Derivation of cross-diffusion models from the multi-species Boltzmann equation in the diffusive scaling

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Context of the study

- Non-reactive mixture of p monoatomic gases
- Isothermal setting $T > 0$ uniform and constant
- Two 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
    - number density $n_i(t, x)$
    - velocity $u_i(t, x)$

  $\rightsquigarrow$ flux of species i : $J_i(t, x) = n_i(t, x)u_i(t, x)$

  $\rightsquigarrow$ vectorial quantities $\mathbf{n} = \begin{bmatrix} n_1 \\ \vdots \\ n_p \end{bmatrix}, \mathbf{J} = \begin{bmatrix} J_1 \\ \vdots \\ J_p \end{bmatrix}$
- Link between the two scales in the diffusive scaling
  - Formal and theoretical convergence
  - Numerical scheme describing both scales

Diffusion models for mixtures: Maxwell-Stefan/Fick

Mass conservation:

$$\partial_t \mathbf{n} + \nabla \cdot \mathbf{J} = 0$$

Diffusion process (link between $\mathbf{J}$ and $\nabla \mathbf{n}$):

Maxwell-Stefan equations

$$\boxed{-\nabla \mathbf{n} = A(\mathbf{n})\mathbf{J}}$$

Fick equations

$$\boxed{\mathbf{J} = -B(\mathbf{n})\nabla \mathbf{n}}$$

- $A(\mathbf{n})$ and $B(\mathbf{n})$ are not invertible (rank $p-1$)
- Using Moore-Penrose pseudo-inverse: structural similarity [Giovangigli '91, '99]

Formal analogy of the two systems,
but Fick and Maxwell-Stefan are not obtained in the same way

Maxwell-Stefan vs. Fick (macroscopic point of view)

Obtention of the Maxwell-Stefan equations

- Mechanical considerations on forces (balance of pressure and friction forces)
- Assumption: different species have different macroscopic velocities on macroscopic time scales

Obtention of the Fick equations

- Thermodynamics of irreversible processes (entropy decay) [Onsager]
- Thermodynamical considerations on fluxes, written (close to equilibrium) as linear combinations of potential gradients
  - nonreactive isothermal setting $\rightsquigarrow$ chemical potential gradients
  - ideal gases $\rightsquigarrow$ (number) density gradients

Mesoscopic point of view

- How to justify these two (different) equations from the (same) kinetic description?
- In which regime are these macroscopic models valid?

Moment method (Maxwell-Stefan)

- Based on the ansatz that the distribution functions are at local Maxwellian states [Levermore], [Müller, Ruggieri]

Perturbative method (Fick)

- Based on the Chapman-Enskog expansion [Bardos, Golse, Levermore], [Bisi, Desvillettes]

Kinetic setting

- Boltzmann equations for mixtures on $\mathbb{R}_+ \times \Omega \times \mathbb{R}^d$

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

[Desvillettes, Monaco, Salvarani, '05]

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

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

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

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

- Cross sections $\mathcal{B}_{ik} = \mathcal{B}_{ki} > 0$

Properties of the collision operator

- Equilibrium: Maxwellian with same bulk velocity and temperature

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

- Conservation properties of the collision operator for $1 \leq i, k \leq p$

$$\int_{\mathbb{R}^d} Q_{ik}(f_i,f_k)(v)\,\mathrm{d}v = 0$$

$$\int_{\mathbb{R}^d} Q_{ii}(f_i,f_i)(v)v\,\mathrm{d}v = 0$$

$$\int_{\mathbb{R}^d}\Big(m_i Q_{ik}(f_i,f_k)(v) + m_k Q_{ki}(f_k,f_i)(v)\Big)v\,\mathrm{d}v = 0$$

- Weak form:

$$\int Q_{ik}(f_i,f_k)(v)\,\psi(v)dv = \iiint \mathcal{B}_{ik}\, f_i(v)\, f_k(v_*)\,\left[\psi(v') - \psi(v)\right]\, d\sigma\, dv_*\, dv$$

Outline of the talk

Moment method

Diffusive scaling: small mean free path and Mach number: Kn $\sim$ Ma $\sim \varepsilon$

Moments of the distribution functions

- Number density of species i

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

- Flux of species i

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

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

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

Macroscopic diffusion equations

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

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

- **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).

