Construction of a *BGK* model from an entropy minimization principle

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Plan

Introduction

Boltzmann equation

$f(t, x, v)$: distribution function, $t \in \mathbb{R}_+$, $x \in \mathbb{R}^3$, $v \in \mathbb{R}^3$
$\Rightarrow$ number of particles having at time t, position x and the velocity v.

$$\underbrace{\frac{\partial f}{\partial t} + v.\nabla_x f}_{transport} = \underbrace{Q(f,f)}_{Collision\quad operator}$$

Collision operator

$$Q(f,f) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B(v - v_*, \omega)[f(t,x,v')f(t,x,v'_*) - f(t,x,v)f(t,x,v_*)]d\omega dv_*,$$

where

$$v' = v - \langle v - v_*\,,\,\omega\rangle\omega, \quad v'_* = v + \langle v - v_*\,,\,\omega\rangle\omega, \quad \omega \in \mathbb{S}^2$$

$\rightarrow$ High complexity

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Properties of $Q(f, f)$.

Orthogonality relations

$$\int_{\mathbb{R}^3} Q(f, f)(1, v, |v|^2)dv = 0,$$

H Theorem

$$\int_{\mathbb{R}^3} f \ln(f)dv \leq 0$$

Resolution of $Q(f, f) = 0$.

$$Q(f, f) = 0 \Leftrightarrow \exists(\rho, u, T)/\, f(t, x, v) = \frac{\rho}{(2\pi T)^{\frac{2}{3}}} \exp(-\frac{|v-u|^2}{2T})$$

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Notations

Macroscopic quantities

ρ, u et T : mass, velocity and temperature

$$\rho = \int_{\mathbb{R}^3} f\,dv, \qquad u = \frac{1}{\rho}\int_{\mathbb{R}^3} vf\,dv, \qquad T = \frac{1}{3\rho}\int_{\mathbb{R}^3} |v-u|^2 f\,dv.$$

Stress tensor

$$\Theta = \frac{1}{\rho}\int_{\mathbb{R}^3} c\otimes c\, fdv, \qquad f = \mathcal{M} \Rightarrow \rho\Theta = \rho T\, Id$$

Boltzmann entropy

$$\mathcal{H}(g) = \int (g\ln g - g)dv.$$

Space of invariants

$\mathbb{K} = \{1, v, |v|^2\}$. $P_{\mathbb{K}}$: projection on $\mathbb{K}$

Aim

- Construct a relaxation operator $R(f) = \lambda(G - f) \approx Q(f, f)$

  - Go beyond the BGK model,

  - As close as possible of $Q(f, f)$,

- Generalization to polyatomic gases : $f(t, x, v, I)$, I : Internal energy

- Generalization to mixtures : $f_i(t, x, v)$ ($\mathbf{f} := (f_1, \cdots, f_p)$)

$$\frac{\partial f_i}{\partial t}(t, x, v) + v \cdot \nabla_x f_i(t, x, v) = \sum_{k=1}^{k=p} Q_{ki}(f_k, f_i) \approx \lambda(G_i - f_i).$$

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Chapman-Enskog expansion

Parameter ε Knudsen number. When $\varepsilon \to 0 \Rightarrow$ fluid model

Rescaled Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f).$$

Chapman-Enskog expansion

- Equilibrium state : $Q(f, f) = 0 \ \Leftrightarrow f = \mathcal{M}$
- $f = \mathcal{M}$ + moments extraction w.r.t. $(1, v, v^2)$
  $\Rightarrow$ Euler system
- $f = \mathcal{M} + \varepsilon f_1$ + moments extraction w.r.t. $(1, v, v^2)$
  $\Rightarrow$ Navier-Stokes system

Euler system

Order 0

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla_x\right)\mathcal{M} = 0 \qquad (1)$$

Integration of (1) w.r.t $(1, v, |v|^2) \Rightarrow$ Euler system

Euler system

$$\begin{aligned} \partial_t \rho + div(\rho u) &= 0 \\ \partial_t(\rho\, u) + div_x(\rho\, u \otimes u) + \nabla_x(\rho T) &= 0 \\ \partial_t\Big(\rho(\frac{1}{2}|u|^2 + \frac{3}{2}T)\Big) + div_x\Big(\rho u(\frac{1}{2}|u|^2 + \frac{5}{2}T)\Big) &= 0. \end{aligned}$$

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\end{aligned}$$

Computation of f_1

Expression of times derivatives w.r.t space derivatives.

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla_x\right)\mathcal{M} = (\mathbb{A}(V) : \mathbb{D}(u) - B(V)\frac{\nabla_x T}{\sqrt{T}})\mathcal{M} = \mathcal{L}(f_1)$$

$$V = \frac{v-u}{\sqrt{T}}, \quad \mathcal{L}(g) = Q(M, Mg) + Q(Mg, M)$$

Inversion of the relation $\Rightarrow f_1$

Sonine polynomials

$$\mathbb{A}(v) = v \otimes v - \frac{1}{3}|v|^2 Id, \quad \mathbf{B}(v) = \frac{v}{2}(v^2 - \frac{5}{2}).$$

$\mathbb{D}(u)$ (viscosity tensor) :

$$\mathbb{D}(u) = \frac{1}{2}(\nabla_x u + \nabla_x u^t) - \frac{1}{3} div(u) Id.$$

