Simulation Monte Carlo (DSMC) method [1, 2], which is a particle stochastic method. However, it is sometimes interesting to have alternative numerical methods, like, for instance, methods based on a direct discretization of the Boltzmann equation (deterministic approaches). This is hardly possible for the full Boltzmann equation (except for monatomic gases, see [3, 4]), since this is still much too computationally expensive for real gases. But BGK like model equations [5] are very well suited for such deterministic codes: indeed, their complexity can be reduced by the well known reduced distribution technique [6], which leads to intermediate models between the full Boltzmann equation and moment models [7]. The Fokker-Planck model [8] is another model Boltzmann equation that can give very efficient stochastic particle methods, see [9].

These model equations have already been extended to polyatomic gases, so that they can take into account the internal energy of rotation of gas molecules. They contains correction terms that lead to correct transport coefficients: the ESBGK or Chekhov’s models [10, 11, 12], and the cubic Fokker-Planck and ES-Fokker-Planck [9, 13, 14, 15].

For high temperature flows, like in space reentry problems, other energies can be activated (like vibrations: [16, 17]) and have a significant influence on energy transfers in the gas flow. It is therefore interesting to extend the model equations to take these energies into account. Several extended BGK models have been recently proposed to do so, for instance [18, 19, 20, 21], and a Fokker-Planck model was proposed earlier in [13].
In this paper, we create BGK and Fokker-Planck models for every thermally perfect gas (perfect gas with energy depending on temperature without knowing the precise form of the dependence). Since no obvious kinetic description of degrees of liberty can be precisely given for such gases, we directly use a reduced model with one function for translation energy and the other one for other degrees of freedom: note that with this reduction, only higher order moments with respect to the vibration energy variable are lost: the macroscopic quantities of interest like pressure, temperature, and heat flux are the same as in the non-reduced model. Moreover, since the reduced variable is not the velocity, this reduction does not require any assumption or special geometries. We prove that these reduced models satisfies the H-theorem as well as conservation properties. This paper is a first step towards the creation of ESBGK or ES-Fokker-Planck models able to reproduce the relaxation of several energies towards equilibrium.

Our paper is organised as follows. In section 2, we present the kinetic description of a thermally perfect gas and we discuss the mathematical properties of the reduced distributions that will be used for our models. Our BGK and Fokker-Planck models are presented in sections 3 and 4 respectively. In section 5, the hydrodynamic limits of our models, obtained by a Chapman-Enskog procedure, are discussed. In section 6 we provide an extension of our framework to several energies. Finally, section 7 gives some perspectives around this work.

2 Kinetic description of a thermally perfect gas

2.1 Some thermodynamics on thermally perfect gases

Before writing any kinetic model, we consider some thermodynamics. A thermally perfect gas is a gas satisfying \( P = \rho RT \) where \( P \) is the pressure, \( \rho \) the density and \( T \) the temperature of a gas with \( R \), constant of the perfect gas. However this law does not give the relation between energy and temperature which can be linear (for simple models of rotations for instance) or non linear (for instance for vibrations in a diatomic molecule can be set to \( e(T) = \frac{5}{2}RT + \frac{RT_0}{\exp(T_0/T) - 1} \) for some \( T_0 \) characteristic temperature of vibrations) or simply tabulated according to temperature. In simple cases when the relation between energy and temperature is well defined one can construct BGK or Fokker-Planck models to capture correctly the physics. We do want to extend these models to any kind of energy. In order to do so we suppose that energy \( e \) can be defined through

\[
e(T) = e_{tr}(T) + e_{int}(T)
\]

where:

\[
e_{tr}(T) = \frac{3}{2}RT, \quad e_{int}(T) = e(T) - e_{tr}(T),
\]

\( e_{tr} \) being the translational kinetic energy and \( e_{int} \) represents all the other internal energies. Moreover we also suppose that \( e_{int} \) is a strictly increasing function of temperature: \( e \) is then also a strictly increasing function so that there exists one-to-one functions \( T \) and \( T_{int} \) such that

\[
T = T(e) \quad , \quad e = e(T) \quad , \quad \frac{d}{dT} e = \frac{3}{2}R + c_v^{int} > 0,
\]

\[
T_{int} = T_{int}(e_{int}) \quad , \quad e_{int} = e_{int}(T_{int}) \quad , \quad \frac{d}{dT_{int}} e_{int} = c_v^{int} > 0,
\]

where \( c_v^{int} \) is the specific heat associated to \( e_{int} \).
We can also define an entropy $s^{\text{int}}$ satisfying $ds^{\text{int}} = \frac{de^{\text{int}}}{T^{\text{int}}(e^{\text{int}})}$ up to some constant by integration (we will give some expressions later for the simple rotational and vibrational case). Similarly an entropy for translations can be defined through $ds^{\text{tr}} = \frac{de^{\text{tr}}}{T^{\text{tr}}(e^{\text{tr}})}$. The second principle now writes:

$$\begin{equation}
ds(\rho, T) = ds^{\text{tr}}(T) + ds^{\text{int}}(T) - R \frac{d\rho}{\rho}.
\end{equation}$$

We now have all the necessary tools to construct our BGK and Fokker-Planck models.

### 2.2 Distribution function and local equilibrium

We consider a thermally perfect gas. Since we only know the relation between temperature and energy, there is no clear extension to other degrees of freedom than the translational ones for an equilibrium state such as the one of polyatomic gases ([11]) or vibrational diatomic gases ([22]). We propose to separate the translational degrees of freedom of molecules with the remaining degrees of freedom: even if there is a loss of information for high order moments in internal energy this reduction will be enough to capture both pressure and thermal flux which are the quantities of interest in our problem. To do that we define $F(t, x, v)$ the mass density of molecules with position $x$, velocity $v$ and $G(t, x, v)$ the internal energy density of molecules with position $x$, velocity $v$. We directly write a two model distribution as it was done in ([11, 22]). The corresponding local equilibrium distributions for $F$ and $G$ are defined by (see [1])

$$\begin{equation}
M^{\text{int}}[F, G](v) = \frac{\rho}{\sqrt{2\pi RT}^3} \exp \left( -\frac{1}{2} \frac{|u - v|^2}{RT} \right),
\end{equation}$$

$$\begin{equation}
e^{\text{int}}(T)M^{\text{int}}[F, G](v) = e^{\text{int}}(T) \frac{\rho}{\sqrt{2\pi RT}^3} \exp \left( -\frac{1}{2} \frac{|u - v|^2}{RT} \right).
\end{equation}$$

Here, $\rho$ is the gas density, $T$ its equilibrium temperature and $u$ its mean velocity, defined through:

$$\begin{equation}
\rho = \langle F \rangle_v, \quad \rho u = \langle vF \rangle_v,
\end{equation}$$

$$\begin{equation}
\rho e^{\text{tr}} = \left\langle \left(\frac{1}{2}(v - u)^2\right)F \right\rangle_v, \quad \rho e^{\text{int}} = \langle G \rangle_v,
\end{equation}$$

$$\begin{equation}
\rho e = \left\langle \left(\frac{1}{2}(v - u)^2\right)F \right\rangle_v + \langle G \rangle_v, \quad T = T(e)
\end{equation}$$

where we use the notation $\langle \psi \rangle_v = \iint \psi(t, x, v) dv$ for any function $\psi$.

