Diffusion models for mixtures using a stiff dissipative hyperbolic formalism

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Workshop on kinetic and fluid Partial Differential Equations
March 7th, 2018

Outline of the talk

Diffusion models for mixtures: Fick/Maxwell-Stefan

- Mixture of $p \geq 2$ species
- ρ_i: mass density of species i
- $N_i = \rho_i u_i$: momentum of species i
- $\rho = \begin{bmatrix} \rho_1 \\ \vdots \\ \rho_p \end{bmatrix}$, $N = \begin{bmatrix} N_1 \\ \vdots \\ N_p \end{bmatrix}$
- Mass conservation: $\partial_t \rho + \nabla \cdot N = 0$

Fick law:

$$\boxed{N = -F(\rho)\nabla_x \rho}$$

Maxwell-Stefan equations:

$$\boxed{-\nabla_x \rho = S(\rho)N}$$

Properties of matrices F and S

- $F(\rho)$ and $S(\rho)$ are not invertible (rank $p-1$).
- Cauchy problem for Maxwell-Stefan's equations [Giovangigli, Bothe, Jüngel & Stelzer]
- Using Moore-Penrose pseudo-inverse: structural similarity

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

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

Obtention of the Fick law

- Thermodynamics of irreversible processes (entropy decay) [Onsager]
- Thermodynamical considerations on fluxes, written as linear combinations of potential gradients
- Stems from mass equations

Obtention of the Maxwell-Stefan equations

- Mechanical considerations on forces (equilibrium of pressure and friction forces)
- Assumption: different species have different macroscopic velocities on macroscopic time scales
- Stems from momentum equations

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

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

Perturbative method (Fick)

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

Moment method (Maxwell-Stefan)

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

The Maxwell-Stefan equations can be written

$$-\frac{1}{m_i}\nabla_{\boldsymbol{x}}\rho_i = \sum_{j\neq i}\frac{\rho_i\rho_j(u_j - u_i)}{D_{ij}},$$

m_i: molecular mass of species i, $D_{ij} > 0$ symmetric.

Outline of the talk

Stiff dissipative model for mixtures

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

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

- Ideal gas law for the partial pressure $P_i(\rho_i) = \rho_i k_B T / m_i$
- Relaxation term: friction force exerted by the mixture on species i

$$R_i = \sum_{j \neq i} a_{ij} \rho_i \rho_j (\boldsymbol{u}_j - \boldsymbol{u}_i) = \sum_{j \neq i} \alpha_{ij} (\boldsymbol{u}_j - \boldsymbol{u}_i) = \sum_{j=1}^{p} \alpha_{ij} \boldsymbol{u}_j.$$

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

Obtain a reduced system involving the aligned velocity $\boldsymbol{u}$ when ε remains small

$$\begin{cases} \partial_t \rho_i + \nabla_{\boldsymbol{x}} \cdot (\rho_i \boldsymbol{u}) = \varepsilon \nabla_{\boldsymbol{x}} \cdot \left(\sum_{j=1}^{p} \ell_{ij} \frac{\nabla_x P_j}{\rho_j} \right), \\ \partial_t (\rho \boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla_{\boldsymbol{x}} P = \boldsymbol{0}, \end{cases}$$

where $P = \sum_j P_j(\rho_j)$ is the total pressure, and (ℓ_{ij}) are real constants.

Stiff dissipative model for mixtures

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

This approach has been used in previous papers for other systems:

- [Kawashima], [Yong], [Kawashima,Yong], ...
- [Giovangigli, Matuszewski], [Giovangigli, Yong], ...