Navier-Stokes system

Integration of $\left(\frac{\partial}{\partial t} + v \cdot \nabla_x\right)(\mathcal{M} + \varepsilon f_1)$ w.r.t $(1, v, |v|^2)$,

$$\partial_t \rho + div_x(\rho u) = 0$$
$$\partial_t(\rho\, u) + div_x(\rho\, u \otimes u + \rho T\, Id - \varepsilon\mu\mathbb{D}(u)) = 0$$
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Transport Coefficients

$\mu = \mu(T, \rho, \mathbb{A}, \mathcal{L}^{-1})$: Viscosity, $\quad \kappa = \kappa(T, \rho, \mathbf{B}, \mathcal{L}^{-1})$: Heat flux

Prandtl number

$$Pr = \frac{5}{2}\frac{\mu}{\kappa} \approx \frac{2}{3}.$$

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Monoatomic case

BGK Models

Relaxation operator

$$Q(f,f) \sim R(f) = \frac{1}{\tau}(\mathcal{M} - f), \quad \tau > 0$$

where $\mathcal{M}$ is defined by

$$\mathcal{M}(v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|v-u|^2}{2T}\right).$$

$$\mathcal{M} = \min_{g \in C_f} \mathcal{H}(g)$$

where

$$C_f = \{g \geq 0 \text{ s.t. } \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ v^2 \end{pmatrix} g\, dv = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ v^2 \end{pmatrix} f\, dv\}$$

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Properties of the *BGK* operator

Conservation laws

$$\int_{\mathbb{R}^3} (\mathcal{M} - f)(1, v, |v|^2) dv = (0, 0, 0),$$

Equilibrium states

$$\int_{\mathbb{R}^3} \rho(\mathcal{M} - f) \ln f \, dv = 0 \Leftrightarrow f = \mathcal{M},$$

H Theorem

$$\int_{\mathbb{R}^3} (\mathcal{M} - f) \ln f \, dv \leq 0.$$

Trend to equilibrium

$$\lim_{t \to +\infty} f(t) = \mathcal{M}.$$

Problem : Prandtl number not correct ≈ 1

Remark : Model coming from an entropy minimization problem

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Minimization principle

<u>Aim :</u> Methodology to construct *BGK* models $\Rightarrow$ correct transport coefficients up to Navier-Stokes.

The models are researched on the form $\lambda(G - f)$

Minimization problem

G is researched as

$$\mathcal{H}(G) = \min_{g \in C_f} \mathcal{H}(g),$$

$$C_f = \{g \, / \int \mathbf{m}(v) g dv = \mathcal{V}(\int \mathbf{m}(v) f dv)\}$$

$span(\mathbf{m}(v)) = \mathbb{P}$

$G = \exp(\alpha \cdot \mathbf{m}(v))$ is expected.

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Realisability problems

Let $\mathcal{V} \in \mathbb{R}^N$. Is there $G \geq 0 \in L^1$ s.t.

$$\mathcal{H}(G) = \min \mathcal{H}(g)$$

under the constraints

$$\int_{\mathbb{R}^3} g\,\mathbf{m}(v) dv = \mathcal{V}?$$

CN : $\mathcal{V}$ corresponds to a nonnegative L^1 function

Characterisation of realisability [M.Junk, 98], [J.Schneider, 2004]

Pb : G is not always equal to $\exp(\alpha \cdot \mathbf{m}(v))$

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Approach by relaxation coefficients

Relaxation coefficents :

$$R(f) = \Sigma_i \lambda_i (G_i - f)$$

[Levermore, J.S.P., 1996]

Problem : We obtain only $Pr \geq 1$.

New approach : One **unique** relaxation coefficient $\lambda > 0$ and **different** relaxation rates $(\lambda)_{i=1 \cdots N} \geq 0$ s.t.

$$\int \lambda (G - f)\, m_i(v) dv = -\lambda_i \int f\, m_i(v) dv, \ \forall m_i \in \mathbb{P}$$

Conserved quantities : $\lambda_i = 0$.

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Explanation of the constraints

Assume $\mathbb{P} = \mathbb{P}_0 \oplus_\perp \mathcal{V}ect[m_{n+1} \ldots m_N]$ for the scalar product

$$\langle \varphi, \psi \rangle = \int \mathcal{M} \varphi \psi \, dv.$$

Hence for $\lambda_i > 0$, and $i > n$

$$\partial_t \int f \, m_i \, dv = \int \lambda (G - f) \, m_i \, dv = -\lambda_i \int f \, m_i \, dv$$

$$\Rightarrow \int f \, m_i \, dv \to 0, \ \forall i > n \text{ when } t \to +\infty.$$

$\mathbb{P} = \mathbb{P}_0 \oplus_\perp \mathbb{A}(c)$, for the scalar product $\langle \varphi, \psi \rangle = \int \mathcal{M} \varphi \psi \, dv$

Aim : Derive a relaxation operator $\lambda(G - f)$, where

$$G = \min_{g \in C_f} \mathcal{H}(g). \tag{2}$$

$\mathcal{C}_f = \{g \geq 0$ s.t.

