Plasma models physically consistent from kinetic scale to hydrodynamic scale

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Workshop on Moment Methods in Kinetic Theory II

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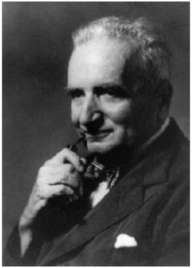
von Karman Institute for Fluid Dynamics



"With the advent of jet propulsion, it became necessary to broaden the field of aerodynamics to include problems which before were treated mostly by physical chemists. . ."

Theodore Kármán, 1958

"Aerothermochemistry" was coined by von Kármán in the 1950s to denote this multidisciplinary field of study shown to be pertinent to the then emerging aerospace era

Team

- Collaborators who contributed to the results presented here
  - **Mike Kapper, Gérald Martins, Alessandro Munafò, JB Scoggins** and **Erik Torres** (VKI)
  - **Benjamin Graille** (Paris-Sud Orsay)
  - **Marc Massot** (Ecole Centrale Paris)
  - **Irene Gamba** and **Jeff Haack** (The University of Texas at Austin)
  - **Anne Bourdon** and **Vincent Giovangigli** (Ecole Polytechnique)
  - **Manuel Torrilhon** (RWTH Aachen University)
  - **Marco Panesi** (University of Illinois at Urbana-Champaign)
  - **Rich Jaffe, David Schwenke, Winifred Huo** (NASA ARC)
  - **Mikhail Ivanov** and **Yevgeniy Bondar** (ITAM)

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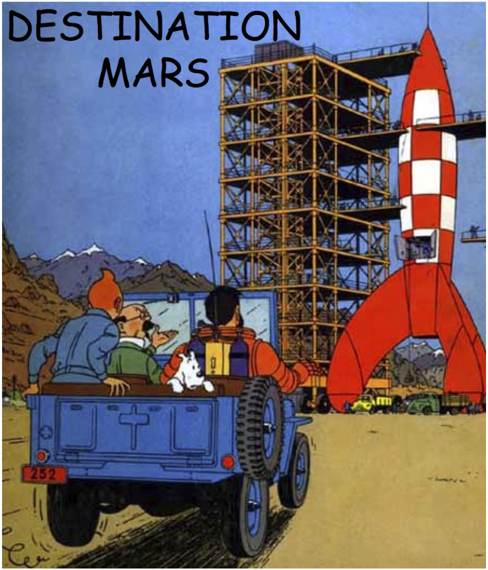
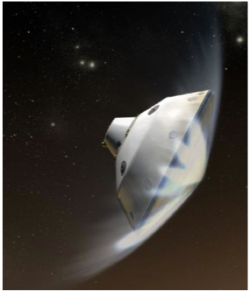
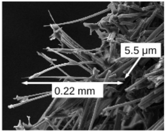
Outline

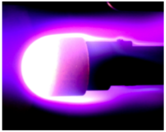
Outline



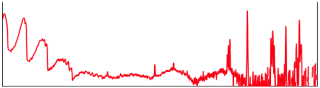




material



flow

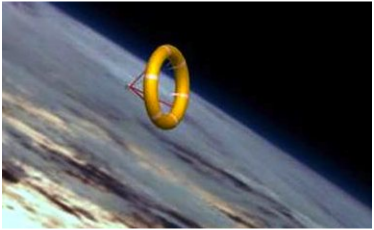


radiation

Motivation: new challenges for aerospace science

- Design of spacecraft heat shields
  - Modeling of the convective and radiative heat fluxes for:
    - Robotic missions aiming at bringing back samples to Earth
    - Manned exploration program to the Moon and Mars

Intermediate eXperimental Vehicle of ESA



Ballute aerocapture concept of NASA

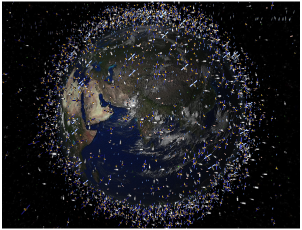
- Hypersonic cruise vehicles
  - Modeling of flows from continuum to rarefied conditions for the next generation of air breathing hypersonic vehicles

Motivation: new challenges for aerospace science

- Electric propulsion
  - Today, 20% of active satellites operate with EP systems

