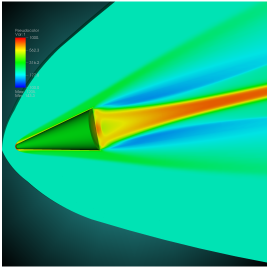
DE LA RECHERCHE À L'INDUSTRIE

Moment models for rarefied gas dynamics at high temperatures



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International Workshop on Simulating Interacting Particles

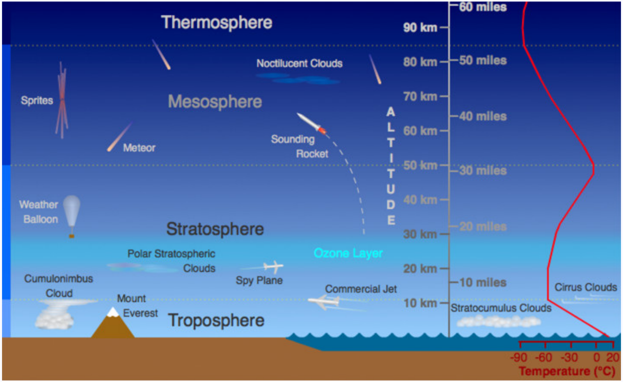
Atmospheric reentry

From rarefied flows to continuous flows

Rarefied Gas dynamics

Continuous laminar flows

Turbulent laminar flows



Outline

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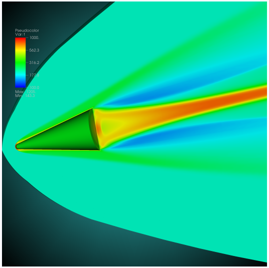
1. Context
2. New results for Fokker-Planck models
3. Models for vibrations
4. New results for BGK models and their extensions
5. Perspectives

Atmospheric re-entry context

Steady flow

- Flow around spacecraft
- Hypersonic flows
- Sphere-cone configuration
- Quantities of interest: heat flux and aerodynamic coefficients



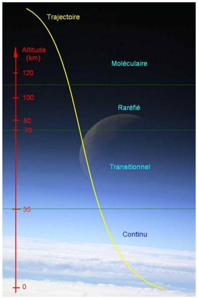
Looking for **steady state solution**: relaxation time scale $\ll$ trajectory time scale

Physical numbers

Knudsen number

Knudsen number:

$$Kn = \frac{\lambda}{L} \quad \left(\frac{\text{mean free path}}{\text{characteristic length}}\right)$$



Free molecular zone (Kn > 10)

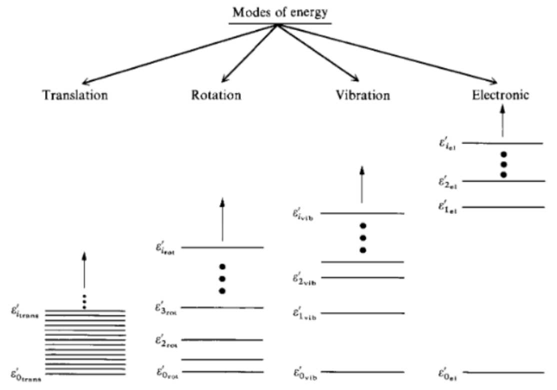
Kinetic theory

Navier-Stokes (Kn < 0.1)

Prandtl number

The Prandtl number characterizes the ratio of the conductivity (λ) and the viscosity (μ) of a gas of specific heat C_p through: $Pr = \dfrac{\mu C_p}{\lambda}$.
In heat transfer problems, the Prandtl number controls the relative thickness of the momentum and thermal boundary layers.It is equal to $2/3$ for monoatomic perfect gases

Modes of energy in the air



	Translation	Rotation	Vibration	Electronic
Typical temperature of activation (K)	1	3	600	10000

Some chemistry in the air

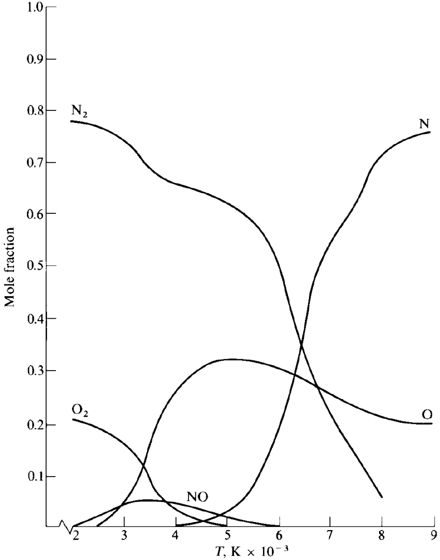


Fig. 11.12 **Composition of equilibrium air vs temperature at 1 atm.**

Zoology of models (1): Boltzmann equation

Boltzmann equation: $f(t,x,v)$

$$\partial_t f + v \cdot \nabla_x f = Q(f,f),$$

$$Q(f,f)(v) = \iint_{v_* \in \mathbb{R}^3, \sigma \in \mathbb{S}^2} \Big(f(v'_*)\, f(v') - f(v_*)\, f(v) \Big)\, r^2\, |v - v_*|\, d\sigma\, dv_*,$$

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma \qquad , \qquad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2}\sigma.$$

Advantages and drawbacks

- \+ Capture the correct physics: in the Chapman expansion one recovers the Prandtl number of Navier-Stokes equation which is equal to $\frac{2}{3}$ for a monoatomic gas
- \- High numerical cost in transitional area between 100km and 60km (6D non linear problem).

