Derivation of relaxation operators

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Plan

The Boltzmann equation

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
$nu = \int vf\, dv$	:	momentum (m=1)
$E = \frac{nu^2}{2} + \frac{3}{2}nT = \frac{1}{2}\int v^2\, dv$	:	total energy
$\mathcal{H}(f) = \int (f \ln f - f)\, dv$	:	Boltzmann Entropy

1) $f(t, x, v) \geq 0$. Preservation of the positivity

2) Collision invariants (mass, momentum and energy)

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

3) $\exists \eta$ entropy density and

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

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

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

4) Extended H theorem

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

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

5) Correctness of the hydrodynamic limit

$\Rightarrow$ Right properties on the linearized operator

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

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

$\Rightarrow$ Euler and Navier-Stokes (transport coefficients)

Summary

$f(t,x,v)$: distribution function

$$\underbrace{\frac{\partial f}{\partial t} + v.\nabla_x f}_{transport} + \underbrace{F.\nabla_v f}_{Force \;\; term} = \underbrace{\mathcal{C}(f,f)}_{Collision\;de\;term}$$

n, u et T : density, velocity and temperature

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

Obtention of fluid models

- Equilibrium states : $\mathcal{C}(f,f) = 0 \;\Leftrightarrow f = \mathcal{M}_f + \mathcal{O}(\varepsilon^2)$
- $f = \mathcal{M}_f + \mathcal{O}(\varepsilon)$ + moments extraction w.r.t. $(1, v, v^2) \Rightarrow$ Euler system
- $f = \mathcal{M}_f(1+\varepsilon g) + \mathcal{O}(\varepsilon^2)$ + moments extraction w.r.t. $(1, v, v^2)$ $\Rightarrow$ Navier-Stokes system

Chapman-Enskog expansion

Parameter ε Knudsen number.

When $\varepsilon \to 0$, Boltzmann $\Rightarrow$ fluid model

Rescaled Boltzmann equation

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

Chapman-Enskog expansion

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

Order 0

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

with

$$\mathcal{L}_B(g) = \frac{1}{\mathcal{M}} Q(\mathcal{M}, \mathcal{M}g) + Q(\mathcal{M}g, \mathcal{M})$$

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.
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Computation of g

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

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

$$V = \frac{v - u}{\sqrt{T}}.$$

Inversion of the relation $\Rightarrow g$

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

$$\partial_t \rho + div_x(\rho u) = 0$$
$$\partial_t(\rho\, u) + div_x(\rho\, u \otimes u + \rho T\, Id - \varepsilon \mu \mathbb{D}(u)) = 0$$
$$\partial_t\Big(\rho(\frac{1}{2}|u|^2 + \frac{3}{2}T)\Big) + div_x\Big(\rho(\frac{1}{2}|u|^2 + \frac{5}{2}T) - \varepsilon\kappa\nabla_x T - \varepsilon\mu\mathbb{D}(u)\cdot u\Big) = 0.$$

Transport Coefficients

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

Prandtl number

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

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Boltzmann 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

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

→ High complexity

⇒ Find a simplified operator

$$Q(f,f) \approx \lambda(G - f)$$

Method of moment relaxation

Relaxation operator

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

where $\mathcal{M}$ is defined by

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

$$\mathcal{M} = \mathrm{Argmin}_{g \in C_f} \mathcal{H}(g)$$

where

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

BGK Models

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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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Motivations

Aim Construct relaxation operator

$$R(f) = \nu(G - f) \approx Q(f, f)$$

that is able to reproduce right the **transport coefficients**.

Requirements

- $R(f)$ « behaves as » linear operator
- "good properties" : Positivity, H-theorem, ...

