# Construction of *BGK* models from an entropy minimization principle

Stéphane BRULL, Jacques SCHNEIDER, Vincent PAVAN

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# Plan

# Introduction

# 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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# Notations

**Macroscopic quantities**

$\rho$, $u$ 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**

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

**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 $\mathbb{K}$

# Chapman-Enskog expansion

Parameter $\varepsilon$ 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 : $Q(f, f) = 0 \ \Leftrightarrow f = \mathcal{M}$
- 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

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

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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# Computation of $f_1$

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

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

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

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 $(1, v, |v|^2)$,

$$\begin{aligned}
&\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 \\
&\partial_t\Big(\rho(\frac{1}{2}|u|^2 + \frac{3}{2}T)\Big) + div_x\Big(\rho(\frac{1}{2}|u|^2 + \frac{5}{2}T) - \varepsilon\kappa\nabla_x T - \varepsilon\mu\mathbb{D}(u)\cdot u\Big) = 0.
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Transport Coefficients

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

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 $\approx 1$

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

$$\begin{aligned} \mathcal{H}(G) &= \min_{g \in C_f} \mathcal{H}(g), \\ C_f &= \{g \geq 0 \;/\; \int \mathbf{m}(v) g dv = \mathcal{V}(\int \mathbf{m}(v) f dv)\} \end{aligned}$$

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

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

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

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

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

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

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

# $\mathbb{P} = \mathbb{P}_0 + v \otimes v$

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

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

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

$C_f = \{g \geq 0$ 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.

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

$\alpha$ Lagrange multipliers 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 $\lambda$ 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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# 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 $\gamma$ and $\delta$

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

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

$\rho$, $u$ 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

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

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Temperatures are associated to these energies

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

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

$R(f) = \lambda(G - f)$, 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.

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

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

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

# 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 $\lambda$, $\lambda_1$, $\lambda_2$.

Tensor for polyatomic Navier-Stokes

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

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 :

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

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

Thermodynamics of Irreversible Processes assumptions.

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

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

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

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

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

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

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

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

# Fluxes and transport coefficients

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

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

Fluxes :

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

Transport coefficients :

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

# 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 :

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

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

# 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 $\lambda_r$ 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 $\nu \geq \max_r \lambda_r$

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

# 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, ...)

Related results

- Fick relaxation model for slow reactive mixtures
- Derivation of an ESBGK model for gas mixtures [Brull, 2015].
- Existence theorems (see Seok-Bae Yun)

# 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 redaction
- Reacting gas mixture
- Numerical implementation of the BGK models : [Brull, Prigent], in revision
- Existence theorems in bounded domains : [Brull, Yun], submitted

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**THANKS FOR YOUR ATTENTION !**