Derivation of cross-diffusion systems from the multispecies Boltzmann equation in the diffusive scaling

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Outline of the presentation

1. Introduction
   - Context of the study and different limit models
   - Emerging questions in this context
2. Hydrodynamic limit of the Boltzmann equation for mixtures
   - Analysis of the macroscopic equations
   - Formal derivation of the macroscopic equations
3. Rigorous convergence in a perturbative setting
   - Comparison between the two macroscopic models
   - Ideas of the proof
4. Prospects

Context of the study

- Non-reactive mixture of N monatomic gases, each with mass m_i
- 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 : $J_i(t, x) = n_i(t, x) u_i(t, x)$
  - vectorial quantities $\boldsymbol{f} = (f_1, \cdots, f_N)^\intercal$, $\boldsymbol{n} = (n_1, \cdots, n_N)^\intercal$, $\boldsymbol{J} = (J_1, \cdots, J_N)^\intercal$
- Link between the two scales in the diffusive scaling
  - Formal and theoretical convergence

Multispecies Boltzmann equation

$$\boxed{\partial_t f_i(t,x,v) + v \cdot \nabla f_i(t,x,v) = \sum_{j=1}^{N} Q_{ij}(f_i, f_j), \qquad 1 \le i \le N}$$

Collision rules & Collision operator

$$v' = \left(m_i v + m_j v_* + m_j |v - v_*| \sigma\right) / (m_i + m_j), \qquad v'_* = \left(m_i v + m_j v_* - m_i |v - v_*| \sigma\right) / (m_i + m_j)$$

$$Q_{ij}(f,g)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} \mathcal{B}_{ij}(v, v_*, \sigma) \left(f(v')g(v'_*) - f(v)g(v_*)\right) \mathrm{d}\sigma \, \mathrm{d}v_*$$

Cross sections $\mathcal{B}_{ij} = \mathcal{B}_{ji} > 0$, hard or Maxwell potentials with Grad's cutoff assumption

H-theorem[1]

Equilibrium distribution functions are the local Maxwellian with bulk velocity u

$$f_i(t,x,v) = n_i(t,x) \left(\frac{m_i}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{m_i |v - u(t,x)|^2}{2 k_B T}\right)$$

[1] [Desvillettes, Monaco, Salvarani 2005]

Multispecies Boltzmann equation

$$\boxed{\partial_t f_i(t,x,v) + v\cdot\nabla f_i(t,x,v) = \sum_{j=1}^{N} Q_{ij}(f_i,f_j), \qquad 1\le i\le N}$$

Conservation properties of the Boltzmann equation

$$\int_{\mathbb{R}^3} Q_{ij}(f,g)(v)\,\mathrm{d}v = 0,$$

$$m_i\int_{\mathbb{R}^3} v\,Q_{ij}(f,g)(v)\,\mathrm{d}v + m_j\int_{\mathbb{R}^3} v\,Q_{ji}(g,f)(v)\,\mathrm{d}v = 0.$$

Moments of the distribution function

$$n_i = \int_{\mathbb{R}^3} f_i\,\mathrm{d}v,$$

$$J_i = n_i u_i = \int_{\mathbb{R}^3} v\,f_i\,\mathrm{d}v.$$

Scaled Multispecies Boltzmann equation

$$\boxed{\varepsilon \partial_t f_i(t,x,v) + v \cdot \nabla f_i(t,x,v) = \frac{1}{\varepsilon} \sum_{j=1}^{N} Q_{ij}(f_i, f_j), \qquad 1 \leq i \leq N}$$

Diffusive scaling: Kn $=$ Ma $= \varepsilon \ll 1 \rightsquigarrow$ cross-diffusion equations (isothermal setting)

Maxwell-Stefan equations	Fick equations

Maxwell-Stefan equations

$$\partial_t n_i + \nabla \cdot J_i = 0,$$

$$\nabla n_i = \sum_{j=1}^{N} \frac{1}{D_{ij}} \left(n_i J_j - n_j J_i \right).$$

Vectorial form

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

Fick equations

$$\partial_t n_i + \nabla \cdot J_i = 0,$$

$$J_i = \sum_{j=1}^{N} \varphi_{ij}(\boldsymbol{n}) \nabla n_j.$$

Vectorial form $\rightsquigarrow$ Parabolic form

$$\boxed{\boldsymbol{J} = \boldsymbol{F}(\boldsymbol{n}) \nabla \boldsymbol{n}} \quad \rightsquigarrow \quad \boxed{\partial_t \boldsymbol{n} + \nabla \cdot (\boldsymbol{F}(\boldsymbol{n}) \nabla \boldsymbol{n}) = 0}$$