Immediate computations of Gaussian functions lead to the following proposition:

**Proposition 2.1** (Conservation properties).

$$\begin{equation}
\rho = \langle M^{\text{int}}[F, G] \rangle_v, \quad \rho u = \langle vM^{\text{int}}[F, G] \rangle_v,
\end{equation}$$

$$\begin{equation}
\rho e^{\text{tr}} = \left\langle \left(\frac{1}{2}(v - u)^2\right)M^{\text{int}}[F, G] \right\rangle_v, \quad \rho e^{\text{int}} = \langle e^{\text{int}}(T)M^{\text{int}}[F, G] \rangle_v,
\end{equation}$$

$$\begin{equation}
\rho e = \left\langle \left(\frac{1}{2}(v - u)^2\right)M^{\text{int}}[F, G] \right\rangle_v + \langle e^{\text{int}}(T)M^{\text{int}}[F, G] \rangle_v, \quad T = T(e).
\end{equation}$$
We now define a reduced entropy as a function of \(F\) and \(G\) in the following proposition:

**Proposition 2.2 (Entropy).** We define the following reduced entropy \(\mathcal{H}(F,G)\) of \(F\) and \(G\) as:

\[
\mathcal{H}(F,G) = \left\langle F \log(F) - F \frac{s_{\text{int}}}{R} \left( \frac{G}{F} \right) \right\rangle_v.
\]

1. The partial derivatives of \(H = F \log(F) - F \frac{s_{\text{int}}}{R} \left( \frac{G}{F} \right)\) computed at \((F,G)\) are:

\[
D_1 H(F,G) = 1 + \log(F) + G \frac{F^3}{c\int_{\text{int}}(G/F)F} - \left( \frac{G}{F} \right), \quad D_2 H(F,G) = - \frac{1}{F \int_{\text{int}}(G/F)}.
\]

2. We note \(\mathbb{H} = \begin{pmatrix} D_{11} H(F,G) & D_{12} H(F,G) \\ D_{12} H(F,G) & D_{22} H(F,G) \end{pmatrix}\) the Hessian matrix of \(H\). Its value is:

\[
\begin{pmatrix}
D_{11} H(F,G) = \frac{1}{F} + \frac{G^2}{F^3 \int_{\text{int}}(G/F)F}, & D_{12} H(F,G) = - \frac{G}{F^2 \int_{\text{int}}(G/F)F} \\
D_{21} H(F,G) = D_{12} H(F,G), & D_{22} H(F,G) = \frac{G}{F^2 \int_{\text{int}}(G/F)F}
\end{pmatrix}
\]

Moreover, the derivatives satisfy the following equality’s:

\[
FD_{11} H(F,G) + GD_{21} H(F,G) = 1, \\
FD_{12} H(F,G) + GD_{22} H(F,G) = 0.
\]

3. The function \((F,G) \mapsto H(F,G)\) is convex.

**Proof.** Points 1 and 2 are given by direct computations. The Hessian matrix is positive definite (trace and determinant are positive) so that \(H\) is convex.

**Proposition 2.3 (Minimisation of entropy).** Let \((F,G)\) be a couple of reduced distributions and \(\rho, \rho u, \) and \(\rho e\) its moments as defined by (6). Let \(S\) be the convex set defined by

\[
S = \left\{ (F_1, G_1) \text{ such that } \langle F_1 \rangle_v = \rho, \; \langle vF_1 \rangle_v = \rho u, \; \left\langle \frac{1}{2} |v|^2 F_1 + G_1 \right\rangle_v = \rho e \right\}.
\]

1. The minimum of \(\mathcal{H}\) on \(S\) is obtained for the couple \((M_{\text{int}}(F,G), e_{\text{int}}(T)M_{\text{int}}(F,G))\) with

\[
M_{\text{int}}[F,G] = \frac{\rho}{\sqrt{2\pi RT}} \exp\left(-\frac{|v-u|^2}{2RT}\right)
\]

where \(e_{\text{int}}(T)\) is the equilibrium internal energy defined by (1).

2. For every \((F_1,G_1)\) in \(S\), we have

\[
0 \geq H(M_{\text{int}}(F,G), e_{\text{int}}(T)M_{\text{int}}(F,G)) - H(F_1,G_1) \geq D_1 H(F,G)(M_{\text{int}}(F,G) - F) + D_2 H(F,G)(e_{\text{int}}(T)M_{\text{int}}(F,G) - G)
\]
Proof. We now compute the minimum of the reduced entropy. First, the set $S$ is clearly convex, and it is non empty, since it is easy to see that $(M_{int}, e_{int}(T)M_{int})$ realises the moments $\rho$, $\rho u$, and $\rho e$, and hence belongs to $S$. Now, we define the following Lagrangian

$$
\mathcal{L}(F_1, G_1, \alpha, \beta, \gamma) = \langle H(F_1, G_1) \rangle_v - \alpha \langle F_1 \rangle_v - \rho - \beta \cdot (\langle vF_1 \rangle_v - \rho u) - \frac{\gamma}{2} \langle \frac{1}{2} |v|^2 F_1 + G_1 \rangle_v - \rho e
$$

for $(F_1, G_1) \in S$, $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$. The reduced entropy can reach a minimum of $S$ when $\mathcal{L}$ has its first derivatives equal to zero. This point, denoted by $(F_1, G_1, \alpha, \beta, \gamma)$ for the moment, is characterised by the fact that the partial derivatives of $\mathcal{L}$ vanish at $(F_1, G_1, \alpha, \beta, \gamma)$. This gives the following relations:

$$
D_1 H(F_1, G_1) = \alpha + \beta \cdot v + \frac{\gamma}{2} |v|^2, 
\quad (13)
$$

$$
D_2 H(F_1, G_1) = \gamma, 
\quad (14)
$$

$$
\langle F_1 \rangle_v - \rho = 0, 
\quad (15)
$$

$$
\langle vF_1 \rangle_v - \rho u = 0, 
\quad (16)
$$

$$
\langle \frac{1}{2} |v|^2 F_1 + G_1 \rangle_v - \rho e = 0, 
\quad (17)
$$

where $D_1 H$ and $D_2 H$ are defined in (10). Combining equations (13) and (14), one gets that there exist real numbers $A$, $B$, $D$ and one vector $E \in \mathbb{R}^3$, independent of $v$, such that:

$$
F_1 = A \exp (E \cdot v + B |v|^2),
$$

$$
G_1 = D F_1,
$$

where $B$ is necessarily non positive to ensure the integrability of $F_1$ and $G_1$. $G/F$ is a constant because the temperature is a bijective function of energy so that $D_2 H(F_1, G_1) = \gamma$ only owns one solution. It is then standard to use equations (15) to get $F_1 = M_{int}(F, G)$ and $G_1 = e_{int}(T)M_{int}(F, G)$.

Finally point 2 is a direct consequence of the convexity of $H$ and of the minimization property.

\[\square\]

3 A BGK model for thermally perfect gases

3.1 A reduced BGK model

For physics considerations, it is interesting to reduce complex kinetic models by using the usual reduced distribution technique [23]. Even for perfect gases, some degenerate models of energy cannot be described easily through equilibrium (extensions of Maxwellians is not very clear when ones deals with partial degrees of freedom of internal energy. In this paper we propose to use two reduced functions $F$ and $G$ that will transport energy. $F$ is transporting the translational energy whereas $G$ transport the reminder of internal energy. More precisely they are defined through:

$$
\partial_t F + v \cdot \nabla_x F = \frac{1}{\tau} (M_{int}[F, G] - F),
$$

$$
\partial_t G + v \cdot \nabla_x G = \frac{1}{\tau} (e_{int} M_{int}[F, G] - G),
$$

(18)
where the reduced Maxwellian is
\[ M_{\text{int}}[F, G] = \frac{\rho}{\sqrt{2\pi RT}} \exp \left(-\frac{|v - u|^2}{2RT}\right), \]
and the macroscopic quantities are defined by
\[ \rho = \langle F \rangle_v, \quad \rho u = \langle vF \rangle_v, \quad \rho e = \langle \frac{1}{2}(v - u)^2 F \rangle_v + \langle G \rangle_v, \]
and \( T \) is still defined by (2).

It is interesting to compare our new model to the work of [16, 22] and [21]: in these recent papers, the authors also proposed, independently, BGK and ES-BGK models for temperature dependent \( \delta \), like in the case of vibrational energy. However, they are not based on an underlying discrete vibrational energy partition, and the authors are not able to prove any H-theorem. Only a local entropy dissipation can be proved. The advantage of our approach is that the reduced model, which is continuous in energy too, has got a H-theorem, as it is shown below.

