A numerical scheme for a kinetic model for mixtures in the diffusive limit using the moment method

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LABORATOIRE MAP5

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Université de Paris

Outline of the talk

1. Introduction
   - Context of the study
   - Kinetic setting
   - Moment method
   - Towards an Asymptotic-Preserving scheme?
2. Numerical scheme
   - Description of the scheme
   - Existence of a solution
3. Numerical results
   - Diffusive behavior
   - AP behavior
4. Properties of the scheme
   - Nonnegativity of the concentrations
   - A posteriori validation of the assumptions
5. Conclusion and prospects

Context of the study

- Non-reactive mixture of p monoatomic gases
- Isothermal setting $T > 0$ uniform and constant
- 2 different scales for the description of the mixture
  - mesoscopic scale (kinetic model): species i described by its distribution function $f_i(t, x, v)$
  - macroscopic scale: species i described by the physical observables (concentration $c_i(t, x)$, velocity $u_i(t, x)$)
- Diffusive scaling: diffusion model at the limit

$$\boxed{\text{Boltzmann equations} \rightsquigarrow \text{Maxwell-Stefan equations}}$$

- Study of the link between the two models: formal and theoretical convergence
- Numerical scheme which describes both scales?

Kinetic setting

- Elastic collision rules, for $\sigma \in \mathbb{S}^{d-1}$

$$\begin{cases} v' = (m_i v + m_k v_* + m_k |v - v_*| \sigma)/(m_i + m_k), \\ v'_* = (m_i v + m_k v_* - m_i |v - v_*| \sigma)/(m_i + m_k) \end{cases}$$

- Boltzmann collision operator, for $v \in \mathbb{R}^d$

$$Q_{ik}(f_i, f_k)(v) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \mathcal{B}_{ik}(v, v_*, \sigma) \Big[f_i(v') f_k(v'_*) - f_i(v) f_k(v_*) \Big] \mathrm{d}\sigma \mathrm{d}v_*$$

- Cross sections $\mathcal{B}_{ik} = \mathcal{B}_{ki} > 0$ (Maxwell molecules)
- Boltzmann equations for mixtures

$$\partial_t f_i + v \cdot \nabla_x f_i = \sum_{k=1}^{p} Q_{ik}(f_i, f_k), \qquad \text{on } \mathbb{R}_+ \times \Omega \times \mathbb{R}^d, \qquad 1 \le i \le p$$

Properties of the collision operator & Diffusive scaling

[Desvillettes, Monaco, Salvarani, '05]

- Equilibrium: Maxwellian with same bulk velocity and temperature

$$M_i(t,x,v) = c_i(t,x)\left(\frac{m_i}{2\pi k_B T}\right)^{d/2} \exp\left(-\frac{m_i|v-u(t,x)|^2}{2k_B T}\right)$$

- Conservation properties of the collision operator

$$\int_{\mathbb{R}^d} Q_{ik}(f_i,f_k)(v)\, m_i \,\mathrm{d}v = 0 \text{ and } \int_{\mathbb{R}^d} Q_{ii}(f_i,f_i)(v)\, m_i v \,\mathrm{d}v = 0, \quad 1 \le i,k \le p.$$

Diffusive scaling

Small mean free path and Mach number: $\mathrm{Kn} \sim \mathrm{Ma} \sim \varepsilon$

$$\varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_{k=1}^{p} Q_{ik}(f_i^\varepsilon, f_k^\varepsilon), \qquad 1 \le i \le p$$

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Moment method

Moments of the distribution functions

- Concentration of species i

$$c_i^\varepsilon(t,x) = \int_{\mathbb{R}^d} f_i^\varepsilon(t,x,v)\mathrm{d}v$$

- Flux of species i

$$F_i^\varepsilon(t,x) = c_i^\varepsilon(t,x)\, u_i^\varepsilon(t,x) = \frac{1}{\varepsilon}\int_{\mathbb{R}^d} v\, f_i^\varepsilon(t,x,v)\mathrm{d}v$$