Vectorial expression of the system

$$\partial_t \mathrm{W} + \nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathrm{W}) + \frac{1}{\varepsilon}\mathrm{R}(\mathrm{W}) = 0 \qquad (*)$$

- Unknown $\mathrm{W} = [W_1, \dots, W_p, \boldsymbol{W}_{p+1}, \cdots, \boldsymbol{W}_{2p}] \in (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp}$, with $W_i = \rho_i$, $\boldsymbol{W}_{p+i} = \rho_i \boldsymbol{u}_i$
- the k-th column of F(W) and R(W) are given by

$$\mathrm{F}_k(\mathrm{W}) = \begin{bmatrix} \boldsymbol{W}_{p+1} \cdot \boldsymbol{e}_k \\ \vdots \\ \boldsymbol{W}_{2p} \cdot \boldsymbol{e}_k \\ \left(\dfrac{\boldsymbol{W}_{p+1} \otimes \boldsymbol{W}_{p+1}}{W_1} + P_1(W_1)\mathbb{I}_d \right) \boldsymbol{e}_k \\ \vdots \\ \left(\dfrac{\boldsymbol{W}_{2p} \otimes \boldsymbol{W}_{2p}}{W_p} + P_p(W_p)\mathbb{I}_d \right) \boldsymbol{e}_k \end{bmatrix}, \quad \mathrm{R}(\mathrm{W}) = \begin{bmatrix} 0_{p\times 1} \\ \displaystyle\sum_{j=1}^{p} \alpha_{1j} \frac{\boldsymbol{W}_{p+j}}{W_j} \\ \vdots \\ \displaystyle\sum_{j=1}^{p} \alpha_{pj} \frac{\boldsymbol{W}_{p+j}}{W_j} \end{bmatrix}.$$

Aim of the work

- Adapt the formalism by Chen, Levermore and Liu in the gaseous mixture framework
- Limiting behavior for small ε
- 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

Analogy with the kinetic theory

- relaxation time $\varepsilon \longleftrightarrow$ mean free path
- unknown $\mathrm{W} \longleftrightarrow$ distribution function f
- friction relaxation term $\mathrm{R} \longleftrightarrow$ collision operator Q (with dissipativity and collisional invariant properties)
- local equilibria $\longleftrightarrow$ Maxwellian functions

Outline of the talk

Building the entropy

$$\partial_t \mathrm{W} + \nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathrm{W}) + \frac{1}{\varepsilon}\mathrm{R}(\mathrm{W}) = 0 \qquad (*)$$

Entropy for Equation $(*)$

The function η defined by

$$\eta(\mathrm{W}) = \frac{1}{2}\frac{\boldsymbol{W}_{p+i}^2}{W_i} + E_i(W_i), \text{ with } E_i(W_i) = \frac{k_B T}{m_i}\left(W_i \ln\left(\frac{W_i}{W_i^0}\right) - W_i\right)$$

is a strictly convex entropy for Equation $(*)$, *i.e.*

- $\nabla^2_{\mathrm{W}}\eta(\mathrm{W})\nabla_{\mathrm{W}}\mathrm{F}_k(\mathrm{W})$ is symmetric for any k
- $\nabla_{\mathrm{W}}\eta(\mathrm{W}) \cdot \mathrm{R}(\mathrm{W}) \geq 0$
- $\nabla^2_{\mathrm{W}}\eta(\mathrm{W})$ is a positive definite quadratic form

$\rightsquigarrow$ Choice of the internal energy $E_i''(W_i) = P_i'(W_i)/W_i$

$\rightsquigarrow$ Nonnegativity of the matrix $\mathbb{A} = (\alpha_{ij})$

Conserved quantities

The matrix

$$\mathbb{Q} = \begin{bmatrix} \mathbb{I}_p & 0_{p\times dp} \\ 0_{d\times p} & [\mathbb{I}_d, \cdots, \mathbb{I}_d] \end{bmatrix} \in \mathbb{R}^{(p+d)\times(p+dp)}$$

satisfies $\mathbb{Q}\mathrm{R}(\mathrm{W}) = 0_{(p+d)\times 1}$. It allows to define

$$\mathrm{w} = \mathbb{Q}\mathrm{W} = \left[W_1, \cdots, W_p, \sum_{j=1}^{p} \boldsymbol{W}_{p+j}^{\mathsf{T}}\right]^{\mathsf{T}} \in \mathbb{R}^{p+d}$$

the $p+d$ independent conserved quantities.