### 3.2 Properties of the reduced model

System (18) naturally satisfies local conservation laws of mass, momentum, and energy. Moreover, the H-theorem holds with the reduced entropy \( H(F, G) \) as defined in (9). Indeed, we have the

**Proposition 3.1.** The reduced BGK system (18) satisfies the H-theorem
\[ \partial_t H(F, G) + \nabla_x \cdot \langle vH(F, G) \rangle_v \leq 0, \]
where \( H(F, G) \) is the reduced entropy defined in (9).

**Proof.**
By differentiation we get
\[
\begin{align*}
\partial_t H(F, G) + \nabla_x \cdot \langle vH(F, G) \rangle_v &= \langle D_1 H(F, G)(\partial_t F + v\nabla_x F) + D_2 H(F, G)(\partial_t G + v\nabla_x G) \rangle_v \\
&= \frac{1}{\tau} \langle D_1 H(F, G)(M_{\text{int}}[F, G] - F) + D_2 H(F, G)(\delta(T)RTM_{\text{int}}[F, G] - G) \rangle_v \\
&\leq 0
\end{align*}
\]
where we have used (18) to replace the transport terms by relaxation ones, and point 2 of proposition 2.3 to obtain the inequality.

### 4 A Fokker-Planck model for thermally perfect gases

It is difficult to derive a Fokker-Planck model for the distribution function \( f \) with discrete energy levels. We find it easier to directly derive a reduced model, by analogy with the reduced BGK model (18) and by using our previous work [15] on a Fokker-Planck model for polyatomic gases. We remind that the original Fokker-Planck model for monoatomic gas can be derived from the Boltzmann collision operator under the assumption of small velocity changes through collisions and additional equilibrium assumptions (see [8]). In practice, the agreement of this model with the Boltzmann equation is observed even when the gas is far from equilibrium (see [9], for instance).
4.1 A reduced Fokker-Planck model

By analogy, now we propose the following reduced Fokker-Planck model for a diatomic gas with vibrations. Note that now, the model is still with variables $x$, $v$, and $\varepsilon$: only the discrete energy levels $i$ are eliminated. This model is

$$
\begin{align*}
\partial_t F + v \cdot \nabla_x F &= D_F(F, G), \\
\partial_t G + v \cdot \nabla_x G &= D_G(F, G),
\end{align*}
$$

(20)

with

$$
\begin{align*}
D_F(F, G) &= \frac{1}{\tau} \left( \nabla_v \cdot \left( (v - u)F + RT \nabla_v F \right) \right), \\
D_G(F, G) &= \frac{1}{\tau} \left( \nabla_v \cdot \left( (v - u)G + RT \nabla_v G \right) \right) + \frac{2}{\tau} (e_{int}(T)F - G),
\end{align*}
$$

(21)

where the macroscopic values are defined as in [19] and (2).

4.2 Properties of the reduced model

Using direct calculations and dissipation properties as in [15] we can prove the following proposition.

**Proposition 4.1.** The collision operator conserves the mass, momentum, and energy:

$$
\langle (1, v)D_F(F, G) \rangle_v = 0 \quad \text{and} \quad \left\langle \left( \frac{1}{2} |v|^2 \right) D_F(F, G) + D_G(F, G) \right\rangle_v = 0,
$$

the reduced entropy $\mathcal{H}(F, G)$ satisfies the H-theorem:

$$
\partial_t \mathcal{H}(F, G) + \nabla_x \cdot \langle v H(F, G) \rangle_v = D(F, G) \leq 0,
$$

and we have the equilibrium property

$$(D_F(F, G) = 0 \; \text{and} \; D_G(F, G) = 0) \iff (F = M_{int}[F, G] \; \text{and} \; G = e_{int}(T)M_{int}[F, G]).$$

**Proof.** The conservation property is the consequence of direct integration of (21). The equilibrium property can be proved as follows. To shorten the notations, $M_{int}[F, G]$ will be simply denoted by $M_{int}$ below, and $e_{int}(T)$ will be simply denoted by $e_{int}$ as well. Then the collision operators can be written in the compact form

$$
\begin{align*}
D_F(F, G) &= \frac{1}{\tau} \nabla_v \cdot \left( M_{int} \nabla_v \frac{F}{M_{int}} \right), \\
D_G(F, G) &= \frac{1}{\tau} \nabla_v \cdot \left( M_{int} \nabla_v \frac{G}{M_{int}} \right) + \frac{2}{\tau} (e_{int}F - G).
\end{align*}
$$

Then an integration by part gives the following identity for $D_F(F, G)$:

$$
\langle D_F(F, G) \frac{F}{M_{int}} \rangle_v = -\frac{1}{\tau} \left\langle \left( \nabla_v \frac{F}{M_{int}} \right)^T M_{int} \nabla_v \frac{F}{M_{int}} \right\rangle_v.
$$
Consequently, if $D_F(F,G) = 0$, since the integrand in the previous relation is a definite positive form, the gradient is necessarily zero, and hence $F = M_{\text{int}}$. For the equilibrium property of $G$, the proof is a bit more complicated. First, we have

$$\left\langle D_G(F,G) \frac{G}{e_{\text{int}} M_{\text{int}}} \right\rangle_v = -\frac{1}{\tau e_{\text{int}}} \left\langle \left( \nabla_v \frac{G}{M_{\text{int}}} \right)^T M_{\text{int}} \nabla_v \frac{G}{M_{\text{int}}} \right\rangle_v + \frac{2}{\tau} \left\langle (e_{\text{int}} F - G) \frac{G}{e_{\text{int}} M_{\text{int}}} \right\rangle_v.$$  

Consequently, if $D_G(F,G) = 0$, and since $F = M_{\text{int}}$, we have

$$\frac{1}{e_{\text{int}}} \left\langle \left( \nabla_v \frac{G}{M_{\text{int}}} \right)^T M_{\text{int}} \nabla_v \frac{G}{M_{\text{int}}} \right\rangle_v = \frac{2}{\tau} \left\langle (e_{\text{int}} M_{\text{int}} - G) \frac{G}{e_{\text{int}} M_{\text{int}}} \right\rangle_v$$

$$= -\frac{2}{\tau} \left\langle (e_{\text{int}} M_{\text{int}} - G)^2 \frac{1}{e_{\text{int}} M_{\text{int}}} \right\rangle_v + \frac{2}{\tau} \left\langle e_{\text{int}} M_{\text{int}} - G \right\rangle_v$$

$$\leq \frac{2}{\tau} \left\langle e_{\text{int}} M_{\text{int}} - G \right\rangle_v = \frac{2}{\tau} (\rho e_{\text{int}} - \left\langle G \right\rangle_v) = 0,$$

which comes from (6) and $F = M_{\text{int}}$. Therefore, we obtain

$$\frac{1}{e_{\text{int}}} \left\langle \left( \nabla_v \frac{G}{M_{\text{int}}} \right)^T M_{\text{int}} \nabla_v \frac{G}{M_{\text{int}}} \right\rangle_v \leq 0,$$

and again this gives $G = e_{\text{int}} M_{\text{int}}$, which concludes the proof of the equilibrium property.