Ansatz

The distribution function of each species i is at a local Maxwellian state with a small velocity of order ε for any $(t,x) \in \mathbb{R}_+ \times \Omega$

$$f_i^\varepsilon(t,x,v) = c_i^\varepsilon(t,x)\left(\frac{m_i}{2\pi k_B T}\right)^{d/2} \exp\left(-\frac{m_i|v-\varepsilon u_i^\varepsilon(t,x)|^2}{2k_B T}\right)$$

Macroscopic diffusion equations

$$\boxed{\varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_k Q_{ik}(f_i^\varepsilon, f_k^\varepsilon), \quad \forall i}$$

- Mass conservation: moment of order 0

$$\varepsilon \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^3} f_i^\varepsilon(v) \, \mathrm{d}v \right) + \nabla_x \cdot \left(\int_{\mathbb{R}^3} v \, f_i^\varepsilon(v) \, \mathrm{d}v \right) = 0,$$

where the collision term vanishes (conservation property).

$$\partial_t c_i^\varepsilon + \nabla_x \cdot F_i^\varepsilon = 0.$$

- Momentum equation: moment of order 1

$$\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^3} v \, f_i^\varepsilon(v) \, \mathrm{d}v + \int_{\mathbb{R}^3} v \, \left(v \cdot \nabla_x f_i^\varepsilon(v) \right) \, \mathrm{d}v = \frac{1}{\varepsilon} \sum_{k \neq i} \int_{\mathbb{R}^3} v \, Q_{ik}(f_i^\varepsilon, f_k^\varepsilon)(v) \, \mathrm{d}v$$

where the mono-species collision term vanishes (conservation property).

Maxwell-Stefan equations

Computing all terms, introducing μ_{ik} the reduced mass

$$\varepsilon^2 m_i \Big(\partial_t(F_i^\varepsilon) + \nabla_x \cdot (F_i^\varepsilon \otimes u_i^\varepsilon)\Big) + k_B T \nabla_x c_i^\varepsilon = \sum_{k \neq i} \mu_{ik} B_{ik} \left(c_i^\varepsilon F_k^\varepsilon - c_k^\varepsilon F_i^\varepsilon\right)$$

- Matrix form of the Maxwell-Stefan equations (limit $\varepsilon \to 0$)

$$k_B T \nabla_x \mathcal{C} = -A(\mathcal{C})\mathcal{F},$$

where $\mathcal{C} = (c_i)_{1 \leq i \leq p}$, $\mathcal{F} = (F_i)_{1 \leq i \leq p}$ and

$$A_{ik} = \begin{cases} -\mu_{ik} B_{ik} c_i, & \text{if } i \neq k, \\ \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} c_\ell, & \text{if } i = k. \end{cases}$$

- Need of a closure relation in the limit $\varepsilon \to 0$, e.g. equimolar diffusion: $\sum_i c_i$ constant (or $\sum_i F_i = 0$)

Towards an Asymptotic-Preserving (AP) scheme?

- Numerical scheme capturing the behavior of both
  - solutions to the Boltzmann equations in a rarefied regime
  - solutions of the Maxwell-Stefan equations in the fluid regime,

  with fixed discretization parameters (independent of ε): AP behavior

  [Filbet, Jin, '10], [Jin, '12], [Jin, Shi, '10], [Jin, Li, '13]

Difficulties

- The collision (and the transport) term in the Boltzmann equation become stiffer when $\varepsilon \to 0$
- The Maxwell-Stefan equations are not invertible (closure relation)

Towards an Asymptotic-Preserving (AP) scheme?

Ideas

1. Following [Jin, Li, '13], penalize the Boltzmann operator with a linear BGK operator (IMEX scheme)

$$\varepsilon \frac{f_i^{\varepsilon,n+1} - f_i^{\varepsilon,n}}{\Delta t} + v \cdot \nabla_x f_i^{\varepsilon,n} = \frac{Q_i^{\varepsilon,n} - P_i^{\varepsilon,n}}{\varepsilon} + \frac{P_i^{\varepsilon,n+1}}{\varepsilon},$$

   BGK operator: $P_i^\varepsilon = \beta_i(M_i - f_i^\varepsilon)$, where M_i is the global Maxwellian with concentration c_i and zero bulk velocity

   Issue: discretization of the transport term $\Rightarrow$ restrictive CFL condition