Formal limit

$$n_i(t,x) = \lim_{\varepsilon \to 0} n_i^\varepsilon(t,x), \qquad J_i(t,x) = \lim_{\varepsilon \to 0} n_i^\varepsilon(t,x) u_i^\varepsilon(t,x)$$

$$\rightsquigarrow \boxed{\partial_t n_i + \nabla_x \cdot J_i = 0}$$

Computation of the divergence term

- Momentum equation: moment of order 1

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

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

- Use of the Ansatz, translation in v

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

- In terms of macroscopic quantities

$$\nabla_x \cdot \left(\int v \otimes v\, f_i^\varepsilon(v)\,\mathrm{d}v \right) = \frac{k_B T}{m_i} \nabla_x n_i^\varepsilon + \varepsilon^2 \nabla_x \cdot \left(n_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon \right)$$

Computation of the divergence term

- Momentum equation: moment of order 1

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

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

- Use of the Ansatz, translation in v + parity argument

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

- In terms of macroscopic quantities

$$\nabla_x \cdot \left(\int v \otimes v\, f_i^\varepsilon(v)\,\mathrm{d}v \right) = \frac{k_B T}{m_i} \nabla_x n_i^\varepsilon + \varepsilon^2 \nabla_x \cdot \left(n_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon \right)$$

Computation of the collision term

For Maxwell molecules : $\mathcal{B}_{ik}(v, v_*, \sigma) = b_{ik}(\theta)$

- Weak form with $\psi(v) = v$ + collision rules

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

- Symmetry and parity arguments: cancellation of the term in blue
- In terms of macroscopic quantities

$$\frac{1}{\varepsilon}\sum_{k\neq i}\int v\, Q_{ik}(f_i^\varepsilon, f_k^\varepsilon)(v)\,\mathrm{d}v = \sum_{k\neq i} \underbrace{\frac{2\pi m_i m_k \|b_{ik}\|_{L^1}}{(m_i + m_k) k_B T}}_{D_{ik}^{-1}} \frac{k_B T}{m_i}\left(n_i^\varepsilon J_k^\varepsilon - n_k^\varepsilon J_i^\varepsilon\right)$$

$$\varepsilon^2 \frac{m_i}{k_B T}\left(\partial_t (n_i^\varepsilon u_i^\varepsilon) + \nabla_x \cdot (n_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon)\right) + \nabla_x n_i^\varepsilon = \sum_{k\neq i} \frac{n_i^\varepsilon J_k^\varepsilon - n_k^\varepsilon J_i^\varepsilon}{D_{ik}}$$

$$\rightsquigarrow \boxed{-\nabla_x n_i = \sum_{k\neq i} \frac{n_k J_i - n_i J_k}{D_{ik}}}$$

Asymptotic-Preserving numerical scheme

- Capture the behavior of the solutions to both
  - the Boltzmann equations in a rarefied regime
  - 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 are stiff when $\varepsilon \to 0$

$$\varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_k Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)$$

- At the limit, the Maxwell-Stefan equations are not invertible

$$\begin{cases} \partial_t n_i^\varepsilon + \nabla_x \cdot J_i^\varepsilon = 0 \\ \varepsilon^2 m_i \Big(\partial_t (n_i^\varepsilon u_i^\varepsilon) + \nabla_x \cdot (n_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon) \Big) + k_B T \nabla_x n_i^\varepsilon = \sum_{k \neq i} \mu_{ik} (n_i^\varepsilon J_k^\varepsilon - n_k^\varepsilon J_i^\varepsilon) \end{cases}$$

Towards an Asymptotic-Preserving (AP) scheme?

Ideas

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

$$\frac{f_i^{\varepsilon,n+1} - f_i^{\varepsilon,n}}{\Delta t} + \frac{1}{\varepsilon} v \cdot \nabla_x f_i^{\varepsilon,n} = \frac{Q_i^{\varepsilon,n} - P_i^{\varepsilon,n}}{\varepsilon^2} + \frac{P_i^{\varepsilon,n+1}}{\varepsilon^2},$$

   BGK operator: $P_i^\varepsilon = \beta_i(M_i - f_i^\varepsilon)$, where M_i is the global Maxwellian

   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:

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

   - Computation of the moments

Description of the 1D scheme

$$\partial_t n_i^\varepsilon + \partial_x J_i^\varepsilon = 0$$

$$\varepsilon^2 m_i \Big(\partial_t J_i^\varepsilon + \partial_x \Big(\frac{(J_i^\varepsilon)^2}{n_i^\varepsilon} \Big) \Big) + k_B T \partial_x n_i^\varepsilon = \sum_{k \neq i} \mu_{ik} (n_i^\varepsilon J_k^\varepsilon - n_k^\varepsilon J_i^\varepsilon)$$