Construction of the model

Linearization of f :

$$f = \mathcal{M}(1+g) \Longrightarrow Q(f,f) \approx \mathcal{M}\mathcal{L}_B(g)$$

$\mathcal{L}_B$: Linearized Boltzmann operator :

$$Q(\mathcal{M}(1+g), \mathcal{M}(1+g)) \;=\; \cancel{Q(\mathcal{M},\mathcal{M})} \;+\; \mathcal{M}\mathcal{L}_B(g) \;+\; \cancel{Q(\mathcal{M}g,\mathcal{M}g)}$$

$\forall \phi$ test function,

$$\int_{\mathbb{R}^3} R(f)\phi dv \approx \int_{\mathbb{R}^3} \mathcal{M}\mathcal{L}_B(g)\phi\, dv = \int_{\mathbb{R}^3} \mathcal{M}g\mathcal{L}_B(\phi)\, dv = \int_{\mathbb{R}^3} f\mathcal{L}_B(\phi)\, dv$$

$$\Rightarrow \int_{\mathbb{R}^3} \nu(G-f)\phi dv = \int_{\mathbb{R}^3} f\mathcal{L}_B(\phi)\, dv$$

Relaxation constraints

Choice of a polynomial space in v : $\mathbb{P} = \mathrm{span}(m_1(v), \ldots, m_N(v))$,
s.t. $\mathbb{K} = \mathrm{span}\{1,\ v,\ v^2\} \subset \mathbb{P}$

$(m_i)_i$ eigenvectors of $\mathcal{L}_B$: $\mathcal{L}_B(m_i) = -\nu_i m_i$

Test function : $\phi = m_i$

$$\int R(f) m_i(v) dv = \int \nu (G - f)\, m_i(v) dv = -\nu_i \int_{\mathbb{R}^3} f\, m_i(v) dv$$

$$\Rightarrow \int G\, m_i(v) dv = (1 - \frac{\nu_i}{\nu}) \int_{\mathbb{R}^3} f\, m_i(v) dv$$

$(-\nu_i)_{i=1,\ldots,N}$ are nonpositive relaxation frequencies (eigenvalues)

First example

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

$$\begin{aligned} \mathbb{K} &= Span\{1,\ v,\ v^2\} \\ \mathbb{A}(v) &= (v-u)\otimes(v-u) - \frac{1}{3}\|v-u\|^2\, I_d \end{aligned}$$

Constraints on G : $\mathcal{C}_f$

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

Conservation laws $\Rightarrow \nu_i = 0$ on $\mathbb{K}$ ($\mathbb{K} \subset \mathbb{P}$)

$\Rightarrow$ Derivation of the ESBGK model [S.B., J. Schneider, 2008] with $\eta(f) = f\ln(f) - f$

Main example

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

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

Constraints : $\mathcal{C}_f$

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

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

How to define ν, $\nu_{\mathbb{A}}$ and ν_b, G ?

Definition of G

Computation of G

$$G = argmin_{g \in C_f} \int_{\mathbb{R}^3} \eta(g)\, dv$$

(C_f set of moments constraints)

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

$$\exists \eta, \quad \int \partial_f \eta\,(f)\, R\,(f)\, d\mathbf{v} \leq 0,$$

$$R\,(f) = 0 \Leftrightarrow \int \partial_f \eta\,(f)\, R(f) d\mathbf{v} = 0 \Leftrightarrow \partial_f \eta\,(f) \in \mathrm{span}\left\{\mathbf{1}, \mathbf{v}, \mathbf{v}^2\right\}.$$

Chapman-Enskog expansion

$\Rightarrow O(\varepsilon)$: Euler and $O(\varepsilon^2)$: Navier-Stokes

Linearized operator/transport coefficients

Linearized operator of the Relaxation operator

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

Transport coefficients for the relaxation operator

$$\begin{aligned}
\mu_R &= -\frac{k_B T}{10}\left\langle \mathcal{L}_R^{-1}(\mathbb{A}), \mathbb{A}\right\rangle = \frac{nk_B T}{\nu_{\mathbb{A}}}, \\
\kappa_R &= -\frac{1}{3k_B T^2}\left\langle \mathcal{L}_R^{-1}(\mathbf{b}), \mathbf{b}\right\rangle = \frac{5}{2}\frac{nk_B^2 T}{m\nu_{\mathbf{b}}}.
\end{aligned}$$

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

Aim : Recover the right viscosity and the heat conductivity

$\mu_R = \mu_{\text{ref}} = \mu_B$ and $\kappa_R = \kappa_{\text{ref}} = \kappa_B$