2. Moment method, in order to mimic the proof of the formal convergence
   - Same ansatz:

$$f_i^\varepsilon(t,x,v) = c_i^\varepsilon(t,x) \left(\frac{m_i}{2\pi k_B T}\right)^{1/2} \exp\left\{-m_i \frac{|v - \varepsilon u_i^\varepsilon(t,x)|^2}{2 k_B T}\right\}$$

   - Computation of the moments

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Description of the scheme

$$\partial_t c_i^\varepsilon + \partial_x F_i^\varepsilon = 0$$

$$\varepsilon^2 m_i \Big(\partial_t F_i^\varepsilon + \partial_x (c_i^\varepsilon (u_i^\varepsilon)^2) \Big) + k_B T \partial_x c_i^\varepsilon = \sum_{k \neq i} \mu_{ik} B_{ik} (c_i^\varepsilon F_k^\varepsilon - c_k^\varepsilon F_i^\varepsilon)$$

- 1D in space (and velocity)
- Dirichlet boundary conditions on the fluxes
- Choice: $c_i^\varepsilon (u_i^\varepsilon)^2 = (F_i^\varepsilon)^2 / c_i^\varepsilon$ for $c_i^\varepsilon \neq 0$
- Implicit treatment of the linear and the Maxwell-Stefan terms (in red)
- $\Delta t, \Delta x > 0$: time and space steps, $\lambda = \Delta t / \Delta x$
- $c_{i,j}^n \approx c_i^\varepsilon (n\Delta t, j\Delta x)$, $F_{i,j+\frac{1}{2}}^n \approx F_i^\varepsilon (n\Delta t, (j+\frac{1}{2})\Delta x)$
- Boundary conditions taken into account via ghost cells: $F_{i,-\frac{1}{2}}^{n+1} = F_{i,N-\frac{1}{2}}^{n+1} = 0$

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Discretization of the equations

$$c_{i,j}^{n+1} + \lambda\left(F_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1}\right) = c_{i,j}^{n}$$

$$\Big(-\Delta t \sum_{k\neq i} \mu_{ik} B_{ik}\, c_{k,j+\frac{1}{2}}^{n+1} - \varepsilon^2 m_i\Big) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t\, c_{i,j+\frac{1}{2}}^{n+1} \sum_{k\neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1}$$
$$= k_B T \lambda\left(c_{i,j+1}^{n+1} - c_{i,j}^{n+1}\right) + \varepsilon^2 m_i\left(\lambda R_{i,j+\frac{1}{2}}^{n} - F_{i,j+\frac{1}{2}}^{n}\right)$$

- Choice of c_i at the center of the cells: $c_{i,j+\frac{1}{2}}^{n+1} := \min\left\{c_{i,j}^{n+1}, c_{i,j+1}^{n+1}\right\}$

Matrix form of the scheme

Vector of unknowns $\mathcal{Y}^n = \begin{pmatrix} \mathcal{C}^n \\ \mathcal{F}^n \end{pmatrix} \in \mathbb{R}^{p(2N+1)}$, where

$$\mathcal{C}^n = \left(c_{1,0}^n, \cdots, c_{1,N}^n, \cdots, c_{p,0}^n, \cdots, c_{p,N}^n\right)^{\mathsf{T}}, \quad \mathcal{F}^n = \left(F_{1,\frac{1}{2}}^n, \cdots, F_{p,N-\frac{1}{2}}^n\right)^{\mathsf{T}}.$$

The system becomes

$$\boxed{\mathbb{S}^{\varepsilon}(\mathcal{C}^{n+1})\,\mathcal{Y}^{n+1} = \mathrm{b}^n}$$

Existence of a solution

$$\mathbb{S}^{\varepsilon}(\mathcal{C}^{n+1})\,\mathcal{Y}^{n+1} = \mathrm{b}^{n}, \text{ where } \mathbb{S}^{\varepsilon}(\mathcal{C}^{n+1}) = \begin{bmatrix} \mathbb{I} & \mathbb{S}_{12} \\ \mathbb{S}_{21} & \mathbb{S}^{\varepsilon}_{22}(\mathcal{C}^{n+1}) \end{bmatrix}$$

The matrix form of the system is solved numerically by a Newton method.