    STO-VKI Lecture Series (2015-16) *Electric Propulsion Systems: from recent research developments to industrial space applications*

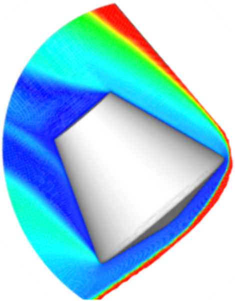

EP system for ESA's gravity mission GOCE


∼20,000 space debris > 10cm

- Space debris
  - Space debris, a threat for satellite and space systems and for mankind when undestroyed debris impact the Earth

    STO-VKI Lecture Series (June 2015) *Space Debris, In Orbit Demonstration, Debris Mitigation*

Engineering design in hypersonics



Blast capsule flow simulation

VKI COOLFLUID platform

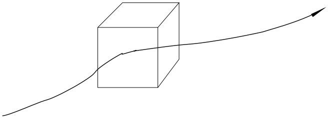
and MUTATION library

- Two quantities of interest relevant to rocket scientists
  - Heat flux
  - Shear stress to the vehicle surface

⇒ Complex multiscale problem
  - Chemical nonequilibrium (gas)
    - Dissociation, ionization, . . .
    - Internal energy excitation
  - Thermal nonequilibrium
    - Translational and internal energy relaxation
  - Radiation
  - Gas / surface interaction
    - Surface catalysis
    - Ablation
  - Rarefied gas effects
  - Turbulence (transition)

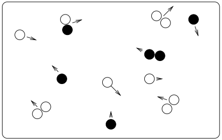
Physico-chemical models for atmospheric entry plasmas

Earth atmosphere: $S = \{N_2, O_2, NO, N, O, NO^+, N^+, O^+, e^-, \ldots\}$



Fluid dynamics

$\rho_i(\mathbf{x}, t),\ i \in S,\ \mathbf{v}(\mathbf{x}, t),\ E(\mathbf{x}, t)$



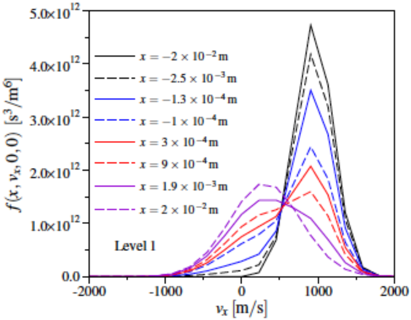
Kinetic theory

$f_i(\mathbf{x}, \mathbf{c}_i, t)\ ,\ i \in S$

- Fluid dynamical description
  - Gas modeled as a continuum in terms of macroscopic variables
  - *e.g.* Navier-Stokes eqs., Boltzmann moment systems
- Kinetic description
  - Gas particles of species $i \in S$ follow a velocity distribution f_i in the phase space $(\mathbf{x}, \mathbf{c}_i)$
  - *e.g.* Boltzmann eq.

$\Rightarrow$ Constraint: descriptions with consistent physico-chemical models

From microscopic to macroscopic quantities



Velocity distribution function for 1D Ar shockwave (Mach 3.38) at different positions $x \in [-1\text{cm}, +1\text{cm}]$

[Munafo et al. 2013]

- Mass density of species $i \in S$:
  $\rho_i(\mathbf{x}, t) = \int f_i \, m_i \, d\mathbf{c}_i$
  Mixture mass density:
  $\rho(\mathbf{x}, t) = \sum_{j \in S} \rho_j(\mathbf{x}, t)$
- Hydrodynamic velocity:
  $\rho(\mathbf{x}, t)\mathbf{v}(\mathbf{x}, t) = \sum_{j \in S} \int f_j \, m_j \mathbf{c}_j \, d\mathbf{c}_j$
- Total energy (point particles):
  $E(\mathbf{x}, t) = \sum_{j \in S} \int f_j \, \frac{1}{2} m_j |\mathbf{c}_j|^2 \, d\mathbf{c}_j$
  Thermal (translational) energy:
  $\rho(\mathbf{x}, t) e(\mathbf{x}, t) = \sum_{j \in S} \int f_j \, \frac{1}{2} m_j |\mathbf{c}_j - \mathbf{v}|^2 \, d\mathbf{c}_j$

$\Rightarrow$ Suitable asymptotic solutions can be derived by means of the Chapman-Enskog perturbative solution method

Objective of this presentation

"Engineers use knowledge primarily to design, produce, and operate artifacts... Scientists, by contrast, use knowledge primarily to generate more knowledge."