$$\int_{\mathbb{R}^3} (1, v, |v|^2) \, g dv = \int_{\mathbb{R}^3} (1, v, |v|^2) \, f dv, \tag{3}$$

$$\int_{\mathbb{R}^3} \lambda(g - f) \mathbb{A}(c) \, dv = -\lambda_1 \int_{\mathbb{R}^3} f \mathbb{A}(c) dv, \quad c = v - u\}. \tag{4}$$

Setting $\nu = 1 - \frac{\lambda_1}{\lambda} \Rightarrow$ (4) can be written

$$\frac{1}{\rho} \int_{\mathbb{R}^3} c \otimes c \, g dv = \nu \Theta + (1 - \nu) T Id = \mathcal{T} \tag{5}$$

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Main result

Theorem

Let $f \neq 0$, $f \geq 0$ s.t. $\int (1+|v|^2)\, f \; < +\infty$ *and* $\nu \in [-\frac{1}{2}, 1[$,
$\Rightarrow$ *the problem (2, 3, 4) has a unique solution G*

$$G(v) = \frac{\rho}{\sqrt{det(2\pi\mathcal{T})}} \exp\left(-\frac{1}{2}\langle c, \mathcal{T}^{-1} c\rangle\right).$$

Conversely, if the problem (2, 3, 4) has a solution for any $f \geq 0$ s.t.
$\int f\,(1+|v|)^2 \; < +\infty$, *then* $\nu \in [-\frac{1}{2}, 1[$.

Arguments : $\mathcal{C}_f \neq \emptyset$. Ex : $G_{ES} \in \mathcal{C}_f$.
M.Junk, J.Schneider $\Rightarrow \exists$ a solution to the minimization problem.

$$G(v) = \exp\left(\alpha \cdot \mathbf{m}(v)\right)$$

α Lagrange associated to constraints

Chapman-Enskog expansion

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla_x\right) f = \frac{\lambda}{\varepsilon}(G - f),$$

f is expanded as

$$f = \mathcal{M}(1 + \varepsilon f^{(1)}).$$

Computation of λ and $\lambda_1 \Rightarrow$ exact expansion up to Navier-Stokes

$$\lambda_1 = \frac{\rho T}{\mu}, \qquad \lambda = \frac{5}{2}\frac{\rho T}{\kappa}.$$

Prandtl number

$$Pr = \frac{5}{2}\frac{\mu}{\kappa} = \frac{\lambda}{\lambda_1} = \frac{1}{1-\nu}. \qquad Pr = \frac{2}{3} \to \nu = -\frac{1}{2}$$

$\Rightarrow$ Result : Ellipsoidal Statistical Model ([Holway, 1964]).

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$$\lambda_1 = \frac{\rho T}{\mu}, \qquad \lambda = \frac{5}{2}\frac{\rho T}{\kappa}.$$

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$$Pr = \frac{5}{2}\frac{\mu}{\kappa} = \frac{\lambda}{\lambda_1} = \frac{1}{1-\nu}. \qquad Pr = \frac{2}{3} \rightarrow \nu = -\frac{1}{2}$$

$\Rightarrow$ Result : Ellipsoidal Statistical Model ([Holway, 1964]).

Chapman-Enskog expansion

$$\left(\frac{\partial}{\partial t} + v \cdot \nabla_x\right) f = \frac{\lambda}{\varepsilon}(G - f),$$

f is expanded as

$$f = \mathcal{M}(1 + \varepsilon f^{(1)}).$$

Computation of λ and λ_1 $\Rightarrow$ exact expansion up to Navier-Stokes

$$\lambda_1 = \frac{\rho T}{\mu}, \qquad \lambda = \frac{5}{2}\frac{\rho T}{\kappa}.$$

Prandtl number

$$Pr = \frac{5}{2}\frac{\mu}{\kappa} = \frac{\lambda}{\lambda_1} = \frac{1}{1-\nu}. \qquad\qquad Pr = \frac{2}{3} \rightarrow \nu = -\frac{1}{2}$$

$\Rightarrow$ Result : Ellipsoidal Statistical Model ([Holway, 1964]).

H Theorem

Theorem

For any $-\frac{1}{2} \leq \nu < 1$,

$$D(f) = \int (G_\nu - f) \ln f \, dv \leq 0$$

Moreover $D(f) < 0$ *for* $-\frac{1}{2} \leq \nu < 1$ *equality iff* $f = \mathcal{M}$.

[Andries-Le Tallec-Perlat-Perthame 1999].
[Brull-Schneider 2008].

Polyatomic case

Borgnakke-Larsen model

Microscopic model : [Borgnakke-Larsen, 1975]

Distribution function → f = f(t,x,v,I)
$I =$ internal energy parameter ($I \geq 0$) with $\varepsilon(I) = I^{\frac{2}{\delta}} =$ internal energy

Discrete energy parameter : Giovangigli

Collision operator : [Bourgat-Desvillettes-Le Tallec-Perthame, 1994].
Conserved moments : $(1, v, \frac{1}{2}|v|^2 + I^{\frac{2}{\delta}})$

$\delta =$ number of internal degrees of freedom.
Link between γ and δ

$$\gamma = \frac{\delta + 5}{\delta + 3}, \quad \delta = 2 \Rightarrow \gamma = \frac{7}{5}$$

