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

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Workshop "Analytical and Computational Problems for Mixtures and Plasma Dynamics"

June 17th, 2019

Outline of the talk

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   - Maxwell-Stefan equations
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3. Properties of the scheme
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   - Matrix form of the scheme
   - Existence of a solution
4. Numerical results
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   - Investigating the assumptions made in the scheme
   - Cross-diffusion for mixtures & AP-like behavior
5. Conclusion and prospects

Kinetic setting

- Non-reactive mixture of p monoatomic gases
- Species i described by its distribution function $f_i(t, x, v)$
- Elastic collision rules, for $\sigma \in \mathbb{S}^{d-1}$

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

- 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, for $\theta \in [0, \pi]$ the deviation angle between $v - v_*$ and σ

$$\mathcal{B}_{ik}(v, v_*, \sigma) = b_{ik} \left(\frac{v - v_*}{|v - v_*|} \cdot \sigma \right) = b_{ik}(\cos \theta), \qquad 1 \le i, k \le p$$

- 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

- Equilibrium: Maxwellian with same bulk velocity and temperature
- The collision operator satisfies conservation properties [Desvillettes, Monaco, Salvarani, '05]

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

- Isothermal setting $T > 0$ uniform and constant

Diffusive scaling

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

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

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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 operator $Q_{ik}(f_i, f_k)$ vanishes by invariance.

$$\partial_t c_i^\varepsilon + \nabla_x \cdot (c_i^\varepsilon u_i^\varepsilon) = 0.$$

- 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 by invariance.

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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Maxwell-Stefan equations

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

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

- Need of a closure relation in the limit $\varepsilon \to 0$
- Equimolar diffusion: $\sum_i c_i$ constant (or $\sum_i F_i = 0$)
- Matrix form of the Maxwell-Stefan equations (limit $\varepsilon \to 0$)

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

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

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

Towards an Asymptotic-Preserving 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.
- Difficulties: the collision term (and the transport term) becomes stiffer when $\varepsilon \to 0$
- Need to use time and space steps independent of the parameter ε (AP behavior) [Filbet, Jin, '10], [Jin, '12], [Jin, Shi, '10], [Jin, Li, '13].
- 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 [Andries, Aoki, Perthame, '02]
- Issue: numerical instability caused by the discretization of the transport term $\frac{1}{\varepsilon} v \cdot \nabla_x f_i^{\varepsilon,n} \Rightarrow$ CFL condition: $C\frac{\Delta t}{\varepsilon \Delta x} < 1$!

Outline of the talk

Moment method

- 1D in space and velocity ($d = 1$)
- Maxwell molecules
- Ansatz $f_i^\varepsilon(t,x,v) = c_i^\varepsilon(t,x)\left(\frac{m_i}{2\pi k_B T}\right)^{1/2} \exp\left\{-m_i \frac{|v-\varepsilon u_i^\varepsilon(t,x)|^2}{2k_B T}\right\}$
- Computation of the moments, with $F_i^\varepsilon = c_i^\varepsilon u_i^\varepsilon$

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

$$\varepsilon^2 m_i \left(\partial_t F_i^\varepsilon + \partial_x (c_i^\varepsilon (u_i^\varepsilon)^2)\right) + k_B T \partial_x c_i^\varepsilon = \sum_{k\neq i} \mu_{ik} B_{ik}(c_i^\varepsilon F_k^\varepsilon - c_k^\varepsilon F_i^\varepsilon) = -[A^\varepsilon \mathcal{F}^\varepsilon]_i$$

- Dirichlet boundary conditions on the fluxes $F_i^\varepsilon(t,\cdot) = 0$ on $\partial\Omega$
- Let $\Delta t > 0$ and $\Delta x > 0$ the time and space steps, and $\lambda = \Delta t/\Delta x$
- $c_{i,j}^n \approx c_i^\varepsilon(t^n, x_j) = c_i^\varepsilon(n\Delta t, j\Delta x)$
- $F_{i,j+\frac{1}{2}}^n \approx F_i^\varepsilon(t^n, x_{j+\frac{1}{2}}) = F_i^\varepsilon(n\Delta t, (j+\frac{1}{2})\Delta x)$.