Walter Vincenti

- ⇒ Enrich mathematical models by adding more physics
- ⇒ Derive mathematical structure and fix ad-hoc terms found in engineering models
- ⇒ Integrate quantum chemistry databases

Outline

Transport collision integrals

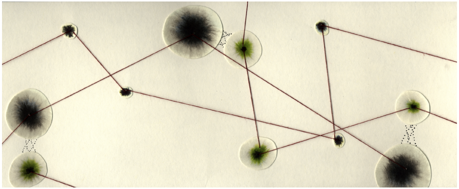
⇒ Closure of the transport fluxes at a microscopic scale

- The transport properties are expressed in terms of collision integrals

$$\bar{Q}_{ij}^{(l,s)}(T) = \frac{2\,(l+1)}{(s+1)!\,\left[2l+1-(-1)^l\right](\mathrm{k_B}\,T)^{s+2}} \int_0^\infty \exp\left(\frac{-E}{\mathrm{k_B}\,T}\right)\,E^{s+1}\,Q_{ij}^{(l)}\,\mathrm{d}E$$

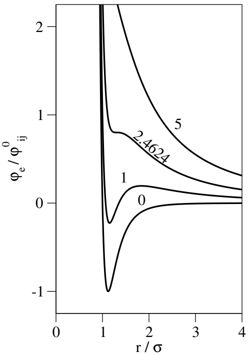
- They represent an average over all possible relative energies of the relevant cross section

$$Q_{ij}^{(l)}(E) = 2\,\pi \int_0^\infty \left[1-\cos^l(\chi)\right]\,b\,\mathrm{d}b,$$

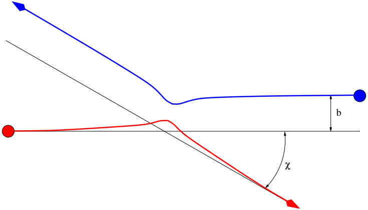


"Boltzmann impression", Losa, Luzern 2004

Deflection angle



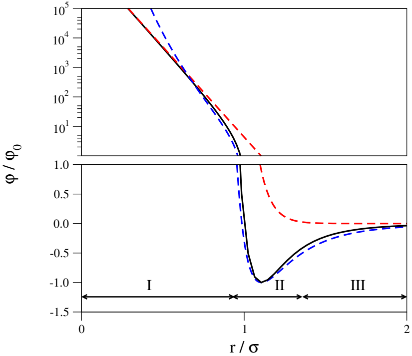
Effective Lennard-Jones potential



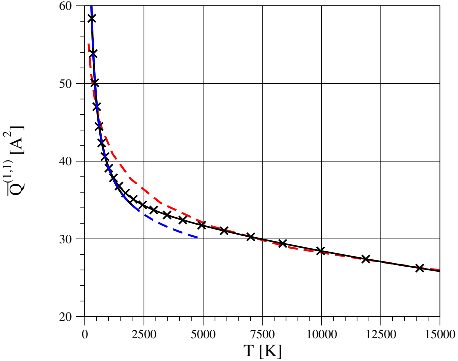
Dynamics of an elastic binary collision

- Effective potential
  $\varphi_e(E, b, r) = \varphi(r) + E\,\frac{b^2}{r^2}$
- Deflection angle
  $\chi\,(E, b) = \pi - 2\; b \int_{r_m}^{\infty} \frac{\mathrm{d}r}{r^2\sqrt{1-\varphi_e/E}}$

Neutral-neutral interactions: sewing method for potentials [M., Degrez, Sokolova 2004]



Potentials models for the $O_2 - O_2$
— Tang-Toennies, – – Born-Mayer, and – – (m,6)
(experimental data of Brunetti)



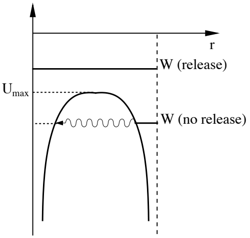
$\bar{Q}^{(1,1)}$ collision integral for the $CO_2 - CO_2$ interaction:
– – (m,6) potential,
– – Born-Mayer potential,
and × combined result