[Giovangigli 1991; Giovangigli 1999; Bothe 2011; Jüngel, Stelzer 2013]

Emerging questions in this context

1. Cauchy problem for the cross-diffusion systems $\rightsquigarrow$ in a perturbative setting[1]
2. Formal derivation of the macroscopic equations from the Boltzmann equation
   - $\rightsquigarrow$ ansatz for the distribution function[2]
   - $\rightsquigarrow$ expansion of the distribution function[3]
3. Rigorous convergence[4]
   - $\rightsquigarrow$ perturbative setting
   - $\rightsquigarrow$ analysis of the kinetic operator
   - $\rightsquigarrow$ hypocoercivity estimates
4. Asymptotic-preserving numerical schemes

[1][Bondesan, Briant 2022; Briant, G. 2023], [2][Levermore 1996; Müller, Ruggeri 1993],
[3][Bardos, Golse, Levermore 1991; Bisi, Desvillettes 2014], [4][Bondesan, Briant 2021; Briant, G. 2023]

Outline of the presentation

Perturbative Cauchy theory for the Fick equations I

$$\boxed{\partial_t \boldsymbol{n} + \nabla \cdot (\boldsymbol{F}(\boldsymbol{n}) \nabla \boldsymbol{n}) = 0, \qquad n_{\text{tot}} = \sum_i n_i = \text{cst.}}$$

- Decomposition of the matrix $\boldsymbol{F}(\boldsymbol{n}) = \boldsymbol{D}(\boldsymbol{n}) \breve{\boldsymbol{F}}(\boldsymbol{n})$, with $\boldsymbol{D}(\boldsymbol{n}) = \mathrm{Diag}(\boldsymbol{n})$.
- Kernel of $\breve{\boldsymbol{F}}$: Span$(\boldsymbol{nm})$

Notation: $\boldsymbol{nm} = (n_1 m_1, \cdots, n_N m_N)^{\intercal}$

- Outside its kernel, the matrix $\breve{\boldsymbol{F}}$ is strictly negative as long as $\boldsymbol{n} > 0$.
  - Perturbative solution $\boldsymbol{n}(t,x) = \bar{\boldsymbol{n}} + \tilde{\boldsymbol{n}}(t,x)$, with $\bar{\boldsymbol{n}}$ cst.
  - Assume $\boldsymbol{n}(0,x) > C > 0$ and $\tilde{\boldsymbol{n}}(0,x)$ small enough in H^2

Proposition

Under suitable assumptions on the matrix $\boldsymbol{F}(\boldsymbol{n})$

- *a perturbative solution of the Fick equation satisfies $\boldsymbol{n} > C > 0$*
- *the perturbation $\|\tilde{\boldsymbol{n}}\|_{H^2}$ decays exponentially in time with an explicit decay rate.*

- Perturbed equation

Notation: $\bar{\boldsymbol{D}} = \boldsymbol{D}(\bar{\boldsymbol{n}})$, $\tilde{\boldsymbol{D}} = \boldsymbol{D}(\tilde{\boldsymbol{n}})$

$$\boxed{\partial_t \tilde{\boldsymbol{n}} + \nabla \cdot (\bar{\boldsymbol{D}} \breve{\boldsymbol{F}}(\boldsymbol{n}) \nabla \tilde{\boldsymbol{n}}) = -\nabla \cdot (\tilde{\boldsymbol{D}} \breve{\boldsymbol{F}}(\boldsymbol{n}) \nabla \tilde{\boldsymbol{n}}), \qquad \sum_i \tilde{n}_i = 0.}$$

Perturbative Cauchy theory for the Fick equations II

$$\boxed{\partial_t \tilde{\boldsymbol{n}} + \nabla \cdot (\bar{\boldsymbol{D}}\breve{\boldsymbol{F}}(\boldsymbol{n})\nabla\tilde{\boldsymbol{n}}) = -\nabla \cdot (\tilde{\boldsymbol{D}}\breve{\boldsymbol{F}}(\boldsymbol{n})\nabla\tilde{\boldsymbol{n}}), \qquad \sum_i \tilde{n}_i = 0.}$$

- Working in the weighted $L^2_x(\bar{\boldsymbol{n}}^{-1/2})$-norm $\rightsquigarrow$ negative feedback on $(\mathrm{Ker}\,\breve{\boldsymbol{F}})^\perp$:

  without nonlinear terms, standard a priori estimate

  Notation: $\pi_{\breve{\boldsymbol{F}}}$ projection on $\mathrm{Ker}\,\breve{\boldsymbol{F}}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{n}}\|^2_{L^2(\bar{\boldsymbol{n}}^{-1/2})} = \langle \breve{\boldsymbol{F}}\nabla\tilde{\boldsymbol{n}}, \nabla\tilde{\boldsymbol{n}}\rangle_{L^2} \leq -\beta\|\pi^\perp_{\breve{\boldsymbol{F}}}(\nabla\tilde{\boldsymbol{n}})\|^2_{L^2} \leq -\beta\|\nabla\tilde{\boldsymbol{n}}\|^2_{L^2} + \beta\|\pi_{\breve{\boldsymbol{F}}}(\nabla\tilde{\boldsymbol{n}})\|^2_{L^2}$$