The proof of the H-theorem is much longer. First, by differentiation one gets that the quantity $\mathcal{D}(F,G) = \partial_t H(F,G) + \nabla_x \cdot \left\langle v H(F,G) \right\rangle_v$ satisfies:

$$\mathcal{D}(F,G) = \left\langle D_1 H(F,G)(\partial_t F + v \cdot \nabla_x F) + D_2 H(F,G)(\partial_t G + v \cdot \nabla_x G) \right\rangle_v$$

$$= \left\langle D_1 H(F,G) D_F(F,G) + D_2 H(F,G) D_G(F,G) \right\rangle_v,$$  

from (18). Then the proof is based on the convexity of $H(F,G)$: while for the BGK we only used the the first derivatives of $H$, we now use the positive-definiteness of the Hessian matrix of $H$. To do so we integrate by parts $\mathcal{D}(F,G)$ and multiply by $\tau$ so that:

$$\tau \mathcal{D}(F,G) = -\sum_{i=1}^3 \left\langle \partial_{v_i}(F) D_{11} H(F,G) (F(v_i - u_i) + RT \partial_{v_i} F) \right\rangle_v$$

$$-\sum_{i=1}^3 \left\langle \partial_{v_i}(G) D_{21} H(F,G) (F(v_i - u_i) + RT \partial_{v_i} F) \right\rangle_v$$

$$-\sum_{i=1}^3 \left\langle \partial_{v_i}(F) D_{12} H(F,G) (G(v_i - u_i) + RT \partial_{v_i} G) \right\rangle_v$$

$$-\sum_{i=1}^3 \left\langle \partial_{v_i}(G) D_{22} H(F,G) (G(v_i - u_i) + RT \partial_{v_i} G) \right\rangle_v$$

$$-2 \left\langle (e_{\text{int}}(T) F - G) \frac{1}{RT(G/F)} \right\rangle_v$$
To use the positive definiteness of the Hessian matrix $\mathbb{H}$ of $H$, we introduce the following vector:

$$V_i = (F(v_i - u_i) + RT\partial_{v_i} F, G(v_i - u_i) + RT\partial_{v_i} G),$$

and we decompose the partial derivatives of $F$ and $G$ in factors of $D_{11} F$, $D_{22} F$, $D_{12} F$ as follows:

$$(\partial_{v_i} (F), \partial_{v_i} (G)) = \frac{1}{RT} V_i - (F \frac{v_i - u_i}{RT}, G \frac{v_i - u_i}{RT}).$$

This gives

$$\tau D(F,G) = \sum_{i=1}^{3} \left( \left\langle \left( \frac{v_i - u_i}{RT} \right) D_{11} H(F,G) \left( F(v_i - u_i) + RT\partial_{v_i} F \right) \right\rangle_v 
+ \sum_{i=1}^{3} \left\langle \left( \frac{v_i - u_i}{RT} \right) D_{21} H(F,G) \left( F(v_i - u_i) + RT\partial_{v_i} F \right) \right\rangle_v 
+ \sum_{i=1}^{3} \left\langle \left( \frac{v_i - u_i}{RT} \right) D_{12} H(F,G) \left( G(v_i - u_i) + RT\partial_{v_i} G \right) \right\rangle_v 
+ \sum_{i=1}^{3} \left\langle \left( \frac{v_i - u_i}{RT} \right) D_{22} H(F,G) \left( G(v_i - u_i) + RT\partial_{v_i} G \right) \right\rangle_v 
- \sum_{i=1}^{3} \left\langle V_i^T \mathbb{H} V_i \right\rangle_v 
- 2 \left\langle (e_{\text{int}}(T) F - G) \frac{1}{RT(G/F)} \right\rangle_v \right).$$

Now this expression can be considerably simplified by using property (11), and we get

$$\tau D(F,G) = \sum_{i=1}^{3} \left( \left\langle \left( \frac{v_i - u_i}{RT} \right) \left( F(v_i - u_i) + RT\partial_{v_i} F \right) \right\rangle_v 
- \sum_{i=1}^{3} \left\langle V_i^T \mathbb{H} V_i \right\rangle_v 
- 2 \left\langle (e_{\text{int}}(T) F - G) \frac{1}{RT(G/F)} \right\rangle_v \right).$$

Then the first two terms are simplified by using an integration by parts and relations (6) and (2) to get

$$\tau D(F,G) = \frac{2}{RT} (\rho e_{\text{int}}(T) - \langle G \rangle_v) - \sum_{i=1}^{3} \left\langle V_i^T \mathbb{H} V_i \right\rangle_v - 2 \left\langle (e_{\text{int}}(T) F - G) \frac{1}{RT(G/F)} \right\rangle_v \right).$$

The terms with the Hessian are clearly negative, since $\mathbb{H}$ is positive definite. Then we have

$$\tau D(F,G) \leq \frac{2}{RT} (\rho e_{\text{int}}(T) - \langle G \rangle_v) - 2 \left\langle (e_{\text{int}}(T) F - G) \frac{1}{RT(G/F)} \right\rangle_v \right).$$

Note that from (5) the first term can be written as

$$\frac{2}{RT} (\rho e_{\text{int}}(T) - \langle G \rangle_v) = \frac{2}{RT} \langle e_{\text{int}}(T) F - G \rangle_v,$$
and can be factorised with the second term to find
\[ \tau D(F,G) \leq 2 \left\langle \left( e_{\text{int}}(T)F - G \right) \left( \frac{1}{RT} - \frac{1}{RT(G/F)} \right) \right\rangle_v. \]

We can now prove that the integrand of the right-hand side is non-positive. Indeed, assume for instance that the second factor is non-positive, that is to say \( \frac{1}{RT} - \frac{1}{RT(G/F)} \leq 0 \). Since \( e_{\text{int}} \) is an increasing function of temperature (see definition (1)), it is now very easy to prove the following relations:
\[ \frac{1}{RT} - \frac{1}{RT(G/F)} \leq 0 \iff \frac{G}{F} \leq e_{\text{int}}(T) \]
that is to say the first factor of the integrand is non-negative. Consequently, we have proved \( \tau D(F,G) \leq 0 \), which concludes the proof.

5 Hydrodynamic limits for reduced models

With a convenient scaling, the relaxation time \( \tau \) of the reduced BGK model (18) and the Fokker-Planck model (20) is replaced by \( Kn \tau \), where \( Kn \) is the Knudsen number, which can be defined as a ratio between the mean free path and a macroscopic length scale. It is then possible to look for macroscopic models derived from BGK and Fokker-Planck reduced models, in the asymptotic limit of small Knudsen numbers. For convenience, these models are re-written below in non-dimensional form. The BGK model is:
\[ \partial_t F + v \cdot \nabla_x F = \frac{1}{Kn \tau} (M_{\text{int}}[F,G] - F), \]
\[ \partial_t G + v \cdot \nabla_x G = \frac{1}{Kn \tau} (e_{\text{int}}(T)M_{\text{int}}[F,G] - G), \]
where \( M_{\text{int}}[F,G] \) can be defined by (12) with \( R = 1 \). Similarly, the relations (1)–(2) between the translational, internal, and total energies and the temperature, have to be read with \( R = 1 \) in non-dimensional variables. The Fokker-Planck model is
\[ \partial_t F + v \cdot \nabla_x F = D_F(F,G), \]
\[ \partial_t G + v \cdot \nabla_x G = D_G(F,G), \]
with
\[ D_F(F,G) = \frac{1}{Kn \tau} \left( \nabla_v \cdot ((v - u)F + T \nabla_v F) \right), \]
\[ D_G(F,G) = \frac{1}{Kn \tau} \left( \nabla_v \cdot ((v - u)G + T \nabla_v G) \right) + \frac{2}{Kn \tau} (e_{\text{int}}(T)F - G). \]

5.1 Euler limit

In this section, we compute the Euler limit of the two models:
Proposition 5.1. The mass, momentum, and energy densities \((\rho, \rho u, E) = \frac{1}{2} \rho u^2 + \rho e\) of the solutions of the reduced BGK and the Fokker-Planck models satisfy the equations
\[
\begin{align*}
\partial_t \rho + \nabla \cdot \rho u &= 0, \\
\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p &= O(Kn), \\
\partial_t E + \nabla \cdot ((E + p)u) &= O(Kn),
\end{align*}
\]
which are the Euler equations, up to \(O(Kn)\). The non-conservative form of these equations is
\[
\begin{align*}
\partial_t \rho + \nabla \cdot \rho u &= 0, \\
\rho (\partial_t u + (u \cdot \nabla)u) + \nabla p &= O(Kn), \\
\partial_t T + u \cdot \nabla T + \frac{T}{c_v(T)} \nabla \cdot u &= O(Kn),
\end{align*}
\]
where \(c_v(T) = \frac{\partial}{\partial T} e(T)\) is the heat capacity at constant volume.