Ion-neutral interactions

- Elastic collisions: $\bar{Q}_{el}^{(l,s)}$
  - Born-Mayer potential: $\varphi(r) = \varphi_0 \exp(-\alpha r)$
  - with parameters recovered from atom-atom model

- Resonant charge-transfer: $\bar{Q}_{res}^{(1,s)}, \; s \in \{1,2,3\}$

  For l odd interaction where atom and ions are parent and child



- $O - O^+$

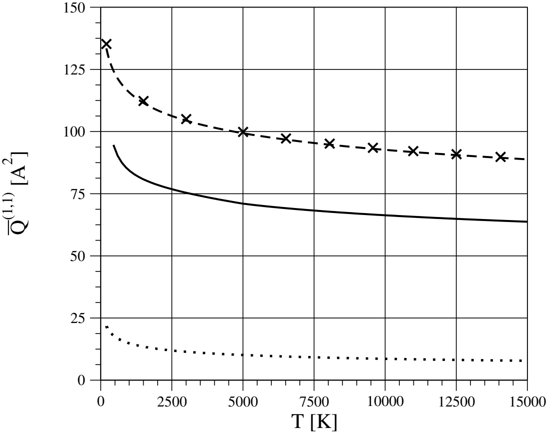
  [Stallcop, Partridge, Levin]
- $C - C^+$

  [Duman and Smirnov]
  - $Q_{exc} = (7.071 - 0.3485 \ln E)^2$
  - $Q_{res}^{(1)} = 2 \; Q_{exc}$

- For $l = 1$

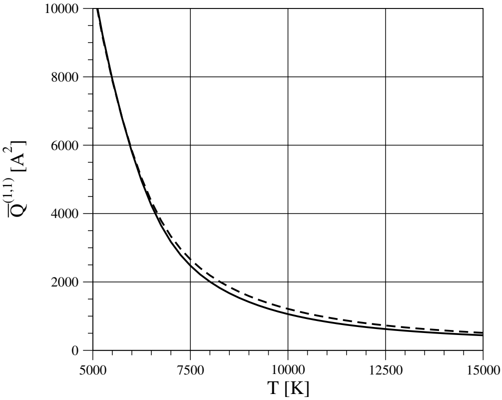
$$\bar{Q}^{(1,s)} = \sqrt{\left(\bar{Q}_{el}^{(1,s)}\right)^2 + \left(\bar{Q}_{res}^{(1,s)}\right)^2}$$

Ion-neutral interactions



$\bar{Q}^{(1,1)}$ collision integrals: $\mathrm{O}-\mathrm{O}^+$, — Stallcop *et al.*; $\mathrm{C}-\mathrm{C}^+$, −− resonant charge transfer, $\cdots$ Born-Mayer, and $\times$ combined result

Charge-charge interactions



$\bar{Q}^{(1,1)}$ for LTE carbon dioxide at 1 atm: −− attractive interaction and — repulsive interaction

- Shielded Coulomb potential [Mason et al] and [Devoto]:

$$\varphi(r) = \pm\varphi_0 \frac{d}{r} \exp\left(-\frac{r}{d}\right)$$

- Debye length

$$\lambda_D = \left(\frac{\varepsilon_0 k_B T_e}{2 n_e q_e^2}\right)^{1/2}$$

Conditions on the kinetic data

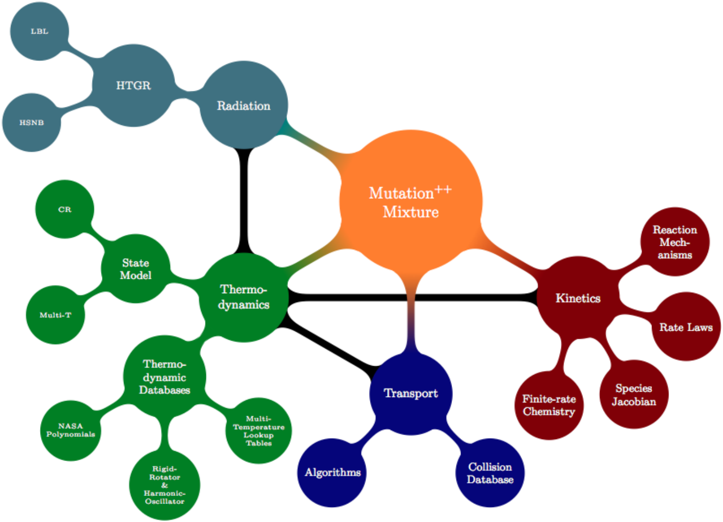
- Well-posedness of the transport properties is established provided that some conditions are met by the kinetic data
- For instance, the electrical conductivity and thermal conductivity reads in the first and second Laguerre-Sonine approximations, respectively
  - $\sigma_e(1) = \frac{4}{25} \frac{(x_e q_e)^2}{k_B^2 T_e} \frac{1}{\Lambda_{ee}^{00}}$
  - $\lambda_e(2) = \frac{x_e^2}{\Lambda_{ee}^{11}}$