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

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Discretization of the equations

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

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

- Choice of n_i at the center of the cells: $n_{i,j+\frac{1}{2}}^{n+1} := \min\left\{n_{i,j}^{n+1}, n_{i,j+1}^{n+1}\right\}$
[Anaya, Bendahmane, Sepúlveda, '15]

Matrix form of the scheme

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

$$\mathcal{N}^n = (n_{1,0}^n, \cdots, n_{1,N}^n, \cdots, n_{p,0}^n, \cdots, n_{p,N}^n)^\intercal, \quad \mathcal{J}^n = \left(J_{1,\frac{1}{2}}^n, \cdots, J_{p,N-\frac{1}{2}}^n\right)^\intercal.$$

The system becomes

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

Existence of a solution

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

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

Fixed-point argument: existence of a solution $\mathcal{Y}^{n+1}$ to the system

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

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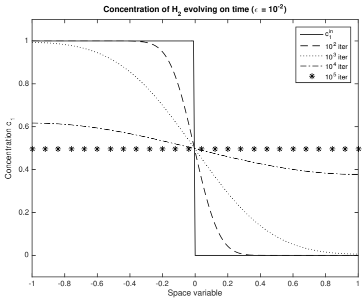
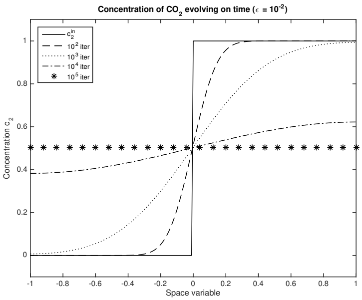
Parameters of the scheme and diffusion of two species

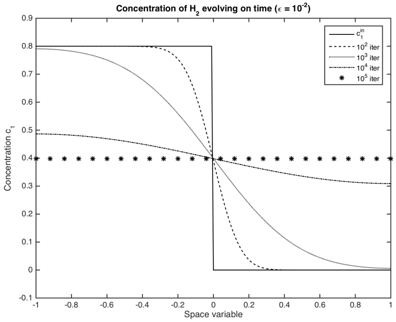
- 3 species: H_2, N_2 and CO_2, molar masses $M_1 = 2$, $M_2 = 28$ and $M_3 = 44\,\text{g} \cdot \text{mol}^{-1}$
- B_{ij} computed from the binary diffusive coefficients: $B_{ij} = \frac{(m_i+m_j)k_B T}{4\pi m_i m_j D_{ij}}$, rescaled by a factor 10^5
- $\Omega = [-1, 1]$, $\Delta t = \Delta x^2 = 10^{-4}$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

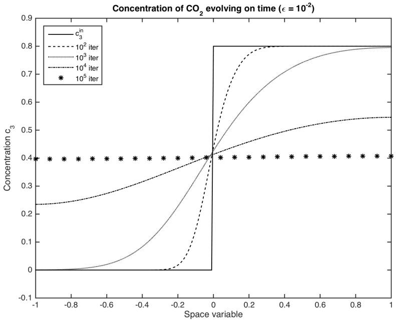




Cross-diffusion for mixtures

- 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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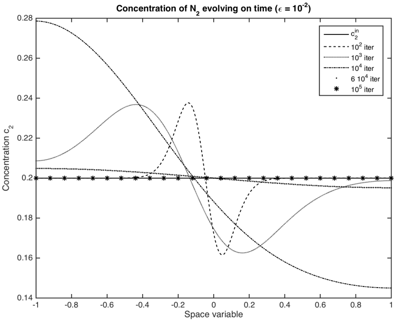
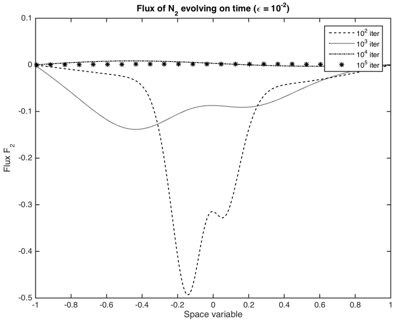
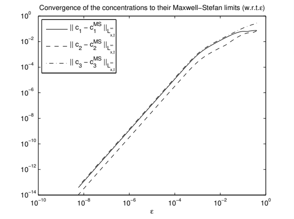