Discretization of the equations

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

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

- Choice of c_i at the center of the cells: $c_{i,j+\frac{1}{2}}^{n+1} := \min\left\{ c_{i,j}^{n+1}, c_{i,j+1}^{n+1} \right\}$
- Discretization of the nonlinear term $R_{i,j+\frac{1}{2}}^{n} = \left[\partial_x (c_i^\varepsilon (u_i^\varepsilon)^2)\right]_{i,j+\frac{1}{2}}^{n}$: centered discretization with $c_i^\varepsilon (u_i^\varepsilon)^2 = (F_i^\varepsilon)^2 / c_i^\varepsilon$ for $c_i^\varepsilon \neq 0$
- Boundary conditions taken into account via ghost cells: $F_{i,-\frac{1}{2}}^{n+1} = F_{i,N-\frac{1}{2}}^{n+1} = 0$

Vectorial form of the momentum equation

$$A\mathcal{F} = k_B T \lambda (\mathcal{C}_{j+1}^{n+1} - \mathcal{C}_{j}^{n+1}) + \varepsilon^2 \mathcal{S}_{j+\frac{1}{2}}^{n}$$

where $\mathcal{C}_j^{n+1} = (c_{i,j}^{n+1})_i$, $\mathcal{S}_{j+\frac{1}{2}}^{n}$ is the vector of the terms in blue, and A is the matrix of the LHS

Outline of the talk

Mass conservation and nonnegativity

Mass conservation

Sum the continuity equations to get

$$\sum_{j=0}^{N} c_{i,j}^{n+1} = \sum_{j=0}^{N} c_{i,j}^{n}, \qquad \forall n \in \mathbb{N}.$$

Nonnegativity of the concentrations

- Use of an auxiliary scheme for the momentum equation [Anaya, Bendahmane, Sepúlveda, '15]

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

- Definition of the corresponding modified matrix $\tilde{A} = ([\tilde{A}]_{ik})_{1\leq i,k\leq p}$

Mass conservation and nonnegativity

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

- Definition of the corresponding modified matrix $\tilde{A} = ([\tilde{A}]_{ik})_{1 \leq i,k \leq p}$

Properties of the matrix $\tilde{A}$

- $\tilde{A}$ is invertible and has positive eigenvalues
- All coefficients of $\tilde{A}^{-1}$ are nonnegative, and $\left[\left(\tilde{A}^{n+1}_{j+\frac{1}{2}}\right)^{-1}\right]_{ik}$ contains a factor $[c^{n+1}_{i,j+\frac{1}{2}}]^+$ if $k \neq i$.

Proof of nonnegativity of the concentrations

- By induction on n, base case obviously true
- The momentum equation gives

$$\mathcal{F}^{n+1}_{j+\frac{1}{2}} = -\left(\tilde{A}^{n+1}_{j+\frac{1}{2}}\right)^{-1}\left(k_B T\lambda(\mathcal{C}^{n+1}_{j+1} - \mathcal{C}^{n+1}_j) + \varepsilon^2 \mathcal{S}^n_{j+\frac{1}{2}}\right).$$

- Substitution into the continuity equation

$$\frac{\mathcal{C}^{n+1}_j - \mathcal{C}^n_j}{\lambda} = \left(\tilde{A}^{n+1}_{j+\frac{1}{2}}\right)^{-1}\left(k_B T\lambda(\mathcal{C}^{n+1}_{j+1} - \mathcal{C}^{n+1}_j) + \varepsilon^2 \mathcal{S}^n_{j+\frac{1}{2}}\right) - \left(\tilde{A}^{n+1}_{j-\frac{1}{2}}\right)^{-1}\left(k_B T\lambda(\mathcal{C}^{n+1}_{j} - \mathcal{C}^{n+1}_{j-1}) + \varepsilon^2 \mathcal{S}^n_{j-\frac{1}{2}}\right)$$