Proposition (M. and Degrez, 2004)

Let $\bar{Q}_{ie}^{(1,1)}$, $\bar{Q}_{ie}^{(1,2)}$, $\bar{Q}_{ie}^{(1,3)}$, $i \in \mathcal{H}$ and $\bar{Q}_{ee}^{(2,2)}$ be positive coefficients such that $5\bar{Q}_{ie}^{(1,2)} - 4\bar{Q}_{ie}^{(1,3)} < 25\bar{Q}_{ie}^{(1,1)}/12$, and assume that $x_i > 0, \ i \in \mathcal{S}$. Then the scalars Λ_{ee}^{00} and Λ_{ee}^{11} are positive

Mutation++ library [Scoggins and M. 2014]

MUTATION++: MUlticomponent Transport And Thermodynamic properties / chemistry for IONized gases written in C++



MUTATION++: library for high enthalpy and plasma flows

- Quantities relevant to engineering design for hypersonic flows
  - Heat flux & shear stress to the surface of a vehicle
  - Their prediction strongly relies on completeness and accuracy of the numerical methods & physico-chemical models

- Why a library for physico-chemical models?
  - Implementation common to several CFD codes
  - Nonequilibrium models, not satisfactory today, are regularly improved
  - Basic data are constantly updated

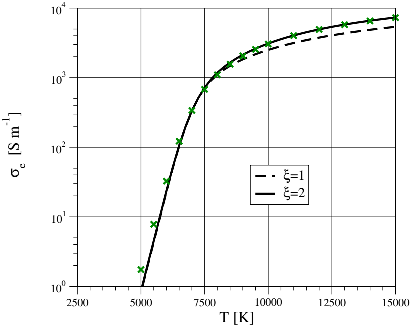
    (Chemical rate coefficients, spectroscopic constants, transport cross-sections,...)

- Constraints for the library implementation
  - High accuracy of the physical models
    - Laws of thermodynamics must be satisfied
    - Validation based on experimental data
  - Low computational cost
  - User-friendly interface

Electron transport coefficients

- Electron conduction current density:

$$\mathbf{J}_{\mathfrak{e}} = n_{\mathfrak{e}} q_e \mathbf{V}_{\mathfrak{e}} = \sigma_e \mathbf{E} + \cdots$$



Electrical conductivity of carbon dioxide at 1 atm

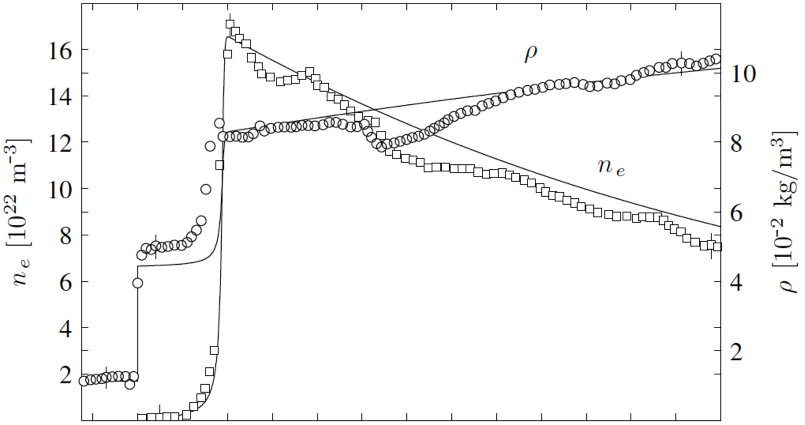
– – $\sigma_e(1)$ Mutation , —— $\sigma_e(2)$ Mutation, and × Andriatis and Sokolova

with $\sigma_e = \dfrac{(n_{\mathfrak{e}} q_e)^2}{p_{\mathfrak{e}}} D_{\mathfrak{e}}$

