

# Relaxation operators in kinetic theory

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- Find deterministic methods for the Boltzmann equation
- Discrete velocity models have good properties but computation of  $Q(f, f)$  for " $N$ " velocities in  $O(N^2 \log N)$ .
- Look for simpler model rather than for numerical method.
- Find a compromise between the numerical cost and the accuracy of the model.

# The Boltzmann equation

## The Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = Q(f, f) = Q^+(f, f) - \nu(f)f, \quad (t, x, v) \in \mathbb{R}^+ \times \mathbb{R}^3 \times \mathbb{R}^3$$

## Notations

- $f(t, x, v)$  : distribution function
- $n = \int f \, dv$  : number of molecules per unit volume
- $nu = \int v f \, dv$  : momentum (m=1)
- $E = \frac{nu^2}{2} + \frac{3}{2}nT = \frac{1}{2} \int v^2 \, dv$  : total energy

# Main properties I

- 1) Preservation of positivity : under suitable assumptions the solution exists and  $f(t, x, v)$  remains a density function i.e.  $f(t, x, v) \geq 0$
- 2) Collision invariants (mass, momentum and energy are conserved during a collision)

$$\int Q(f, f)(1, v, v^2) dv = 0$$

- 3)  $\exists \eta$  entropy density and

$$H(f) = \int \eta(f) dv \quad \text{s.t.} \quad \int \eta'(f) Q(f, f) dv \leq 0.$$

- 3') For the Boltzmann equation  $\eta(x) = x \ln(x) - x$ ,

$$\partial_t H(f) + \operatorname{div} \int v \eta(f) dv \leq 0$$

# Main properties II

## 4) Extended $H$ theorem

$$\int_{\mathbb{R}^3} \eta'(f) Q(f, f) dv = 0 \Leftrightarrow Q(f, f) = 0 \Leftrightarrow \eta'(f) \in \text{Span}\{1, v, v^2\}$$

$$\Rightarrow f = \mathcal{M} = \frac{n}{(2\pi T)^{\frac{3}{2}}} \exp\left(-\frac{(v-u)^2}{2T}\right)$$

## 5) Galilean invariance

6) Correctness of the hydrodynamic limit : Right properties on the linearized operator (Fredholm, kernel =  $\mathbb{K}$ )

Chapmann-Engskog expansion :  $f = \mathcal{M}(1 + \varepsilon g) + O(\varepsilon^2)$  into

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

$\Rightarrow$  Euler and Navier-Stokes

# Entropic approximation and first models



# A hierarchy of models

**Main idea** :E. M. Shakhov,MEKHIANIKA ZHIDKOSTI I GAZA, 1968

Replace  $Q(f, f) = Q^+(f, f) - \nu f$  with  $R(f) = \nu(G - f)$  where  $G \approx Q^+(f, f)/\nu$ .

**Constraints for Maxwell molecules :**

$$\int G \mathbf{m}(v) = \nu^{-1} \int Q^+(f, f) \mathbf{m}(v)$$

where  $\mathbf{m}(v) = (m_0, \dots, m_N)$  is a generating vector of a (suitable) polynomial space  $\mathbb{P}$

**"Closure"** :  $G = \mathcal{M} * p(v)$  where  $p(v) \in \mathbb{P}$

**Problem** :  $G$  is not nonnegative everywhere and the solution might become negative !

[Levermore, JSP, 1996]

- Replace  $f \rightarrow G = \exp(\alpha \cdot \mathbf{m}(v))$  solution of

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

with

$$C_f = \{g \geq 0, \int g \mathbf{m}(v) = \int f \mathbf{m}(v) dv\}.$$

[Levermore, JSP, 1996]

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**Question :**  $f \rightarrow G$  well-defined ?

# Entropic Approximation 2

Junk says not always ! M3AS, 2000.

But it is possible if the constraint of highest degree is relaxed  
J.S., M2AN, 2004.

- 1 Example :  $\mathbb{P} = \mathbb{P}_{N-1} \oplus \mathbb{R} \cdot |v|^N$ , just ask  $\int g |v|^N \leq \int f |v|^N$
- 2 The **entropic "approximation"**  $f \rightarrow G(f)$  is well defined.
- 3 **New closure in Shakhov model** :  $G =$  entropic approximation  $Q^+(f, f)/\nu$ . The model satisfies all properties !  
 $\implies$  **model restricted to Maxwellian molecules.**

# Method of moment relaxation

Aim : Construct relaxation operator

$$R(f) = \nu(G - f)$$

that « behaves as » linear operator while pertaining positivity

## Definition

If  $R(f)$  satisfies properties 1 – 6,  $R(f)$  is a well defined operator.

## Remark

*We do not ask  $H(f) = \int \eta(f)dv$  to be a Lyapounov Functional.*

Let  $\mathbf{m}(v) = (m_1(v), \dots, m_N(v))$  be a set of tensors.

$$\int R(f) m_i(v) dv = -v_i \int_{\mathbb{R}^3} f m_i(v) dv$$

$(v_i)_{i=1, \dots, N}$  are nonnegative relaxation coefficients (frequency)

## First example

Set of tensors :  $\mathbb{P} = \mathbb{K} \oplus^\perp \mathbb{A}$ , where

$$\mathbb{A}(v) = (v - u) \otimes (v - u) - \frac{1}{3} \|v - u\|^2 I_d$$

⇒ Rigorous derivation of the ESBGK model [S. Brull, J.S., 2008]

# Main example

Set of tensors :  $\mathbb{P} = \mathbb{K} \oplus^\perp \mathbb{A} \oplus^\perp \mathbf{b}$ , where

$$\mathbf{b}(v) = (v - u) \left( \frac{1}{2}(v - u)^2 - \frac{5}{2}T \right)$$

Constraints

$$\begin{aligned} \int_{\mathbb{R}^3} G(1, v, v^2) dv &= \int_{\mathbb{R}^3} f(1, v, v^2) dv \\ \int_{\mathbb{R}^3} G \mathbb{A}(v - u) dv &= \left(1 - \frac{\nu_{\mathbb{A}}}{\nu}\right) \int_{\mathbb{R}^3} f \mathbb{A}(v - u) dv \\ \int_{\mathbb{R}^3} G \mathbf{b}(v - u) dv &= \left(1 - \frac{\nu_{\mathbf{b}}}{\nu}\right) \int_{\mathbb{R}^3} f \mathbf{b}(v - u) dv \end{aligned}$$

Conservation laws  $\Rightarrow \nu_i = 0$  on  $\mathbb{K}$

How to define  $\nu$ ,  $G$ ,  $\nu_{\mathbb{A}}$  and  $\nu_{\mathbf{b}}$  ?