- Similar relations for the boundary terms $j = 0$ and $j = N$
- Scalar product (in $\mathbb{R}^p$) with $[\mathcal{C}^n_j]^-$, discrete integration by parts using the BC

$$\sum_{j=0}^{N}\left\langle \frac{\mathcal{C}_j^{n+1}-\mathcal{C}_j^n}{\lambda},[\mathcal{C}_j^{n+1}]^-\right\rangle_p$$

$$=-\sum_{j=0}^{N}\left\langle \left(\tilde{A}_{j+\frac12}^{n+1}\right)^{-1}\left(k_BT\lambda(\mathcal{C}_{j+1}^{n+1}-\mathcal{C}_j^{n+1})+\varepsilon^2\mathcal{S}_{j+\frac12}^n\right),([\mathcal{C}_{j+1}^{n+1}]^- - [\mathcal{C}_j^{n+1}]^-)\right\rangle_p$$

Component-wise, we consider

$$\left[\left(\tilde{A}_{j+\frac12}^{n+1}\right)^{-1}\right]_{ik}\left(k_BT\lambda(c_{k,j+1}^{n+1}-c_{k,j}^{n+1})+\varepsilon^2\mathcal{S}_{k,j+\frac12}^n\right)([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-)$$

- if $k\neq i$, these terms contain a factor $[c_{i,j+\frac12}^{n+1}]^+$; the definition of $c_{i,j+\frac12}$ implies that they contain a factor $\min\{[c_{i,j}^{n+1}]^+,[c_{i,j+1}^{n+1}]^+\}([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-)=0.$
- if $k=i$
  - the terms in red are nonpositive, since $\left[\left(\tilde{A}_{j+\frac12}^{n+1}\right)^{-1}\right]_{ii}\geq 0$ and $(a-b)(a^- - b^-)\leq 0$
  - the terms in blue have an undefined sign: uniform boundedness assumption of $\mathcal{S}$ with respect to ε ensures that they are controlled by the red terms for ε small enough

$$\sum_{j=0}^{N}\left\langle \frac{\mathcal{C}_j^{n+1}-\mathcal{C}_j^{n}}{\lambda}, [\mathcal{C}_j^{n+1}]^- \right\rangle_p$$

$$= -\sum_{j=0}^{N}\left\langle \left(\tilde{A}_{j+\frac{1}{2}}^{n+1}\right)^{-1}\left(k_B T\lambda(\mathcal{C}_{j+1}^{n+1}-\mathcal{C}_j^{n+1})+\varepsilon^2\mathcal{S}_{j+\frac{1}{2}}^{n}\right), ([\mathcal{C}_{j+1}^{n+1}]^- - [\mathcal{C}_j^{n+1}]^-) \right\rangle_p$$

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$$\left[\left(\tilde{A}_{j+\frac{1}{2}}^{n+1}\right)^{-1}\right]_{ik}\left(k_B T\lambda(c_{k,j+1}^{n+1}-c_{k,j}^{n+1})+\varepsilon^2\mathcal{S}_{k,j+\frac{1}{2}}^{n}\right)([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-)$$

- if $k \neq i$, these terms contain a factor $[c_{i,j+\frac{1}{2}}^{n+1}]^+$; the definition of $c_{i,j+\frac{1}{2}}$ implies that they contain a factor $\min\{[c_{i,j}^{n+1}]^+, [c_{i,j+1}^{n+1}]^+\}([c_{i,j+1}^{n+1}]^- - [c_{i,j}^{n+1}]^-) = 0$.
- if $k = i$
  - the terms in red are nonpositive, since $\left[\left(\tilde{A}_{j+\frac{1}{2}}^{n+1}\right)^{-1}\right]_{ii} \geq 0$ and $(a-b)(a^- - b^-) \leq 0$
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Conclusion of the proof

For ε small enough, we thus have, using that $\mathcal{C}_j^{n+1} = [\mathcal{C}_j^{n+1}]^+ - [\mathcal{C}_j^{n+1}]^-$

$$\sum_{j=0}^{N} \left\langle [\mathcal{C}_j^{n+1}]^-, [\mathcal{C}_j^{n+1}]^- \right\rangle_p \leq - \sum_{j=0}^{N} \left\langle \mathcal{C}_j^{n}, [\mathcal{C}_j^{n+1}]^- \right\rangle_p .$$

Since $c_{i,j}^n \geq 0$ by induction hypothesis, this implies that

$$\sum_{j=0}^{N} \left\| [\mathcal{C}_j^{n+1}]^- \right\|_p^2 \leq 0$$

Therefore $c_{i,j}^{n+1} \geq 0$ for any i, j, n.