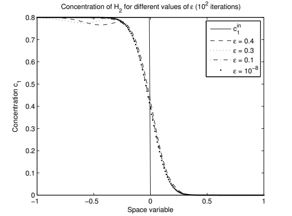


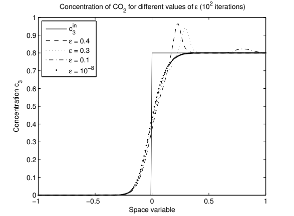
AP behavior

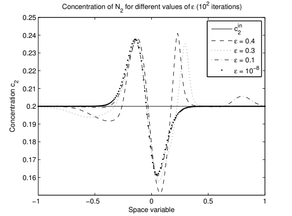
- Fixed discretization parameters for arbitrary small values of ε
- Convergence of the number densities to the solutions of Maxwell-Stefan



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







Outline of the talk

Perturbative method

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

- Expansion around the global Maxwellian with zero bulk velocity (equilibrium) with number density n_i

$$f_i^\varepsilon = n_i\mu_i + \varepsilon g_i^\varepsilon$$

$$\mu_i = (m_i/2\pi k_B T)^{d/2} e^{-m_i|v|^2/2k_B T}$$

- Moments

$$J_i(t,x) = \frac{1}{\varepsilon}\int v\, f_i^\varepsilon(t,x,v)\mathrm{d}v = \int v\, g_i^\varepsilon(t,x,v)\mathrm{d}v$$

- Mass conservation, order ε: $\partial_t n_i + \nabla_x \cdot J_i = 0$
- Inject expansion in the Boltzmann equation, order ε^0

$$\mu_i v \cdot \nabla_x n_i = \sum_k Q_{ik}(n_i\mu_i, g_k^\varepsilon) + Q_{ki}(g_i^\varepsilon, n_k\mu_k) =: \mathcal{L}_i(\mathbf{g}^\varepsilon),$$

where $\mathbf{g}^\varepsilon = (g_i^\varepsilon)_i \rightsquigarrow$ defines the linearized Boltzmann operator $\mathbf{L} = (\mathcal{L}_i)_i$

- In a vectorial form, defining $W_i = \mu_i v \cdot \nabla_x n_i$ and $\mathbf{W} = (W_i)_i$

$$\mathbf{W} = \mathbf{L}(\mathbf{g}^\varepsilon) \quad \underset{(\star)}{\rightsquigarrow} \quad \mathbf{g}^\varepsilon = \mathbf{L}^{-1}\mathbf{W}$$

- Inject this expression for g_i^ε in the definition of J_i

$$J_i = \int v[\mathbf{L}^{-1}\mathbf{W}]_i \mathrm{d}v = \int n_i\mu_i v[\mathbf{L}^{-1}\mathbf{W}]_i (n_i\mu_i)^{-1} \mathrm{d}v$$

- With $\mathbf{C}_i = (\mu_k v \delta_{ik})_k$, we get

$$J_i = n_i \langle \mathbf{C}, \mathbf{L}^{-1}\mathbf{W} \rangle_{L^2((n\mu)^{-1/2})}$$

- $\mathbf{L}^{-1}$ is self-adjoint on $(\mathrm{Ker}\,\mathbf{L})^\perp$. Let $\mathbf{\Gamma}$ be the projection of $\mathbf{C}$ on $\mathrm{Ker}\,\mathbf{L}$. Thus

$$J_i = n_i \sum_k \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_k, W_k \rangle_{L^2((n\mu)^{-1/2})}$$

- Since $W_j = \mu_j v \cdot \nabla_x n_j =$ "$\mathbf{C}_j \cdot \nabla_x n_j$"

$$J_i = \sum_k \underbrace{n_i \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_k, \mathbf{C}_k \rangle_{L^2((n\mu)^{-1/2})}}_{b_{ik}(n_i)} \nabla_x n_k$$

$\rightsquigarrow$ Fick equation: $\mathbf{J} = -B(\mathbf{n})\nabla_x \mathbf{n}$

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$\rightsquigarrow$ Fick equation: $\mathbf{J} = -B(\mathbf{n})\nabla_x \mathbf{n}$