Zoology of models (2): BGK equation and Fokker Planck equation

BGK equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau}\left(M(f) - f\right),$$

$M(f) = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(\frac{|v-u|^2}{2RT}\right)$ is the Maxwellian of equilibrium satisfying:

$$< f > \quad = \quad \int f dv = \rho, < fv >= \int fv dv = \rho u, < f\frac{1}{2}(v-u)^2 >= \int f\frac{1}{2}(v-u)^2 dv = \frac{3}{2}\rho T$$

τ: characteristic time of collisions.

Fokker Planck equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau}\nabla_v \cdot \left((v-u)f + T\nabla_v f\right),$$

Zoology of models (2): BGK equation and Fokker Planck equation

Advantages and drawbacks

- \- Physics only approximated: thermal flux underestimated. The Prandtl number is equal to 1 for BGK model and $\frac{3}{2}$ for *FP* model.
- \+ Numerical cost less important in transitional area between 100km and 60km.

How to recover the correct Prandtl number?

For BGK models it has been done using the ESBGK model:

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\tau} \left(G(f) - f \right),$$

with $G(f)$ anisotropic Gaussian defined as:

$$G(f) = \frac{\rho}{\sqrt{\det(2\pi\Pi)}} \exp\left(-\frac{(v-u)\Pi^{-1}(v-u)}{2} \right).$$

Π being a tensor linked to the different temperatures of thermal agitation.

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Polyatomic model

Equations

We consider a gas described by the particle mass density $f(t,x,v,I)$ that at time t have the position x, the velocity v and an internal energy parameter I (of internal energy $I^{2/\delta}$:

$$\partial_t f + v\cdot\nabla_x f = \underbrace{\frac{1}{\tau}\left(\nabla_v\cdot\left((v-u)f+\Pi\nabla_v f\right)+\partial_I\left(\delta f I+\frac{\delta^2}{2}RT_{rel}I^{2-\frac{2}{\delta}}\partial_I f\right)\right)}_{D(f)},$$

with:

$$\begin{aligned}
&\Theta := \frac{1}{\rho}\left\langle (v-u)\otimes(v-u)f\right\rangle,\\
&E_{tr} = \frac{3}{2}\rho RT_{tr} = \left\langle \tfrac{1}{2}|v-u|^2 f\right\rangle, E_{int} = \frac{\delta}{2}\rho RT_{int} = \left\langle \varepsilon(I)f\right\rangle,\\
&T = \frac{3}{3+\delta}T_{tr} + \frac{\delta}{3+\delta}T_{int},\\
&\Pi = (1-\theta)\left((1-\nu)RT_{tr}Id+\nu\Theta\right)+\theta RTId,\\
&T_{rel} = (1-\theta)T_{int}+\theta T.
\end{aligned}$$

where the coefficients ν and θ are some free parameters to be fitted.

Conservation properties

Proposition

We assume ν satisfies a positiveness condition for Π and that $\nu < 1$. The collision operator D conserves mass, momentum, and energy:

$$\left\langle \left(1, v, \tfrac{1}{2}|v|^2 + I^{2/\delta}\right) D(f) \right\rangle = 0,$$

It satisfies the dissipation of the entropy:

$$\langle D(f) \log f \rangle \leq 0,$$

and the equilibrium property:

$$D(f) = 0 \Leftrightarrow f = G_p(f) \Leftrightarrow f = M_p(f).$$

with:

$$M_p(f) = \frac{\rho \Lambda_\delta}{(2\pi)^{3/2} \left(RT\right)^{(3+\delta)/2}} \exp\left(-\frac{|v-u|^2}{2RT} - \frac{I^{2/\delta}}{RT} \right),$$

$$G_p(f) = \frac{\rho \Lambda_\delta}{\sqrt{\det(2\pi\Pi)} (RT_{rel})^{\delta/2}} \exp\left(-\frac{1}{2} \begin{pmatrix} v-u \\ \delta I \end{pmatrix}^T \left(\begin{array}{c|c} \Pi & 0 \\ \hline 0 & \frac{\delta^2}{2} RT_{rel} I^{2-\frac{2}{\delta}} \end{array} \right)^{-1} \begin{pmatrix} v-u \\ \delta I \end{pmatrix} \right).$$

Navier-Stokes limit through Chapmann-Enskog expansion

The moments of f satisfy, up to $O(Kn^2)$, the Navier-Stokes equations:

$$\begin{aligned}
&\partial_t\rho + \nabla\cdot\rho u = 0,\\
&\partial_t\rho u + \nabla\cdot(\rho u\otimes u) + \nabla p = -\nabla\cdot\sigma,\\
&\partial_t E + \nabla\cdot(E+p)u = -\nabla\cdot q - \nabla\cdot(\sigma u),
\end{aligned}$$

where the shear stress tensor and the heat flux are given by

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

with the following values of the viscosity and heat transfer coefficients (in dimensional variables).