Polyatomic Maxwellian distribution

$$\mathcal{M} = \frac{\rho \Lambda_\delta}{(2\pi T_{eq})^{\frac{3}{2}} (T_{eq})^{\frac{\delta}{2}}} \exp\left(-\frac{|v-u|^2}{2T_{eq}} - \frac{I^{\frac{2}{\delta}}}{T_{eq}} \right), \quad \Lambda_\delta^{-1} = \int_{\mathbb{R}_+} e^{-I^{\frac{2}{\delta}}} dI.$$

Macroscopic quantities

ρ, u defined as in the monoatomic case

Specific internal energy

$$e = \frac{1}{\rho}\int_{\mathbb{R}^3\times\mathbb{R}_+}(\frac{1}{2}|v-u|^2 + I^{\frac{2}{\delta}})\, f\, dvdI.$$

$e = e_{tr} + e_{int}$

$$e_{tr} = \frac{1}{2\rho}\int_{\mathbb{R}^3\times\mathbb{R}_+}|v-u|^2 f\, dvdI, \quad e_{int} = \frac{1}{\rho}\int_{\mathbb{R}^3\times\mathbb{R}_+} I^{\frac{2}{\delta}} f\, dvdI.$$

Temperatures are associated to these energies

$$e = \frac{3+\delta}{2}T_{eq}, \qquad e_{tr} = \frac{3}{2}T_{tr}, \qquad e_{int} = \frac{\delta}{2}T_{int}.$$

Macroscopic quantities

ρ, u defined as in the monoatomic case

Specific internal energy

$$e = \frac{1}{\rho} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{1}{2}|v-u|^2 + I^{\frac{2}{\delta}}\right) f \, dv dI.$$

$e = e_{tr} + e_{int}$

$$e_{tr} = \frac{1}{2\rho} \int_{\mathbb{R}^3 \times \mathbb{R}_+} |v-u|^2 f \, dv dI, \quad e_{int} = \frac{1}{\rho} \int_{\mathbb{R}^3 \times \mathbb{R}_+} I^{\frac{2}{\delta}} f \, dv dI.$$

Temperatures are associated to these energies

$$e = \frac{3+\delta}{2} T_{eq}, \quad e_{tr} = \frac{3}{2} T_{tr}, \quad e_{int} = \frac{\delta}{2} T_{int}.$$

$R(f) = \lambda(G - f)$, where G is solution of the minimization problem

$$G = \min_{g \in \mathcal{C}_f} \mathcal{H}(g). \tag{6}$$

$\mathcal{C}_f = \{g \geq 0$ s.t.

$$\int_{\mathbb{R}^3\times\mathbb{R}_+} g\,(1, v, \frac{1}{2}|c|^2 + I^{\frac{2}{\delta}})\,dvdI = \int_{\mathbb{R}^3\times\mathbb{R}_+} f\,(1, v, \frac{1}{2}|c|^2 + I^{\frac{2}{\delta}})\,dvdI, \tag{7}$$

$$\int_{\mathbb{R}^3\times\mathbb{R}_+} \Big(\frac{1}{3}|c|^2 - \frac{2}{3+\delta}(\frac{|c|^2}{2} + I^{\frac{2}{\delta}})\Big)\lambda(g - f)\,dvdI$$
$$= -\lambda_2 \int_{\mathbb{R}^3\times\mathbb{R}_+} \Big(\frac{1}{3}|c|^2 - \frac{2}{3+\delta}(\frac{|c|^2}{2} + I^{\frac{2}{\delta}})\Big) f\,dvdI, \tag{8}$$

$$\int_{\mathbb{R}^3\times\mathbb{R}_+}\Big(c \otimes c - \frac{1}{3}|c|^2 Id\Big)\lambda(g - f)\,dvdI = -\lambda_1 \int_{\mathbb{R}^3\times\mathbb{R}_+}\Big(c \otimes c - \frac{1}{3}|c|^2 Id\Big) f\,dvdI\} \tag{9}$$

Construction of G

$$\theta = 1 - \frac{\lambda_2}{\lambda}, \quad \frac{\lambda_1}{\lambda} = 1 - \nu(1-\theta).$$

$$\mathcal{T} = \frac{1}{\rho}\int_{\mathbb{R}^3} c \otimes c\, g\, dv\, dI = (1-\theta)\left((1-\nu)\, T_{tr}\, Id + \nu\Theta\right) + \theta\, T_{eq}\, Id$$

Stress tensor

$$\Theta = \frac{1}{\rho}\int c \otimes c\, f\, dv\, dI.$$

Interpretation : $\mathcal{T}$ is a “double convex combinaison”.
Comparison with the Ellipsoidal Statistical Model in the polyatomic case [P.Andries-P.LeTallec-J.P.Perlat-B.Perthame, 2000]

Main theorem

Relaxation temperature : $T_{rel} = \theta T_{eq} + (1-\theta) T_{int}$,

Theorem

Let f ($f \neq 0$), $f \geq 0$ s.t. $\int f\,(1+|v|^2+I^{\frac{2}{\delta}})\,dvdI < +\infty$, $\nu \in [-\frac{1}{2}, 1[$ *and* $\theta \in [0,1]$. *Then the problem (6, 7, 8, 9) has a unique solution G,*

$$G = \frac{\rho \Lambda_\delta}{\sqrt{det(2\pi\mathcal{T})(T_{eq})^{\frac{\delta}{2}}}} \exp\Big(-\frac{1}{2}\langle c, \mathcal{T}^{-1} c\rangle - \frac{I^{\frac{2}{\delta}}}{T_{rel}}\Big).$$

Conversely, if (6, 7, 8, 9) has a unique solutio for any $f \geq 0$ s.t. $\int f\,(1+|v|^2+I^{\frac{2}{\delta}})\,dvdI < +\infty$, *then* $\nu \in [-\frac{1}{2}, 1[$ *and* $\theta \in [0,1]$.