By a fixed-point argument, we can prove the existence of a solution $\mathcal{Y}^{n+1}$ to this matrix form of the system.

- Auxiliary system: replace the concentrations $\mathcal{C}^{n+1}$ by their positive parts $\tilde{\mathcal{C}}^{n+1}$
- $\mathbb{S}^{\varepsilon}(\tilde{\mathcal{C}}^{n+1})$ is invertible
- Write $\tilde{\mathcal{C}}^{n+1} = f(\tilde{\mathcal{C}}^{n+1})$, with f continuous and compact
- Bound on any ξf, for $\xi \in [0,1]$, by using a L^1-estimate: $\|\tilde{\mathcal{C}}^{n+1}\|_{L^1} \leq \|\tilde{\mathcal{C}}^{n}\|_{L^1}$
- Schaefer's fixed-point theorem: existence of $\tilde{\mathcal{C}}^{n+1}$, and thus of $\mathcal{F}^{n+1} = g(\tilde{\mathcal{C}}^{n+1})$.
- By nonnegativity, a solution to the auxiliary system is also solution of the initial system.

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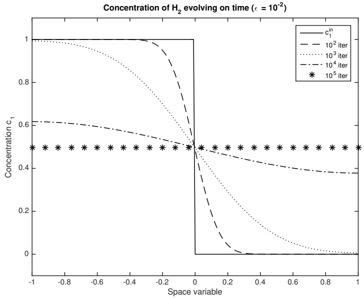
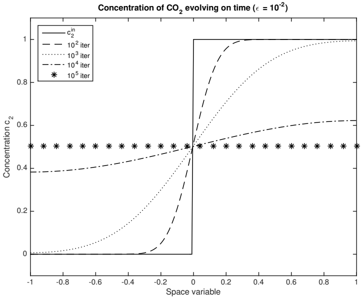
Parameters of the scheme and diffusion of two species

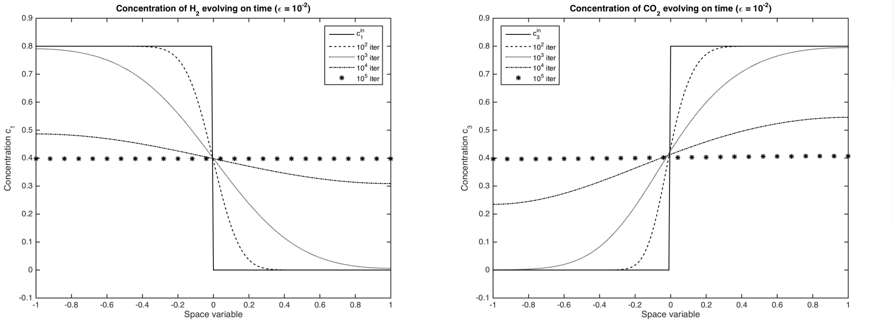
- 3 species: H_2, N_2 and CO_2
- Molar masses $M_1 = 2$, $M_2 = 28$ and $M_3 = 44\,\mathrm{g} \cdot \mathrm{mol}^{-1}$
- B_{ij} computed from the binary diffusive coefficients: $B_{ij} = \frac{(m_i + m_j) k_B T}{4\pi m_i m_j D_{ij}}$
- Rescaling of the cross sections by a factor 10^5
- $\Omega = [-1, 1]$, $\Delta t = \Delta x^2 = 10^{-4}$
- Diffusion of two species
  - Diffusion of H_2 and CO_2 for $\varepsilon = 10^{-2}$
  - Plots of the concentrations for $t = 0, 10^{-2}, 10^{-1}, 1, 10$





Cross-diffusion for mixtures

- 3 species test case, classical diffusion H_2 and CO_2
- N_2, although being at equilibrium, moves (uphill diffusion)
- Diffusion barrier: classical diffusion takes over