⚠ Control of the kernel quantity $\pi_{\breve{\boldsymbol{F}}}(\nabla\tilde{\boldsymbol{n}}) = \langle\nabla\tilde{\boldsymbol{n}}, \mathbf{nm}\rangle$, even at the main order $\langle\nabla\tilde{\boldsymbol{n}}, \bar{\boldsymbol{n}}\mathbf{m}\rangle$

- Rescaling in time and space $\mathfrak{n}_i = \tilde{n}_i(t/m_i\bar{n}_i^2, \sqrt{m_i\bar{n}_i}x)$

  $\rightsquigarrow$ use of the coercivity of $\breve{\boldsymbol{F}}$

  $\rightsquigarrow$ main order of the projection on the kernel: $\langle\nabla\mathfrak{n}, \mathbf{1}\rangle = 0$ (closure condition)

- Other terms are nonlinear
  - $\rightsquigarrow$ remain small (for small initial data) by Sobolev controls on $\breve{\boldsymbol{F}}$
- Use Poincaré inequality and apply Grönwall's lemma

[Briant, G. 2023]

Perturbative Cauchy theory for the Fick equations II

$$\boxed{\partial_t \tilde{\boldsymbol{n}} + \nabla \cdot (\bar{\boldsymbol{D}}\breve{\boldsymbol{F}}(\boldsymbol{n})\nabla \tilde{\boldsymbol{n}}) = -\nabla \cdot (\tilde{\boldsymbol{D}}\breve{\boldsymbol{F}}(\boldsymbol{n})\nabla \tilde{\boldsymbol{n}}), \qquad \sum_i \tilde{n}_i = 0.}$$

- Working in the weighted $L^2_x(\bar{\boldsymbol{n}}^{-1/2})$-norm $\rightsquigarrow$ negative feedback on $(\mathrm{Ker}\, \breve{\boldsymbol{F}})^\perp$:

  without nonlinear terms, standard a priori estimate

  Notation: $\pi_{\breve{\boldsymbol{F}}}$ projection on $\mathrm{Ker}\, \breve{\boldsymbol{F}}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{n}}\|^2_{L^2(\bar{\boldsymbol{n}}^{-1/2})} = \langle \breve{\boldsymbol{F}}\nabla\tilde{\boldsymbol{n}}, \nabla\tilde{\boldsymbol{n}}\rangle_{L^2} \leq -\beta\|\pi^\perp_{\breve{\boldsymbol{F}}}(\nabla\tilde{\boldsymbol{n}})\|^2_{L^2} \leq -\beta\|\nabla\tilde{\boldsymbol{n}}\|^2_{L^2} + \beta\|\pi_{\breve{\boldsymbol{F}}}(\nabla\tilde{\boldsymbol{n}})\|^2_{L^2}$$

⚠ Control of the kernel quantity $\pi_{\breve{\boldsymbol{F}}}(\nabla\tilde{\boldsymbol{n}}) = \langle \nabla\tilde{\boldsymbol{n}}, \mathbf{nm}\rangle$, even at the main order $\langle \nabla\tilde{\boldsymbol{n}}, \bar{\boldsymbol{n}}\mathbf{m}\rangle$

- Rescaling in time and space $\mathfrak{n}_i = \tilde{n}_i(t/m_i\bar{n}_i^2, \sqrt{m_i\bar{n}_i}x)$

  $\rightsquigarrow$ use of the coercivity of $\breve{\boldsymbol{F}}$

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- Other terms are nonlinear
  - $\rightsquigarrow$ remain small (for small initial data) by Sobolev controls on $\breve{\boldsymbol{F}}$
- Use Poincaré inequality and apply Grönwall's lemma

[Briant, G. 2023]

Hydrodynamic limit of the Boltzmann equation for mixtures

$$\boxed{\varepsilon \partial_t f_i(t,x,v) + v \cdot \nabla f_i(t,x,v) = \frac{1}{\varepsilon} \sum_{j=1}^{N} Q_{ij}(f_i, f_j), \qquad 1 \le i \le N}$$