[S.B-J.Schneider], 2009

Definition of λ, λ_1, λ_2.

Tensor for polyatomic Navier-Stokes

$$\sigma_{ij} = \mu\,(\partial_{x_j} u_i + \partial_{x_i} u_j - \alpha div(u)\delta_{ij}).$$

Chapman-Enskog expansion
$\Rightarrow$ Definition of $\lambda(\rho, T, \kappa)$, $\lambda_1(\rho, T, \mu)$ et $\lambda_2(\rho, T, \mu, \alpha)$.

Result : Ellipsoidal Statistical Model for polyatomic gases
[P.Andries-P.LeTallec-J.P.Perlat-B.Perthame, 2000]

Generalization to gas mixtures

Setting of the problem

Aim : Construct a relaxation operator for multi-species basing on (true) hydrodynamic limit and right kinetic coefficients
(Fick, Soret, Duffour, Fourier, Newton).
⇒ [Brull-Pavan-Schneider, 2012] Fick law.
[Brull, 2015] ES-BGK

Up to now : Approx. of moments exchanges of Boltzmann equation

- [Garzò-Santos-Brey, 1989]
- [Kosuge, 2009] (approximation on the Grad 13 moments).

Pb : loss of positivity, no H theorem, uncorrect transport coefficients.

One particular model : [Andries-Aoki-Perthame, 2002]
Good mathematical properties : H theorem, positivity.
Valid only for Maxwellian molecules ⇒ uncorrect transport coefficients.

Application to reacting mixtures (Bisi, Groppi, Spiga).

Navier-Stokes system for a mixture

Navier-Stokes system :

$$\forall i \in [1,p]\,,\ \partial_t n^i + \nabla\cdot(n^i\mathbf{u} + \mathbf{J}_i) = 0,$$
$$\partial_t(\rho\,\mathbf{u}) + \nabla\cdot(\mathbb{P} + \rho\,\mathbf{u}\otimes\mathbf{u} + \mathbb{J}_{\mathbf{u}}) = 0,$$
$$\partial_t E + \nabla\cdot(E\mathbf{u} + \mathbb{P}\,[\mathbf{u}] + \mathbb{J}_{\mathbf{u}}\,[\mathbf{u}] + \mathbf{J}_q) = 0,$$

$\mathbf{J}_i$, $\mathbb{J}_{\mathbf{u}}$ $\mathbf{J}_{\mathbf{q}}$: mass, momentum and heat fluxes.

Thermodynamics of Irreversible Processes assumptions.

$$\begin{aligned}
\mathbf{J}_i &= \sum_{j=1}^{j=p} L_{ij}\nabla\left(\frac{-\mu_j}{T}\right) + L_{i\mathbf{q}}\nabla\left(\frac{1}{T}\right),\\
\mathbf{J}_{\mathbf{q}} &= \sum_{j=1}^{j=p} L_{\mathbf{q}j}\nabla\left(\frac{-\mu_j}{T}\right) + L_{\mathbf{qq}}\nabla\left(\frac{1}{T}\right),\\
\mathbb{J}_{\mathbf{u}} &= L_{\mathbf{uu}}\mathbb{D}\left(\mathbf{u}\right),
\end{aligned}$$

μ_i : chemical potential : $\dfrac{\mu_i}{T} = k_B\left(\ln\left(n_i\right) - \dfrac{3}{2}\ln\left(\dfrac{2\pi k_B T}{m_i}\right)\right).$

Fick, Dufour, Soret, Fourier coefficients

Phenomenological point of view :
[Chapman-Cowling], [Kurochkin-Makarenko-Tirskii]

$$J_i = \sum_{j=1}^{j=p} D_{ij} \nabla n_j + D_{iT} \nabla T, \quad J_{\mathbf{q}} = \sum_{j=1}^{j=p} D_{\mathbf{q}j} \nabla n_j - D_{\mathbf{qq}} \nabla T.$$

D_{ij} : Fick coefficient : Diffusion

D_{iT} : Soret coefficient : Thermal diffusion

$D_{\mathbf{q}j}$: Duffour coefficient : Diffusion thermo-effect

$D_{\mathbf{qq}}$: Fourier coefficient

Relation between diffusion and Onsager matrixes

$$D_{ij} = -\frac{n k_B L_{ij}}{n_i n_j}$$

Notations

Distribution function : $\mathbf{f} := (f_1, \cdots, f_p) \to n^i, u^i, T^i$.
Maxwellians distributions : $\boldsymbol{M} := (\mathcal{M}_1, \cdots, \mathcal{M}_p)$.