Remark

Because of the nonnegativity of the concentrations, a solution $(c_{i,j}^n)_j$, $(F_{i,j+\frac{1}{2}}^n)_j$ of the auxiliary scheme is also solution of the initial system.

Matrix form of the scheme

Introduce the following vector of unknowns $\mathrm{y}^n = \begin{pmatrix} \mathrm{y}_1^n \\ \mathrm{y}_2^n \end{pmatrix} \in \mathbb{R}^{p(2N+1)}$, where

$$\mathrm{y}_1^n = \left(c_{1,0}^n, \cdots, c_{1,N}^n, \cdots, c_{p,0}^n, \cdots, c_{p,N}^n\right)^\mathsf{T} \in \mathbb{R}^{p(N+1)},$$
$$\mathrm{y}_2^n = \left(F_{1,\frac{1}{2}}^n, \cdots, F_{1,N-\frac{1}{2}}^n, \cdots, F_{p,\frac{1}{2}}^n, \cdots, F_{p,N-\frac{1}{2}}^n\right)^\mathsf{T} \in \mathbb{R}^{pN}.$$

The system becomes

$$\boxed{\mathbb{S}^\varepsilon(\mathrm{y}_1^{n+1})\,\mathrm{y}^{n+1} = \mathrm{b}^n}$$

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

Auxiliary system

Let $\tilde{\mathrm{y}} = (\tilde{\mathrm{y}}_1, \mathrm{y}_2)^\mathsf{T} = ([c_{1,0}]^+, \cdots, [c_{1,N}]^+, \cdots, [c_{p,0}]^+, \cdots, [c_{p,N}]^+, \mathrm{y}_2)^\mathsf{T}$.

$$\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathrm{y}}_1^{n+1})\tilde{\mathrm{y}}^{n+1} = \mathrm{b}^n, \text{ where } \tilde{\mathbb{S}}^\varepsilon(\tilde{\mathrm{y}}_1) = \begin{bmatrix} \mathbb{I} & \mathbb{S}_{12} \\ \mathbb{S}_{21} & \tilde{\mathbb{S}}_{22}^\varepsilon(\tilde{\mathrm{y}}_1) \end{bmatrix}$$

Existence of a solution

- Use of block determinant computation and the Schur complement: $\tilde{\mathbb{S}}^\varepsilon(\tilde{\mathrm{y}}_1^{n+1})$ is invertible
$$\tilde{\mathrm{y}}^{n+1} = \left(\mathbb{S}^\varepsilon(\tilde{\mathrm{y}}_1^{n+1})\right)^{-1}\mathrm{b}^n$$
- Use of Schaefer's fixed-point theorem on the first part $\tilde{\mathrm{y}}_1$ of $\tilde{\mathrm{y}}$, by exploring the structure of $\left(\mathbb{S}^\varepsilon(\tilde{\mathrm{y}}_1^{n+1})\right)^{-1}$
$$\tilde{\mathrm{y}}_1^{n+1} = f(\tilde{\mathrm{y}}_1^{n+1}) = \mathrm{b}_1^n + \mathbb{S}_{12}\left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathrm{y}}_1^{n+1})\right)^{-1}\mathbb{S}_{21}\mathrm{b}_1^n - \mathbb{S}_{12}\left(\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathrm{y}}_1^{n+1})\right)^{-1}\mathrm{b}_2^n$$
where $\tilde{\mathbb{P}}^\varepsilon(\tilde{\mathrm{y}}_1) = \tilde{\mathbb{S}}_{22}^\varepsilon(\tilde{\mathrm{y}}_1) - \mathbb{S}_{21}\mathbb{S}_{12}$ and $\mathrm{y}_2^{n+1} = g(\tilde{\mathrm{y}}_1^{n+1})$.
- $f : \mathbb{R}_+^{p(N+1)} \to \mathbb{R}_+^{p(N+1)}$ (nonnegativity), continuous thus compact.
- Prove that the set E is bounded, where
$$E = \left\{\tilde{\mathrm{y}}_1 \in (\mathbb{R}_+)^{p(N+1)} \mid \exists \xi \in [0,1] \text{ such that } \tilde{\mathrm{y}}_1 = \xi f(\tilde{\mathrm{y}}_1)\right\}$$
- Sum the continuity equations to obtain an a priori estimate in L^1: $\|\tilde{\mathrm{y}}_1^{n+1}\|_{L^1} \leq \|\tilde{\mathrm{y}}_1^n\|_{L^1}$ and conclude the existence.
- By nonnegativity, a solution to the auxiliary system is also solution of the initial system.