Scaled moments of the distribution function

$$n_i = \int_{\mathbb{R}^3} f_i \, \mathrm{d}v, \qquad J_i = \frac{1}{\varepsilon} \int_{\mathbb{R}^3} v \, f_i \, \mathrm{d}v.$$

Moment of order 0 of the Boltzmann equation $\rightsquigarrow$ mass conservation

$$\partial_t n_i + \nabla \cdot J_i = 0$$

Maxwell-Stefan limit

Moment method: prescribing the moments with entropy minimization

Scaled ansatz: local Maxwellian $n_i M_i^{\varepsilon}$

$$f_i(t,x,v) \propto n_i(t,x) e^{-\frac{m_i}{2k_B T}|v - \varepsilon u_i(t,x)|^2}$$

Fick limit

Global Maxwellian $\mu_i(v) \propto e^{-\frac{m_i}{2k_B T}|v|^2}$

Perturbative method: expansion around the global Maxwellian $n_i \mu_i$

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

Macroscopic cross-diffusion effect

- Scaled ansatz $f_i \propto n_i(t,x) \exp\left(-\frac{m_i}{2k_B T}|v - \varepsilon u_i(t,x)|^2\right)$
- Moment of order 1 of the Boltzmann equation

$$\boxed{\int_v v \times \left(\varepsilon \partial_t f_i + v \cdot \nabla f_i = \frac{1}{\varepsilon} \sum_{j=1}^{N} Q_{ij}(f_i, f_j)\right)}$$

  - Use of the ansatz

$$\varepsilon^2 \partial_t(n_i u_i) + \varepsilon^2 \nabla \cdot (n_i u_i \otimes u_i) + \frac{k_B T}{m_i} \nabla n_i = \frac{1}{\varepsilon} \sum_{j=1}^{N} \int_{\mathbb{R}^3} v\, Q_{ij}(f_i, f_j)\, \mathrm{d}v$$

  - Computation of the collision term for Maxwell molecules

$$\frac{1}{\varepsilon} \sum_{j=1}^{N} \int_{\mathbb{R}^3} v\, Q_{ij}(f_i, f_j)\, \mathrm{d}v = \sum_{j=1}^{N} \frac{2\pi m_j \|b_{ij}\|_{L^1}}{m_i + m_j} \underbrace{n_i n_j (u_j - u_i)}_{= n_i J_j - n_j J_i}$$

  - $\rightsquigarrow$ Maxwell-Stefan system [Boudin, G., Salvarani 2015]

Obtention of the Fick system: perturbative method

- Expansion $\mathbf{f} = \mathbf{n}\boldsymbol{\mu} + \varepsilon \mathbf{g}$ in the Boltzmann equation, at leading order (ε^0)

$$\boldsymbol{\mu} v \cdot \nabla_x \boldsymbol{n} = \boldsymbol{\mathcal{L}} \mathbf{g}$$

Linearized Boltzmann operator $\boldsymbol{\mathcal{L}}$ around the global Maxwellian $\boldsymbol{\mu}$

- Fluxes: $\boldsymbol{J} = \dfrac{1}{\varepsilon} \displaystyle\int v \, \boldsymbol{f} \, \mathrm{d}v = \int v \mathbf{g} \, \mathrm{d}v$

Notation: $\mathbf{W} = \boldsymbol{\mu} v \cdot \nabla_x \boldsymbol{n}$

$$\mathbf{W} = \boldsymbol{\mathcal{L}} \mathbf{g} \quad \underset{(\star)}{\rightsquigarrow} \quad \mathbf{g} = \boldsymbol{\mathcal{L}}^{-1} \mathbf{W} + \chi, \qquad \chi \in \operatorname{Ker} \boldsymbol{\mathcal{L}}$$

Weighted function space $L^2_v((\boldsymbol{n}\boldsymbol{\mu})^{-1/2})$

Notation: scalar product $\langle \cdot, \cdot \rangle_{\boldsymbol{n}\boldsymbol{\mu}}$ and norm $\| \cdot \|_{\boldsymbol{n}\boldsymbol{\mu}}$

- $\operatorname{Ker} \boldsymbol{\mathcal{L}}$ is spanned by $N + d + 1$ explicit functions

Notation: $\pi_{\boldsymbol{\mathcal{L}}}(\cdot)$ projection on $\operatorname{Ker} \boldsymbol{\mathcal{L}}$

- $\boldsymbol{\mathcal{L}}$ is a closed, self-adjoint operator in $L^2_v((\boldsymbol{n}\boldsymbol{\mu})^{-1/2})$, which is bounded and displays a spectral gap (with a gain of weight)[1]
- $\boldsymbol{\mathcal{L}}^{-1}$ is a self-adjoint operator on $(\operatorname{Ker} \boldsymbol{\mathcal{L}})^{\perp}$ which is bounded and displays a spectral gap