Outline of the talk

Stiff dissipative model for mixtures

For any species i with density n_i and velocity $\boldsymbol{u}_i$, we write mass and momentum conservation

$$(*)\begin{cases}\partial_t n_i + \nabla_{\boldsymbol{x}} \cdot (n_i \boldsymbol{u}_i) = 0,\\ \partial_t (n_i \boldsymbol{u}_i) + \nabla_{\boldsymbol{x}} \cdot (n_i \boldsymbol{u}_i \otimes \boldsymbol{u}_i) + \nabla_{\boldsymbol{x}} n_i + \dfrac{1}{\varepsilon} R_i = 0\end{cases}$$

- Ideal gas law for the partial pressure $P_i(n_i) \propto n_i$
- Relaxation term of Maxwell-Stefan's type: friction force exerted by the mixture on species i

$$R_i = \sum_{k \neq i} a_{ik} n_i n_k (\boldsymbol{u}_k - \boldsymbol{u}_i)$$

Using the formalism of Chen, Levermore, Liu, CPAM, '94

Obtain a reduced system when ε remains small

- Derive an approximation of the local equilibrium and its first-order correction
  - Build a relevant entropy which ensures...
  - ... the hyperbolicity of the local equilibrium approximation...
  - ... and the dissipativity of its first-order correction

Maxwell-Stefan vs. Fick

Reduced system involving the bulk velocity $\boldsymbol{u}$ for small ε

Let $n = \sum_i n_i$, and $\boldsymbol{u}$ the mass-weighted averaged (aligned) velocity.

System $(*)$ formally reduces to

$$\begin{cases} \partial_t n_i + \nabla_{\boldsymbol{x}} \cdot \left(n_i \boldsymbol{u} - \varepsilon \sum_{k=1}^{p} \beta_{ik} \frac{\nabla_{\boldsymbol{x}} n_k}{n_k} \right) = 0, \\ \partial_t (n\boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (n\boldsymbol{u} \otimes \boldsymbol{u}) + \nabla_{\boldsymbol{x}} P = \boldsymbol{0}. \end{cases}$$

where $P = \sum_i P_i(n_i)$ is the total pressure, and (β_{ik}) are positive constants.

- Diffusion correction term of Fick's type (on the mass equation)
  - Fick equations model mass diffusion in a continuous regime
- No viscosity term on the momentum equation (convective $\gg$ diffusive fluxes)
- Maxwell-Stefan equations needed in a moderately rarefied regime

Conclusion and prospects

Conclusions

- Formal derivation of Maxwell-Stefan and Fick equations from the Boltzmann equation for mixtures in the diffusive regime
- Numerical scheme able to capture the Maxwell-Stefan diffusion asymptotic of Boltzmann equation for mixtures, via the moment method

Prospects

- AP property, higher space and velocity dimensions
- AP scheme for the full distribution function (without the ansatz)
- AP scheme for the Fick equations
- Numerical simulations for the stiff dissipative model
- Non isothermal setting

Thank you for your attention!

Nonnegativity of the concentrations I

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

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

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

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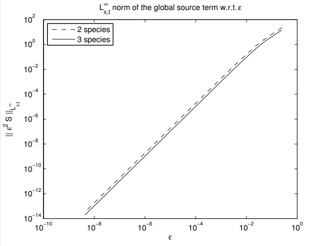
$$\min(\mathcal{C}_j^+, \mathcal{C}_{j+1}^+)(\mathcal{C}_{j+1}^- - \mathcal{C}_j^-) = 0.$$

- 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.

A posteriori validation of the assumptions

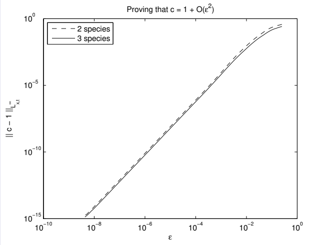
Smallness of the source terms $\varepsilon^2 \mathcal{S}$

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



Closure relation for Maxwell-Stefan

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



Closure relation (1)

Maxwell-Stefan equation $-\nabla \mathbf{n} = A(\mathbf{n})\mathbf{J}$

- Summing over i the equations (A has rank $p-1$) implies that $\nabla_x \sum_i n_i = 0$
- Ansatz (local Maxwellian) implies

$$\int m_i |v|^2 f_i^\varepsilon \mathrm{d}v = 3k_B T n_i^\varepsilon + o(\varepsilon), \qquad \int m_i |v|^2 v f_i^\varepsilon \mathrm{d}v = 5\varepsilon k_B T J_i^\varepsilon + o(\varepsilon).$$

- Moment of order 2 (order ε^1), summing over i, and taking the limit $\varepsilon \to 0$

$$3\partial_t \sum_i n_i + 5\nabla_x \cdot \sum_i J_i = 0,$$

where the collision operator disappears by symmetry when summing over i.