Proof.

The reduced BGK model \((18)\) is multiplied by \(1, v,\) and \(\frac{1}{2} |v|^2\) and integrated with respect to \(v\), which gives the following conservation laws (with \(\sigma(F) = \langle F(v - u) \otimes (v - u) \rangle_v\) the stress tensor, and \(q(F,G) = \langle (F(\frac{1}{2}|v - u|^2) + G) (v - u) \rangle_v\) the heat flux):
\[
\begin{align*}
\partial_t \rho + \nabla \cdot \rho u &= 0, \\
\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla \sigma(F) &= 0, \\
\partial_t E + \nabla \cdot Eu + \nabla \cdot \sigma(F)u + \nabla \cdot q(F,G) &= 0.
\end{align*}
\]

When \(Kn\) is very small, if all the time and space derivatives of \(F\) and \(G\) are \(O(1)\) with respect to \(Kn\), then \((23)-(24)\) imply \(F = M_{int}[F,G] + O(Kn)\) and \(G = e_{int}(T)M_{int}[F,G] + O(Kn)\) so that \(\sigma(F) = \sigma(M_{int}[F,G]) + O(Kn)\) and \(\rho I + O(Kn)\), where \(I\) is the unit tensor, and \(q(F,G) = q(M_{int}[F,G], e_{int}(T)M_{int}[F,G]) + O(Kn) = O(Kn)\), which gives the Euler equations \((29)\). The same analysis can be applied for the reduced Fokker-Planck model \((25)-(27)\). Finally, the non conservative form is readily obtained from the conservative form. We also get from the non conservative temperature equation:
\[
\partial_t e_{int}(T) + u \cdot \nabla e_{int}(T) + T \frac{e_{int}}{c_v} \nabla \cdot u = O(Kn).
\]

5.2 Compressible Navier-Stokes limit

In this section, we shall prove the following proposition:

Proposition 5.2. The moments of the solution of the BGK and Fokker-Planck kinetic models \((18)\) and \((20)\) satisfy, up to \(O(Kn^2)\), the Navier-Stokes equations
\[
\begin{align*}
\partial_t \rho + \nabla \cdot \rho u &= 0, \\
\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p &= -\nabla \cdot \sigma, \\
\partial_t E + \nabla \cdot ((E + p)u) &= -\nabla \cdot q - \nabla \cdot (\sigma u),
\end{align*}
\]
where the shear stress tensor and the heat flux are given by
\[
\sigma = -\mu (\nabla u + (\nabla u)^T - a \nabla \cdot u), \quad \text{and} \quad q = -\kappa \nabla \cdot T, \tag{32}
\]
and the values of the viscosity and heat transfer coefficients (in dimensional variables) are:
\[
\mu = \tau_p, \quad \text{and} \quad \kappa = \mu c_p(T) \quad \text{for BGK},
\]
\[
\mu = \frac{1}{2} \tau_p, \quad \text{and} \quad \kappa = \frac{2}{3} \mu c_p(T) \quad \text{for Fokker-Planck}, \tag{33}
\]
while the volume viscosity coefficient is \( \alpha = \frac{c_v(T)}{c_v(T)} - 1 \) for both models, and \( c_p(T) = \frac{d}{dT}(e(T) + p/\rho) = c_v(T) + R \) is the heat capacity at constant pressure. Moreover, the corresponding Prandtl number is
\[
\Pr = \frac{\mu c_p(T)}{\kappa} = 1 \quad \text{for BGK, and} \quad \frac{3}{2} \quad \text{for Fokker-Planck}. \tag{34}
\]

### 5.2.1 Proof for the BGK model

The usual Chapman-Enskog method is applied as follows. We decompose \( F \) and \( G \) as \( F = M_{int}[F,G] + Kn F_1 \) and \( G = \varepsilon_{int}(T) M_{int}[F,G] + Kn G_1 \), which gives
\[
\sigma(F) = p I + Kn \sigma(F_1), \quad \text{and} \quad q(F,G) = Kn q(F_1,G_1).
\]
Then we have to approximate \( \sigma(F_1) \) and \( q(F_1,G_1) \) up to \( O(Kn) \). This is done by using the previous expansions and (18) to get
\[
F_1 = -\tau (\partial_t M_{int}[F,G] + v \cdot \nabla_x M_{int}[F,G]) + O(Kn),
\]
\[
G_1 = -\tau (\partial_t \varepsilon_{int}(T) M_{int}[F,G] + v \cdot \nabla_x \varepsilon_{int}(T) M_{int}[F,G]) + O(Kn).
\]
This gives the following approximations
\[
\sigma(F_1) = -\tau \langle (v - u) \otimes (v - u) (\partial_t M_{int}[F,G] + v \cdot \nabla_x M_{int}[F,G]) \rangle_v + O(Kn), \tag{35}
\]
and
\[
q(F_1,G_1) = -\tau \langle (v - u) \frac{1}{2} |v - u|^2 (\partial_t M_{int}[F,G] + v \cdot \nabla_x M_{int}[F,G]) \rangle_v
\]
\[
-\tau \langle (v - u) \partial_t \varepsilon_{int}(T) M_{int}[F,G] + v \cdot \nabla_x \varepsilon_{int}(T) M_{int}[F,G] \rangle_v + O(Kn). \tag{36}
\]

Now it is standard to write \( \partial_t M_{int}[F,G] \) and \( \nabla_x M_{int}[F,G] \) as functions of derivatives of \( \rho, u, \) and \( T \), and then to use Euler equations (28) to write time derivatives as functions of the space derivatives only. After some algebra, we get
\[
\partial_t (M_{int}(F,G)) + v \cdot \nabla_x (M_{int}(F,G)) = \frac{\rho}{T^2} M_0(V) \left( A \cdot \frac{\nabla T}{\sqrt{T}} + B : \nabla u \right) + O(Kn), \tag{37}
\]
where
\[
V = \frac{v - u}{\sqrt{T}}, \quad M_0(V) = \frac{1}{(2\pi)^{\frac{d}{2}}} \exp\left(-\frac{|V|^2}{2}\right)
\]
\[
A = \left( \frac{|V|^2}{2} - \frac{5}{2} \right) V, \quad B = V \otimes V - \left( \frac{1}{c_v} \frac{|V|^2}{2} + \frac{\varepsilon'(T)}{c_v(T)} \right) I.
\]
Then we introduce (37) into (35) to get
\[
\sigma_{ij}(F_1) = -\tau \rho T \langle V_i V_j B_{kl} M_0 \rangle_V \partial_{x_l} u_k + O(Kn),
\]
where we have used the change of variables \( v \mapsto V \) in the integral (the term with \( A \) vanishes due to the parity of \( M_0 \)). Then standard Gaussian integrals (see appendix A) give
\[
\sigma(F_1) = -\mu \left( \nabla u + (\nabla u)^T - \alpha \nabla \cdot u I \right) + O(Kn),
\]
with \( \mu = \tau \rho T \) and \( \alpha = \frac{\Delta c_p}{c_v} - 1 \), which is the announced result, in a non-dimensional form.