[1] [Briant, Daus 2016]

- Inject the expression for g_i in the definition of J_i

$$J_i = \int v[\mathcal{L}^{-1}\mathbf{W} + \chi]_i \mathrm{d}v = \int n_i\mu_i v[\mathcal{L}^{-1}\mathbf{W}]_i (n_i\mu_i)^{-1} \mathrm{d}v + \int v\chi_i \,\mathrm{d}v$$
$$= n_i \langle \mathbf{C}^{(i)}, \mathcal{L}^{-1}\mathbf{W}\rangle_{\boldsymbol{n\mu}} + X_i$$

Notation: $\mathbf{C}^{(i)} = (\mu_i v \delta_{ij})_j$, $X_i = \int v\chi_i \,\mathrm{d}v$

- $\mathcal{L}^{-1}$ is self-adjoint on $(\mathrm{Ker}\,\mathcal{L})^{\perp}$

$$J_i = n_i \sum_j \langle [\mathcal{L}^{-1}(\mathbf{C}^{(i)} - \boldsymbol{\Gamma}^{(i)})]_j, W_j\rangle_{n_j\mu_j} + X_i$$
$$= \sum_j \underbrace{n_i \langle [\mathcal{L}^{-1}(\mathbf{C}^{(i)} - \boldsymbol{\Gamma}^{(i)})]_j, \mathbf{C}^{(j)}\rangle_{n_j\mu_j}}_{\varphi_{ij}(\boldsymbol{n})} \nabla_x n_j + X_i$$

- $\rightsquigarrow$ Fick equation: $\mathbf{J} = \boldsymbol{F}(\mathbf{n})\nabla\mathbf{n} + \mathbf{X}(\boldsymbol{n})$
- Closure relation from inversion in $(\star)$: orthogonality with $\sqrt{n_k}\mu_k \mathbf{e}_k$, $v_k \boldsymbol{mn\mu}$, $|v|^2 \boldsymbol{mn\mu}$

$$0 = \langle \mu_i v \cdot \nabla_x n_i, m_i n_i \mu_i v\rangle_{\boldsymbol{n\mu}} = \sum_i \int \mu_i v \cdot \nabla_x n_i \, m_i v \mathrm{d}v \propto \nabla_x \sum_i n_i$$

- Summing mass conservation for each species

$$0 = \frac{\mathrm{d}}{\mathrm{dt}} \int \sum_i n_i \mathrm{d}x \quad \rightsquigarrow \quad \sum_i n_i \text{ cst}$$

- Inject the expression for g_i in the definition of J_i

$$J_i = \int v[\mathcal{L}^{-1}\mathbf{W} + \chi]_i \mathrm{d}v = \int n_i\mu_i v[\mathcal{L}^{-1}\mathbf{W}]_i (n_i\mu_i)^{-1} \mathrm{d}v + \int v\chi_i \,\mathrm{d}v$$
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Notation: $\boldsymbol{\Gamma}^{(i)} = \pi_{\mathcal{L}}(\mathbf{C}^{(i)})$

$$J_i = n_i \sum_j \langle [\mathcal{L}^{-1}(\mathbf{C}^{(i)} - \boldsymbol{\Gamma}^{(i)})]_j, W_j\rangle_{n_j\mu_j} + X_i$$
$$= \sum_j \underbrace{n_i \langle [\mathcal{L}^{-1}(\mathbf{C}^{(i)} - \boldsymbol{\Gamma}^{(i)})]_j, \mathbf{C}^{(j)}\rangle_{n_j\mu_j}}_{\varphi_{ij}(\boldsymbol{n})} \nabla_x n_j + X_i$$

since $W_j = \mu_j v \cdot \nabla n_j =$“$\mathbf{C}^{(j)} \cdot \nabla n_j$”

- $\rightsquigarrow$ Fick equation: $\mathbf{J} = \boldsymbol{F}(\mathbf{n})\nabla\mathbf{n} + \mathbf{X}(\boldsymbol{n})$
- Closure relation from inversion in $(\star)$: orthogonality with $\sqrt{n_k}\mu_k \mathbf{e}_k$, $v_k \boldsymbol{mn\mu}$, $|v|^2 \boldsymbol{mn\mu}$

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- Summing mass conservation for each species

$$0 = \frac{\mathrm{d}}{\mathrm{dt}} \int \sum_i n_i \mathrm{dx} \quad \rightsquigarrow \quad \sum_i n_i \text{ cst}$$