Conversely, to any $\mathrm{w} = \left[w_1, \cdots, w_p, \boldsymbol{w}_{p+1}^{\mathsf{T}}\right]^{\mathsf{T}}$, we associate, via the equilibrium function $\mathcal{E}$, the equilibrium $\mathrm{W}_{\mathrm{eq}} = \mathcal{E}(\mathrm{w})$ such that $\mathrm{R}(\mathrm{W}_{\mathrm{eq}}) = 0$, where

$$\mathcal{E}(\mathrm{w}) = \left[w_1, \cdots, w_p, \frac{w_1}{\sigma(\mathrm{w})}\boldsymbol{w}_{p+1}^{\mathsf{T}}, \cdots, \frac{w_p}{\sigma(\mathrm{w})}\boldsymbol{w}_{p+1}^{\mathsf{T}}\right]^{\mathsf{T}}, \text{ with } \sigma(\mathrm{w}) = \sum_{i=1}^{p} w_i.$$

Characterization of the local equilibria

Equilibrium function

$$\mathcal{E}(\mathrm{w}) = \left[w_1, \cdots, w_p, \frac{w_1}{\sigma(\mathrm{w})} \boldsymbol{w}_{p+1}^\mathsf{T}, \cdots, \frac{w_p}{\sigma(\mathrm{w})} \boldsymbol{w}_{p+1}^\mathsf{T} \right]^\mathsf{T}, \text{ with } \sigma(\mathrm{w}) = \sum_{i=1}^{p} w_i.$$

⇝ Characterization of the equilibrium

- $\mathrm{R}(\mathrm{W}_{\mathrm{eq}}) = 0$
- there exists $\boldsymbol{u} \in \mathbb{R}^d$ such that $\mathrm{W}_{\mathrm{eq}} = [W_1, \cdots, W_p, W_1 \boldsymbol{u}^\mathsf{T}, \cdots, W_p \boldsymbol{u}^\mathsf{T}]^\mathsf{T}$
  ⇝ this corresponds to saying that all species velocities are aligned
- there exists $\mathrm{v} \in \mathbb{R}^{p+d}$ such that $\nabla_{\mathrm{W}} \eta(\mathrm{W}_{\mathrm{eq}}) = \mathrm{v}^\mathsf{T} \mathbb{Q}$

⇝ Use of the Legendre-Fenchel transform of η

- there exists $\mathrm{v} \in \mathbb{R}^{p+d}$ such that $\mathrm{W}_{\mathrm{eq}} = \nabla_{\mathrm{V}} \eta^*(\mathrm{v}^\mathsf{T} \mathbb{Q})$

In terms of the physical variables,

$$\mathcal{E}(\mathrm{w}) = [\rho_1, \cdots, \rho_p, \rho_1 \boldsymbol{u}^\mathsf{T}, \cdots, \rho_p \boldsymbol{u}^\mathsf{T}]^\mathsf{T}.$$

Define $\mathbb{P}(\mathrm{w}) = \nabla_{\mathrm{w}} \mathcal{E}(\mathrm{w}) \mathbb{Q}$, which is a projection matrix.

Outline of the talk

Look for an expansion $\mathsf{W} = \mathcal{M}[\mathsf{w}]$ (with $\mathsf{w} = \mathbb{Q}\mathsf{W}$), such that

$$\partial_t \mathsf{w} + \nabla_{\boldsymbol{x}} \cdot \mathbb{Q}\mathsf{F}(\mathcal{M}[\mathsf{w}]) \simeq 0.$$

Then

$$\partial_t \mathsf{W} + \nabla_{\boldsymbol{x}} \cdot \mathsf{F}(\mathsf{W}) + \frac{1}{\varepsilon}\mathsf{R}(\mathsf{W}) \simeq (\mathbb{I} - \nabla_{\mathsf{w}}\mathcal{M}[\mathsf{w}]\mathbb{Q})\nabla_{\boldsymbol{x}} \cdot \mathsf{F}(\mathcal{M}[\mathsf{w}]) + \frac{1}{\varepsilon}\mathsf{R}(\mathcal{M}[\mathsf{w}]).$$