Outline of the talk

Parameters of the scheme and validation

- 3 species: H_2, N_2 and CO_2 with respective molar masses $M_1 = 2$, $M_2 = 28$ and $M_3 = 44\,\mathrm{g}\cdot\mathrm{mol}^{-1}$
- Cross sections computed from the binary diffusive coefficients D_{ij}

$$B_{ij} = \frac{(m_i + m_j)k_B T}{4\pi m_i m_j D_{ij}}$$

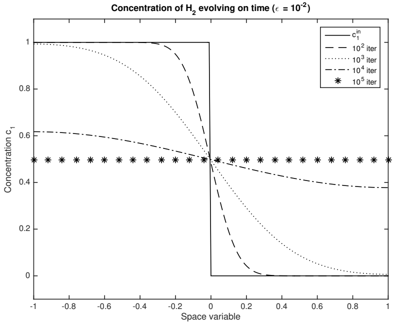
- Rescaling of the cross sections by a factor 10^5
- $\Omega = [-1, 1]$, $\Delta t = \Delta x^2 = 10^{-4}$

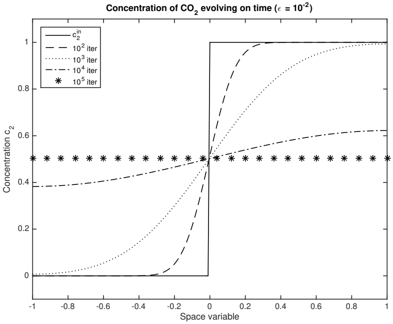
Validation

Preservation of constant states with zero initial fluxes

Diffusion of two species

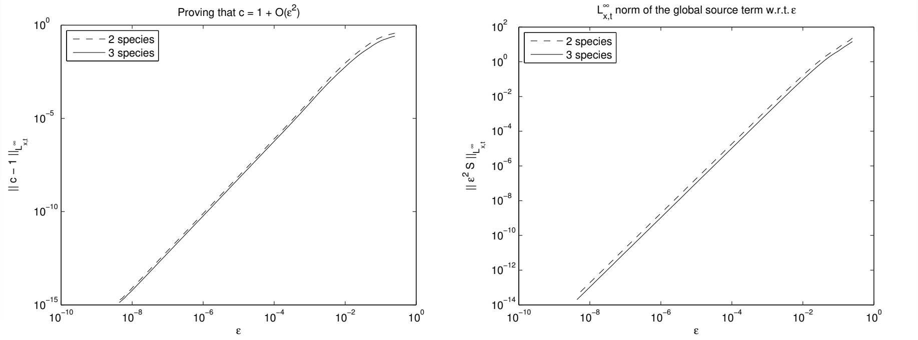
- Diffusion of H_2 and CO_2 for $\varepsilon = 10^{-2}$
- No cross-diffusion effects in the Maxwell-Stefan equations due to the symmetry of the binary diffusion coefficients
- Plots of the concentrations for $t = 0$, $t = 10^{-2}$, $t = 10^{-1}$, $t = 1$ and $t = 10$





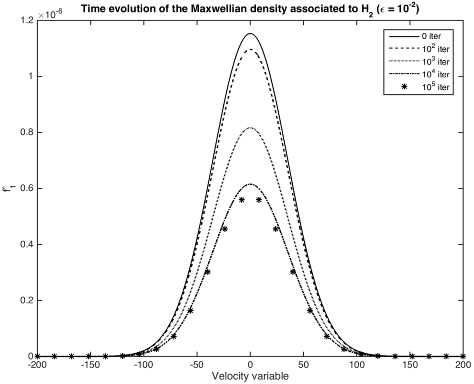
Discussion on the closure relation for Maxwell-Stefan and the smallness assumption on the source terms