- Inject the expression for g_i in the definition of J_i

$$J_i = \int v[\boldsymbol{\mathcal{L}}^{-1}\mathbf{W} + \chi]_i \mathrm{d}v = \int n_i\mu_i v[\boldsymbol{\mathcal{L}}^{-1}\mathbf{W}]_i (n_i\mu_i)^{-1}\mathrm{d}v + \int v\chi_i \,\mathrm{d}v$$
$$= n_i\langle \mathbf{C}^{(i)}, \boldsymbol{\mathcal{L}}^{-1}\mathbf{W}\rangle_{\boldsymbol{n\mu}} + X_i$$

Notation: $\mathbf{C}^{(i)} = (\mu_i v \delta_{ij})_j$, $X_i = \int v\chi_i \,\mathrm{d}v$

- $\boldsymbol{\mathcal{L}}^{-1}$ is self-adjoint on $(\mathrm{Ker}\,\boldsymbol{\mathcal{L}})^{\perp}$

Notation: $\boldsymbol{\Gamma}^{(i)} = \pi_{\boldsymbol{\mathcal{L}}}(\mathbf{C}^{(i)})$

$$J_i = n_i \sum_j \langle [\boldsymbol{\mathcal{L}}^{-1}(\mathbf{C}^{(i)} - \boldsymbol{\Gamma}^{(i)})]_j, W_j\rangle_{n_j\mu_j} + X_i$$
$$= \sum_j \underbrace{n_i\langle [\boldsymbol{\mathcal{L}}^{-1}(\mathbf{C}^{(i)} - \boldsymbol{\Gamma}^{(i)})]_j, \mathbf{C}^{(j)}\rangle_{n_j\mu_j}}_{\varphi_{ij}(\boldsymbol{n})} \nabla_x n_j + X_i$$

since $W_j = \mu_j v \cdot \nabla n_j =$"$\mathbf{C}^{(j)} \cdot \nabla n_j$"

- $\rightsquigarrow$ Fick equation: $\mathbf{J} = \boldsymbol{F}(\mathbf{n})\nabla\mathbf{n} + \mathbf{X}(\boldsymbol{n})$
- Closure relation from inversion in $(\star)$: orthogonality with $\sqrt{n_k}\mu_k\mathbf{e}_k$, $v_k\boldsymbol{mn\mu}$, $|v|^2\boldsymbol{mn\mu}$

$$0 = \langle \mu_i v \cdot \nabla_x n_i, m_i n_i \mu_i v\rangle_{\boldsymbol{n\mu}} = \sum_i \int \mu_i v \cdot \nabla_x n_i \, m_i v \mathrm{d}v \propto \nabla_x \sum_i n_i$$

- Summing mass conservation for each species

$$0 = \frac{\mathrm{d}}{\mathrm{dt}} \int \sum_i n_i \mathrm{d}x \qquad \rightsquigarrow \qquad \sum_i n_i \text{ cst}$$

[Briant, G. 2023]

Outline of the presentation

Rigorous convergence in a perturbative setting

Maxwell-Stefan limit

All macroscopic quantities are contained in the local Maxwellian $\boldsymbol{nM}^\varepsilon$

Expansion around $\boldsymbol{nM}^\varepsilon$

$$\boldsymbol{f} = \boldsymbol{nM}^\varepsilon + \varepsilon \boldsymbol{g}$$

Insert expansion in the Boltzmann equation

$$\varepsilon \partial_t \boldsymbol{g} + v \cdot \nabla_x \boldsymbol{g} = \frac{1}{\varepsilon} \boldsymbol{L}^\varepsilon \boldsymbol{g} + \boldsymbol{Q}(\boldsymbol{g}, \boldsymbol{g}) + \boldsymbol{S}^\varepsilon$$

Linearized operator $\boldsymbol{L}^\varepsilon$ around $\boldsymbol{nM}^\varepsilon$

$\boldsymbol{S}^\varepsilon$ contains several terms in $\boldsymbol{M}^\varepsilon$ up to order $1/\varepsilon^2$

$\rightsquigarrow$ Prove that $\boldsymbol{g}$ is small for macroscopic quantities $\boldsymbol{n}$, $\boldsymbol{J}$ being perturbative solutions of Maxwell-Stefan equations

Rigorous convergence in a perturbative setting

Maxwell-Stefan limit

All macroscopic quantities are contained in the local Maxwellian $\boldsymbol{n}\boldsymbol{M}^{\varepsilon}$

Expansion around $\boldsymbol{n}\boldsymbol{M}^{\varepsilon}$

$$\boldsymbol{f} = \boldsymbol{n}\boldsymbol{M}^{\varepsilon} + \varepsilon \boldsymbol{g}$$