Satisfying equation $(*)$ leads to cancelling the RHS.
Introduce the formal expansion

$$\mathsf{W} = \mathcal{M}[\mathsf{w}] = \mathcal{E}(\mathsf{w}) + \varepsilon\mathcal{M}^{(1)}[\mathsf{w}] + \cdots$$

Linearizing, order 1 in ε becomes

$$(\mathbb{I} - \nabla_{\mathsf{w}}\mathcal{E}(\mathsf{w})\mathbb{Q})\nabla_{\boldsymbol{x}} \cdot \mathsf{F}(\mathcal{E}(\mathsf{w})) + \nabla_{\mathsf{W}}\mathsf{R}(\mathcal{E}(\mathsf{w}))\mathcal{M}^{(1)}[\mathsf{w}] = 0$$

Provided that the inversion of $\nabla_{\mathsf{W}}\mathsf{R}(\mathcal{E}(\mathsf{w}))$ is possible in some sense,

$$\mathcal{M}^{(1)}[\mathsf{w}] = -\left(\nabla_{\mathsf{W}}\mathsf{R}(\mathcal{E}(\mathsf{w}))\right)^{-1}(\mathbb{I} - \underbrace{\nabla_{\mathsf{w}}\mathcal{E}(\mathsf{w})\mathbb{Q}}_{=\mathbb{P}(\mathsf{w})})\nabla_{\boldsymbol{x}} \cdot \mathsf{F}(\mathcal{E}(\mathsf{w}))$$

and the equation on w becomes, with $\mathsf{f}(\mathsf{w}) = \mathbb{Q}\mathsf{F}(\mathcal{E}(\mathsf{w}))$

$$\partial_t \mathsf{w} + \nabla_{\boldsymbol{x}} \cdot \mathsf{f}(\mathsf{w}) + \varepsilon\nabla_{\boldsymbol{x}} \cdot \left[\mathbb{Q}\nabla_{\mathsf{W}}\mathsf{F}(\mathcal{E}(\mathsf{w}))\mathcal{M}^{(1)}[\mathsf{w}]\right] = 0.$$

Local equilibrium approximation

Formal expansion

$$\mathsf{W}^{\varepsilon} = \mathcal{E}(\mathsf{w}) + \varepsilon \mathcal{M}^{(1)}[\mathsf{w}] + \cdots$$

Chen, Levermore and Liu's computations

The first-order correction is given by

$$\mathcal{M}^{(1)}[\mathsf{w}] = -\mathbb{B}\left[\mathbb{I}_{p+dp} - \mathbb{P}(\mathsf{w})\right] \nabla_{\boldsymbol{x}} \cdot \mathsf{F}(\mathcal{E}(\mathsf{w})), \text{ with } \mathbb{P}(\mathsf{w}) = \nabla_{\mathsf{w}} \mathcal{E}(\mathsf{w}) \mathbb{Q}.$$

The system $(*)$ becomes

$$\partial_t \mathsf{w} + \nabla_{\boldsymbol{x}} \cdot \mathsf{f}(\mathsf{w}) = \varepsilon \nabla_{\boldsymbol{x}} \cdot \mathsf{g}(\mathsf{w}),$$

where

$$\mathsf{f}_k(\mathsf{w}) = \mathbb{Q} \mathsf{F}_k(\mathcal{E}(\mathsf{w})),$$

$$\mathsf{g}_k(\mathsf{w}) = \mathbb{Q} \nabla_{\mathsf{W}} \mathsf{F}_k(\mathcal{E}(\mathsf{w})) \mathbb{B}\left[\mathbb{I}_{p+dp} - \mathbb{P}(\mathsf{w})\right] \nabla_{\boldsymbol{x}} \cdot \mathsf{F}(\mathcal{E}(\mathsf{w})),$$

where $\mathbb{B}$ is the pseudo-inverse of $\nabla_{\mathsf{W}} \mathsf{R}(\mathcal{E}(\mathsf{w}))$ such that $\operatorname{im} \mathbb{B} = \ker \mathbb{Q}$.