# Variational principle

Choose a strictly convex function  $\eta$  with domain in  $\mathbb{R}_+$  and set

$$H(g) = \int \eta(g) dv$$

For  $\rho_f = \int f \mathbf{m}(v) dv$ , define  $L(\rho_f)$ , with the relaxation constraints

$$(L(\rho_f))_i = \left(1 - \frac{v_i}{v}\right) \int_{\mathbb{R}^3} f m_i(v) dv$$

## Problem

For  $\rho_f \in \mathbb{R}^q$  ( $q$  : dimension of  $\text{span}\{m_i\}$ ), find if possible a function  $G$  such that

- 1  $\int G \mathbf{m}(v) dv = L(\rho_f)$
- 2  $H(G) = \min_{\int g \mathbf{m}(v) dv = L(\rho_f)} H(g).$

## Definition of $\nu_A$ and $\nu_b$

If  $f \mapsto G$  is sufficiently smooth and  $R(f)$  is well-posed (H theorem)

$$\partial_t f^\varepsilon + v \cdot \nabla f^\varepsilon = \frac{1}{\varepsilon} R(f^\varepsilon).$$

Order  $-1$  : H theorem  $\Rightarrow f_0 = \mathcal{M} \Rightarrow$  Euler equation in  $O(\varepsilon)$

Setting  $f_1 = \mathcal{M}g_1$

Equation at order 0 :

$$\mathcal{L}_R(g_1) = \mathbb{A}(v - u) : \mathbb{D}(u) + \mathbf{b}(v - u) \cdot \nabla_x \left(-\frac{1}{T}\right),$$

where  $\mathbb{D}(u)$  is the Reynolds tensor and

$$\mathcal{L}_R(g) = \frac{1}{\mathcal{M}} \lim_{\varepsilon \rightarrow 0} \frac{R(\mathcal{M}(1 + \varepsilon g))}{\varepsilon}$$

# Definition of $\nu_{\mathbb{A}}$ and $\nu_{\mathbb{b}}$

Compute

$$\mathcal{L}_R(g) = \nu \left( \sum (1 - \frac{\nu_i}{\nu}) \mathbb{P}_{m_i} + \mathbb{P}_{\mathbb{K}} - Id \right) (g)$$

$$\mu_R = \frac{T}{10} \langle \mathcal{L}_R^{-1}(\mathbb{A}), \mathbb{A} \rangle = \frac{nT}{\nu_{\mathbb{A}}}, \quad \kappa_R = \frac{5nT}{2\nu_{\mathbb{b}}}$$

where  $\langle \cdot, \cdot \rangle$  is the  $L^2(\mathcal{M})$  dot product with the full contraction for tensor.

**Definition of  $\nu_{\mathbb{A}}$  and  $\nu_{\mathbb{b}}$**

$$\nu_{\mathbb{A}} = \frac{nT}{\mu}, \quad \nu_{\mathbb{b}} = \frac{5nT}{2\kappa} \implies Pr = \frac{5\mu}{2\kappa} = \frac{\nu_{\mathbb{b}}}{\nu_{\mathbb{A}}}$$

**$R$  is designed such that  $\mathcal{L}_R^{-1} \sim \mathcal{L}_B^{-1}$  and **not**  $\mathcal{L}_R \sim \mathcal{L}_B$**

# Problems to be solved

We assume that  $f \geq 0$  and

$$\int_{\mathbb{R}^3} f |m_i(v)| dv < +\infty, \quad \forall i = 1, \dots, N.$$

$G$  must satisfy  $G \geq 0$  and  $\int Gm(v) = L(\rho_f)$

## Condition

$$C_f = \left\{ g \geq 0 / \int_{\mathbb{R}^3} g m_i(v) dv = \left(1 - \frac{v_i}{v}\right) \int_{\mathbb{R}^3} f m_i(v) dv \right\} \neq \emptyset.$$

- 1 What is the shape of the set of realizable moments

$$\mathcal{R}_m^+ = \left\{ \int_{\mathbb{R}^3} f \mathbf{m}(v) dv, f \geq 0, \int_{\mathbb{R}^3} f |m_i(v)| dv < +\infty \right\}$$

- 2 Optimization problem :  
Solve

$$\min_{g \in \mathcal{C}_f} \int_{\mathbb{R}^3} \eta(g) dv$$

for some entropy density  $\eta$ .

The choice of  $\eta$  is crucial for

- The existence of a (unique) minimizer
- The H theorem

No solution (in general) when  $\eta(x) = x \ln(x)$  under the constraints

$$\begin{aligned}\int_{\mathbb{R}^3} g(1, \mathbf{v}, \mathbf{v}^2) d\mathbf{v} &= \int_{\mathbb{R}^3} f(1, \mathbf{v}, \mathbf{v}^2) d\mathbf{v} \\ \int_{\mathbb{R}^3} g \mathbf{A}(\mathbf{v} - u) d\mathbf{v} &= \left(1 - \frac{\lambda_{\mathbf{A}}}{\nu}\right) \int_{\mathbb{R}^3} f \mathbf{A}(\mathbf{v} - u) d\mathbf{v} \\ \int_{\mathbb{R}^3} g \mathbf{b}(\mathbf{v} - u) d\mathbf{v} &= \left(1 - \frac{\lambda_{\mathbf{b}}}{\nu}\right) \int_{\mathbb{R}^3} f \mathbf{b}(\mathbf{v} - u) d\mathbf{v}\end{aligned}$$

Artificial condition on  $\int g|\mathbf{v}|^4 d\mathbf{v}$  ?

The problem might not be well posed ?