For the heat flux, we use the same technique. First for \( e_{int} M_{int}(F, G) \) we obtain
\[
\partial_t (e_{int} M_{int}(F, G)) + v \cdot \nabla_x (e_{int} M_{int}(F, G)) = \frac{\rho}{T^2} M_0(V) \left( \tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tilde{B} : \nabla u \right) + O(Kn),
\]
where
\[
\tilde{A} = \left( \frac{|V|^2}{2} - \frac{5}{2} + \frac{T e'_{int}(T)}{e_{int}} \right) V,
\]
\[
\tilde{B} = V \otimes V - \left( \frac{1}{c_v} \frac{|V|^2}{2} + \frac{e'_{int}(T)}{c_v(T)} + \frac{T e'_{int}(T)}{c_v(T)e_{int}} \right) I.
\]

Then \( q(F_1, G_1) \) as given in (36) can be reduced to
\[
q_i(F_1, G_1) = -\tau \rho T \left( \frac{1}{2} |V|^2 V_i A_j M_0 \right)_V + \langle V_i J A_j M_0 \rangle_V \partial_{x_j} T
\]
\[
- \tau \rho \langle V_i \tilde{A}_j M_0 \rangle_V \partial_{x_j} T.
\]
Using again Gaussian integrals, we get
\[
q(F_1, G_1) = -\kappa \nabla_x T,
\]
where \( \kappa = \mu c_p(T) \) with \( c_p(T) = \frac{d}{dT} (e(T) + \frac{\rho}{\rho}) = \frac{5}{2} + e'_{int}(T) = 1 + c_v(T) \) in a non-dimensional form.

5.2.2 Proof for the Fokker-Planck model

Here, we rather use the decomposition \( F = M_{int}(1 + Kn F_1) \) and \( G = e_{int} M_{int}(1 + Kn G_1) \), which gives
\[
\sigma(F) = p I + Kn \sigma(M_{int} F_1) \quad \text{and} \quad q(F, G) = Kn q(M_{int} F_1, e_{int} M_{int} G_1),
\]
in which, for clarity, the dependence of \( M_{int} \) on \( F \) and \( G \) has been omitted, and the dependence of \( e_{int} \) on \( T \) as well. Finding \( F_1 \) and \( G_1 \) is less simple than for the BGK model: however, the computations are very close to what is done in the standard monatomic Fokker-Planck model (see [14] for instance), so that we only give the main steps here (see appendix A for details).

First, the decomposition is injected into (27) to get
\[
D_F(F, G) = \frac{1}{\tau} M_{int} L_F(F_1) + O(Kn),
\]
\[
D_G(F, G) = \frac{1}{\tau} e_{int} M_{int} L_G(F_1, G_1) + O(Kn),
\]
13
where $L_F$ and $L_G$ are linear operators defined by

$$
L_F(F_1) = \frac{1}{M_{int}} \left( \nabla_v \cdot (TM_{int} \nabla_v F_1) \right),
$$

$$
L_G(F_1, G_1) = \frac{1}{e_{int} M_{int}} \left( \nabla_v \cdot (Te_{int} M_{int} \nabla_v G_1) + 2(F_1 - G_1) \right).
$$

Then the Fokker-Planck equations (25)-(26) suggest to look for an approximation of $F_1$ and $G_1$ up to $O(Kn)$ as solutions of

$$
\partial_t M_{int} + v \cdot \nabla_x M_{int} = \frac{1}{\tau} M_{int}(F,G)L_F(F_1)
$$

$$
\partial_t e_{int} M_{int} + v \cdot \nabla_x e_{int} M_{int} = \frac{1}{\tau} e_{int} M_{int}(F,G)L_G(F_1, G_1).
$$

By using (37)-(38), these relations are equivalent, up to another $O(Kn)$ approximation, to

$$
L_F(F_1) = \tau \left( A \cdot \frac{\nabla T}{\sqrt{T}} + B : \nabla u \right), \quad \text{and} \quad L_G(F_1, G_1) = \tau \left( \tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tilde{B} : \nabla u \right),
$$

where $A, B, \tilde{A},$ and $\tilde{B}$ are the same as for the BGK equation in the previous section.

Now, we rewrite $L_F(F_1)$ and $L_G(F_1, G_1)$, defined in (39), by using the change of variables $V = \frac{v - u}{\sqrt{T}}$ to get

$$
L_F(F_1) = -V \cdot \nabla V F_1 + \nabla V \cdot (\nabla V F_1),
$$

$$
L_G(F_1, G_1) = L_F(G_1) + 2(F_1 - G_1).
$$

Then simple calculation of derivatives show that $A, B, \tilde{A},$ and $\tilde{B}$ satisfy the following properties

$$
L_F(A) = -3A, \quad L_F(B) = -2B, \quad L_G(A, \tilde{A}) = -3\tilde{A}, \quad L_G(B, \tilde{B}) = -2\tilde{B}.
$$

Therefore, we look for $F_1$ and $G_1$ as solution of (40) under the following form

$$
F_1 = aA \cdot \frac{\nabla T}{\sqrt{T}} + bB : \nabla u \quad \text{and} \quad G_1 = \tilde{a}\tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tilde{b}\tilde{B} : \nabla u,
$$

and we find $\tilde{a} = a = -1/3$ and $\tilde{b} = b = 1/2$.

Finally, using these relations into $\sigma$ and $q$ and using some Gaussian integrals (see appendix A) give

$$
\sigma(M_{int} F_1) = -\mu \left( \nabla u + (\nabla u)^T - \alpha \nabla \cdot u I \right) \quad \text{and} \quad q(M_{int} F_1, e_{int} M_{int} G_1) = -\kappa \nabla_x T,
$$

where $\alpha = \frac{\alpha_v}{c_v} - 1$, $\mu = \frac{\tau}{2} \rho T$, and $\kappa = \frac{2}{3} \mu c_p(T)$, which is the announced result, in a non-dimensional form.
6 Extension of the model

6.1 Extension to several type of energies

The model we present in this paper recovers Navier-Stokes with potentially false Prandtl number for both BGK and Fokker-Planck models as usual. If one wants to describe more precisely relaxation phenomena of molecules, one has to consider each independent internal energies which means for instance that rotational energy and vibrational energies have to be separated to capture them correctly. Before going to ESBGK or ES Fokker-Planck models we now present the framework that should allow to go further. Let us define $e_{\text{int}}^i, e_{\text{int}}^n$, $n$ independent terms of the internal energy (rotation energy, vibrations energy, electronic energy..) depending on temperature through strictly increasing functions. We can define entropy’s $s_{\text{int}}^a, s_{\text{int}}^n$ associated to each energy satisfying $T_{\text{int}}^{i} ds_{\text{int}}^{i} = e_{\text{int}}^{i}$. As before we define $F$ the function transporting the velocities as well as $G^a, ..., G^n$ the functions that transport other energies. The macroscopic variables are now obtained through $F$ and $G^a, ..., G^n$ only, as it is shown in the following proposition.

**Proposition 6.1** (Moments of the reduced distributions). The macroscopic variables $\rho, u,$ and $e$ are defined through

$$ \rho = \langle F \rangle_v, \quad \rho u = \langle vF \rangle_v, \quad \rho e = \left( \frac{1}{2} (v - u)^2 F \right)_v + \langle (G^a + ... + G^n) \rangle_v. \quad (41) $$

Now it is possible to write a reduced entropy as a function of $F$ and $G^a, ..., G^n$ only, as it is shown in the following proposition.