Explicit computations

⇝ Expression of the equilibrium, definition of $\mathbb{P}(\mathrm{w}) = \nabla_{\mathrm{w}}\mathcal{E}(\mathrm{w})\mathbb{Q}$

$$(\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w})) = \begin{bmatrix} 0_{p\times 1} \\ \nabla_{\boldsymbol{x}} P_1(\rho_1) - \dfrac{\rho_1}{\rho}\nabla_{\boldsymbol{x}} P \\ \vdots \\ \nabla_{\boldsymbol{x}} P_p(\rho_p) - \dfrac{\rho_p}{\rho}\nabla_{\boldsymbol{x}} P \end{bmatrix},$$

where $\rho = \sum_i \rho_i$ and $P = \sum_i P_i(\rho_i)$.

⇝ Computation of $\mathrm{X} = \mathbb{B}(\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w}))$:

- $\mathbb{B}$ pseudo-inverse of $\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w}))$ such that $\operatorname{im}\mathbb{B} = \ker\mathbb{Q}$
- $\ker\mathbb{Q} = \left\{ \left[0, \cdots, 0, \boldsymbol{X}_{p+1}^{\mathsf{T}}, \cdots, \boldsymbol{X}_{2p}^{\mathsf{T}}\right]^{\mathsf{T}}, \sum_{i=1}^{p} \boldsymbol{X}_{p+i} = 0_{d\times 1} \right\}$
- $\mathrm{X} \in \operatorname{im}\mathbb{B} = \ker\mathbb{Q}$ thus $X_i = 0$ and $\sum_{j=1}^{p} \boldsymbol{X}_{p+j} = 0$
- $\operatorname{im}(\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w}))) = \ker\mathbb{Q} \implies (\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{x} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w})) \in \operatorname{im}(\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w})))$
- $\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w}))\mathrm{X} = (\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{x} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w}))$

$$\sum_{j=1}^{p} \alpha_{ij}\frac{\boldsymbol{X}_{p+j}}{\rho_j} = \nabla_x P_i(\rho_i) - \frac{\rho_i}{\rho}\nabla_x P \quad \rightsquigarrow \quad \text{Pseudo-invert } \mathbb{A} = (\alpha_{ij})$$

Explicit computations

⇝ Expression of the equilibrium, definition of $\mathbb{P}(\mathrm{w}) = \nabla_{\mathrm{w}}\mathcal{E}(\mathrm{w})\mathbb{Q}$

$$(\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w})) = \begin{bmatrix} 0_{p\times 1} \\ \nabla_{\boldsymbol{x}} P_1(\rho_1) - \dfrac{\rho_1}{\rho}\nabla_{\boldsymbol{x}} P \\ \vdots \\ \nabla_{\boldsymbol{x}} P_p(\rho_p) - \dfrac{\rho_p}{\rho}\nabla_{\boldsymbol{x}} P \end{bmatrix},$$

where $\rho = \sum_i \rho_i$ and $P = \sum_i P_i(\rho_i)$.

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- $\mathrm{X} \in \operatorname{im}\mathbb{B} = \ker\mathbb{Q}$ thus $X_i = 0$ and $\sum_{j=1}^{p} \boldsymbol{X}_{p+j} = 0$
- $\operatorname{im}(\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w}))) = \ker\mathbb{Q} \implies (\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{x} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w})) \in \operatorname{im}(\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w})))$
- $\nabla_{\mathrm{W}}\mathrm{R}(\mathcal{E}(\mathrm{w}))\mathrm{X} = (\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w}))\nabla_{x} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w}))$

$$\sum_{j=1}^{p} \alpha_{ij}\frac{\boldsymbol{X}_{p+j}}{\rho_j} = \nabla_x P_i(\rho_i) - \frac{\rho_i}{\rho}\nabla_x P \quad ⇝ \quad \text{Pseudo-invert } \mathbb{A} = (\alpha_{ij})$$