See [Junk, 1998, 2000], [J.S., 2004], [Hauck et al, 2008], [Pavan, 2011]

## Shape of the set $\mathcal{R}_m^+$

## In 1d : Hamburger moment problem

Given  $\rho_0, \dots, \rho_n \in \mathbb{R}$  and  $m_i(x) = x^i$  is there a measure  $\mu$  such that

$$\int_{\mathbb{R}} x^i d\mu = \rho_i$$

**Theorem (Akhiezer, Krein, 1962)**

*If  $n = 2p$  there exists a measure  $\mu$  iff the Hankel matrix*

$$H := (\rho_{i+j})_{0 \leq i, j \leq p}$$

*is positive definite.*

The measure  $d\mu$  can be changed into  $f(x) dx$  with  $f \in L^1$



## Definition

Let  $\mathbf{m}(\mathbf{v}) := (\mathbf{m}_0(\mathbf{v}), \dots, \mathbf{m}_k(\mathbf{v}), \dots, \mathbf{m}_n(\mathbf{v}))$  be a list of tensors where  $\mathbf{v} \in \mathbb{R}^d$ .  $(\mathbf{m}_k)_k$  is pseudo-Haar when :

$$\forall \boldsymbol{\alpha} = (\alpha_0, \dots, \alpha_n), [\boldsymbol{\alpha} \neq \mathbf{0} \Rightarrow \boldsymbol{\alpha} \cdot \mathbf{m}(\mathbf{v}) \neq 0], \text{ l.a.e } \mathbf{v} \in \mathbb{R}^d \quad (1)$$

$$\boldsymbol{\alpha} \cdot \mathbf{m}(\mathbf{v}) := \sum_k \alpha_k : \mathbf{m}_k(\mathbf{v}) \quad (2)$$

## Problem

Let  $\boldsymbol{\rho} = (\rho_0, \dots, \rho_n)$  a list of tensor. Is there a nonnegative function  $f$  in  $L^1(\mathbb{R}^d)$  s.t.

$$\int f m_i(\mathbf{v}) d\mathbf{v} = \rho_i$$

## Example

One may consider the following Pseudo-Haar basis :

- 1 "Euler"  $\mathbf{m}(\mathbf{v}) = (1, \mathbf{v}, \mathbf{v}^2)$
- 2 "Gauss" :  $\mathbf{m}(\mathbf{v}) = (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v})$
- 3 Grad :  $\mathbf{m}(\mathbf{v}) = (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2 \mathbf{v})$
- 4 Levermore :  $\mathbf{m}(\mathbf{v}) = (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2 \mathbf{v}, \mathbf{v}^4)$

## Theorem

[Junk, 2000]

- 1  $\rho \in \mathcal{R}_m^+ \setminus \{0\} \Leftrightarrow \forall \alpha \neq 0$  such that  $\alpha \cdot m(v) \leq 0$  a.e. there is  $\rho \cdot \alpha < 0$
- 2  $\mathcal{R}_m^{+,*}$  is an open convex set
- 3  $\forall \rho \in \mathcal{R}_m^+, \exists \psi \geq 0, \in C_c^\infty(\mathbb{R}^3))$  such that  $\rho = \int_{\mathbb{R}^3} m(v) \psi(v) dv$

## Remark

The set of realizable moment  $\mathcal{R}_m^+ \setminus \{0\}$  is characterized by the set of (non positive) nonnegative polynomials : all  $\alpha \neq 0$  such that  $\alpha \cdot m(v) \geq 0$ .

## Definition (Cone spanned by the pseudo-Haar basis)

Let  $\mathbf{m}(\mathbf{v})$  pseudo-Haar on  $\mathbb{R}^d$  and  $q$  dimension of  $\text{span}(m_0(\mathbf{v}), \dots, m_N(\mathbf{v}))$ . Define  $C$  the positive cone spanned by  $\mathbf{m}(\mathbf{v})$  in  $\mathbb{R}^q$  :

$$C = \left\{ \sum_i \lambda_i \mathbf{m}(\mathbf{v}_i), \lambda_i \geq 0, \mathbf{v}_i \in \mathbb{R}^d \right\} \quad (3)$$

## First remark

If  $m(\mathbf{v})$  is continuous w.r.t  $\mathbf{v}$  and  $\psi_\epsilon \in C_0^\infty$  such that  $\psi_\epsilon \rightarrow \delta$  then

$$\rho_\epsilon := \int m(\mathbf{w}) \psi_\epsilon(\mathbf{w} - \mathbf{v}) d\mathbf{v} \in \mathcal{R}_m^+ \quad \text{et} \quad \rho_\epsilon \longrightarrow m(\mathbf{v}). \quad (4)$$

Same thing for each element of  $C \implies C \subset \overline{\mathcal{R}_m^+}$ .

Converse statement ?

## Second remark

Let  $\alpha \neq 0$  such that  $\alpha \cdot \mathbf{m}(\mathbf{v}) \leq 0, \forall \mathbf{v}$  and  $f \geq 0$  ( $\neq 0$ )  $f \in \mathbb{L}_m^1$  then

$$\alpha \cdot \rho_f = \int \alpha \cdot \mathbf{m}(\mathbf{v}) f(\mathbf{v}) d\mathbf{v} < 0 \quad (5)$$

## Definition (Polar cone of $C$ )

$$\begin{aligned} C^\circ &:= \{\boldsymbol{\alpha} : \boldsymbol{\alpha} \cdot \boldsymbol{\eta} \leq 0 \quad \forall \boldsymbol{\eta} \in C\}, \\ &= \{\boldsymbol{\alpha} : \boldsymbol{\alpha} \cdot \mathbf{m}(\mathbf{v}) \leq 0 \quad \forall \mathbf{v} \in \mathbb{R}^d\} \end{aligned}$$

## Theorem (Interior of a solid convex cone)

If  $\mathcal{X}$  is a convex cone with non-empty interior in  $\mathbb{R}^q$ , then

$$x \in \text{int}(\mathcal{X}) \Leftrightarrow \forall \mathbf{y} \in \mathcal{X}^\circ, [\mathbf{y} \neq \mathbf{0} \Rightarrow \mathbf{y} \cdot \mathbf{x} < 0] \quad (6)$$

$\Rightarrow$  if  $\text{int}(C) \neq \emptyset$  then  $\mathcal{R}_{\mathbf{m}}^{*+} \subset \text{int}(C)$

## Proposition

Let  $\mathbf{m}(\mathbf{v})$  pseudo-Haar basis and  $C$  the positive cone associated to it, then

- 1  $\text{int}(C) \neq \emptyset \implies \mathcal{R}_{\mathbf{m}}^{*+} \subset \text{int}(C)$
- 2  $\forall \rho \in \text{int}(C), \exists \psi \geq 0, \in C_c^\infty(\mathbb{R}^3))$  such that

$$\rho = \int \mathbf{m}(\mathbf{v}) \psi(\mathbf{v}) d\mathbf{v} \quad (7)$$

$$\implies \text{int}(C) \subset \mathcal{R}_{\mathbf{m}}^{*+}$$

## XVIIth Hilbert's problem

Show that every nonnegative polynomial with coefficient in  $\mathbb{R}$  is a sum of square rational functions.