$$\mu = \frac{\tau p}{2(1-(1-\theta)\nu)}, \quad \alpha = (\gamma-1) - \frac{(1-\nu)(1-\theta)}{\theta}\left(\frac{5}{3}-\gamma\right) \quad \text{and} \quad \kappa = \frac{5+\delta}{6}\tau p R,$$

and $\gamma = \frac{\delta+5}{\delta+3}$. Moreover, the corresponding Prandtl number is

$$\mathrm{Pr} = 3/(2(1-(1-\theta)\nu)).$$

Numerical 0-D scheme

Ornstein-Uhlenbeck process

The Ornstein-Uhlenbeck process reads:

$$\begin{aligned} dV_i(t) &= -\frac{dt}{\tau}\left(V_i(t)-u\right)+A_v dB_v(t), \\ d\varepsilon_i(t) &= -\frac{2dt}{\tau}\left(\varepsilon_i(t)-\frac{\delta}{2}RT_{rel}\right)+2\sqrt{RT_{rel}\varepsilon_i(t)}\,dB_\varepsilon(t), \end{aligned}$$

$$V_i^{n+1}=\left(1-\frac{\Delta t}{\tau}\right)\left(V_i^n-u\right)+\sqrt{\frac{2\Delta t}{\tau}}A\begin{pmatrix} B_1 \\ B_2 \\ B_3 \end{pmatrix}$$

$$\varepsilon_i^{n+1}=\left(\left(\sqrt{\varepsilon_i^n}+\sqrt{\frac{dt}{\tau}RT_{rel}}B_\varepsilon\right)^2+(\delta-1)RT_{rel}\frac{dt}{\tau}\right)\Big/\left(1+\frac{2dt}{\tau}\right),$$

Numerical results: 0D and 2D

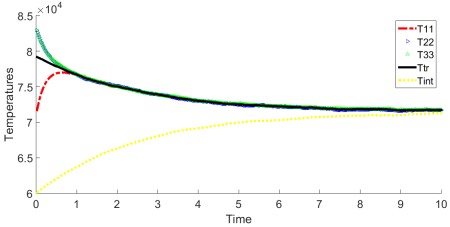

Figure: Convergence of the directional translational temperatures and the internal temperature to their equilibrium value.

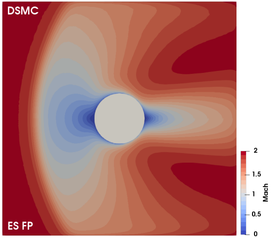

Figure: Comparison at Mach 2, Kn=0.05 between DSMC and FP in collaboration with H. Gorji (RWTH Aachen, Germany)

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3 **Models for vibrations**

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Simple vibratory models

Definition

Let $f(t, x, v, \varepsilon, i)$ be the mass density distribution of particles with position x, velocity v, internal energy ε, and in the i-th vibrational energy level, such that its vibrational energy is iRT_0 (T_0: characteristic vibrational temperature of the molecule). The corresponding local equilibrium distribution is defined by:

$$M_{vib}[f](v, \varepsilon, i) = \frac{\rho}{\sqrt{2\pi RT}^3} \frac{1 - e^{-T_0/T}}{RT} \exp\left(- \frac{\frac{1}{2}|u - v|^2 + \varepsilon + iRT_0}{RT} \right)$$

$$\rho = \langle f \rangle_{v,\varepsilon,i}\,, \qquad \rho u = \langle vf \rangle_{v,\varepsilon,i}\,, \qquad \rho e = \left\langle \left(\frac{1}{2}|v - u|^2 + \varepsilon + iRT_0 \right) f \right\rangle_{v,\varepsilon,i}\,,$$

where we use the notation $\langle \phi \rangle_{v,\varepsilon,i} = \sum_{i=0}^{\infty} \iint \phi(t, x, v, \varepsilon, i)\, dv d\varepsilon$ for any function ϕ.

The temperature T can be recovered by inverting the relation $e = \left(\frac{5}{2} + \frac{T_0/T}{e^{T0/T} - 1} \right) RT$ so that there exists T^{-1} such that $T = T^{-1}(e)$.

The entropy $H(f)$ of f is naturally defined through $H(f) = \langle f \log f \rangle_{v,\varepsilon,i}\,.$

Some properties and notations

Properties of the equilibrium

$$\langle M_{vib}[f]\rangle_{v,\varepsilon,i} = \rho, \quad \langle vM_{vib}[f]\rangle_{v,\varepsilon,i} = \rho u, \quad \left\langle (\frac{1}{2}(v-u)^2 + \varepsilon + iRT_0)M_{vib}[f]\right\rangle_{v,\varepsilon,i} = \rho e.$$

Energies at equilibrium

At equilibrium, we define the following energies of translation, rotation, and vibration:

$$e_{tr}(T) = \left\langle (\frac{1}{2}(v-u)^2)M_{vib}[f]\right\rangle_{v,\varepsilon,i} = \frac{3}{2}\rho RT, \tag{1}$$

$$e_{rot(T)} = \langle \varepsilon M_{vib}[f]\rangle_{v,\varepsilon,i} = \rho RT, \tag{2}$$

$$e_{vib}(T) = \langle (iRT_0)M_{vib}[f]\rangle_{v,\varepsilon,i} = \rho\frac{RT_0}{e^{T_0/T}-1} = \rho\frac{\delta(T)}{2}RT, \tag{3}$$

with $\delta(T) = 2\frac{T_0/T}{e^{T0/T}-1}$.