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

Transport coefficients for Boltzmann

$$\mu_B = -\frac{k_B T}{10} \left\langle \mathcal{L}_B^{-1}(\mathbb{A}), \mathbb{A} \right\rangle, \qquad \kappa_B = -\frac{1}{3 k_B T^2} \left\langle \mathcal{L}_B^{-1}(\mathbf{b}), \mathbf{b} \right\rangle$$

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

$$\mu_R = \mu_B, \quad \kappa_R = \kappa_B \Rightarrow \nu_{\mathbb{A}} = \frac{nT}{\mu_B}, \quad \nu_{\boldsymbol{b}} = \frac{5}{2}\frac{nT}{\kappa_B} \Rightarrow Pr = \frac{5}{2}\frac{\mu}{\kappa} = \frac{\nu_{\boldsymbol{b}}}{\nu_{\mathbb{A}}}$$

Remark : 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

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

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

2. Relaxation frequencies ν, $(\nu_i)_i$ are such that $C_f \neq \emptyset$?

3. Optimization problem : choose η such that
   - Existence of a (unique) minimizer
   - H theorem, positivity ...

Remark

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

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

Artificial condition on $\int g|v|^4 dv$?

The problem might not be well posed ?

See [Junk, 1998, 2000], [J.Schneider, 2004], [Hauck et all, 2008], [Pavan, 2011]

Variational principle

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

$$\mathcal{H}(g) = \int \eta(g)\, dv$$

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

$$(L(\boldsymbol{\rho}_f))_i = (1 - \frac{\nu_i}{\nu}) \int_{\mathbb{R}^3} f\, m_i(v)\, dv$$

Problem

For $\boldsymbol{\rho}_f \in \mathbb{R}^q$ (q= dim (span$\{m_i\}$)), find if possible a function G such that

1. $\int G\mathbf{m}(v)\, dv = L(\boldsymbol{\rho}_f)$
2. $H(G) = \min_{\int g\mathbf{m}(v)\, dv = L(\boldsymbol{\rho}_f)} H(g).$

Shape of the set $\mathcal{R}^+_{\mathbf{m}}$

Realizability

Assume $\mathbf{m}(\mathbf{v}) := (\mathbf{m}_0(\mathbf{v}), \cdots, \mathbf{m}_k(\mathbf{v}), \cdots, \mathbf{m}_n(\mathbf{v}))^T$: be a vector of tensors polynomial in $v \in \mathbb{R}^3$ (pseudo Haar basis)

Realizability problem : $\boldsymbol{\rho} = (\rho_0, \ldots, \rho_n)$ list of tensor.

Is there a function $f \geq 0$ in $L^1(\mathbb{R}^d)$ s.t.

$$\int f\, m_i(v) dv = \rho_i \ \ ?$$

Hamburger, Riesz, Haviland, Curto-Fialkow, Junk, Lasserre, Pichard, ...

Junk's theorem

Theorem (Junk, 2000)

1. $\boldsymbol{\rho} \in \mathcal{R}^{+}_{\mathbf{m}} \backslash \{0\} \Leftrightarrow \forall\, \boldsymbol{\alpha} \neq 0$ *s.t.* $\boldsymbol{\alpha} \cdot \boldsymbol{m}(v) \geq 0$ *a.e. there is* $\boldsymbol{\rho} \cdot \boldsymbol{\alpha} > 0$
2. $\mathcal{R}^{+,*}_{\mathbf{m}}$ *is an open convex set*

Remark

$\mathcal{R}^{+}_{\mathbf{m}} \backslash \{0\}$ *is characterized by the set of (negative) positive polynomials : all* $\boldsymbol{\alpha}$ *such that* $\boldsymbol{\alpha} \cdot \boldsymbol{m}(v) \geq 0$.

Issue : Characterize the set of nonnegative polynomials (tractable way ?)

Examples in kinetic theory

Example

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

Characterizing nonnegative polynomials

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

Exemple : [Lasserre, 2009]

$p(x) = 2x_1^4 + 2x_1^3 x_2 - x_1^2 x_2^2 + 5x_2^4 = \frac{1}{2}(2x_1^2 - 3x_2^2 + x_1 x_2)^2 + \frac{1}{2}(x_2^2 + x_1 x_2)^2$

But $p(x) = x_1^2 x_2^2 (x_1^2 + x_2^2 - 1) + 1$ is nonnegative but not S.O.S.