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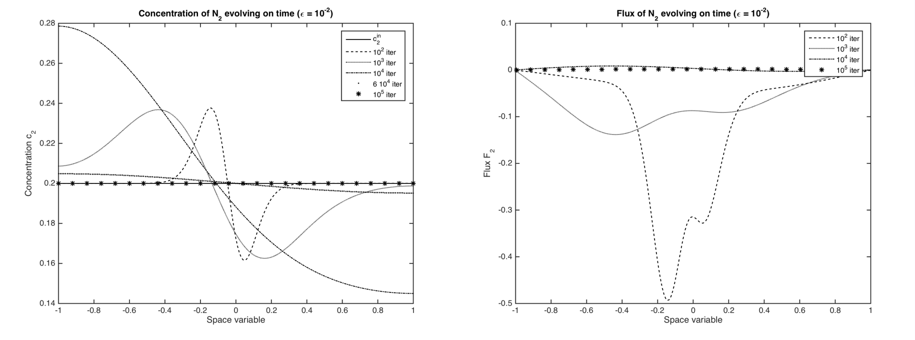
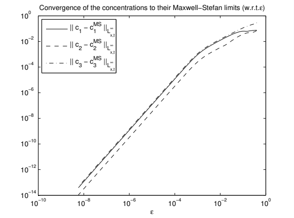
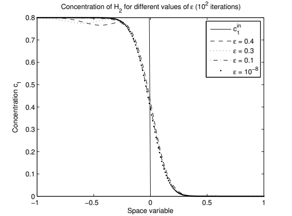


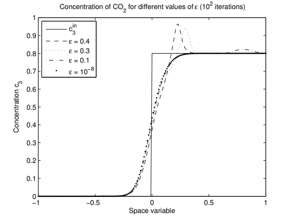
AP behavior

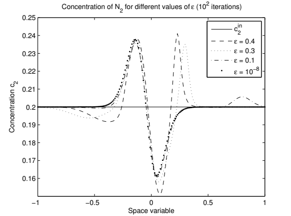
- Fixed discretization parameters for arbitrary small values of ε
- Convergence of the concentrations to the solutions of Maxwell-Stefan



- Influence of the value of ε on the diffusion process (plot at $t = 10^{-2}$)







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Nonnegativity of the concentrations I

$$c_{i,j}^{n+1} + \lambda(F_{i,j+\frac{1}{2}}^{n+1} - F_{i,j-\frac{1}{2}}^{n+1}) = c_{i,j}^{n}$$

$$\Big(- \Delta t \sum_{k \neq i} \mu_{ik} B_{ik} c_{k,j+\frac{1}{2}}^{n+1} - \varepsilon^2 m_i \Big) F_{i,j+\frac{1}{2}}^{n+1} + \Delta t \, c_{i,j+\frac{1}{2}}^{n+1} \sum_{k \neq i} \mu_{ik} B_{ik} F_{k,j+\frac{1}{2}}^{n+1}$$
$$= k_B T \lambda (c_{i,j+1}^{n+1} - c_{i,j}^{n+1}) + \varepsilon^2 m_i (\lambda R_{i,j+\frac{1}{2}}^{n} - F_{i,j+\frac{1}{2}}^{n})$$

Vectorial form of the equations, with $\mathcal{S}$ the source term

$$\partial_t \mathcal{C} = \partial_x \mathcal{F}$$
$$\mathcal{A}\mathcal{F} = \partial_x \mathcal{C} + \varepsilon^2 \mathcal{S}$$

Nonnegativity of the concentrations II

$$\partial_t \mathcal{C} = \partial_x \mathcal{F}$$
$$\mathcal{A}\mathcal{F} = \partial_x \mathcal{C} + \varepsilon^2 \mathcal{S}$$

- Auxiliary equations: replace $\mathcal{C}$ by $\mathcal{C}^+$ in $\mathcal{A} \rightsquigarrow \tilde{\mathcal{A}}$ (invertible)
- Use the momentum equation in the mass equation
- Multiply by $\mathcal{C}^-$, integration by parts [Anaya, Bendahmane, Sepúlveda, '15]
- Nondiagonal terms of $\tilde{\mathcal{A}}^{-1}$ contain $\mathcal{C}^+_{j+1/2}$:

$$\min(\mathcal{C}_j^+, \mathcal{C}_{j+1}^+)(\mathcal{C}_{j+1}^- - \mathcal{C}_j^-) = 0.$$

- Diagonal terms of $\tilde{\mathcal{A}}^{-1}$ are nonnegative
  - We have $< \partial_x \mathcal{C}, \partial_x \mathcal{C}^- > \leq 0$,
  - and for ε small enough, the $\mathcal{S}$-term is controlled by the previous one.
- Thus $< \partial_t \mathcal{C}, \mathcal{C}^- > \leq 0$: $\mathcal{C}$ is nonnegative.