Scalar product $\langle \mathbf{f}, \mathbf{g} \rangle = \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} f_i g_i \mathcal{M}_i \, dv \;\Rightarrow\;$ Euclidiean norm : $\| \, \|$.

Collision invariants $\mathbb{K}$ de $\mathbb{L}^2(\boldsymbol{M})$ spanned by :

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} m_1 v_x \\ m_2 v_x \\ \vdots \\ m_p v_x \end{pmatrix}, \begin{pmatrix} m_1 v_y \\ m_2 v_y \\ \vdots \\ m_p v_y \end{pmatrix}, \begin{pmatrix} m_1 v_z \\ m_2 v_z \\ \vdots \\ m_p v_z \end{pmatrix}, \begin{pmatrix} m_1 \mathbf{v}^2 \\ m_2 \mathbf{v}^2 \\ \vdots \\ m_p \mathbf{v}^2 \end{pmatrix}$$

denoted ϕ^l, $l \in \{1, \ldots, p+4\}$.
Notation : $(\mathbf{C}_i)_j = \delta_{ij} (\mathbf{v} - \mathbf{u})$.

Chapman-Enskog expansion

$\mathcal{P}_{\mathbb{K}} =$ Orthogonal projection on $\mathbb{K}$ and $\mathcal{I}$ unit operator

$$\mathcal{L}_B(g) = \frac{1}{k_B} \sum_{j=1}^{j=p} \left(\mathcal{I} - \mathcal{P}_{\mathbb{K}}\right) \left(\mathbf{C}_j\right) \cdot \nabla \left(-\frac{\mu_j}{T}\right) + \mathbb{A} : \mathbb{D}\left(\mathbf{u}\right) + \widetilde{\mathbf{B}} \cdot \nabla \left(\frac{1}{T}\right),$$

$$\begin{aligned}
\left(\mathbb{A}\right)_i &= m_i \left[\left(\mathbf{v} - \mathbf{u}\right) \otimes \left(\mathbf{v} - \mathbf{u}\right) - \frac{1}{3} \left(\mathbf{v} - \mathbf{u}\right)^2 \mathbb{I} \right], \\
\left(\mathbf{B}\right)_i &= \left(\mathbf{v} - \mathbf{u}\right) \left[\frac{1}{2} m_i \left(\mathbf{v} - \mathbf{u}\right)^2 - \frac{5}{2} k_B T \right], \\
\left(\widetilde{\mathbf{B}}\right)_i &= \left(\mathbf{v} - \mathbf{u}\right) \left[\frac{1}{2} m_i \left(\mathbf{v} - \mathbf{u}\right)^2 - \frac{5n}{2\rho} k_B T \right].
\end{aligned}$$

New space $\mathbb{C} = span \left(\mathcal{I} - \mathcal{P}_{\mathbb{K}}\right) \left(\mathbf{C}_i\right), i \in [1, p]$.

$\left(\mathcal{I} - \mathcal{P}_{\mathbb{K}}\right) \left(\mathbf{C}_i\right), i \in [1, p-1]$ basis of $\mathbb{C} \Longrightarrow \dim(\mathbb{C}) = 3\left(p - 1\right)$.

Fluxes and transport coefficients

[Chapman, Cowling], [Brull, Pavan, Schneider]

$$\mathcal{L}_B(g) = \frac{1}{k_B}\sum_{j=1}^{j=p}\left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)\left(\mathbf{C}_j\right)\cdot\nabla\left(-\frac{\mu_j}{T}\right) + \mathbb{A}:\mathbb{D}\left(\mathbf{u}\right) + \widetilde{\mathbf{B}}\cdot\nabla\left(\frac{1}{T}\right).$$

Fluxes :

$$\mathbf{J}_i = \langle \mathbf{g}, \mathbf{C}_i\rangle = \langle \mathbf{g}, \left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)\left(\mathbf{C}_i\right)\rangle, \quad \mathbb{J}_u = \langle \mathbf{g}, \mathbb{A}\rangle, \quad \mathbf{J}_{\mathbf{q}} = \left\langle \mathbf{g}, \widetilde{\mathbf{B}}\right\rangle.$$

Transport coefficients :

$$\begin{aligned}
L_{ij} &= \frac{1}{3k_B}\left\langle \mathcal{L}_B^{-1}\left[\left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)\left(\mathbf{C}_i\right)\right], \left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)\left(\mathbf{C}_j\right)\right\rangle \\
L_{i\mathbf{q}} = L_{\mathbf{q}i} &= \frac{1}{3}\left\langle \mathcal{L}_B^{-1}\left(\widetilde{\mathbf{B}}\right), \left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)\left(\mathbf{C}_i\right)\right\rangle \\
L_{\mathbf{uu}} &= \frac{1}{10}\left\langle \mathcal{L}_B^{-1}\left(\mathbb{A}\right), \mathbb{A}\right\rangle \\
L_{\mathbf{qq}} &= \frac{1}{3}\left\langle \mathcal{L}_B^{-1}\left(\widetilde{\mathbf{B}}\right), \widetilde{\mathbf{B}}\right\rangle.
\end{aligned}$$

Properties of the matrix $L_{i,j}$.