Explicit computations

- ⇝ Expression of the equilibrium, definition of $\mathbb{P}(\mathrm{w}) = \nabla_{\mathrm{w}} \mathcal{E}(\mathrm{w}) \mathbb{Q}$

$$(\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w})) \nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w})) = \begin{bmatrix} 0_{p\times 1} \\ \nabla_{\boldsymbol{x}} P_1(\rho_1) - \dfrac{\rho_1}{\rho} \nabla_{\boldsymbol{x}} P \\ \vdots \\ \nabla_{\boldsymbol{x}} P_p(\rho_p) - \dfrac{\rho_p}{\rho} \nabla_{\boldsymbol{x}} P \end{bmatrix},$$

  where $\rho = \sum_i \rho_i$ and $P = \sum_i P_i(\rho_i)$.
- ⇝ Computation of $\mathrm{X} = \mathbb{B}(\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w})) \nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w}))$:
  - $\mathbb{B}$ pseudo-inverse of $\nabla_{\mathrm{W}} \mathrm{R}(\mathcal{E}(\mathrm{w}))$ such that $\operatorname{im} \mathbb{B} = \ker \mathbb{Q}$
  - $\ker \mathbb{Q} = \left\{ \left[0, \cdots, 0, \boldsymbol{X}_{p+1}^{\mathsf{T}}, \cdots, \boldsymbol{X}_{2p}^{\mathsf{T}}\right]^{\mathsf{T}}, \sum_{i=1}^{p} \boldsymbol{X}_{p+i} = 0_{d\times 1} \right\}$
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  - $\operatorname{im}(\nabla_{\mathrm{W}} \mathrm{R}(\mathcal{E}(\mathrm{w}))) = \ker \mathbb{Q} \Longrightarrow (\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w})) \nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w})) \in \operatorname{im}(\nabla_{\mathrm{W}} \mathrm{R}(\mathcal{E}(\mathrm{w})))$
  - $\nabla_{\mathrm{W}} \mathrm{R}(\mathcal{E}(\mathrm{w})) \mathrm{X} = (\mathbb{I}_{p+dp} - \mathbb{P}(\mathrm{w})) \nabla_{\boldsymbol{x}} \cdot \mathrm{F}(\mathcal{E}(\mathrm{w}))$

$$\sum_{j=1}^{p} \alpha_{ij} \frac{\boldsymbol{X}_{p+j}}{\rho_j} = \nabla_{\boldsymbol{x}} P_i(\rho_i) - \frac{\rho_i}{\rho} \nabla_{\boldsymbol{x}} P \quad \rightsquigarrow \quad \text{Pseudo-invert } \mathbb{A} = (\alpha_{ij})$$

Pseudo-inversion of $\mathbb{A}$

- Let $\mathbb{1} = (1, \cdots, 1)^\intercal$
- $\ker \mathbb{A} = \operatorname{Span} \mathbb{1}$ and $\operatorname{im} \mathbb{A} = (\operatorname{Span} \mathbb{1})^\perp$
- Let $\mathrm{r} = [\rho_1, \cdots, \rho_p]^\intercal$, which is not orthogonal to $\mathbb{1}$
- Decompositions

$$\mathbb{R}^p = (\operatorname{Span} \mathbb{1}) \oplus (\operatorname{Span} \mathrm{r})^\perp = (\operatorname{Span} \mathbb{1})^\perp \oplus (\operatorname{Span} \mathrm{r})$$

- Existence of a unique pseudo-inverse $\mathbb{L} = (\lambda_{ij})_{1 \le i,j \le p}$ of $\mathbb{A}$ with $\operatorname{im} \mathbb{L} = (\operatorname{Span} \mathrm{r})^\perp$ and $\ker \mathbb{L} = \operatorname{Span} \mathrm{r}$
- $\mathbb{L}$ is symmetric
- Since $\mathbb{A} = (\alpha_{ij}) = (\rho_i \rho_j a_{ij})$, we have that $\mathbb{L} = (\lambda_{ij}) = \left(\frac{1}{\rho_i \rho_j} \ell_{ij} \right)$