Reduced models for vibrations: construction

Reduced distributions

For computational efficiency, it is interesting to define marginal, or reduced, distributions F and G by :

$$F(t,x,v,\varepsilon) = \sum_i f(t,x,v,\varepsilon,i),$$
$$G(t,x,v,\varepsilon) = \sum_i iRT_0 f(t,x,v,\varepsilon,i).$$

The macroscopic variables defined by f can be obtained through F and G only

$$\rho = \langle F\rangle_{v,\varepsilon}, \qquad \rho u = \langle vF\rangle_{v,\varepsilon}, \qquad \rho e = \left\langle (\frac{1}{2}(v-u)^2+\varepsilon)F \right\rangle_{v,\varepsilon} + \langle G\rangle_{v,\varepsilon}.$$

where we use the notation $\langle \psi\rangle_{v,\varepsilon} = \iint \psi(t,x,v,\varepsilon)\, dv d\varepsilon$ for any function ψ.

Reduced models: entropy

Entropy

The reduced entropy $\mathcal{H}(F,G)$ of the system is:

$$\mathcal{H}(F,G) = \left\langle F\log(F) + F\log\left(\frac{RT_0F}{RT_0F+G}\right) + \frac{G}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)\right\rangle_{v,\varepsilon}.$$

Proof (1)

The set $\{f > 0 \text{ such that } \sum_i f_i = F, \quad \sum_i iRT_0f_i = G\}$ is clearly convex, so that we can use a Lagrangian multiplier approach by finding a saddle point of the function $\mathcal{I}$ defined through :

$$\mathcal{I}(f,\alpha,\beta) = \sum_i f_i\log f_i - \alpha\left(\sum_i f_i - F\right) - \beta\left(\sum_i iRT_0f_i - G\right),$$

where α and β are real numbers.

Reduced models: entropy

Proof (2)

The saddle point satisfies $\dfrac{\partial \mathcal{I}}{\partial f} = 0$, and one deduces that f can be written $f_i(v, \varepsilon) = A(v, \varepsilon)\exp\left(-iB(v, \varepsilon)T_0\right)$. The linear constraints give:

$$F = \sum_i f_i = \frac{A}{1-\exp\left(-BT_0\right)} \quad , \quad G = \sum_i f_i iRT_0 = \frac{ART_0\exp\left(-BT_0\right)}{\left(1-\exp\left(-BT_0\right)\right)^2}.$$

Solving this linear system gives:

$$H(F, G) = F\log(F) + F\log\left(\frac{RT_0F}{RT_0F+G}\right) + \frac{G}{RT_0}\log\left(\frac{G}{RT_0F+G}\right),$$

using that $G/F = e_{vib}(1/B)$.

A final integration with respect to v and ε gives the final result:

$$\mathcal{H}(F, G) = \langle H(F, G)\rangle_{v,\varepsilon}$$

Reduced models: H-theorem

Proposition

We have the following properties

- the function $(F, G) \mapsto H(F, G)$ is convex.
- the minimum of $\mathcal{H}(F_1, G_1)$ on $\mathcal{S}$ is obtained on $(M_{vib}(F, G), N_{vib}(F, G))$ with:

$$M_{vib}(F, G) = \frac{\rho}{\sqrt{2\pi RT}^3} \exp\left(-\frac{\rho|u - v|^2}{2RT}\right) \frac{1}{RT} \exp\left(-\frac{\varepsilon}{RT}\right),$$

$$N_{vib}(F, G) = e_{vib}(T) M_{vib}(F, G)),$$

where $e_{vib}(T)$ is the equilibrium vibrational energy.

Mathematical properties of the entropy

Properties

- We note $\mathbb{H}(F,G)$ be the positive-definite Hessian matrix of H.

$$\mathbb{H}(F,G) = \begin{pmatrix} \frac{2}{F} - \frac{RT_0}{RT_0F+G} & -\frac{1}{RT_0F+G} \\ -\frac{1}{RT_0F+G} & \frac{F}{G(RT_0F+G)} \end{pmatrix} \tag{4}$$

  It satisfies: $1 = F\mathbb{H}_{11}(F,G) + G\mathbb{H}_{21}(F,G) \quad , \quad 0 = F\mathbb{H}_{12}(F,G) + G\mathbb{H}_{22}(F,G).$

- Using $D_1(H)(F,G) = 1 + \log\left(\frac{RT_0F^2}{RT_0F+G}\right)$, $D_2(H)(F,G) = \frac{1}{RT_0}\log\left(\frac{G}{RT_0F+G}\right)$, we have:

$$\begin{aligned} &\mathcal{H}(M_{vib}(F,G), N_{vib}(F,G)) - \mathcal{H}(F,G) \\ &\qquad \geq D_1(H)(F,G)(M_{vib}(F,G) - F) + D_2(H)(F,G)(N_{vib}(F,G) - G) \end{aligned} \tag{5}$$

Consequences

Equations (4) and (5) respectively give the second principle for the Fokker-Planck model and the BGK model we are going to construct.