One of the important question about this problem :

- If  $p(\mathbf{v}) = \boldsymbol{\alpha} \cdot \mathbf{m}(\mathbf{v})$  is nonnegative, is it a sum of square (S.O.S) polynomials ?



# Hilbert problem for quadratic structured space

## Example (Levermore space)

The Levermore space can be identified as a product of

$$(1, \mathbf{v}, \mathbf{v}^2) \vee (1, \mathbf{v}, \mathbf{v}^2) = (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2 \mathbf{v}, \mathbf{v}^4)$$

A square polynomial  $P(v) = (a + \mathbf{b} \cdot \mathbf{v} + c\mathbf{v}^2)^2$  can be written as

$$\boldsymbol{\beta}^T M \boldsymbol{\beta}, \text{ with } \boldsymbol{\beta} = (a, \mathbf{b}, c)^T \in \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}$$

$$M = \begin{bmatrix} 1 & \mathbf{v}^T & \mathbf{v}^2 \\ \mathbf{v} & \mathbf{v} \otimes \mathbf{v} & \mathbf{v}^2 \mathbf{v} \\ \mathbf{v}^2 & \mathbf{v}^2 \mathbf{v}^T & \mathbf{v}^4 \end{bmatrix}$$

## What about Grad space ?

$\text{Gr}(\mathbf{v}) = (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2 \mathbf{v})$  has no quadratic structure

## Definition

Likewise, for  $f \geq 0$  in  $L^1_{Lev}$  define a Hankel matrix  $H$  as

$$H = \int_{\mathbb{R}^3} M f(v) dv.$$

$$\Rightarrow \int (a + \mathbf{b} \cdot \mathbf{v} + c\mathbf{v}^2)^2 f dv = \boldsymbol{\beta}^T H \boldsymbol{\beta} > 0$$

**Necessary condition :**

$H$  must be definite positive.

**Converse statement ?**

True if every positive polynomial is a SOS ( $\Leftarrow \boldsymbol{\beta}^T H \boldsymbol{\beta} = \boldsymbol{\rho}_f \cdot \boldsymbol{\alpha}_\beta$ )

Known results between positive polynomials and S.O.S in  $\mathbb{R}^d$

- 1  $d = 1$  : every positive polynomial is a SOS
- 2  $d = 2$  : true for polynomial of degree  $n \leq 4$  but not always if  $n \geq 6$  (Hilbert 1893)
- 3  $d \geq 3$  : true for polynomial of degree  $n = 2$  but not always if  $n \geq 4$

The first explicit counterexample for non S.O.S polynomial in dimension 2 was only found in 1966!

## Theorem

*Artin (1927) Every nonnegative polynomial is a sum of square rational functions.*

# The Grad space

Every positive polynomial  $\alpha \cdot \mathbf{m}(v)$  writes as

$$(\boldsymbol{\beta}, 0) \cdot (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2 \mathbf{v})$$

with  $\boldsymbol{\beta} = (\alpha_0, \alpha_1, \boldsymbol{\alpha}_2)$  and  $\alpha_0 \in \mathbb{R}$ ,  $\alpha_1 \in \mathbb{R}^3$ ,  $\boldsymbol{\alpha}_2 \in \mathbb{R}^3 \times \mathbb{R}^3$

$\Rightarrow$  Characterization by S.O.S. in the Gauss space **and** of realizable moment by the Hankel matrix

## Proposition

$\rho = (n, nu, \Pi, Q) \in \mathcal{R}_{\text{Grad}}^+$  iff  $n > 0$ ,  $\Pi - u \otimes u > 0$ .

$$\Pi = \int \mathbf{v} \otimes \mathbf{v} f dv, \quad Q = \int \mathbf{v}^2 \mathbf{v} f dv.$$

# Grad basis

For  $f \geq 0$  s.t.  $\int_{\mathbb{R}^3} f(1 + |v|^3) < +\infty$ ,  $\text{span} (1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2 \mathbf{v})$  is the space generated by

$$\mathbf{a}(\mathbf{v} - \mathbf{u}) := (1, (\mathbf{v} - \mathbf{u}), (\mathbf{v} - \mathbf{u})^2 - 3T, \mathbb{A}(\mathbf{v} - \mathbf{u}), \mathbf{b}(\mathbf{v} - \mathbf{u}))$$

$$\boldsymbol{\rho}_f = (n, 0, 0, \bar{\mathbb{P}}, \mathbf{q})$$

where  $\bar{\mathbb{P}}$  is the traceless pressure tensor and  $\mathbf{q}$  is the heat flux

## Proposition

$(n, 0, 0, \lambda_{\mathbb{A}} \bar{\mathbb{P}}, \lambda_{\mathbf{b}} \mathbf{q}) \in \mathcal{R}_{Grad}^{+,*} \forall 0 \leq \lambda_{\mathbb{A}} \leq 1$  and  $\forall \lambda_{\mathbf{b}} \in \mathbb{R}$   
 $\forall -\frac{1}{2} \leq \lambda_{\mathbb{A}} \leq 1, \lambda_{\mathbf{b}} = 0$  (Ellipsoidal)

## Remark

*The heat flux can take any value*

# Variational problem

## Remark

*The study of « complex » variational or dual principle in kinetic theory is quite recent (1990') compared to the study of variational problem in general*

- have a look at earlier results
- opens a wide and rich field of research

**Rational Extended Thermodynamics** and its connection with kinetic and its connections with kinetic theory (Muller-Ruggeri)

Formulation of duality on a moment closure : [Levermore, JSP, 1996]

Study of the dual expression  $\rho \leftrightarrow \alpha$  ?

