

Construction of *BGK* models from an entropy minimization principle

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9th november 2018

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- Construction of the model
- Definition of the relaxation coefficients

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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 .

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

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

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

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

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

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Notations

Macroscopic quantities

ρ , u et T : mass, velocity and temperature

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

Stress tensor

$$\Theta = \frac{1}{\rho} \int_{\mathbb{R}^3} (v - u) \otimes (v - u) f \, dv, \quad f = \mathcal{M} \Rightarrow \rho\Theta = \rho T \, Id$$

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 : $f_i(t, x, v)$ ($\mathbf{f} := (f_1, \dots, f_p)$)

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

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Chapman-Enskog expansion

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

Rescaled Boltzmann equation

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

Chapman-Enskog expansion

- Equilibrium state : $Q(f, f) = 0 \Leftrightarrow f = \mathcal{M}$
- Choice of the Maxwellian

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ v^2 \end{pmatrix} \mathcal{M} dv = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ v \\ v^2 \end{pmatrix} f dv$$

- $f = \mathcal{M}$ + 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

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

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

Euler system

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

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Computation of f_1

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

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

Inversion of the relation $\Rightarrow f_1$

Sonine polynomials

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

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

$$\partial_t \rho + \operatorname{div}_x(\rho \mathbf{u}) = 0$$

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Transport Coefficients

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

Prandtl number

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

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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

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

Problem : Prandtl number not correct ≈ 1

Remark : Model coming from an entropy minimization problem

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Minimization principle

Aim : 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

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

$$C_f = \{g \geq 0 / \int \mathbf{m}(v)g dv = \mathcal{V}(\int \mathbf{m}(v)f dv)\}$$

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

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

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

NC : \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 coefficients :

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

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

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

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

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

Conserved quantities : $\lambda_i = 0$.

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Explanation of the constraints

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

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

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

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

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

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

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

$C_f = \{g \geq 0 \text{ s.t.}$

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

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

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

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

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Main result

Theorem

Let $f \neq 0$, $f \geq 0$ s.t. $\int (1 + |v|^2) f < +\infty$ and $v \in [-\frac{1}{2}, 1[$,
 \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 $v \in [-\frac{1}{2}, 1[$.

Arguments : $C_f \neq \emptyset$. Ex : $G_{ES} \in C_f$.

M.Junk, J.Schneider $\Rightarrow \exists$ a solution to the minimization problem.

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

α Lagrange multipliers associated to constraints

Chapman-Enskog expansion

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

f is expanded as

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

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

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

Prandtl number

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

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

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Prandtl number

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

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

Chapman-Enskog expansion

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

f is expanded as

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

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

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\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 $\rightarrow \mathbf{f} = \mathbf{f}(t, \mathbf{x}, \mathbf{v}, I)$

$I =$ 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 : $(1, \mathbf{v}, \frac{1}{2}|\mathbf{v}|^2 + I^{\frac{2}{\delta}})$

$\delta =$ 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

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

Macroscopic quantities

ρ , u defined as in the monoatomic case

Specific internal energy

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

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

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

Temperatures are associated to these energies

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

Macroscopic quantities

ρ , u defined as in the monoatomic case

Specific internal energy

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

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

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

Temperatures are associated to these energies

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

$$\mathbb{P} = \{1, v, v \otimes v, l^{\frac{2}{\delta}}\}$$

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

$$G = \min_{g \in C_f} \mathcal{H}(g). \quad (6)$$

$$C_f = \{g \geq 0 \text{ s.t.}$$

$$\int_{\mathbb{R}^3 \times \mathbb{R}_+} g(1, v, \frac{1}{2}|c|^2 + l^{\frac{2}{\delta}}) dv dl = \int_{\mathbb{R}^3 \times \mathbb{R}_+} f(1, v, \frac{1}{2}|c|^2 + l^{\frac{2}{\delta}}) dv dl, \quad (7)$$

$$\begin{aligned} & \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{1}{3}|c|^2 - \frac{2}{3+\delta} \left(\frac{|c|^2}{2} + l^{\frac{2}{\delta}} \right) \right) \lambda(g - f) dv dl \\ &= -\lambda_2 \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(\frac{1}{3}|c|^2 - \frac{2}{3+\delta} \left(\frac{|c|^2}{2} + l^{\frac{2}{\delta}} \right) \right) f dv dl, \end{aligned} \quad (8)$$

$$\int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(c \otimes c - \frac{1}{3}|c|^2 Id \right) \lambda(g - f) dv dl = -\lambda_1 \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left(c \otimes c - \frac{1}{3}|c|^2 Id \right) f dv dl \quad (9)$$

Construction of G

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

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

Stress tensor

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

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. $\int f (1 + |v|^2 + l^{\frac{2}{\delta}}) dv dl < +\infty$, $\nu \in [-\frac{1}{2}, 1[$ and $\theta \in [0, 1]$. Then the problem (6, 7, 8, 9) has a unique solution G ,

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

Conversely, if (6, 7, 8, 9) has a unique solution for any $f \geq 0$ s.t. $\int f (1 + |v|^2 + l^{\frac{2}{\delta}}) dv dl < +\infty$, 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

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

Chapman-Enskog expansion

⇒ 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 :

$$\begin{aligned}\forall i \in [1, \rho], \quad \partial_t n^i + \nabla \cdot (n^i \mathbf{u} + \mathbf{J}_i) &= 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\mathbb{P} + \rho \mathbf{u} \otimes \mathbf{u} + \mathbb{J}_u) &= 0, \\ \partial_t E + \nabla \cdot (E \mathbf{u} + \mathbb{P}[\mathbf{u}] + \mathbb{J}_u[\mathbf{u}] + \mathbf{J}_q) &= 0,\end{aligned}$$

$\mathbf{J}_i, \mathbb{J}_u, \mathbf{J}_q$: mass, momentum and heat fluxes.