Outline

UTIAS shock-tube experiments [Glass and Liu, 1978]

(Mach=15.9, p=5.14 Torr, T=293.6 K, α=0.14)



Mass density and electron number density

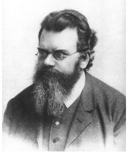
[Kapper and Cambier, 2011]

Boltzmann equation with reactive collisions

- Assumptions
  - Plasma spatially uniform, at rest, no external forces
  - Composed of electrons, neutral particles, and ions: $\mathsf{S} = \{\mathfrak{e}, \mathfrak{n}, \mathfrak{i}\}$
  - Ionization mechanism: reaction $\mathfrak{r}_i$

$$\mathfrak{n} + i \rightleftharpoons \mathfrak{i} + \mathfrak{e} + i, \ \ i \in \mathsf{S}$$

  - Maxwellian regime for reactive collisions (chemistry characteristic times larger than the mean free times)
  - Boltzmann collision operator



- Boltzmann eq.[1] : $\partial_{t^\star} f_i^\star = \sum_{j \in \mathsf{S}} \mathcal{J}_{ij}^\star \left(f_i^\star, f_j^\star \right) + \mathcal{C}_i^\star(f^\star), \quad i \in \mathsf{S}$
- Reactive collision operator for particle i: $\mathcal{C}_i^\star = \mathcal{C}_i^{\mathfrak{r}_\mathfrak{e}\star} + \mathcal{C}_i^{\mathfrak{r}_\mathfrak{n}\star} + \mathcal{C}_i^{\mathfrak{r}_\mathfrak{i}\star}$

[1] Dimensional quantities are denoted by the superscript *

Reactive collision operator [Giovangigli 1998]

- *e.g.*, e-impact ionization reaction $r_{\mathfrak{e}}$

$$\mathfrak{n} + \mathfrak{e} \rightleftharpoons \mathfrak{i} + \mathfrak{e} + \mathfrak{e}$$

- For electrons

$$\begin{aligned}\mathcal{C}_{\mathfrak{e}}^{r_{\mathfrak{e}}\star}(f^\star) = &\int \left(f_{\mathfrak{i}}^\star f_{\mathfrak{e}_1}^\star f_{\mathfrak{e}_2}^\star \frac{\beta_{\mathfrak{i}}^\star \beta_{\mathfrak{e}}^\star}{\beta_{\mathfrak{n}}^\star} - f_{\mathfrak{n}}^\star f_{\mathfrak{e}}^\star \right) \mathcal{W}_{\mathfrak{ne}}^{\mathfrak{iee}\star} \mathrm{d}\mathbf{c}_{\mathfrak{n}}^\star \mathrm{d}\mathbf{c}_{\mathfrak{i}}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_1}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_2}^\star \\ &- 2 \int \left(f_{\mathfrak{i}}^\star f_{\mathfrak{e}}^\star f_{\mathfrak{e}_2}^\star \frac{\beta_{\mathfrak{i}}^\star \beta_{\mathfrak{e}}^\star}{\beta_{\mathfrak{n}}^\star} - f_{\mathfrak{n}}^\star f_{\mathfrak{e}_1}^\star \right) \mathcal{W}_{\mathfrak{ne}}^{\mathfrak{iee}\star} \mathrm{d}\mathbf{c}_{\mathfrak{n}}^\star \mathrm{d}\mathbf{c}_{\mathfrak{i}}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_1}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_2}^\star,\end{aligned}$$

with the statistical weight $\beta_i^\star = [\mathrm{h_P}/(a_i m_i^\star)]^3$, $a_{\mathfrak{e}} = 2, a_{\mathfrak{n}} = a_{\mathfrak{i}} = 1$