- Initial conditions compatible with $\sum_i c_i = 1$ and $\sum_i F_i = 0$ (equimolar diffusion)
- We observe numerically that $c = 1 + O(\varepsilon^2)$
- Uniform boundedness assumption of the source terms with respect to ε numerically verified



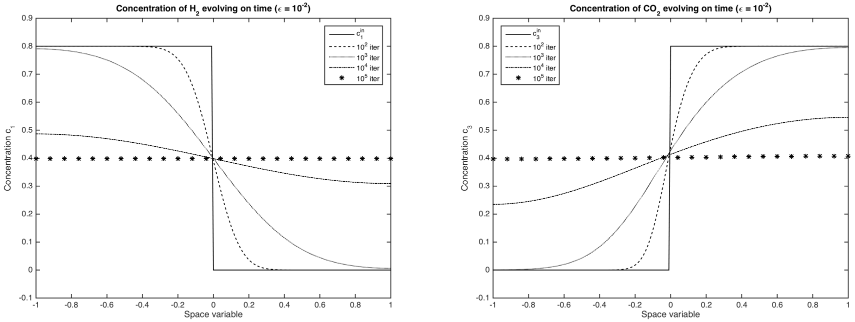
Reconstruction of the velocity distribution

- Species H_2 at $x = -0.21$ (concentration initially equal to 1, decreasing)
- Use of the Ansatz (local Maxwellian)
- Plots of the velocity distribution for $t = 0,\ 10^{-2},\ 10^{-1},\ 1$ and $t = 10$
- $\varepsilon = 10^{-2}$, so that $\varepsilon u_i = O(10^{-2})$



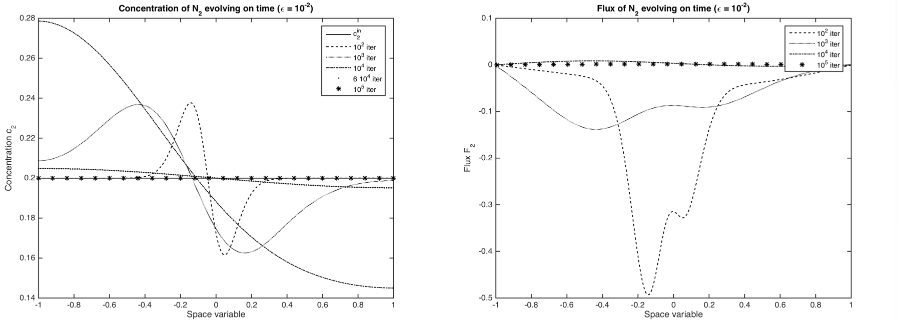
Cross-diffusion for mixtures I

- 3 species test case, appearance of uphill diffusion



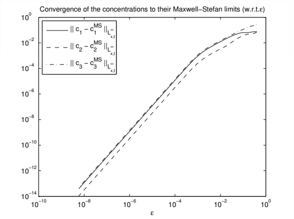
Cross-diffusion for mixtures II

- N_2, although being at equilibrium, moves because of the movement of other species
- Diffusion barrier: classical diffusion takes over

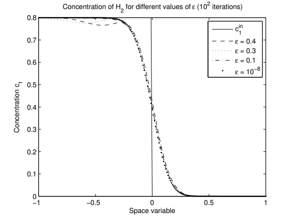


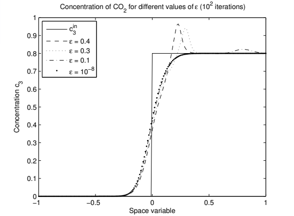
AP-like behavior

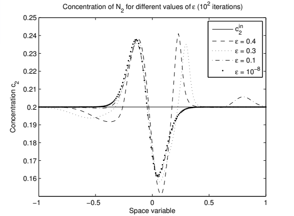
- Fixed discretization parameters for arbitrary small values of ε
- Convergence of the concentrations to the solutions of Maxwell-Stefan



- Influence of the value of ε on the diffusion process







Outline of the talk

Conclusion and prospects

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

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

Thank you for your attention!