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Nonnegativity of the concentrations II

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- Auxiliary equations: replace $\mathcal{C}$ by $\mathcal{C}^+$ in $\mathcal{A} \rightsquigarrow \tilde{\mathcal{A}}$ (invertible)
- Use the momentum equation in the mass equation
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Nonnegativity of the concentrations II

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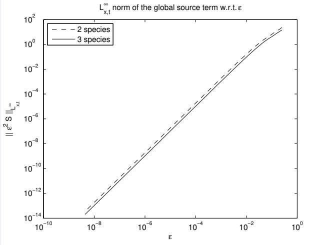
A posteriori validation of the assumptions

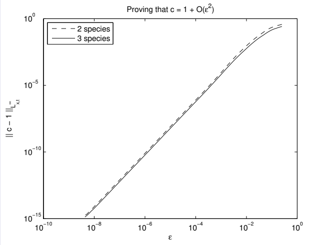
Smallness of the source terms $\varepsilon^2\mathcal{S}$

- Numerically, uniform boundedness w. r. t. ε



Closure relation for Maxwell-Stefan

- Numerically, $\sum_{i=1}^{p} c_i = 1 + O(\varepsilon^2)$



Outline of the talk

1 Introduction
- Context of the study
- Kinetic setting
- Moment method
- Towards an Asymptotic-Preserving scheme?

2 Numerical scheme
- Description of the scheme
- Existence of a solution

3 Numerical results
- Diffusive behavior
- AP behavior

4 Properties of the scheme
- Nonnegativity of the concentrations
- A posteriori validation of the assumptions

5 Conclusion and prospects

Conclusion and prospects

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Conclusions

- Suitable numerical scheme able to capture the Maxwell-Stefan diffusion asymptotic of Boltzmann equation for mixtures, via the moment method
- A priori nonnegativity of the concentrations, existence of a solution to the scheme
- A posteriori validation of the assumptions (closure relation, smallness assumption)

Prospects

- Higher space and velocity dimensions
- L^2 a priori estimates
- AP-property
- Uniqueness of the scheme

Thank you for your attention!

Computations of the different terms

- Divergence term: use of the Ansatz, translation in v + parity argument

$$\nabla \cdot \left(\int v \otimes v \, f_i^\varepsilon(v) \, \mathrm{d}v \right) \propto \nabla \cdot \left(c_i^\varepsilon \int \left(v \otimes v + \varepsilon^2 u_i{}^\varepsilon \otimes u_i^\varepsilon \right) e^{-m_i |v|^2 / 2kT} \mathrm{d}v \right)$$

$$= \frac{kT}{m_i} \nabla c_i^\varepsilon + \varepsilon^2 \nabla \cdot \left(c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon \right)$$

- Collision term: explicit computations or algebraic arguments [Boudin, G., Salvarani, '15], [Hutridurga, Salvarani, '17], [Boudin, G., Pavan, '17]
- For Maxwell molecules: weak form, collision rules, symmetry and parity arguments:

$$\int v Q_{ik}(f_i^\varepsilon, f_k^\varepsilon)(v) \, \mathrm{d}v = \frac{m_k}{m_i + m_k} \int b_{ik}(\cos\theta) \, f_i^\varepsilon f_{k*}^\varepsilon \left(v_* - v + |v - v_*| \sigma \right) \mathrm{d}\sigma \, \mathrm{d}v_* \, \mathrm{d}v$$

In terms of macroscopic quantities

$$\frac{1}{\varepsilon} \sum_{k \neq i} \int v \, Q_{ik}(f_i^\varepsilon, f_k^\varepsilon)(v) \, \mathrm{d}v = \sum_{k \neq i} \underbrace{\frac{2\pi m_k \|b_{ij}\|_{L^1}}{m_i + m_k}}_{D_{ij}^{-1}} \left(c_i^\varepsilon c_k^\varepsilon u_k{}^\varepsilon - c_k^\varepsilon c_i^\varepsilon u_i{}^\varepsilon \right)$$

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