Thermodynamics of Irreversible Processes assumptions.

$$\begin{aligned}\mathbf{J}_i &= \sum_{j=1}^{j=\rho} L_{ij} \nabla \left(\frac{-\mu_j}{T} \right) + L_{iq} \nabla \left(\frac{1}{T} \right), \\ \mathbf{J}_q &= \sum_{j=1}^{j=\rho} L_{qj} \nabla \left(\frac{-\mu_j}{T} \right) + L_{qq} \nabla \left(\frac{1}{T} \right), \\ \mathbb{J}_u &= L_{uu} \mathbb{D}(\mathbf{u}),\end{aligned}$$

$$\mu_j : \text{chemical potential} : \frac{\mu_j}{T} = k_B \left(\ln(n_j) - \frac{3}{2} \ln \left(\frac{2\pi k_B T}{m_j} \right) \right).$$

Fick, Dufour, Soret, Fourier coefficients

Phenomenological point of view :

[Chapman-Cowling], [Kurochkin-Makarenko-Tirskii]

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

D_{ij} : Fick coefficient : Diffusion

D_{iT} : Soret coefficient : Thermal diffusion

D_{qj} : Duffour coefficient : Diffusion thermo-effect

D_{qq} : Fourier coefficient

Relation between diffusion and Onsager matrixes

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

Notations

Distribution function : $\mathbf{f} := (f_1, \dots, f_p) \rightarrow n^i, u^i, T^i$.

Maxwellians distributions : $\mathbf{M} := (\mathcal{M}_1, \dots, \mathcal{M}_p)$.

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

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

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

denoted $\phi^l, l \in \{1, \dots, p + 4\}$.

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

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

$$(\mathbb{A})_i = m_i \left[(\mathbf{v} - \mathbf{u}) \otimes (\mathbf{v} - \mathbf{u}) - \frac{1}{3} (\mathbf{v} - \mathbf{u})^2 \mathbb{I} \right],$$

$$(\mathbf{B})_i = (\mathbf{v} - \mathbf{u}) \left[\frac{1}{2} m_i (\mathbf{v} - \mathbf{u})^2 - \frac{5}{2} k_B T \right],$$

$$(\tilde{\mathbf{B}})_i = m_i (\mathbf{v} - \mathbf{u}) \left[\frac{1}{2} (\mathbf{v} - \mathbf{u})^2 - \frac{5n}{2\rho} k_B T \right].$$

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

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

Fluxes and transport coefficients

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

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

Fluxes :

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

Transport coefficients :

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

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

Casimir-Onsager relations :

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

Total mass conservation :

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

$$\text{Ker}(\mathbf{L}) = \text{Vect}(m_1, \dots, m_p, 0) \Rightarrow \text{Rank}(\mathbf{L}) = p - 1$$

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.

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

Space of constraints : C_f .

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

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

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

\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^* : $(l_r^*, \mathbf{w}_r)_{r \in \{1, \dots, p-1\}} \cup (0, \mathbf{w}_p)$

Theorem

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

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

Properties of the BGK model

The Fick relaxation operator satisfies the fundamental properties :

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

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

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

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

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

Computation of transport coefficients

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

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

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

⇒ correct **viscosity** if $\nu \geq \max_r \lambda_r$

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

Physical context

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



Collisional models

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

$$\int (\mathcal{R}_i^{CE}(\mathbf{f}) + \mathcal{R}_j^{CE}(\mathbf{f})) d\mathbf{v} = 0, \quad (i, j) = (1, 3), (1, 4), (2, 4),$$
$$\sum_{i=1}^4 \int m_i \mathbf{v} \mathcal{R}_i^{CE}(\mathbf{f}) d\mathbf{v} = 0, \quad \sum_{i=1}^4 \int \left(\frac{1}{2} m_i v^2 + E^i \right) \mathcal{R}_i^{CE}(\mathbf{f}) d\mathbf{v} = 0.$$

+ $\tilde{n}_1, \dots, \tilde{n}_4, \tilde{\mathbf{u}}, \tilde{T}$ 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].
- Existence theorems (see Seok-Bae Yun)
- Slip boundary conditions, shock waves : see Aoki et al

Perspectives

- Fit other laws : Pb of realisability (See Junk, Schneider)
 - ⇒ Higher moments constraints
 - ⇒ phi divergence approach based on an approach entropy : see Abdel Malik, Van Brummelen,
Application to BGK models : Pavan, Schneider
- Generalize BGK models to mixture of polyatomic setting (ESBGK, ...). Brull, in progress
- Reacting gas mixture
- Numerical implementation

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THANKS FOR YOUR
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