[Junk, 1998, 2000], [Schneider, 2004], [Hauck et al, 2008], [Pavan, 2011]

# The classical problem

$\mathbf{m}(v) = (1, v, v^2, m_3(v), \dots, m_N(v))$  pseudo-Haar basis

$$f \in L_{\mathbf{m}}^1 \Leftrightarrow \int |f|(1 + |v|^{2p}) dv < +\infty$$

$$\eta : x \mapsto \begin{cases} x \ln(x) & \text{if } x \geq 0 \\ +\infty & \text{else} \end{cases}$$

Entropy

$$H(g) = \int \eta(g) dv$$



## Definition (Entropy density)

( $q$  : dimension of  $\text{span}\{m_i\}$ ), for  $\rho \in \mathbb{R}^q$ ,  $h : \mathbb{R}^q \rightarrow \overline{\mathbb{R}}$

$$h(\rho) = \min_{\int g \mathbf{m}(v) dv = \rho} H(g).$$

## Definition (Primal problem)

For  $\rho \in \text{dom}(h)$  find if possible a function  $G$  such that

- $\int G \mathbf{m}(v) dv = \rho$
- $H(G) = h(\rho)$

# Domain of definition

- If  $\rho \in \mathcal{R}_m^+$ , from Junk's theorem  $\exists \Psi \in C_c^\infty(\mathbb{R}^d)$  s.t.  $\int m(v) \Psi dv = \rho$   
 $\Rightarrow H(\Psi) < +\infty$
- $H$  is bounded from below (and above) in the set

$$D(\rho) = \{g \geq 0, \int g m(v) dv = \rho, \int g \ln(g) dv \leq H(\Psi)\}$$

## Proposition

$dom(h) = \mathcal{R}_m^+$  i.e. the infimum exists  $\forall \rho \in \mathcal{R}_m^+$  ( $= +\infty$  outside) and  $h$  is convex l.s.c. in  $\mathbb{R}^q$

# Solution of the primal problem

Let  $g_n$  be a minimizing sequence in  $D(\rho)$  i.e.  $\lim_{n \rightarrow +\infty} H(g_n) = h(\rho)$

Dunford-Pettis in  $D(\rho) \Rightarrow g_n \rightharpoonup G$  in  $L^1$  but not in  $L^1_{\mathbf{m}}$

$$\Rightarrow \int g_n \mathbf{m}(v) dv \rightarrow \int G \mathbf{m}(v) dv$$

The infimum may not satisfy  $\int G \mathbf{m}(v) dv = \rho$

« Formally »,

$$\frac{\partial}{\partial g} \left( H(g) - \boldsymbol{\alpha} \cdot \left( \int \mathbf{m}g \, dv - \boldsymbol{\rho} \right) \right) = 0$$

at the infimum, where  $\boldsymbol{\alpha}$  = Lagrange multipliers.

$$\Rightarrow \eta'(G) = \boldsymbol{\alpha} \cdot \mathbf{m}(v)$$

$$G = (\eta')^{-1}(\boldsymbol{\alpha} \cdot \mathbf{m}(v)) = (\eta^*)'(\boldsymbol{\alpha} \cdot \mathbf{m}(v))$$

Legendre-Fenchel transform :  $\eta^*(x^*) = \max_x (x \cdot x^* - h(x)) = \exp(x^*)$

## Fenchel-Legendre transform of $h$

$$h^*(\boldsymbol{\alpha}) = \max_{\boldsymbol{\rho}}(\boldsymbol{\alpha} \cdot \boldsymbol{\rho} - h(\boldsymbol{\rho}))$$

**Computation** :  $h^*(\boldsymbol{\alpha}) = \int \exp(\boldsymbol{\alpha} \cdot \mathbf{m}(v)) dv$  defined only for  $\exp(\boldsymbol{\alpha} \cdot \mathbf{m}(v)) \in L^1$

**Duality** :  $\forall \boldsymbol{\alpha}, \boldsymbol{\rho}$  s.t.  $h^*(\boldsymbol{\alpha}) + h(\boldsymbol{\rho}) = \boldsymbol{\alpha} \cdot \boldsymbol{\rho}$

$\boldsymbol{\rho} \in \partial h^*(\boldsymbol{\alpha}) =$  "slopes of the lines below  $h^*$ " at  $\boldsymbol{\alpha}$  in 1D  
and  $\boldsymbol{\alpha} \in \partial h(\boldsymbol{\rho})$ .

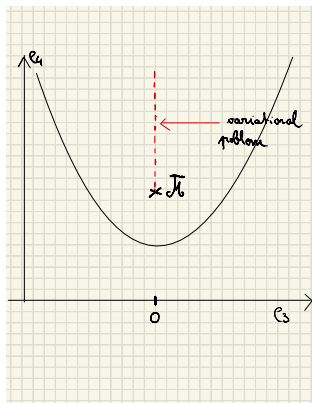
If  $\nabla h^*(\boldsymbol{\alpha})$  exists,  $\boldsymbol{\rho} = \nabla h^*(\boldsymbol{\alpha})$

**Problem** : converse statement i.e if  $\boldsymbol{\rho} \in \mathcal{R}_m^+$ ,  $\exists \boldsymbol{\alpha}$  such that  $\boldsymbol{\rho} = \nabla h^*(\boldsymbol{\alpha})$ ?

# Problem on the boundary

If  $\text{dom}(h^*) = \Lambda$  and  $\Lambda \cap \partial\Lambda \neq \emptyset$ , then  $\nabla h^*$  is not defined on  $\Lambda \cap \partial\Lambda \neq \emptyset$ .

Figure – Domain of definition 5 moments [Junk, 1998]



Normalized Gaussian  $\overline{\mathcal{M}} = \exp(\alpha_{\overline{\mathcal{M}}} \cdot \mathbf{m}(v))$ ,

$\partial h^*(\alpha_{\overline{\mathcal{M}}}) = \text{half-line above } \overline{\mathcal{M}}$

# Comparison with classical projection

$$\forall \rho \in \mathcal{R}_m^{+,*}, \quad D(\rho) = \left\{ f \geq 0, \int f m(v) dv = \rho \right\}$$

- $\mathcal{M}$  = Maxwellian such that  $\int \mathcal{M}(1, \mathbf{v}, \mathbf{v}^2) dv = (\rho_0, \rho_1, \rho_2)$
- $\forall f \in D(\rho)$  define the distance  $d(f, \mathcal{M}) = \int f \ln\left(\frac{f}{\mathcal{M}}\right) dv$  (Csiszar, 1972).