Properties of $\tilde{A}$

- $\tilde{A}$ diagonally dominant $\Rightarrow$ invertible

$$|[\tilde{A}]_{ii}| = \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+ + \varepsilon^2 m_i > \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+ = \sum_{\ell \neq i} |[\tilde{A}]_{i\ell}|,$$

- Positivity of the eigenvalues of $\tilde{A}$
  - if all $[c_i]^+ > 0$, the matrix $\tilde{A}$ can be written $\tilde{A} = \Delta S \Delta^{-1} + D$, where $D = \varepsilon^2 \mathrm{diag}(m_1, \cdots, m_p)$, $\Delta = \mathrm{diag}(\sqrt{[c_1]^+}, \cdots, \sqrt{[c_p]^+})$ and $S = (S_{ik})_{1 \leq i,k \leq p}$ is symmetric

$$S_{ik} = \begin{cases} -\Delta t \mu_{ik} B_{ij} \sqrt{[c_i]^+ [c_k]^+}, & \text{if } i \neq k, \\ \Delta t \sum_{\ell \neq i} \mu_{i\ell} B_{i\ell} [c_\ell]^+, & \text{if } i = k. \end{cases}$$

    and also positive semidefinite
  - if $[c_p]^+ = 0$, $[\tilde{A}]_{pk} = 0$, for any $1 \leq k \leq p-1$, and the cofactor expansion of the determinant gives

$$\det(\tilde{A} - \sigma \mathbb{I}_p) = \left(\Delta t \sum_{k \neq p} \mu_{pk} B_{pk} [c_k]^+ + \varepsilon^2 m_p - \sigma \right) \pi(\sigma),$$

    $\pi(\sigma)$: characteristic polynomial of the first $p-1$ lines and columns of $\tilde{A}$
  - backward induction reasoning if more than one $[c_i]^+$ is equal to zero

Properties of $\tilde{A}^{-1}$ & Matrix form of the scheme

- Non-singular M-matrices theory for matrices with nonpositive extra-diagonal terms
  - $\tilde{A}$ has positive eigenvalues $\Rightarrow \tilde{A}^{-1} \geq 0$
- Determinant formula for inversion: $[\tilde{A}^{-1}]_{ik} = \mathring{A}_{ki} / \det(\tilde{A})$, $\mathring{A}_{ki}$ being the cofactor of matrix $\tilde{A}$, thus contains $[c_i]^+$

$$\boxed{\mathbb{S}^\varepsilon(\mathrm{y}_1^{n+1})\,\mathrm{y}^{n+1} = \mathrm{b}^n, \text{ where } \mathbb{S}^\varepsilon(\mathrm{y}_1^{n+1}) = \begin{bmatrix} \mathbb{I} & \mathbb{S}_{12} \\ \mathbb{S}_{21} & \mathbb{S}_{22}^\varepsilon(\mathrm{y}_1^{n+1}) \end{bmatrix}}$$

$$\mathbb{S}_{12} = \mathrm{Diag}(S_{12}) = \lambda \begin{bmatrix} S_{12} & & \\ & \ddots & \\ & & S_{12} \end{bmatrix}, \text{ where } (S_{12})_{ij} = \delta_{ij} - \delta_{i,j+1},\ \mathbb{S}_{21} = k_B T\, \mathbb{S}_{12}.$$

$$\mathbb{S}_{22}^\varepsilon(\mathrm{y}_1) = \begin{bmatrix} \mathbb{B}_{11}^\varepsilon(\mathrm{y}_1) & \cdots & \mathbb{B}_{1p}(\mathrm{y}_1) \\ \vdots & \ddots & \vdots \\ \mathbb{B}_{p1}(\mathrm{y}_1) & \cdots & \mathbb{B}_{pp}^\varepsilon(\mathrm{y}_1) \end{bmatrix}, \quad \begin{cases} \mathbb{B}_{ij} = \Delta t \mu_{ij} B_{ij}\, \mathrm{Diag}\left(c_{i,\ell+\frac{1}{2}}^{n+1} \right) \\ \mathbb{B}_{ii}^\varepsilon = -\Delta t\, \mathrm{Diag}\left(\sum_{k \neq i} \mu_{ik} B_{ik} c_{k,\ell+\frac{1}{2}}^{n+1} + \varepsilon^2 \dfrac{m_i}{\Delta t} \right) \end{cases}$$