**Proposition 6.2** (Entropy). We define the following reduced entropy for $F, G^a, ..., G^n$ $\mathcal{H}(F,G)$:

$$ \mathcal{H}(F,G^a,..,G^n) = \left< F \log(F) - F \frac{s_{\text{int}}^a}{R} \frac{G^a}{F} - ... - F \frac{s_{\text{int}}^n}{R} \frac{G^n}{F} \right>_v. \quad (42) $$

1. The partial derivatives of $H$ computed at $(F,G)$ are:

$$ D_F H(F,G) = 1 + \log(F) + \sum_{i=a}^n \left( \frac{G^a}{RT_{\text{int}}^a(G^a/F)F} - \frac{s_{\text{int}}^a}{R} \frac{G^a}{F} \right), \quad (43) $$

$$ D_{G^a} H(F,G) = -\frac{1}{RT_{\text{int}}^a(G^a/F)}. \quad (44) $$

2. We note $\mathbb{H}$ the Hessian matrix of $H$ which can be computed through:

$$ \begin{align*}
D_{F,F} H &= \frac{1}{F} + \sum_{i=a}^n \frac{G^i}{F^2 c_{\text{vint}} RT_{\text{int}}^i (G^i/F)} \quad (45) \\
D_{G^a,F} &= D_{F,G^a} H = -\frac{G^a}{F^2 c_{\text{vint}} RT_{\text{int}}^a (G^a/F)} \quad (46) \\
D_{G^a,G^b} H &= 0 (a \neq b), \quad (47) \\
D_{G^a,G^b} H &= 1 \frac{1}{F c_{\text{vint}} RT_{\text{int}}^a (G^a/F)} \quad (48)
\end{align*} $$
Moreover, we have the following equality’s:

\[ FD_{F,F}H + \sum_{i=a}^{n} G^i D_{F,G^i}H = 1 \quad , \quad FD_{F,G^a}H + G^a D_{G^a,G^a}H = 0. \]  

(49)

3. The function \((F, G^a, \ldots, G^n) \mapsto H(F, G^a, \ldots, G^n)\) is convex.

4. Let \((F, G^a, \ldots, G^n)\) be reduced distributions and \(\rho, pu\), and \(pe\) their moments as defined by (41).

Let \(\mathcal{S}\) be the convex set defined by

\[ \mathcal{S} = \{ (F, G^a_1, \ldots, G^n_a) \text{ such that } (F^i)_v = \rho, \quad (vF^i)_v = pu, \quad \left< \frac{1}{2} |v|^2 F^i + G^a_1 + \ldots + G^n_1 \right>_v = \rho e \}. \]

The minimum of \(H\) on \(\mathcal{S}\) is obtained for \((M_{int}(F, G), e_{int}^a(T)M_{int}(F, G), \ldots, e_{int}^n(T)M_{int}(F, G))\) with

\[ M_{int}[F, G] = \frac{\rho}{\sqrt{2\pi RT}} \exp \left( -\frac{|v - u|^2}{2RT} \right) \]  

(50)

where \(e_{int}^a(T)\) is the equilibrium internal energy obtained for \(T\).

5. For every \((F_1, G^a_1, \ldots, G^n_1)\) in \(\mathcal{S}\), we have

\[ 0 \geq H(M_{int}(F, G^a, \ldots, G^n), e_{int}^a(T)M_{int}(F, G^a, \ldots, G^n) - H(F_1, G^a_1, \ldots, G^n_1) \]

\[ \geq D_1 H(F, G)(M_{int}(F, G^a, \ldots, G^n) - F) \]

\[ + \sum_{i=a}^{n} D_{G^i}(F, G^a, \ldots, G^n)(e_{int}^i(T)M_{int}(F, G^a, \ldots, G^n) - G^i) \]  

(51)

Proof. The proof is the same as the one with one energy. The only tricky part (that we prove here) is that the Hessian is positive definite. The quadratic form associated to \(\mathcal{H}\) is clearly positive definite on vectors of the form \((0, x_1, \ldots, x_n)\) because the diagonal terms of the matrix are strictly positive on this subspace so the Hessian have at least \(n\) strictly positive eigenvalues. To ensure that the Hessian matrix is positive definite it is sufficient to have a strictly positive determinant. Developing the determinant one gets:

\[ \det(\mathcal{H}) = D_{F,F}(H) \prod_{i=a}^{n} D_{G^a,G^a}(H) - \sum_{i=a}^{n} D_{G^i,F}(H) \prod_{i \neq j} D_{G^j,G^j}(H) \]

\[ = \frac{1}{F} \prod_{i=a}^{n} D_{G^a,G^a}(H) - \sum_{i=a}^{n} \frac{G^i}{F} D_{G^i,F}(H) D_{G^a,G^a}(H) \]

\[ - \sum_{i=a}^{n} \left( -\frac{G^i}{F} D_{G^i,F}(H) D_{G^a,F}(H) \right) \prod_{i \neq j} D_{G^j,G^j}(H) \]

\[ = \frac{1}{F} \prod_{i=a}^{n} D_{G^a,G^a}(H) - \sum_{i=a}^{n} \frac{G^i}{F} D_{G^i,F}(H) \prod_{i=a}^{n} D_{G^a,G^a}(H) + \left( \sum_{i=a}^{n} \frac{G^i}{F} D_{G^i,F}(H) \right) \prod_{i=a}^{n} D_{G^i,G^i}(H) \]

\[ = \frac{1}{F} \prod_{i=a}^{n} D_{G^a,G^a}(H) > 0 \]
so that the Hessian is positive definite. Equilibrium property is the same as with one energy and convex properties are obtained thanks to the Hessian.

Thanks to this framework we are able to give the BGK model and the Fokker-Planck model associated to \( n \) energies as well as their Chapman-Enskog expansion. We do not give the proof since there are exactly the same as before.

6.2 BGK model and its hydrodynamic limit for \( n \) energies

For physics considerations, it is interesting to reduce complex kinetic models by using the usual reduced distribution technique [23]. Even for perfect gases, some degenerate models of energy cannot be described easily through equilibrium (extensions of Maxwellians is not very clear when ones deals with partial degrees of freedom of internal energy. In this paper we propose to use two reduced functions \( F \) and \( G \) that will transport energy. \( F \) is transporting the translational energy whereas \( G \) transport the reminder of internal energy. More precisely they are defined through:

\[
\frac{\partial_t F}{\tau} + v \cdot \nabla_x F = \frac{1}{\tau} (M_{int}[F,G] - F),
\]

(52)

\[
\frac{\partial_t G^i}{\tau} + v \cdot \nabla_x G^i = \frac{1}{\tau} (e^n_{int}M_{int}[F,G^n,...,G^n] - G^i) \quad \forall a \leq i \leq n
\]

(53)

where the reduced Maxwellian is

\[
M_{int}[F,G] = \frac{\rho}{\sqrt{2\pi RT}} \exp \left( -\frac{|v - u|^2}{2RT} \right),
\]

and the macroscopic quantities are defined by

\[
\rho = \langle F \rangle_v, \quad \rho u = \langle vF \rangle_v, \quad \rho e = \left( \frac{1}{2}(v-u)^2 \right)_v F + \sum_{i=a}^{n} \langle G_i \rangle_v,
\]

(54)

and \( T \) is still defined by [22].

System (52-53) naturally satisfies local conservation laws of mass, momentum, and energy. Moreover, the H-theorem holds with the reduced entropy \( H(F,G) \) as defined in (42). Indeed, we recover the two following propositions:

**Proposition 6.3.** The reduced BGK system (52-53) satisfies the H-theorem

\[
\frac{\partial_t \mathcal{H}(F,G^a,...,G^n)}{\tau} + \nabla_x \cdot \langle vH(F,G^a,...,G^n) \rangle_v \leq 0,
\]

where \( \mathcal{H}(F,G^n,...,G^n) \) is the reduced entropy defined in (42).