Vibrationnal BGK model with correct second principle

Model

$$
\begin{aligned}
\partial_t F + v\cdot\nabla_x F &= \frac{1}{\tau}\left(M_{vib}[F,G] - F\right),\\
\partial_t G + v\cdot\nabla_x G &= \frac{1}{\tau}\left(N_{vib}[F,G] - G\right).
\end{aligned}
$$

with:

$$
\begin{aligned}
F &= \sum_i f(t,x,v,\varepsilon,i),\, G = \sum_i iRT_0 f(t,x,v,\varepsilon,i),\\
M_{vib}[F,G] &= \frac{\rho}{\sqrt{2\pi RT}^3}\exp\left(-\frac{\rho|u-v|^2}{2p}\right)\frac{1}{RT}\exp\left(-\frac{\varepsilon}{RT}\right),\\
\rho &= \langle F\rangle_{v,\varepsilon}, \rho u = \langle Fv\rangle_{v,\varepsilon}, \rho e = \left\langle F\left(\frac{1}{2}(v-u)^2+\varepsilon\right)\right\rangle_{v,\varepsilon} + \langle G\rangle_{v,\varepsilon},\\
T &= T^{-1}(e).
\end{aligned}
$$

Hydrodynamic limit

Let (F, G) be solutions of BGK equations up to $O(\mathrm{Kn}^2)$. Then the moments of (F, G) satisfy the following Navier-Stokes equations up to $O(\mathrm{Kn}^2)$:

$$\begin{cases} \partial_t\rho + \mathrm{div}_{\mathbf{x}}(\rho u) = 0 \\ \partial_t(\rho u) + \mathrm{div}_{\mathbf{x}}(\rho u \otimes u) + \nabla_x p = -\mathrm{div}_{\mathbf{x}}(\sigma) + O(\mathrm{Kn}^2) \\ \partial_t E + \mathrm{div}_{\mathbf{x}}((E+p)u) = -\mathrm{div}_{\mathbf{x}}(q) - \mathrm{div}_{\mathbf{x}}(\sigma u) + O(\mathrm{Kn}^2)\,, \end{cases}$$

with:

$$E = \left\langle \left(\frac{1}{2}|v|^2 + \varepsilon\right) F + G \right\rangle_{v,\varepsilon} = \rho e + \frac{1}{2}\rho|u|^2\,,$$

$$\sigma = -\mu\left(\nabla_x u + \nabla_x u^T - \mathcal{C}\,\mathrm{div}_{\mathbf{x}}(u)\,Id\right)\,,$$

$$q = -\mu\nabla_x h\,,$$

where $h = e + RT$, $\mathcal{C} = \partial_e(RT) = \frac{R}{C_v(T)}$, $C_v(T) = \frac{5}{2}R + \frac{(T_0/T)^2 e^{T_0/T}}{(e^{T_0/T}-1)^2}R$.

By defining $C_p = C_v + R$ the specific heat at constant pressure, one gets:

$$q = -\mu C_p \nabla_x T,$$

so that as usual only a gas with a Prandtl number of one is obtained.

Vibrationnal Fokker-Planck model with correct second principle

Model

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

with:

$$\begin{aligned}
F &= \sum_i f(t,x,v,\varepsilon,i), G = \sum_i iRT_0 f(t,x,v,\varepsilon,i),\\
D_F(F,G) &= \frac{1}{\tau}\left(\nabla_v \cdot \left((v-u)F + T\nabla_v F\right) + 2\nabla_\varepsilon (F\varepsilon + RT\varepsilon\nabla_\varepsilon F)\right),\\
D_G(F,G) &= \frac{1}{\tau}\left(\nabla_v \cdot \left((v-u)G + T\nabla_v G\right) + 2\nabla_\varepsilon (G\varepsilon + RT\varepsilon\nabla_\varepsilon Gf)\right)\\
&+ \frac{2}{\tau}\left(e_{vib}(T)F - G\right),\\
\rho &= \langle F \rangle_{v,\varepsilon}, \rho u = \langle Fv \rangle_{v,\varepsilon}, \rho e = \left\langle F\left(\frac{1}{2}(v-u)^2 + \varepsilon\right)\right\rangle_{v,\varepsilon} + \langle G \rangle_{v,\varepsilon},\\
T &= T^{-1}(e).
\end{aligned}$$

Hydrodynamic limit for Fokker-Planck model

Hydrodynamic limit

Let (F, G) be solutions of BGK equations up to $O(\mathrm{Kn}^2)$. Then the moments of (F, G) satisfy the following Navier-Stokes equations up to $O(\mathrm{Kn}^2)$:

$$\begin{cases} \partial_t \rho + \mathrm{div}_{\mathbf{x}}(\rho u) = 0 \\ \partial_t(\rho u) + \mathrm{div}_{\mathbf{x}}(\rho u \otimes u) + \nabla_x p = -\mathrm{div}_{\mathbf{x}}(\sigma) + O(\mathrm{Kn}^2) \\ \partial_t E + \mathrm{div}_{\mathbf{x}}((E+p)u) = -\mathrm{div}_{\mathbf{x}}(q) - \mathrm{div}_{\mathbf{x}}(\sigma u) + O(\mathrm{Kn}^2)\,, \end{cases}$$

with:

$$E = \left\langle \left(\frac{1}{2}|v|^2 + \varepsilon\right) F + G \right\rangle_{v,\varepsilon} = \rho e + \frac{1}{2}\rho |u|^2\,,$$

$$\sigma = -\mu\left(\nabla_x u + \nabla_x u^T - \mathcal{C}\,\mathrm{div}_{\mathbf{x}}(u) Id\right)\,, q = -\frac{2}{3}\mu \nabla_x h\,,$$

where $h = e + RT$, $\mathcal{C} = \partial_e(RT) = \frac{R}{C_v(T)}$, $C_v(T) = \frac{5}{2}R + \frac{(T_0/T)^2 e^{T_0/T}}{(e^{T_0/T}-1)^2}R$.