Quadratic structured space

Example (Levermore space)

The Levermore space can be identified as a product of
$\left(1, \mathbf{v}, \mathbf{v}^2\right) \vee \left(1, \mathbf{v}, \mathbf{v}^2\right) = \left(1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2\mathbf{v},\ \mathbf{v}^4\right)$

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

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

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

What about Grad space ?

$\left(1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2\mathbf{v}\right)$ has no quadratic structure

Hankel matrix

Definition

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

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

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

Necessary condition :
H must be definite positive.

Converse statement ?
True if every positive polynomial is a Sum Of Square (S.O.S.)
$(\boldsymbol{\beta}^T H \boldsymbol{\beta} = \boldsymbol{\alpha} \cdot \boldsymbol{\rho})$

Known results

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

1. $d = 1$: every positive polynomial is a S.O.S
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.

Grad space

Positive polynomials in Grad space $\in \mathrm{span}\,(1, \mathbf{v}, \mathbf{v}\otimes\mathbf{v})$ (Gauss space)

i.e. Every positive polynomial $\boldsymbol{\alpha}\cdot\boldsymbol{m}(v)$ writes as $(\boldsymbol{\beta}, 0)\cdot(1,\ \boldsymbol{v},\ \boldsymbol{v}\otimes\boldsymbol{v},\ \boldsymbol{v}^2\boldsymbol{v})$

In Gauss space, S.O.S $\Leftrightarrow$ Non negative polynomials

Characterization by S.O.S. in the Gauss space and of realizable moment by the Hankel matrix

Proposition

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

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

Relaxation in Grad basis

$\mathrm{span}\left(1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, \mathbf{v}^2\mathbf{v}\right)$ is generated by

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

Moments of f

$$\int_{\mathbb{R}^3} f\,\mathbf{a}\left(\mathbf{v}-\mathbf{u}\right)\,dv = \left(n,\,0,\,0,\,\overline{\mathbb{P}},\,\boldsymbol{q}\right)$$

where $\overline{\mathbb{P}}$: traceless pressure tensor and $\boldsymbol{q}$: heat flux

Proposition

$\left(n,\,0,\,0,\,\lambda_{\mathbb{A}}\,\overline{\mathbb{P}},\,\lambda_{\boldsymbol{b}}\,\boldsymbol{q}\right) \in \mathcal{R}^{+,*}_{Grad}\ \forall\lambda_{\mathbb{A}} \in [-\frac{1}{2}, 1]$ *and* $\forall\lambda_{\boldsymbol{b}} \in \mathbb{R}$

Remark : The heat flux can take any value

Legendre transform

Problem

Legendre dual function $h^* : \mathbb{R}^q \longrightarrow \overline{\mathbb{R}} = \mathbb{R} \bigcup \{+\infty, -\infty\}$ *:*

$$\forall \boldsymbol{\alpha} \in \mathbb{R}^q, \quad h^*(\boldsymbol{\alpha}) = \sup_{\boldsymbol{\rho} \in \mathbb{R}^q} (\boldsymbol{\rho} \cdot \boldsymbol{\alpha} - h(\boldsymbol{\rho})) .$$

Example : $\phi(x) = x \ln(x) - x \Rightarrow \phi^*(y) = \exp(y)$

$$\int_{\mathbb{R}^3} (f \ln f - f)\, dv \Longrightarrow \text{Maxwellian distribution function : } \mathcal{M}$$

Property : If η is convex, $(\eta')^{-1} = \eta^{*\prime}$

Ex : If $\eta(x) = x \ln x - x$, $(\eta')^{-1} = \exp$, $\eta^* = \exp$, $(\eta^*)' = \exp$

Problem

Definition (Entropy, Entropy density)

$$\mathcal{H}(g) = \int \eta(g)dv, \quad h(\boldsymbol{\rho}) = \min_{\int g\mathbf{m}(v)\,dv = \boldsymbol{\rho}} \mathcal{H}(g).$$

Problem

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

- $\mathcal{H}(G) = h(\boldsymbol{\rho})$
- $\int G\,\mathbf{m}(v)\,dv = \boldsymbol{\rho}$
- $G = (\eta')^{-1}(\boldsymbol{\alpha} \cdot \mathbf{m}(v)) = (\eta^*)'(\boldsymbol{\alpha} \cdot \mathbf{m}(v))$ *(analytical form)*
- $G = \mathcal{M}$ *for* $\boldsymbol{\rho} = \int \mathcal{M}\mathbf{m}(v)\,dv$ *(hydrodynamic limit)*