**Proposition 6.4.** The moments of the solution of the BGK models (52)-(53) satisfy, up to \( O(Kn^2) \), the Navier-Stokes equations

\[
\begin{align*}
\frac{\partial_t \rho}{\tau} + \nabla \cdot \rho u &= 0, \\
\frac{\partial_t \rho u}{\tau} + \nabla \cdot (\rho u \otimes u) + \nabla p &= -\nabla \cdot \sigma, \\
\frac{\partial_t E}{\tau} + \nabla \cdot (E + p)u &= -\nabla \cdot q - \nabla \cdot (\sigma u),
\end{align*}
\]

(55)
where the shear stress tensor and the heat flux are given by

\[
\sigma = -\mu (\nabla u + (\nabla u)^T - \alpha \nabla \cdot u), \quad \text{and} \quad q = -\kappa \nabla \cdot T,
\]

and where the following values of the viscosity and heat transfer coefficients (in dimensional variables) are

\[
\mu = \tau p, \quad \text{and} \quad \kappa = \mu c_p(T),
\]

while the volum viscosity coefficient is \(\alpha = \frac{c_v(T)}{c_v(T)} - 1\) and \(c_p(T) = \frac{d}{dT}(e(T) + p/\rho) = c_v(T) + R\) is the heat capacity at constant pressure. Moreover, the corresponding Prandtl number is

\[
\Pr = \frac{\mu c_p(T)}{\kappa} = 1
\]

6.3 Fokker-Planck model and its hydrodynamic limit for \(n\) energies

By analogy, we propose the following reduced Fokker-Planck model:

\[
\begin{align*}
\partial_t F + v \cdot \nabla_x F &= D_F(F, G^a, ..., G^n), \\
\partial_t G^i + v \cdot \nabla_x G^i &= D_G(F, G^i, ..., G^n) \quad \forall a \leq i \leq n,
\end{align*}
\]

with

\[
\begin{align*}
D_F(F, G^a, ..., G^n) &= \frac{1}{\tau} \left( \nabla_v \cdot \left( (v - u)F + RT \nabla_v F \right) \right), \\
D_G(F, G^i, ..., G^n) &= \frac{1}{\tau} \left( \nabla_v \cdot \left( (v - u)G^i + RT \nabla_v G^i \right) \right) + \frac{2}{\tau} \left( e^{i \Omega}(T)F - G^i \right),
\end{align*}
\]

where the macroscopic values are defined as in (54) and (2). Using direct calculations and dissipation properties we can prove the following propositions.

**Proposition 6.5.** The collision operator conserves the mass, momentum, and energy:

\[
\langle (1, v)D_F(F, G^a, ..., G^n) \rangle_v = 0 \quad \text{and} \quad \left\langle \frac{1}{2}|v|^2 D_F((F, G^a, ..., G^n) + D_G(F, G^a, ..., G^n) \right\rangle_v = 0,
\]

the reduced entropy \(\mathcal{H}(F, G^a, ..., G^n)\) satisfies the H-theorem:

\[
\partial_t \mathcal{H}(F, G^a, ..., G^n) + \nabla_x \cdot \langle vH(F, G^a, ..., G^n) \rangle_v \leq 0,
\]

and we have the equilibrium property

\[
(D_F(F, G^a, ..., G^n) = 0 \text{ and } \forall i, D_G(F, G^a, ..., G^n) = 0)
\]

\[
\Leftrightarrow (F = M_{\text{int}}(F, G^a, ..., G^n) \text{ and } \forall i, G^i = e^{i \Omega}(T)M_{\text{int}}(F, G^a, ..., G^n)).
\]

**Proposition 6.6.** The moments of the solution of the Fokker-Planck kinetic model (59)-(60) satisfy, up to \(O(\text{Kn}^2)\), the Navier-Stokes equations

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho u) &= 0, \\
\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p &= -\nabla \cdot \sigma, \\
\partial_t E + \nabla \cdot (E + p)u &= -\nabla \cdot q - \nabla \cdot (\sigma u),
\end{align*}
\]
where the shear stress tensor and the heat flux are given by
\[ \sigma = -\mu (\nabla u + (\nabla u)^T - \alpha \nabla \cdot u), \quad \text{and} \quad q = -\kappa \nabla \cdot T, \]
and where the following values of the viscosity and heat transfer coefficients (in dimensional variables) are
\[ \mu = \frac{1}{2} \tau p, \quad \text{and} \quad \kappa = \frac{2}{3} \mu c_p(T), \]
while the volumic viscosity coefficient is \( \alpha = c_v(T)/c_v(T) - 1 \) for both models, and \( c_p(T) = \frac{d}{dT} (e(T) + p/\rho) = c_v(T) + R \) is the heat capacity at constant pressure. Moreover, the corresponding Prandtl number is
\[ \text{Pr} = \frac{\mu c_p(T)}{\kappa} = \frac{3}{2} \]

### 6.4 Comments and application to the vibrational case

In the previous subsection we have explained how we can try to capture every kind of energy as long as they are strictly increasing functions of temperatures. We also have constructed an entropy adapted to this situation but to fully use the result one will have to create ESBGK or ES-Fokker Planck like models to capture different relaxations times. We now explain how to use this extension for a diatomic vibrational gas. Such a gas owns a translational, a rotational and a vibrational energy defined as functions of temperatures through:
\[ e_{tr}(T) = \frac{3}{2} RT, \quad e_{rot}(T) = RT, \quad e_{vib}(T) = \frac{RT_0}{e^{T_0/T} - 1}. \]
The associated macroscopic entropy’s for internal degrees of freedom are
\[ s_{\text{rot}}(e) = R \ln(e), \quad s_{\text{vib}}(e) = \left( \frac{e}{T_0} + R \right) \ln \left( \frac{e + RT_0}{RT_0} \right) - \frac{e}{T_0} \ln \left( \frac{e}{RT_0} \right), \]
which leads to the following kinetic entropy:
\[ \mathcal{H}(F,G^{\text{rot}},G^{\text{vib}}) = \left\langle F \log(F) - F \frac{s^{\text{rot}}}{R} \left( \frac{G^{\text{rot}}}{F} \right) - F \frac{s^{\text{vib}}}{R} \left( \frac{G^{\text{vib}}}{F} \right) \right\rangle_v \]
\[ = \left\langle F \log(F) + F \ln \left( \frac{F}{G^{\text{rot}}} \right) + F \ln \left( \frac{RT_0 F}{RT_0 F + G^{\text{vib}}} \right) + \frac{G^{\text{vib}}}{RT_0} \ln \left( \frac{G^{\text{vib}}}{RT_0 F + G^{\text{vib}}} \right) \right\rangle_v. \]
The expression of the vibration’s entropy recovers the one given in [16, 22] and the expression for rotations the one in [11].

### 7 Conclusion and perspectives

In this paper, we have proposed to different models (BGK and Fokker-Planck) of the Boltzmann equation that allow for thermally perfect gases. These models satisfy the conservation and entropy
property (H-theorem) and are using reduced distribution functions with only velocity as a kinetic variable. The low complexity of the reduced BGK model can make it attractive to be implemented in a deterministic code, while the Fokker-Planck model can be easily simulated with a stochastic method. Of course, since these models are based on a single time relaxation, they cannot allow for multiple relaxation times scales but we have made ground for standard procedures like the ellipsoidal-statistical approach, already used to correct the Prandtl number of the BGK model [11] and Fokker-Planck models [16] by already defining models with one equation for each kind of energy in the last section of this paper.

A Gaussian integrals and other summation formula

In this section, we give some integrals and summation formula that are used in the paper.

First, we remind the definition of the absolute Maxwellian $M_0(V) = \frac{1}{(2\pi)^{3/2}} \exp(-\frac{|V|^2}{2})$. We denote by $\langle \phi \rangle = \int_{\mathbb{R}^3} \phi(V) dV$ for any function $\phi$. It is standard to derive the following integral relations (see [24], for instance and note that some computations are redundant), written with the Einstein notation:

$$
\langle M_0 \rangle_V = 1,
\langle V_i V_j M_0 \rangle_V = \delta_{ij},
\langle V_i^2 M_0 \rangle_V = 1,
\langle |V|^2 M_0 \rangle_V = 3,
\langle V_i^2 V_j^2 M_0 \rangle_V = 1 + 2 \delta_{ij},
\langle V_i V_j V_k V_l M_0 \rangle_V = \delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk},
\langle V_i V_j |V|^2 M_0 \rangle_V = 5 \delta_{ij},
\langle |V|^4 M_0 \rangle_V = 15,
\langle V_i V_j |V|^4 M_0 \rangle_V = 35 \delta_{ij},
\langle |V|^6 M_0 \rangle_V = 105,
$$

while all the integrals of odd power of $V$ are zero. From the previous Gaussian integrals, it can be shown that for any $3 \times 3$ matrix $C$, we have

$$
\langle V_i V_j C_{kl} V_k V_l M_0 \rangle_V = C_{ij} + C_{ji} + C_{ii} \delta_{ij}.
$$

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