$\implies$  I-projection of  $\mathcal{M}$  onto  $D(\rho)$  (Csiszar, 1975)

$$d(G, \mathcal{M}) = \inf_{f \in D(\rho)} d(f, \mathcal{M})$$

is not always in  $D(\rho)$ .

Classical entropy is not compatible with moments approach

## $\phi$ divergence



« Renormalisation » map of Abdel-Malik and Van Brummelen [2015, JSP]

One starts from  $(1 + \frac{x}{N})^N \rightarrow \exp(x)$  and looks for solutions of the form

$$G = \overline{\mathcal{M}}(1 + \frac{g}{N})_+^N,$$

$g \in \text{span}\{m_0, \dots, m_N\}$ ,  $(x)_+ = \frac{1}{2}(x + |x|)$

$\overline{\mathcal{M}}$  : prescribed Gaussian

## Remark

- 1 polynomial growth  $(1 + \frac{g}{N})_+^N$  instead of exponential.
- 2 measure  $\rightarrow \overline{\mathcal{M}}dv$

## $\phi$ divergence

Inverse function of  $(1 + \frac{x}{N})_+^N : \widetilde{\ln}(y) = Ny^{1/N} - N$ .

$H$  is replaced by

$$H_N = \int \overline{\mathcal{M}} \phi_N(f/\overline{\mathcal{M}}) dv, \quad \text{with } \phi_N(x) = x\widetilde{\ln}(x)$$

### Theorem (Csiszar 1995)

Let  $\phi$  strictly convex, differentiable on  $\mathbb{R}^{+,*}$ ,

$\phi(1) = \phi'(1) = 0$ ,  $\phi'(x) \rightarrow +\infty$ ,

$\phi^*(\alpha \cdot \mathbf{m}(v)) \in L^1(\overline{\mathcal{M}} dv)$ .

For  $\rho \in \mathcal{R}_m^+$ , there exists a unique solution to the primal problem

$$\inf_{\int g\mathbf{m}(v) dv = \rho} \int \overline{\mathcal{M}} \phi(f/\overline{\mathcal{M}}) dv$$

Moreover, this solution satisfies all constraints.

- 1  $\eta(x) = x \ln(x)$  does not satisfy  $\phi^*(\boldsymbol{\alpha} \cdot \mathbf{m}(v)) \in L^1(\overline{\mathcal{M}} dv)$  for any  $\boldsymbol{\alpha}$ .
- 2 Very general but difficult proof
- 3 No strict proof as concerns the shape of the solution
- 4 For the above approximation

$$\int \overline{\mathcal{M}} \phi_N(f/\overline{\mathcal{M}}) dv \sim \int \overline{\mathcal{M}} (f/\overline{\mathcal{M}})^{1+\frac{1}{N}} dv$$

i.e. weighted  $L^{1+\frac{1}{N}}$  space.

Hölder inequality for  $g_n \in D(\boldsymbol{\rho}) \Rightarrow$  minimizing sequence  $g_n \rightarrow G$  in  $L_{\mathbf{m}}^1$

## Theorem

- 1  $\phi : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\}$  *strictly convex and differentiable of  $\mathbb{R}^+$*
- 2  $\phi(0) = 0, \lim_{\rho \rightarrow 0} \frac{\phi(\rho)}{\rho} \in \mathbb{R},$
- 3  $\forall \alpha, \phi^*(\alpha \cdot \mathbf{m}(v)) \in L^1(\overline{\mathcal{M}} dv)$

Then

- 1  $\forall \rho \in \mathcal{R}_m^{+,*}, \exists ! \alpha$  such that  $\nabla h^*(\alpha) = \rho, \nabla h(\rho) = \alpha$
- 2  $G = \overline{\mathcal{M}}(\phi^*)'(\alpha \cdot \mathbf{m}(v))$  is the unique solution to the primal problem.  
Moreover  $h(\rho)$  is strictly convex on  $\mathcal{R}_m^+$ .

# Sketch of the proof

- 1  $dom(h) = \mathcal{R}_m^+$ , with  $\mathcal{R}_m^{+,*}$  convex and open  $\Rightarrow h$  is continuous on  $\mathcal{R}_m^{+,*}$
- 2  $h^*(\alpha) = \int \overline{\mathcal{M}}\phi^*(\alpha \cdot m(v)) dv$  is differentiable in  $\mathbb{R}^q$
- 3  $h$  is continuous at  $\rho \Rightarrow \exists \alpha \in \partial h(\rho) \neq \emptyset$  (subdifferential at  $\rho$ ) s.t.  
$$\Leftrightarrow h(\rho) + h^*(\alpha) = \rho \cdot \alpha$$
$$\Leftrightarrow \rho \in \partial h^*(\alpha) \text{ is reduced to one point } \rho = \nabla h^*(\alpha)$$

## Remark

*The highest degree in  $m(v)$  is not necessary even*

# Method of construction

Step 1 : For  $f \geq 0$ ,  $f \in L^1_{Grad}$ , consider  $\rho_f = \int f \mathbf{a}(v - u) dv$  and the Maxwellian

$$\mathcal{M}_f = \frac{n}{(2\pi T)^{\frac{3}{2}}} \exp\left(-\frac{(v - u)^2}{2T}\right)$$

Step 2 : Consider a given relaxation on  $\rho_f : L(\rho_f) = (n, 0, 0, \lambda_A \bar{P}, \lambda_B \mathbf{q})$

Step 3 : Change  $\bar{M}$  with  $\mathcal{M}_f$  for some  $\phi$  divergence Theorem  $\Rightarrow \exists ! \alpha$  s.t.

$$G = \mathcal{M}_f(\phi^*)'(\alpha \cdot \mathbf{a}(v - u)),$$

with

$$\int G \mathbf{a}(v - u) dv = L(\rho_f), \quad \text{and} \quad H(G) = h(L(\rho_f))$$

- 1  $L(\rho_f)$  chosen such as mass, momentum and energy are conserved
- 2  $G \geq 0$ , as soon as  $\phi$  satisfies the assumptions of theorem  $\Rightarrow (\phi^*)'(x) \geq 0$  on  $\mathbb{R}$ .
- 3 (Extended) H theorem :  $h$  is strictly convex in  $\mathcal{R}_{Grad}^+$

$$\implies (\lambda_A, \lambda_b) \in [0, 1]^2 \longrightarrow h(n, 0, 0, \lambda_A \bar{P}, \lambda_b q)$$

is strictly convex with a unique minimum in

$$h(n, 0, 0, 0, 0) = H(\mathcal{M}_f)$$

- $\int \mathcal{M}_f \phi(f/\mathcal{M}_f) dv$  is **not a Lyapunov functional** (in general) **in inhomogeneous case**