End of the computations

$$\sum_{j=1}^{p} \alpha_{ij} \frac{\boldsymbol{X}_{p+j}}{\rho_j} = \left(\nabla_{\boldsymbol{x}} P_i(\rho_i) - \frac{\rho_i}{\rho} \nabla_{\boldsymbol{x}} P \right)$$

- $\mathrm{r} = [\rho_1, \cdots, \rho_p]^\mathsf{T}$ spans $\ker \mathbb{L}$, *i.e.* $\sum_j \lambda_{ij} \rho_j = 0$

$$\boldsymbol{X}_{p+i} = \rho_i \sum_{j=1}^{p} \lambda_{ij} \nabla_{\boldsymbol{x}} P_j(\rho_j)$$

⇝ Expression of the equilibrium, and the fact that $\sum_i \boldsymbol{X}_{p+i} = 0$ allow to compute $\mathrm{g}_k(\mathrm{w}) = \mathbb{Q} \nabla_{\mathrm{W}} \mathrm{F}_k(\mathcal{E}(\mathrm{w})) \mathrm{X}$

$$\mathrm{g}_k(\mathrm{w}) = \begin{bmatrix} \rho_1 \sum_{j=1}^{p} \lambda_{1j} \partial_{x_k} P_j(\rho_j) \\ \vdots \\ \rho_p \sum_{j=1}^{p} \lambda_{pj} \partial_{x_k} P_j(\rho_j) \\ 0_{d\times 1} \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{p} \frac{\ell_{1j}}{\rho_j} \partial_{x_k} P_j(\rho_j) \\ \vdots \\ \sum_{j=1}^{p} \frac{\ell_{pj}}{\rho_j} \partial_{x_k} P_j(\rho_j) \\ 0_{d\times 1} \end{bmatrix}$$

End of the computations

$$\frac{\boldsymbol{X}_{p+i}}{\rho_i} = \sum_{j=1}^{p} \lambda_{ij} \left(\nabla_{\boldsymbol{x}} P_j(\rho_j) - \frac{\rho_j}{\rho} \nabla_{\boldsymbol{x}} P \right)$$

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$$\boldsymbol{X}_{p+i} = \rho_i \sum_{j=1}^{p} \lambda_{ij} \nabla_{\boldsymbol{x}} P_j(\rho_j)$$

⇝ Expression of the equilibrium, and the fact that $\sum_i \boldsymbol{X}_{p+i} = 0$ allow to compute $\mathrm{g}_k(\mathrm{w}) = \mathbb{Q} \nabla_{\mathrm{W}} \mathrm{F}_k(\mathcal{E}(\mathrm{w}))\mathrm{X}$

$$\mathrm{g}_k(\mathrm{w}) = \begin{bmatrix} \rho_1 \sum_{j=1}^{p} \lambda_{1j} \partial_{x_k} P_j(\rho_j) \\ \vdots \\ \rho_p \sum_{j=1}^{p} \lambda_{pj} \partial_{x_k} P_j(\rho_j) \\ 0_{d\times 1} \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{p} \frac{\ell_{1j}}{\rho_j} \partial_{x_k} P_j(\rho_j) \\ \vdots \\ \sum_{j=1}^{p} \frac{\ell_{pj}}{\rho_j} \partial_{x_k} P_j(\rho_j) \\ 0_{d\times 1} \end{bmatrix}$$

Outline of the talk

Conclusion and prospects

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

$$\begin{cases}\partial_t \rho_i + \nabla_{\boldsymbol{x}} \cdot (\rho_i \boldsymbol{u}) = \varepsilon \nabla_{\boldsymbol{x}} \cdot \left(\sum_{j=1}^{p} \ell_{ij} \frac{\nabla_{\boldsymbol{x}} P_j}{\rho_j} \right), \\ \partial_t (\rho \boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla_{\boldsymbol{x}} P = \boldsymbol{0}. \end{cases}$$

- Hyperbolicity & dissipativity
- Diffusion correction term of Fick's type (on the equation of mass conservation)
- No viscosity term on the momentum equation (convective $\gg$ diffusive fluxes)
- Maxwell-Stefan can describe a moderate rarefied regime more than Fick

Prospects

- Obtain an explicit form of Fick's coefficients from the Maxwell-Stefan's ones
- Compare the experimental and theoretical relaxation times (experiments being designed at IUSTI)
- Taking into account the non isothermal effects

Thank you for your attention!