ϕ divergence

ϕ divergence

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

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

$$G = \mathcal{M}(1 + \frac{\boldsymbol{\alpha}\cdot \boldsymbol{m}(v)}{N})_+^N,$$

$(x)_+$ = positive part

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

$\mathcal{H}$ is replaced by

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

Remark : polynomial growth of $(1+\frac{x}{N})^N$ instead of exponential

General result by convex analysis

Theorem

1. $\phi : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ *stricly convex and differentiable of* $\mathbb{R}^+$
2. $\phi(0) = 0$, $\lim_{p \to 0} \dfrac{\phi(p)}{p} \in \mathbb{R}$, ϕ *superlinear*
3. $\forall \boldsymbol{\alpha}$, $\phi^*(\boldsymbol{\alpha} \cdot \mathbf{m}(v)) \in L^1(\mathcal{M}\, dv)$: **Csiszar assumption**

Then

$G = \mathcal{M}(\phi^*)'(\boldsymbol{\alpha} \cdot \mathbf{m}(v))$ *: unique solution to the variational problem :*

$$\mathcal{H}(G) = h(\boldsymbol{\rho}) = \min_{\int g\mathbf{m}(v)\, dv = \boldsymbol{\rho}} \mathcal{H}(g)$$

$\phi_N^*(x) = (1 + \frac{x}{N})_+^N$ satisfies Csiszar assumption

$\phi(x) = x \ln(x) - x$ with $\phi^*(x) = \exp(x)$ does not satisfy Csiszar assumption

Back to the model

In the Grad space

Step 1 : For $f \geq 0$, $f \in L^1_{Grad}$, consider $\boldsymbol{\rho}_f = \int f\, \boldsymbol{a}(v-u)dv$

Step 2 : Relaxation :

$$\nu \geq \nu_{\mathbb{A}}, \nu_{\boldsymbol{b}} \geq 0$$
$$L(\boldsymbol{\rho}_f) = (n, 0, 0, (1 - \frac{\nu_{\mathbb{A}}}{\nu})\overline{\mathbb{P}}, (1 - \frac{\nu_{\mathbf{b}}}{\nu})\boldsymbol{q})$$

$(n,\ 0,\ 0,\ \lambda_{\mathbb{A}}\, \overline{\mathbb{P}},\ \lambda_{\boldsymbol{b}}\, \boldsymbol{q}) \in \mathcal{R}^{+,*}_{Grad}\ \forall \lambda_{\mathbb{A}} \in [-\frac{1}{2}, 1]$ and $\forall \lambda_{\boldsymbol{b}} \in \mathbb{R}$

Step 3 : Solve the variational problem for some ϕ divergence

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

with

$$\int G\, \boldsymbol{a}(v-u)\, dv = L(\boldsymbol{\rho}_f), \quad \text{and} \quad \mathcal{H}(G) = h(L(\boldsymbol{\rho}_f))$$

Properties

Equation

$$\partial_t f + v \cdot \nabla_x f = \nu(G - f)$$

1. Positivity, conservation laws, H-theorem, Galilean invariance
2. Exact hydrodynamic limit if $\nu \geq \nu_{\mathbb{A}},\ \nu_{\boldsymbol{b}}$

$$\nu_{\mathbb{A}} = \frac{nT}{\mu_B}, \quad \nu_{\boldsymbol{b}} = \frac{5}{2}\frac{nT}{\kappa_B}$$

Remark

$\int f \ln f$ is almost a Lyapunov functional for the inhomogeneous equation if $\phi(x) \approx x \ln x$ (ex : $\phi_N(x) = N(x^{1+1/N} - x)$)

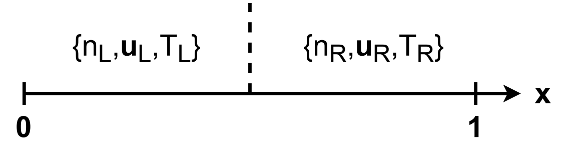
$$\int R(f)\,\phi_N'(f/\mathcal{M})dv \longrightarrow \int R(f)\,\ln(f/\mathcal{M})dv$$