Insert expansion in the Boltzmann equation

$$\varepsilon \partial_t \boldsymbol{g} + v \cdot \nabla_x \boldsymbol{g} = \frac{1}{\varepsilon} \boldsymbol{L}^{\varepsilon} \boldsymbol{g} + \boldsymbol{Q}(\boldsymbol{g}, \boldsymbol{g}) + \boldsymbol{S}^{\varepsilon}$$

Linearized operator $\boldsymbol{L}^{\varepsilon}$ around $\boldsymbol{n}\boldsymbol{M}^{\varepsilon}$

$\boldsymbol{S}^{\varepsilon}$ contains several terms in $\boldsymbol{M}^{\varepsilon}$ up to order $1/\varepsilon^2$

$\rightsquigarrow$ Prove that $\boldsymbol{g}$ is small for macroscopic quantities $\boldsymbol{n}$, $\boldsymbol{J}$ being perturbative solutions of Maxwell-Stefan equations

Fick limit

Global Maxwellian $\boldsymbol{n}\boldsymbol{\mu}$ contains $\boldsymbol{n}$ only

Expansion around $\boldsymbol{n}\boldsymbol{\mu}$

$$\boldsymbol{f} = \boldsymbol{n}\boldsymbol{\mu} + \varepsilon \boldsymbol{g}$$

The fluxes are related to $\boldsymbol{g}$

$\rightsquigarrow$ define $\boldsymbol{F}(\boldsymbol{n})$ and $\boldsymbol{J}$ (through $\boldsymbol{\mathcal{L}}^{-1}$)

$\rightsquigarrow$ handle $\boldsymbol{n}$ only

Insert expansion in the Boltzmann equation

$$\varepsilon \partial_t \boldsymbol{g} + v \cdot \nabla_x \boldsymbol{g} = \frac{1}{\varepsilon} \boldsymbol{\mathcal{L}} \boldsymbol{g} + \boldsymbol{Q}(\boldsymbol{g}, \boldsymbol{g}) + \boldsymbol{\mathcal{S}}$$

Linearized operator $\boldsymbol{\mathcal{L}}$ around $\boldsymbol{n}\boldsymbol{\mu}$

$\rightsquigarrow$ Prove that $\boldsymbol{g}$ is small for macroscopic quantities $\boldsymbol{n}$ being perturbative solutions of Fick equations

Rigorous convergence in a perturbative setting

Theorem (Stability of the Fick system)

With suitable assumptions on the cross sections, if $\mathbf{g}^{(\mathrm{in})}$ *and* $\tilde{\mathbf{n}}^{(\mathrm{in})}$ *are small enough, the multispecies Boltzmann equation admits a unique global perturbative solution* $\mathbf{f}(t,x,v) = (\bar{\boldsymbol{n}} + \varepsilon \tilde{\boldsymbol{n}}(t,x))\boldsymbol{\mu}(v) + \varepsilon \mathbf{g}(t,x,v)$*, and*

$$\|\mathbf{f} - \boldsymbol{n}\boldsymbol{\mu}\|_{\mathcal{H}^s_\varepsilon}(t) \leq C\varepsilon.$$

- Definition of a hypocoercive norm[1] depending on ε

$$\|\cdot\|^2_{\mathcal{H}^s_\varepsilon} \sim \sum_{|\ell|\leq s} \|\partial_x^\ell \cdot\|_{L^2_{x,v}(\boldsymbol{\mu}^{-1/2})} + \varepsilon^2 \sum_{|\ell|+|j|\leq s, |j|\geq 1} \|\partial_x^\ell \partial_v^j \cdot\|_{L^2_{x,v}(\boldsymbol{\mu}^{-1/2})}$$

- A priori estimates on $\boldsymbol{g}$ in the norm $\mathcal{H}^s_\varepsilon$
  - Spectral gap on the linearized operator $\rightsquigarrow$ control of the non kernel part
  - Poincaré inequality for the kernel part
  - Control of the source term
  - Estimates for the commutator

Result of [Bondesan, Briant 2021] for Maxwell-Stefan can be applied here

[1] [Mouhot, Neumann 2006; Briant 2015]

Rigorous convergence in a perturbative setting

Theorem (Stability of the Fick system)

With suitable assumptions on the cross sections, if $\mathbf{g}^{(\mathrm{in})}$ *and* $\tilde{\mathbf{n}}^{(\mathrm{in})}$ *are small enough, the multispecies Boltzmann equation admits a unique global perturbative solution* $\mathbf{f}(t,x,v) = (\bar{\boldsymbol{n}} + \varepsilon \tilde{\boldsymbol{n}}(t,x))\boldsymbol{\mu}(v) + \varepsilon \mathbf{g}(t,x,v)$, *and*

$$\|\mathbf{f} - \boldsymbol{n}\boldsymbol{\mu}\|_{\mathcal{H}^s_\varepsilon}(t) \leq C\varepsilon.$$