By defining $C_p = C_v + R$ the specific heat at constant pressure, one gets:

$$q = -\frac{2}{3}\mu C_p \nabla_x T,$$

so that as usual only a gas with a Prandtl number of $3/2$ is obtained.

Perspectives

Recovering Prandtl number: the easy part

As usual there is a need for a Gaussian equilibrium to correct the characteristics times of relaxation . So we will need to go to an ESBGK or an ESFP model...

Recovering Prandtl number: the tricky part

Since relaxation times for rotation and vibration are not of the same order there is a need for a model with more equations (3 probably) to capture correctly the relaxation phenomena: the Prandtl number cannot be the only criterion to correct the model.

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Model

Equations

$$\partial_t f + v \cdot \nabla f = \frac{M[f] - f}{\tau}, \tag{6}$$

where the Maxwellian equilibrium is $M[f] = M[\rho, u, e]$ defined by

$$M[f](v, \varepsilon) = \frac{\rho}{\sqrt{2\pi \frac{p}{\rho}}^3} \exp\left(- \frac{\rho |u - v|^2}{2p} \right) \Lambda(\delta) \left(\frac{\rho \varepsilon}{p} \right)^{\frac{\delta}{2} - 1} \frac{\rho}{p} \exp\left(- \frac{\rho \varepsilon}{p(\rho, e)} \right).$$

The macroscopic quantities are given by

$$\begin{aligned} \rho &= \langle\langle f \rangle\rangle, \\ u &= \frac{1}{\rho} \langle\langle f v \rangle\rangle, \\ e &= \frac{1}{\rho} \left\langle\left\langle \left(\frac{|v - u|^2}{2} + \varepsilon \right) f \right\rangle\right\rangle, \end{aligned}$$

with $\langle\langle \cdot \rangle\rangle = \int\int_{\mathbb{R}^3 \times \mathbb{R}^+} \cdot \, \mathrm{d}v \mathrm{d}\varepsilon$, and the closure relation on the pressure $p = p(\rho, e)$.

Chapman-Enskog expansion

Prandtl and Schmidt numbers

Let f be the solution of BGK equation up to $O(\mathrm{Kn}^2)$.I Its moments satisfy the following Navier-Stokes equations up to $O(\mathrm{Kn}^2)$:

$$\begin{cases} \partial_t \rho + \mathrm{div}_{\mathbf{x}}(\rho u) = 0 \\ \partial_t(\rho u) + \mathrm{div}_{\mathbf{x}}(\rho u \otimes u) + \nabla_x p = -\mathrm{div}_{\mathbf{x}}(\sigma) + O(\mathrm{Kn}^2) \\ \partial_t E + \mathrm{div}_{\mathbf{x}}((E+p)u) = -\mathrm{div}_{\mathbf{x}}(q) - \mathrm{div}_{\mathbf{x}}(\sigma u) + O(\mathrm{Kn}^2)\,, \end{cases}$$

with: $E = \rho e + \frac{1}{2}\rho|u|^2 \quad , \quad \sigma = -\mu\left(\nabla_x u + \nabla_x u^T - \mathcal{C}\mathrm{div}_{\mathbf{x}}(u) Id\right) \quad , \quad q = -\mu \nabla_x h\,.$

$$h = e + p/\rho \quad , \quad \mathcal{C} = \frac{\rho}{p}\left(\partial_1 p + \frac{p}{\rho^2}\partial_2 p - \frac{p}{\rho}\right).$$

For reacting perfect gases at equilibrium $h(\rho, T) = \sum_i c_i(\rho, T) h_i(T)$ with c_i mass concentration of the $i-th$ gas and h_i its enthalpy. We get that:

$$\mu \nabla h = \mu\left((\sum_i c_i c_{p_i})\nabla T + \sum_i h_i(T)\nabla c_i\right).$$

The Prandtl number is equal to **one**. We also note that D_i the multicomponent diffusion coefficient of the i_{th} component is $\frac{\mu}{\rho}$ so that the Schmidt number $\frac{\mu}{\rho D_i}$ is equal to **one** .