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 : $\{n_R, u_R, T_R\}$

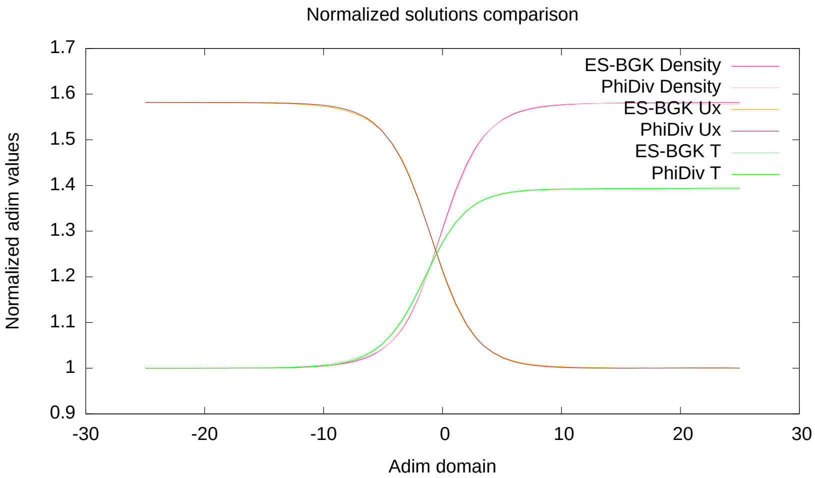
Stationary normal shock wave

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

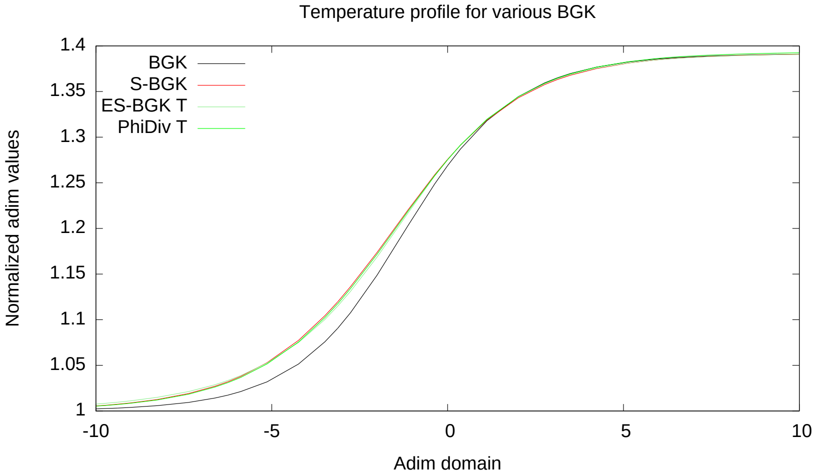
Code characteristics

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

Stationary normal shock wave - Results



Stationary normal shock wave - Results



Existing results

- Fick matrix gas mixtures : [S.B, V. Pavan, J. Schneider., 2012]
- ESBGK models for mono and polyatomic gas mixtures : viscosity (and shear viscosity), heat conductivity : [S.B., J. Schneider, 2008] (mono), [S.B., J. Schneider, 2009] (poly), [S.B., 2015, 2021]
- Polyatomic reacting gases, discrete energy, Fick matrix [S.B., J.Schneider., 2014], [J.Schneider. 2015]
- Fick matrix poly (and mono) gas mixtures : 2 viscosities and Fick matrix [S.B., Guillon, Thieullen, 2024]
- ESBGK model with a general formalism for microscopic energy introduced by [Borsoni, Bisi, Groppi] : [S.B., Pollino, 2025]

Perspectives

- Relaxation model for multispecies (mono and poly) leading to the full set of transport coefficients (Phenomenological or Onsager matrix)

- Numerical method to simulate phi-divergence operators
  Developpement of a code : [S. B., Y. Jobic, V. Pavan, J. Schneider]
  In progress

- BGK model for Enskog.
  [S. B., A. Derro, A. Takahashi]
  In progress

THANKS FOR YOUR ATTENTION !