Pseudo-inverses

Proposition

Let $\mathbb{A} \in \mathbb{R}^{p\times p}$*.Let* S *and* T *be two subspaces of* $\mathbb{R}^p$ *such that* $\mathbb{R}^p = \ker \mathbb{A} \oplus S$ *and* $\mathbb{R}^p = \operatorname{im} \mathbb{A} \oplus T$*. Then there exists a unique matrix* $\mathbb{B}$ *such that:*

1. $\mathbb{A}\mathbb{B}\mathbb{A} = \mathbb{A}$,
2. $\mathbb{B}\mathbb{A}\mathbb{B} = \mathbb{B}$,
3. $\ker \mathbb{B} = T$ *and* $\operatorname{im} \mathbb{B} = S$*.*

This matrix $\mathbb{B}$ *is then called the pseudo-inverse of* $\mathbb{A}$ *with prescribed range* S *and null space* T*.*

Corollary

Let $\mathrm{Y} \in \operatorname{im} \mathbb{A}$*. Then there exists a unique* $\mathrm{X} \in \operatorname{im} \mathbb{B}$ *such that* $\mathbb{A}\mathrm{X} = \mathrm{Y}$*, it is given by* $\mathrm{X} = \mathbb{B}\mathrm{Y}$*.*

Symmetric case

Consider a symmetric matrix $\mathbb{A} \in \mathbb{R}^{p\times p}$, and a subspace N such that $\mathbb{R}^p = \operatorname{im} \mathbb{A} \oplus N$. Then the only symmetric pseudo-inverse of $\mathbb{A}$ is the one with prescribed range $N^\perp$ and null space N.

Legendre-Fenchel transform

We introduce the following domain

$$\mathcal{V} = \left\{ \mathsf{V} \in \mathbb{R}^{p+dp} \mid \mathsf{V} = \nabla_{\mathsf{W}} \eta(\mathsf{W}) \text{ for some } \mathsf{W} \in (\mathbb{R}_+^*)^p \times \mathbb{R}^{dp} \right\}.$$

The Legendre-Fenchel transform η^* of η is the convex function satisfying

$$\eta(\mathsf{W}) + \eta^*(\mathsf{V}) = \mathsf{V} \cdot \mathsf{W}.$$

We can compute

$$\eta^*(\mathsf{V}) = \mathsf{V} \cdot \mathsf{W} - \eta(\mathsf{W}) = \sum_{i=1}^{p} \frac{k_B T}{m_i} W_i^0 \exp\left(\frac{m_i}{k_B T} \left(V_i + \frac{1}{2} \boldsymbol{V}_{p+i}^2 \right) \right).$$

Let $\phi^* : \mathbb{R}^{p+d} \to \mathbb{R}$, $\mathsf{v} \mapsto \eta^*(\mathsf{v}^\intercal \mathbb{Q})$. Denote by ϕ the Legendre-Fenchel transform of ϕ^*, we compute

$$\phi(\mathsf{w}) = \sum_{i=1}^{p} \frac{k_B T}{m_i} w_i \left[\ln\left(\frac{w_i}{W_i^0} \right) - 1 \right] + \frac{1}{2} \frac{\boldsymbol{w}_{p+1}^2}{\sigma(\mathsf{w})}.$$

Then, following [Chen, Levermore, Liu]

$$\mathcal{E}(\mathsf{w}) = \nabla_{\mathsf{V}} \eta^*(\nabla_{\mathsf{w}} \phi(\mathsf{w})^\intercal \mathbb{Q}).$$