In few words,  $\mathbb{P} = \{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, |\mathbf{v}|^2 \mathbf{v}\}$  is invariant under the action of

$$T = \begin{cases} \tau_u \mathbf{v} = \mathbf{v} - u & \forall u \in \mathbb{R}^3 \\ \Theta \mathbf{v} & \forall \Theta \text{ rotation} \end{cases}$$

and

$$H(g(Tv)) = \int \mathcal{M}_f(T(v)) \phi\left(\frac{g(Tv)}{\mathcal{M}_f(T(v))}\right) dv = \int \mathcal{M}_f(v) \phi\left(\frac{g(v)}{\mathcal{M}_f(v)}\right) dv$$

$$\Rightarrow TG(v) = G(T(v))$$

Invariance of the measure in the entropy under Galilean transform



## Theorem

$$\mathcal{L}_{\mathcal{M}}(g) = \nu \left( \sum_i \left(1 - \frac{\nu_i}{\nu}\right) \mathbb{P}_{m_i} + \mathbb{P}_{\mathbb{K}} - Id \right)(g)$$

$\Rightarrow \mathcal{L}_{\mathcal{M}}$  is Fredholm, self-adjoint and negative on  $\mathbb{K}^{\perp}$

Consequences :  $\mathcal{L}_{\mathcal{M}}^{-1}$  is defined on  $\mathbb{K}^{\perp}$  and  $\mu_{\mathbb{K}} = \frac{P}{\nu_A}$ ,  $\kappa_{\mathbb{K}} = \frac{5}{2} \frac{P}{\nu_B}$

Multiple choices for the relaxations (i.e on  $\nu$ )  $\left(1 - \frac{\nu_A}{\nu}\right)$ ,  $\left(1 - \frac{\nu_B}{\nu}\right)$  as soon as :  
 $\mu_{\mathbb{K}} = \mu$ ,  $\kappa_{\mathbb{K}} = \kappa$ ,  $\frac{\nu_B}{\nu_A} = Pr$

Also one can prove from the properties of  $\mathcal{L}_{\mathcal{M}}$  that

$$\int_{\mathbb{R}^3} K(g)\phi(v)dv = 0 \quad \forall g \quad \Rightarrow \phi \in \mathbb{K}$$

## Examples

$$\phi(x) = x \ln(x),$$

$$\int_{\mathbb{R}^3} \mathcal{M} \phi\left(\frac{f}{\mathcal{M}}\right) dv = \int_{\mathbb{R}^3} f \ln\left(\frac{f}{\mathcal{M}}\right) dv$$

the variational problem well-posed in  $\mathbb{P} = \{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}\}$  for

$$L(\rho_f) = (n, 0, 0, \lambda_A \bar{\mathbb{P}}), \quad \text{with} \quad -\frac{1}{2} \leq \lambda_A \leq 1$$

$\lambda_A = 0 \Leftrightarrow \nu_A = \nu$  : BGK model (1954)

Else : ESBGK model [Holway, 1966] from  $Pr = \frac{2}{3}$  to  $+\infty$

$\Rightarrow$  ESBGK mono and poly [Andries et al, 2000], [Brull, J.S. 2008, 2009]

Possibility to extend the variational principle to  $\nu(c)$  ( $c = v - u$ ) dependant collision frequency [Bouchut, Perthame, 1993], [Struchtrup, 1997]

$\phi$  divergence for the Shakhov model

$$\phi_{\chi^2}(x) = \frac{1}{2}(x-1)^2, \quad \forall x \in \mathbb{R}$$

$$(\phi_{\chi^2}^*)'(x^*) = 1 + x^* \quad \forall x^* \in \mathbb{R}$$

Minimization « problem » : projection of  $\frac{f}{M} - 1$  on Grad space in  $\mathcal{L}^2(\mathcal{M})$   
In the Grad space, the choice

$$v_{\mathbf{A}} = v = \frac{P}{\mu} \quad \text{and} \quad v_{\mathbf{b}} = vPr$$

$$\Rightarrow G_S = \mathcal{M} \left( 1 + \frac{1-Pr}{\rho T} (v-u) \cdot \vec{q} \left( \frac{(v-u)^2}{T} - 5 \right) \right)$$

- 1 Contrarily to ESBGK model

$$\int_{\mathbb{R}^3} G_s \mathbf{a}(v - u) dv = \frac{1}{v} \int_{\mathbb{R}^3} Q^+(f, f) \mathbf{a}(v - u) dv$$

for Maxwellian molecules.

- 2 H Theorem  $\forall Pr > 0$

- 3  $\overline{\rho_{Gs}} \in \mathcal{R}_{Grad}^+ \Rightarrow$  this may bring some stability (at least close to a given  $\overline{\mathcal{M}}$ )

# Polynomial approximation of exp

$$\phi_N(x) = Nx^{1/N} - N$$

$$\forall \rho_f \in \mathcal{R}_{Grad}^+, \exists! \alpha \text{ s.t. } G = \mathcal{M} \left(1 + \frac{\alpha \cdot \mathbf{a}(v-u) - 1}{N}\right)_+^N$$

$$H(G) = H(L(\rho_f)), \quad \int G \mathbf{a}(v-u) dv = L(\rho_f)$$

Well-posed operator not restricted to polynomial space with even higher order rank

## Remark

$\int f \ln f$  is almost a Lyapunov functional for the inhomogeneous equation since

$$\int R(f) \widetilde{\ln}(f/\mathcal{M}) dv \approx \int R(f) \ln(f/\mathcal{M}) dv$$

# The Levermore operator

Let  $\mathbb{M} = \mathbb{M}_1 \subset \mathbb{M}_2 \subset \dots \subset \mathbb{M}_N$  and  $0 < \nu_1 < \nu_2 < \dots < \nu_N$  and

$$\mathcal{M}_k = \operatorname{Argmin} \left\{ \int g \ln(g) / \int g m_i(v) dv = \int f m_i(v) dv, \forall m_i \in \mathbb{M}_k \right\}$$

$$K(f) = \nu_1(\mathcal{M} - f) + \sum_{k=2}^N (\nu_k - \nu_{k-1})(\mathcal{M}_k - f)$$