- Combining with mass conservation implies

$$\partial_t \sum_i n_i = \nabla_x \cdot \sum_i J_i = 0$$

- Constant total number of molecules $\sum_i n_i$
- Compatible with equimolar diffusion $\sum_i J_i(t,x) = 0$

Closure relation (2)

Fick equation $\mathbf{J} = -B(\mathbf{n})\nabla\mathbf{n}$

- Summing over i the equations (B has rank $p-1$) implies that $\sum_i m_i J_i = 0$
- Inversion giving the perturbation $\mathbf{g}^\varepsilon$ (relation $(\star)$) only valid if the RHS $W_i = \mu_i v \cdot \nabla_x n_i \in (\mathrm{Ker}\,\mathbf{L})^\perp$.
- $\mathrm{Ker}\,\mathbf{L}$ spanned by $(\sqrt{n_i}\mu_i \mathbf{e}_i)_i$, $m_i n_i \mu_i v$, $m_i n_i \mu_i |v|^2$
- Orthogonality

$$0 = \sum_i \int \mu_i v \cdot \nabla_x n_i \, m_i v \mathrm{d}v = \nabla_x \sum_i m_i n_i$$

- Mass conservation for each species implies (when summing with weights m_i)

$$0 = \frac{\mathrm{d}}{\mathrm{dt}} \int \sum_i m_i n_i \mathrm{d}x$$

- Constant mass $\sum_i m_i n_i$

Steps of the computations

- Internal energy $E_i''(\rho_i) = P_i'(\rho_i)/\rho_i$
- (Strictly convex) entropy $\eta = \sum_{j=1}^{p} \frac{1}{2}\rho_j \boldsymbol{u}_j^2 + E_j(\rho_j)$
- $(p+d)$ independent conserved quantities : $\left[\rho_1, \cdots, \rho_p, \sum_{j=1}^{p} \rho_j \boldsymbol{u}_j\right]$
- Equilibrium: $[\rho_1, \cdots, \rho_p, \rho_1 \boldsymbol{u}, \cdots, \rho_p \boldsymbol{u}]$ for some $\boldsymbol{u}$

Formal expansion around the equilibrium & linearization

$\rightsquigarrow$ expression of the correction provided (pseudo-)inversion of "the gradient of the relaxation term", involving the "flux terms"

$$\sum_{j=1}^{p} \alpha_{ij} \frac{X_j}{\rho_j} = \nabla_x P_i(\rho_i) - \frac{\rho_i}{\rho} \nabla_x P$$

with $\rho = \sum_i \rho_i$, $P = \sum_i P_i$

$\rightsquigarrow$ equation on the conserved quantities with the correction term

Steps of the computations

- Internal energy $E_i''(\rho_i) = P_i'(\rho_i)/\rho_i$
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Formal expansion around the equilibrium & linearization

⇝ expression of the correction provided (pseudo-)inversion of "the gradient of the relaxation term", involving the "flux terms"

$$X_i = \sum_{j=1}^{p} \frac{\beta_{ij}}{\rho_j}\left(\nabla_x P_j(\rho_j) - \frac{\rho_j}{\rho}\nabla_x P\right)$$

with $\rho = \sum_i \rho_i$, $P = \sum_i P_i$

⇝ equation on the conserved quantities with the correction term

Justification of the Ansatz for the Maxwell-Stefan equations

In a moderately rarefied regime (not so dominant collision process)

- Significant deviation from local equilibrium described by the moment method
- Moment method: approach to compute Galerkin solutions to the Boltzmann equation

[Levermore, JSP '96]

1. First finite dimensional subspace $\mathbb{M}_0 = \mathrm{Ker}\, Q$ spanned by $e_1, \cdots, e_p$, $[m_1 v, \cdots, m_p v]$ and $[m_1 v^2, \cdots, m_p v^2]$

$\rightsquigarrow$ equilibrium with one bulk velocity

2. Second finite dimensional subspace $\mathbb{M}_1 \supset \mathbb{M}_0$ spanned by $e_1, \cdots, e_p$, $m_1 v e_1, \cdots, m_p v e_p$ and $[m_1 v^2, \cdots, m_p v^2]$

$\rightsquigarrow$ local Maxwellian with different macroscopic velocities