- For ions

$$\mathcal{C}_{\mathfrak{i}}^{r_{\mathfrak{e}}\star}(f^\star) = -\int \left(f_{\mathfrak{i}}^\star f_{\mathfrak{e}_2}^\star f_{\mathfrak{e}_3}^\star \frac{\beta_{\mathfrak{i}}^\star \beta_{\mathfrak{e}}^\star}{\beta_{\mathfrak{n}}^\star} - f_{\mathfrak{n}}^\star f_{\mathfrak{e}_1}^\star \right) \mathcal{W}_{\mathfrak{ne}}^{\mathfrak{iee}\star} \mathrm{d}\mathbf{c}_{\mathfrak{n}}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_1}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_2}^\star \mathrm{d}\mathbf{c}_{\mathfrak{e}_3}^\star$$

Scaling parameter based on electron / heavy-particle mass ratio:

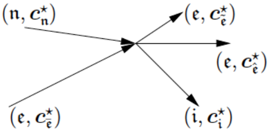
$$\varepsilon = \left(\frac{m_{\mathfrak{e}}^0}{m_{\mathfrak{h}}^0}\right)^{1/2} \ll 1$$

Dynamics of the reactive collisions

[Graille, M., Massot, CTR SP 2008]

- e-impact ionization

$$\mathfrak{n} + \bar{\mathfrak{e}} \rightleftharpoons \mathfrak{i} + \hat{\mathfrak{e}} + \tilde{\mathfrak{e}}$$

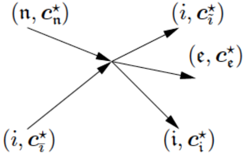


$$|\mathbf{c}_\mathfrak{n}|^2 = |\mathbf{c}_\mathfrak{i}|^2 + \mathcal{O}(\varepsilon)$$
$$|\mathbf{c}_{\bar{\mathfrak{e}}}|^2 = |\mathbf{c}_{\hat{\mathfrak{e}}}|^2 + |\mathbf{c}_{\tilde{\mathfrak{e}}}|^2 + 2\Delta\mathcal{E} + \mathcal{O}(\varepsilon),$$

with the ionization energy $\Delta\mathcal{E} = \mathcal{U}^\mathsf{F}_\mathfrak{e} + m_\mathfrak{i}\mathcal{U}^\mathsf{F}_\mathfrak{i} - m_\mathfrak{n}\mathcal{U}^\mathsf{F}_\mathfrak{n}$

- Heavy-particle impact ionization

$$\mathfrak{n} + \bar{i} \rightleftharpoons \mathfrak{i} + \hat{\mathfrak{e}} + \tilde{i}, \quad i \in \mathrm{H}$$



$$\frac{1}{2} m_i |\mathbf{g}_{\mathfrak{n}i}|^2 - 2\Delta\mathcal{E} = \frac{1}{2} m_i |\mathbf{g}'_{\mathfrak{i}i}|^2 + \mathcal{O}(\varepsilon), \quad i \in \mathrm{H}$$
$$|\mathbf{g}'_{\mathfrak{h}\mathfrak{e}}|^2 = \mathcal{O}(\varepsilon)$$

$\Rightarrow$ the electron pulled from the neutral particle is cold

Euler conservation equations (order ε^{-1})

- Mass

$$\begin{aligned} \mathrm{d}_t \rho_{\mathfrak{e}} &= \omega_{\mathfrak{e}}^{0} \\ \mathrm{d}_t \rho_i &= m_i\, \omega_i^{0}, \quad i \in \mathrm{H} \end{aligned}$$

- Energy

$$\begin{aligned} \mathrm{d}_t(\rho_{\mathfrak{e}} e_{\mathfrak{e}}^{\mathrm{T}}) &= -\Delta E_{\mathfrak{h}}^{0} - \Delta\mathcal{E}\, \omega_{\mathfrak{e}}^{\mathfrak{r}_{\mathfrak{e}}\,0} \\ \mathrm{d}_t(\rho_{\mathfrak{h}} e_{\mathfrak{h}}^{\mathrm{T}}) &= \Delta E_{\mathfrak{h}}^{0} + \Delta\mathcal{E}\, \omega_{\mathfrak{n}}^{\mathfrak{r}_{\mathfrak{n}}\,0} - \Delta\mathcal{E}\, \omega_{\mathfrak{i}}^{\mathfrak{r}_{\mathfrak{i}}\,0} \end{aligned}$$

  - Chemical loss rate controlling energy [Panesi *et. al*, JTHT 23 (2009) 236]
  - Standard derivation [Appleton & Bray] does not account for mass disparity