Results on a mixture of two non-reacting gases

Mach 10, Knudsen 0.1

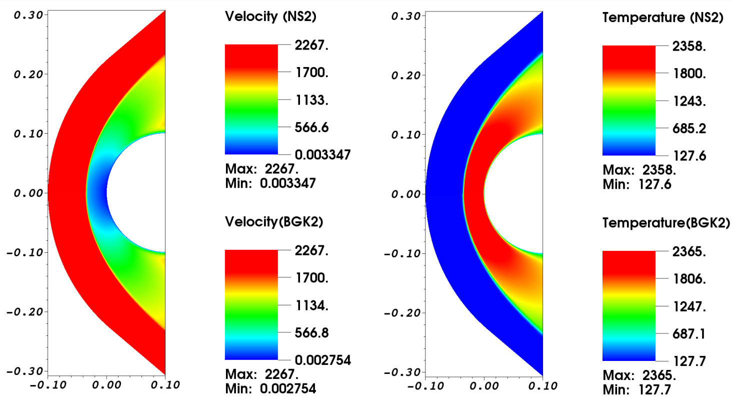

Figure: Velocity field and Temperature field (Top:Navier-Stokes solver NS2, bottom: new model BGK2)

Results on a mixture of two non-reacting gases

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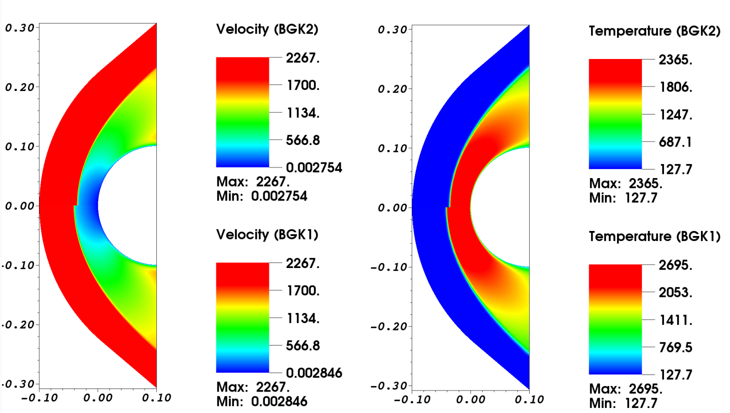

Figure: Velocity field and Temperature field (Top: new model BGK2, bottom: old model BGK1)

Results on a mixture of two non-reacting gases

Mach 10, Knudsen 0.1

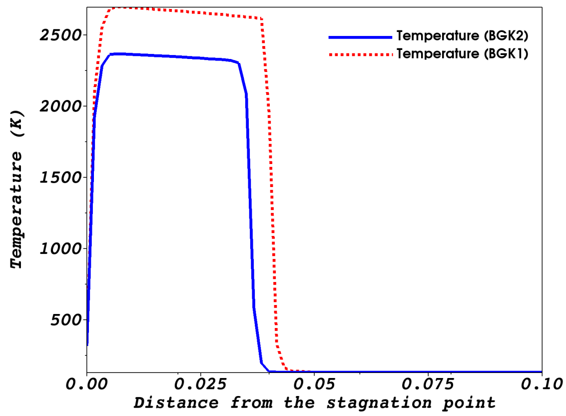

Figure: Temperature along the axis

The MultiGaussian equilibrium model: notations

Notations

For every species of the mixture, numbered with index i:

- its concentration c_i depends on ρ and e only: $c_i = c_i(\rho, e)$;
- its pressure p_i satisfies the usual perfect gas law: $p_i = \rho_i R_i T$, where R_i is the gas constant of the species and $\rho_i = c_i(\rho, e)\rho$, so that $p_i = p_i(\rho, e)$;
- its specific energy e_i and enthalpy h_i depend on T only: $e_i = e_i(T)$ and $h_i = h_i(T)$, where $e_i(T) = \frac{3+\delta_i(T)}{2} R_i T + e_i^{f,0}$, with $e_i^{f,0}$ is the energy of formation of the ith molecule and $\delta_i(T)$ is the number of activated internal degrees of freedom of the molecule that might depend on the temperature, see the previous sections.

For compressible Navier-Stokes equations for an equilibrium chemically reacting mixture, these quantities are not necessary. Instead, it is sufficient to define (with analytic formulas or tables):

- the total pressure $p = \sum_i p_i(\rho, e)$ so that $p = p(\rho, e) = \rho R(\rho, e) T$, with $R(\rho, e) = \sum_i c_i(\rho, e) R_i$;
- the temperature T, though the relation $e = \sum_i c_i(\rho, e) e_i(T)$, so that $T = T(\rho, e)$;
- the total specific enthalpy $h = \sum_i c_i h_i$, so that $h = h(\rho, e) = e + \frac{p(\rho, e)}{\rho}$.

The MultiGaussian equilibrium model: model

Equations

$$
\begin{aligned}
&\partial_t f + v\cdot\nabla_x f = \frac{1}{\tau}(MGE[f,g]-f), \text{with: } MGE[f,g] = \sum_{1\le i\le N} M_i[f,g] \\
&\partial_t g + v\cdot\nabla_x g = \frac{1}{\tau}(NMGE[f,g]-g), \text{with: } NMGE[f,g] = \sum_{N_m+1\le i\le N} N_i[f,g]
\end{aligned}
\tag{7}
$$

with the following definitions for reduced Maxwellians:

$$
\text{for } 1\le i\le N, M_i[f,g] = \frac{\rho c_i}{(2\pi R_i T)^{\frac{3}{2}}}\exp\left(-\frac{|v-u|^2}{2R_iT}\right),
$$

$$
\text{for } N_m+1\le i\le N, N_i[f,g] = \left(\frac{\delta_i(T)}{2}R_iT + e_i^{f,0}\right)\frac{\rho c_i}{(2\pi R_i T)^{\frac{3}{2}}}\exp\left(-\frac{|v-u|^2}{2R_iT}\right),
$$