Then

$$(\forall \phi \in \mathbb{M}_k \setminus \mathbb{M}_{k-1}), \quad \mathcal{L}_{\mathcal{M}}(m) = -\nu_{k-1} m(v)$$

$\Leftrightarrow$  Grad's relaxation

# Problems and questions

- 1 Variational problem may be not well posed
- 2  $\mathbb{M} = \mathbb{K} +$  Gauss space :  $\nu_1 < \nu_2$  does not give the right Prandtl number. (Mieussens Phd Thesis 1999)
- 3 If  $\phi \in \mathbb{M}_k \setminus \mathbb{M}_{k-1}$ , ( $k \geq 2$ )

$$\int K(f)\phi(v)dv \neq -\nu_{k-1} \int f\phi dv$$

(( $\phi_i$ ) orthogonal in  $L^2(\mathcal{M})$ , not in  $L^2(\mathcal{M}_{k-1})$ )

- 4 however

$$\mathcal{L}_{\mathcal{M}}(g) = \nu_N \left( \sum_{k=1}^N \left( 1 - \frac{\nu_{k-1}}{\nu} \right) \mathbb{P}_{\mathbb{M}_k \setminus \mathbb{M}_{k-1}} + \mathbb{P}_{\mathbb{K}} - Id \right)(g)$$

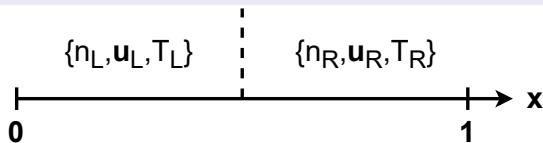


# Stationary shock wave

# Stationary normal shock wave - 1

Purpose : the 1D domain is divided in 2 regions, with different gas states, and let the gas relaxed to the stationary state.

## Domain initialization



## Boundary conditions

- Left at  $0$  :  $\{n_L, u_L, T_L\}$
- Right at  $1$  :  $\{n_R, u_R, T_R\}$

# Stationary normal shock wave - 2

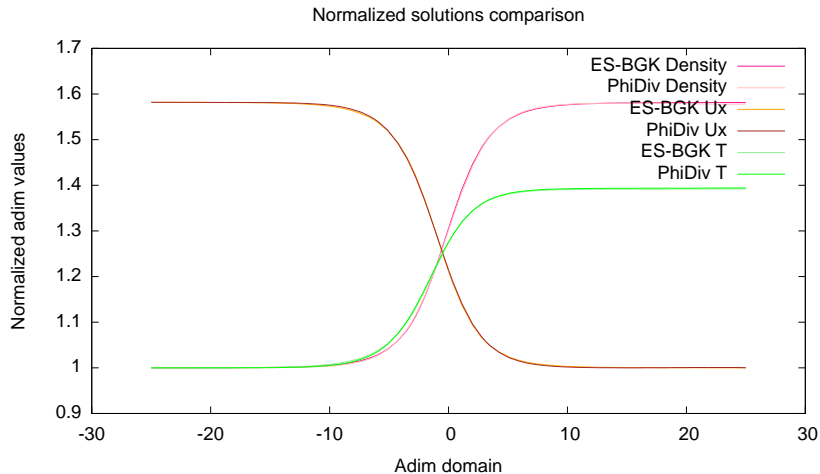
Values :

Mach	Boundary	n	u	T
1.4	left	1	1.278	1
	right	1.581	0.808	1.392

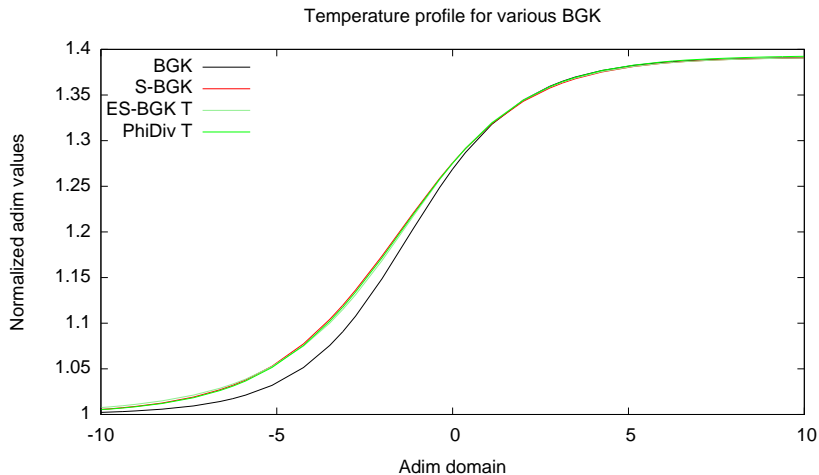
## Code characteristics

- DVM on top of a Discontinuous Galerkin Advection solver
- 1D physical, 3D molecular velocities
- BGK model : BGK, S-BGK, ES-BGK, phi-div

# Stationary normal shock wave - Results



# Stationary normal shock wave - Results



## Existing results and opened problems

- Fick matrix gas mixtures : [Brull, Pavan, J.S., 2012]
- ESBGK models for mono and polyatomic gas mixtures : viscosity (and shear viscosity), heat conductivity : [Brull, 2015, 2021]
- Polyatomic reacting gases, discrete energy, Fick matrix [S. Brull, J.S., 2014], [J.S. 2015]
- Fick matrix poly (and mono) gas mixtures : 2 viscosities and Fick matrix (see talk of K. Guillon)

## Existence theorem

- BGK [Perthame 1989], [Perthame-Pulvirenti 1993], ...
- The many results on ESBGK : Yun et al.  $Pb Pr = 2/3$ ?
- Shakhov near global equilibrium (see talk of Gi-Chan Bae)

- Numerical comparisons between the different relaxation models  
Developpement of a code (in progress)
- Relaxation model for multispecies (mono and poly) leading to the full set of transport coefficients (Phenomenological or Onsager matrix)
- Can we construct a single operator based on general Grad's relaxation  $L(\boldsymbol{\rho}) \in \mathcal{R}_m^+$ ?
- Existence theorem of solutions based on relaxation and variational principles.



**THANKS FOR YOUR**  
**ATTENTION!**