Casimir-Onsager relations :

$$\mathbf{L} := \begin{bmatrix} L_{ij} & L_{i\mathbf{q}} & 0 \\ L_{\mathbf{q}i} & L_{\mathbf{qq}} & 0 \\ 0 & 0 & L_{\mathbf{uu}} \end{bmatrix}$$ is symmetric and non negative.

Total mass conservation :

$$\sum_{i=1}^{i=p} m_i \mathbf{J}_i = 0 \Rightarrow \forall j \in [1, p], \; \sum_{i=1}^{i=p} m_i L_{ij} = 0 \;\Rightarrow\; rank(\, L_{ij}\,) = p - 1.$$

$$Ker(\mathbf{L}) = \; Vect(m_1, \ldots, m_p, 0) \Rightarrow Rank(\mathbf{L}) = p$$

Idea of the relaxation

Idea : Linear relaxation of non conserved moments

1. Aim : New constraint in the space $\mathbb{C} \Rightarrow$ Fick law.

$$\nu \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} (G_j - f_j)\, w_j^r = -\lambda_r \sum_{j=1}^{j=p} \int_{\mathbb{R}^3} f_j w_j^r, \quad (\mathbf{w}_r)_{r\in\{1,\dots,p-1\}} \text{ basis of } \mathbb{C}.$$

   Important coefficients : Fick, viscosity.

   Choice of λ_r and of $w^r \in \mathbb{C} \Rightarrow$ correct Fick coefficients.
   Choice of $\nu \Rightarrow$ correct viscosity if $\nu \geq \max_r \lambda_r$.

2. Resolution of an entropy minimization problem

$$\text{Entropy} \quad \mathcal{H}(\mathbf{f}) = \sum_{i=1}^{p} \int_{\mathbb{R}^3} (f_i \ln(f_i) - f_i)\, d\mathbf{v}.$$

Entropy minimization principle.

$(\boldsymbol{\phi}^l)_{l\in\{1,p+4\}}$ basis of $\mathbb{K}$.

Space of constraints : $C_{\mathbf{f}}$.

$$\mathbf{g} \in C_{\mathbf{f}} \Leftrightarrow \begin{cases} \forall l \in [1, p+4], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \phi_i^l (g_i - f_i)\, d\mathbf{v} = 0, \\ \forall r \in [1, p-1], \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathbf{w}_i^r (g_i - f_i) d\mathbf{v} = -\lambda_r \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathbf{w}_i^r f_i d\mathbf{v}. \end{cases}$$

$$\Rightarrow \ \exists !\ \mathbf{G} = \min_{g \in C_{\mathbf{f}}(\mathbf{f})} \mathcal{H}(\mathbf{f}) \quad s.t.$$

$$\forall i \in [1, p], \ G_i = \frac{n^i}{(2\pi k_B T^*/m_i)^{3/2}} \exp\left(-\frac{m_i (\mathbf{v} - \mathbf{u}_i)^2}{2 k_B T^*}\right).$$

$\mathbf{u}_i$: linear combinations of $\mathbf{u}^i$, u_i : velocity of g_i

Choice of T^* $\Rightarrow$ Energy conservation : $T^* \geq 0$ if $\nu \geq \max_r \lambda_r$.

Computation of the relaxation coefficients

- Introduction of L^*_{ij}

$$(L_{ij})_{i,j\in[1,p]} \Rightarrow \forall i,j \in [1,p]\,,\ L^*_{ij} = \frac{L_{ij}}{\|\mathbf{C}_i\|\,\|\mathbf{C}_j\|}.$$

- Diagonalization of L^* : spectrum of L^* : $(l^*_r, \mathbf{w}_r)_{r\in\{1,\dots,p-1\}} \cup (0, w_p)$

Theorem

$$\lambda_r = l_r^{*-1} \Rightarrow \quad \textit{Fick laws}\ , \quad \lambda_p = 0 \Rightarrow \textit{Conservation of impulsion.}$$

$$\textit{Density fluxes :}\quad \boldsymbol{J}_i = \sum_{j=1}^{j=p} L_{ij}\nabla\left(\frac{-\mu_j}{T}\right) + L_{iq}\nabla\left(\frac{1}{T}\right)$$

Properties of the BGK model

The Fick relaxation operator satisfies the fundamental properties :

$$\forall \mathbf{f}, f_i \geq 0, \forall \boldsymbol{\phi}, \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \phi_i d\mathbf{v} = 0 \Leftrightarrow \boldsymbol{\phi} \in \mathbb{K},$$

$$\forall \mathbf{f}, f_i \geq 0, \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \ln(f_i) \, d\mathbf{v} \leq 0,$$

$$\mathcal{R}(\mathbf{f}) = 0 \Leftrightarrow \exists n^i, \mathbf{u}, T \; s.t. \; \forall i \in [1, p], f_i = \mathcal{M}_i,$$

$$\mathcal{L} = \nu \left(\mathcal{P}_{\mathbb{K}} + \Lambda \circ \mathcal{P}_{\mathbb{C}} - \mathcal{I} \right), \; \Lambda(\mathbf{w}_r) = \left(1 - \frac{\lambda_r}{\nu} \right) \mathbf{w}_r, \; r \in \{1, p-1\}$$

is self adjoint and negative on $\mathbb{K}^\perp$ and $Ker \mathcal{L} = \mathbb{K}$.