The MultiGaussian equilibrium model: closure relations

Closure

We define $c_i(\rho, e)$ as the mass concentration of $i-th$ molecule, $T := T(\rho, e)$ as the mean temperature depending on internal energy and density which are defined through the following relations:

$$\begin{aligned}
\rho(t,x) &= \int_{\mathbb{R}^3} f\,dv = \int_{\mathbb{R}^3} MGE[f,g]\,dv \\
\rho u(t,x) &= \int_{\mathbb{R}^3} vf\,dv = \int_{\mathbb{R}^3} vMGE[f,g]\,dv, \\
\rho e(t,x) &= \int_{\mathbb{R}^3} (\frac{1}{2}|v-u|^2 f + g)\,dv, \\
&= \int_{\mathbb{R}^3} \left(\frac{1}{2}|v-u|^2 MGE[f,g] + NMGE[f,g]\right) dv
\end{aligned}$$

Through the "real gas closure" we have:
$e = \sum_{1\le i\le N_m+N_d} c_i(\rho,e)\left(\frac{3+\delta_i(T(\rho,e))}{2} R_i T(\rho,e) + e_i^{f,0}\right)$, where $e_i^{f,0}$ is the energy of formation of the i_{th} molecule and δ_i the number of activated degrees of freedom of this molecule ($\delta_i = 0$ for $i \le N_m$).

The MultiGaussian equilibrium model: Chapman Enskog

NS equations

The moments of f, g, solution of the MGE model (7), satisfy the following Navier-Stokes equations, up to $O(\mathrm{Kn}^2)$:

$$\begin{aligned}
&\partial_t\rho + \nabla\cdot\rho u = 0,\\
&\partial_t\rho u + \nabla\cdot(\rho u\otimes u) + \nabla p = -\nabla\cdot\sigma,\\
&\partial_t E + \nabla\cdot(E+p)u = -\nabla\cdot q - \nabla\cdot(\sigma u),
\end{aligned} \tag{8}$$

where Kn is the Knudsen number (defined below), E is the total energy density defined by $E = \left\langle\left\langle(\frac{1}{2}|v|^2+\varepsilon)F\right\rangle\right\rangle = \frac{1}{2}\rho|u|^2 + \rho e$.

The MultiGaussian equilibrium model: Chapman Enskog

NS equations

σ and q are the shear stress tensor and heat flux vector defined by

$$\sigma = -\mu \left(\nabla u + (\nabla u)^T + (1 - \mathcal{C}_p) \nabla \cdot u \, Id \right),$$

$$q = -\mu \left(\frac{\sum_i c_i R_i {c_p}^i + \sum_{i<j} c_i c_j \frac{(h_i - h_j)^2}{T^2}}{\sum_i c_i R_i} \right) \nabla T - \mu \sum_{i<j} \frac{c_i c_j}{\sum_i c_i R_i} (h_i - h_j) \nabla \left(\frac{\mu_i - \mu_j}{T} \right).$$

with $h_i = e_i + R_i T(\rho, e)$ is the enthalpy, $\mu_i := \mu_i(\rho, e)$ is the mass chemical potential of the $i-th$ specie depending on ρ and e (we recall that μ defines the viscosity and not a chemical potential), and $\mathcal{C}_p = \frac{\rho}{p} \partial_\rho p + \frac{p}{\rho} \frac{\partial_e p}{p}$

The MultiGaussian equilibrium model

Some remarks

- if $N_m + N_d = 1$, we recover the classical BGK model for monoatomic or polyatomic model with two distributions so that we capture the correct hydrodynamic limit with a Prandtl number of one.
- We are still unable to prove something close to a second principle for such a model even if it can capture more physics like equilibrium of two inert gases.
- The role of chemical potential in the formula is still under investigation: this term does not appear for classical Navier-Stokes equations for Atmospheric reentry with a ”real gas” closure but it appears under various forms in papers for kinetic mixtures models and is linked to Onsager's relations ($\frac{1}{T}$ and $-\frac{u_i}{T}$ are conjugate variables for u and ρ).

Outline

1 Context

2 New results for Fokker-Planck models

3 Models for vibrations

4 New results for BGK models and their extensions

5 Perspectives

Perspectives

Numeric

- Testing the BGK model with a law of real gas
- Pursuing tests on Fokker-Planck Models

Models

- Capturing the different relaxation times for energies,
- Going to non equilibrium chemistry with a ”simple model”

Contributions

[Bar + 18] Baranger,C., Marois,G., Mathé,J., Mathiaud, J. and Mieussens,L. “A BGK model for high temperature rarefied gas flows”. In: Work in progress (2018).

[MM16] J. Mathiaud and L. Mieussens. “A Fokker–Planck Model of the Boltzmann Equation with Correct Prandtl Number”. In: Journal of Statistical Physics 162.2 (Jan. 2016), pp. 397–414.

[MM17] J. Mathiaud and L. Mieussens. “A Fokker–Planck Model of the Boltzmann Equation with Correct Prandtl Number for Polyatomic Gases”. In: Journal of Statistical Physics 168.5 (Sept. 2017), pp. 1031–1055.

[MM18] J. Mathiaud and L. Mieussens. “Vibrational models of Boltzmann equation with correct second principle: BGK and Fokker-Planck”. In: Work in progress (2018).