For the estimates:

- Choice of the Maxwellian $(\bar{\boldsymbol{n}} + \varepsilon \tilde{\mathbf{n}}(t,x))\boldsymbol{\mu}(v)$ with the "good" macroscopic quantities[1]
- Cauchy theory for $\tilde{\mathbf{n}}$
  - Smallness of the macroscopic perturbation: $\|\tilde{\mathbf{n}}\|_{L^\infty_t H^s_x} \leq \delta$
  - Control of $\boldsymbol{\mathcal{S}} = \frac{1}{\varepsilon}\partial_t \boldsymbol{n}\boldsymbol{\mu} + \frac{1}{\varepsilon^2} v \cdot \nabla_x \boldsymbol{n}\boldsymbol{\mu}$:

$$\pi_{\boldsymbol{\mathcal{L}}}(\boldsymbol{\mathcal{S}}) \leq \delta \quad \text{and} \quad \pi^\perp_{\boldsymbol{\mathcal{L}}}(\boldsymbol{\mathcal{S}}) \leq \frac{\delta}{\varepsilon}$$

  This corresponds to the control of $\partial_t \tilde{\mathbf{n}} + \frac{1}{\varepsilon} v \cdot \nabla_x \tilde{\mathbf{n}}$.

For Maxwell-Stefan[2], handle additionally

- the non-equilibrium Maxwellian $\boldsymbol{n}\boldsymbol{M}^\varepsilon$
- the fluxes $\boldsymbol{J}$ (no parabolic writing of the equations)

[1][Caflisch 1980; De Masi, Esposito, Lebowitz 1989], [2][Bondesan, Briant 2021]

Outline of the presentation

Prospects

Open questions

- Non perturbative setting
- Non isothermal case
- Comparison between theoretical and experimental relaxation times

Other complex gases

- Polyatomic gases
  - Compactness of the Boltzmann operator

Coupling of the two description scales

- Spatial coupling of the Boltzmann equations for mixtures and a cross-diffusion model
- Numerical scheme selecting the right model depending on the regime

Thank you for your attention!

Spectral analysis of the linearized operator $\boldsymbol{L}^{\varepsilon}$

- Choice of the weighted function spaces $L^2(\boldsymbol{\mu}^{-1/2})$, and for $\langle v\rangle^{\gamma} = (1+|v|^2)^{\gamma/2}$, $L^2(\langle v\rangle^{\gamma}\boldsymbol{\mu}^{-1/2})$ with scalar product $\langle\cdot,\cdot\rangle_{\gamma,\boldsymbol{\mu}}$
- Projection $\boldsymbol{\pi}_{\boldsymbol{\mathcal{L}}}$ on the kernel of $\boldsymbol{\mathcal{L}}$
- Benefit from the spectral gap of $\boldsymbol{\mathcal{L}}$ (with $\boldsymbol{n}=1$): $\boldsymbol{L}^{\varepsilon} = \boldsymbol{\mathcal{L}} + (\boldsymbol{L}^{\varepsilon} - \boldsymbol{\mathcal{L}})$

Theorem

There exists $\delta > 0$ such that for any $\boldsymbol{g} \in L^2(\boldsymbol{\mu}^{-1/2})$, we have

$$\langle \boldsymbol{L}^{\varepsilon}\boldsymbol{g}, \boldsymbol{g}\rangle_{\boldsymbol{\mu}} \leq -\left(\lambda_{\boldsymbol{\mathcal{L}}} - \varepsilon R^{\varepsilon}\right) \|\boldsymbol{g} - \boldsymbol{\pi}_{\boldsymbol{\mathcal{L}}}\boldsymbol{g}\|^2_{\gamma,\boldsymbol{\mu}} + \varepsilon R^{\varepsilon}\|\boldsymbol{\pi}_{\boldsymbol{\mathcal{L}}}\boldsymbol{g}\|^2_{\gamma,\boldsymbol{\mu}},$$

where

$$R^{\varepsilon} \propto \max_{1\leq i\leq N}\left\{ n_i^{1-\delta}|u_i|\left(1+\varepsilon|u_i|e^{\frac{4m_i}{1-\delta}\varepsilon^2|u_i|^2}\right)\right\}.$$

- $|\boldsymbol{M}^{\varepsilon}(w) - \boldsymbol{\mu}(w)| \leq \varepsilon R^{\varepsilon}\boldsymbol{\mu}^{\delta}(w)$, for $\delta \in (0,1)$
- Kernel form from a Carleman representation, pointwise bounds on the kernel $\rightsquigarrow$ full Maxwellian decay

[Bondesan, Boudin, Briant, G. 2020]

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