Computation of transport coefficients

$$
\begin{aligned}
L_{ij}(\mathcal{R}) &= L_{ij}(\text{Boltzmann or experimental}) \\
&= \frac{1}{3}\left\langle \mathcal{L}^{-1}\left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)(\mathbf{C}_i), \left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)(\mathbf{C}_j)\right\rangle,
\end{aligned}
$$

$$
\frac{1}{3}\left\langle \mathcal{L}^{-1}(\widetilde{\mathbf{B}}), \left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)(\mathbf{C}_i)\right\rangle = L_{iq} = L_{qi} = \frac{5}{2}k_B T \sum_{j=1}^{p} L_{ij},
$$

$$
\frac{1}{10}\left\langle \mathcal{L}^{-1}(\mathbb{A}), \mathbb{A}\right\rangle = \frac{1}{10\nu}\langle \mathbb{A}, \mathbb{A}\rangle = L_{\mathbf{uu}} = \frac{n k_B T}{\nu}
$$

$\Rightarrow$ correct viscosity if $\nu \geq \max_r \lambda_r$

$$
\left\langle \mathcal{L}^{-1}(\widetilde{\mathbf{B}}), \left(\mathcal{I}-\mathcal{P}_{\mathbb{K}}\right)(\mathbf{C}_i)\right\rangle = L_{qq} = -\frac{5k_B^2 T^3}{2\rho}\sum_{i=1}^{p}\frac{n_i}{m_i} + \left(\frac{5k_B^2 T}{2\rho}\right)^2 \sum_{i,j=1}^{p} L_{ij}
$$

Physical context

Mixture with 4 reacting species : A_1, A_2, A_3 A_4

Binary reversible reaction $A_1 + A_2 \leftrightharpoons A_3 + A_4$

Collisional models

- [Rossani, Spiga, 99] : Discrete energy variable
- [Ern, Giovangigli, 99] : Discrete energy variable : several reactions
- [Desvilettes, Monaco, Salvarani, 05] : Continous energy variable

BGK models : Discrete energy variable

- [M.Groppi, G.Spiga, 04] : Generalisation of [Aoki, Andries, Perthame]
  No H theorem.
- $\Rightarrow$ [M.Groppi, Rjasanov, G.Spiga, 09]

Chemical term

[Groppi, Rjasanov, Spiga, 09] $\mathcal{R}_i^{CE}(\mathbf{f}) = \nu_i^C(\tilde{\mathcal{M}}_i - f_i)$,

with

$$\tilde{\mathcal{M}}_i = \tilde{n}^i \left(\frac{m_i}{2\pi k_B \tilde{T}}\right)^{\frac{3}{2}} \exp\left(-\frac{m_i}{2k_B \tilde{T}}(\mathbf{v} - \tilde{\mathbf{u}})^2\right).$$

$\tilde{n}^i$, $\tilde{\mathbf{u}}$ and $\tilde{T}$ are computed to have the conservations

$$\int (\mathcal{R}_i^{CE}(\mathbf{f}) + \mathcal{R}_j^{CE}(\mathbf{f}))\, d\mathbf{v} = 0, \qquad (i,j) = (1,3),\ (1,4),\ (2,4),$$

$$\sum_{i=1}^{4} \int m_i \mathbf{v}\, \mathcal{R}_i^{CE}(\mathbf{f})\, d\mathbf{v} = 0, \qquad \sum_{i=1}^{4} \int \left(\frac{1}{2} m_i v^2 + E^i\right) \mathcal{R}_i^{CE}(\mathbf{f})\, d\mathbf{v} = 0.$$

+ $\tilde{n}_1, \cdots, \tilde{n}_4$, $\tilde{\mathbf{u}}$, $\tilde{T}$ coupled to mass action law

Results

The model $\mathcal{R}_i^{ME}(\mathbf{f}) + \mathcal{R}_i^{CE}(\mathbf{f})$ satisfies the properties

- Conservation laws
- Non-negativity of the solution, H theorem
- Correct equilibrium states

Slow reacting regime

$$\partial_t f_i^\varepsilon + \mathbf{v} \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon}\mathcal{R}_i^{ME}(\mathbf{f}) + \mathcal{R}_i^{CE}(\mathbf{f}).$$

Derivation of a reacting Navier-Stokes model

Conclusions and perspectives

Conclusion

- New way to derive BGK models
- Methodology based on the hydrodynamic limit (exact up to order 1)
- Based on the relaxation of some appropriate moments
- Resolution of an entropy minimization problem under moments constraints
- Application to complex gases (polyatomic, gas mixtures, . . .)
- Fick relaxation model for slow reactive mixtures

Related results

- Derivation of an ESBGK model for gas mixtures [Brull, 2015].

Perspectives

- Fit other laws : Pb of realisability (See Junk)
- Chapman-Enskog expansion to Navier Stokes for polyatomic gases
  For Euler, [Desvillettes, Monaco, Salvarani]
  For Navier-Stokes [Baranger, Bisi, Brull, Desvillettes], Diatomic case
  For discrete energy variable, [Giovangigli]
- Generalize BGK models to polyatomic setting (ESBGK, . . .).
- Reacting gas mixture
- Numerical implementation

THANKS FOR YOUR ATTENTION !