- Using the property $\omega_{\mathfrak{e}}^{r0} = \omega_{\mathfrak{i}}^{r0} = -\omega_{\mathfrak{n}}^{r0}$, $r \in R$, the mixture mass and energy are conserved, i.e.,

$$\mathrm{d}_t \rho = 0, \qquad \mathrm{d}_t(\rho e^{\mathrm{T}} + \rho\,\mathfrak{U}^{\mathrm{F}}) = 0$$

Two temperature Saha law

- e-impact ionization

$$\mathfrak{n} + \bar{\mathfrak{e}} \rightleftharpoons \mathfrak{i} + \hat{\mathfrak{e}} + \tilde{\mathfrak{e}}$$

$$\mathcal{K}^{eq}_{r_\mathfrak{e}}(T_\mathfrak{e}) = \left(\frac{m_\mathfrak{i}}{m_\mathfrak{n}}\right)^{3/2} Q^T_\mathfrak{e}(T_\mathfrak{e}) \exp\left(-\frac{\Delta\mathcal{E}}{T_\mathfrak{e}}\right)$$

- Heavy-particle impact ionization

$$\mathfrak{n} + \bar{i} \rightleftharpoons \mathfrak{i} + \hat{\mathfrak{e}} + \tilde{i}$$

$$\mathcal{K}^{eq}_{r_i}(T_\mathfrak{h}, T_\mathfrak{e}) = \left(\frac{m_\mathfrak{i}}{m_\mathfrak{n}}\right)^{3/2} Q^T_\mathfrak{e}(T_\mathfrak{e}) \exp\left(-\frac{\Delta\mathcal{E}}{T_\mathfrak{h}}\right), \quad i \in \mathrm{H}$$

[M., Graille, Massot, CTR ARB 2009]

[Massot, Graille, M., RGD 2010]

Law of mass action for plasmas

- e-impact ionization

$$\mathfrak{n} + \bar{\mathfrak{e}} \rightleftharpoons \mathfrak{i} + \hat{\mathfrak{e}} + \tilde{\mathfrak{e}}$$

$$\mathcal{K}^{\mathrm{f}}_{r_{\mathfrak{e}}} = \mathcal{K}^{\mathrm{f}}_{r_{\mathfrak{e}}}(T_{\mathfrak{e}}), \qquad \mathcal{K}^{\mathrm{b}}_{r_{\mathfrak{e}}} = \mathcal{K}^{\mathrm{b}}_{r_{\mathfrak{e}}}(T_{\mathfrak{e}})$$

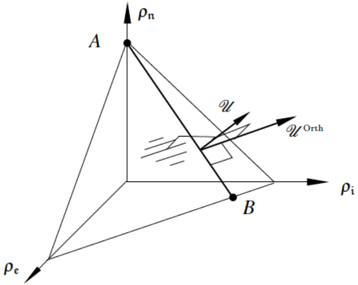
- Heavy-particle impact ionization

$$\mathfrak{n} + \bar{i} \rightleftharpoons \mathfrak{i} + \hat{\mathfrak{e}} + \tilde{i}$$

$$\mathcal{K}^{\mathrm{f}}_{r_i} = \mathcal{K}^{\mathrm{f}}_{r_i}(T_{\mathfrak{h}}), \qquad \mathcal{K}^{\mathrm{b}}_{r_i} = \mathcal{K}^{\mathrm{eq}}_{r_i}(T_{\mathfrak{h}}, T_{\mathfrak{e}})\mathcal{K}^{\mathrm{f}}_{r_i}(T_{\mathfrak{h}}), \quad i \in \mathrm{H}$$

[Graille, M., Massot, CTR SP 2008]
[M., Graille, Massot, CTR ARB 2009]
[Massot, Graille, M., RGD 2010]

Thermo-chemical dynamics and chemical quasi-equilibrium



- The species Gibbs free energy is defined as
  $\rho_i g_i = n_i T_i \ln\left(\frac{n_i}{Q_i^{\mathrm{T}}(T_i)}\right) + \rho_i \mathfrak{U}_i^{\mathrm{F}}, \quad i \in \mathrm{S}$
- Modified Gibbs free energy for thermal non-equilibrium
  $\rho_i \tilde{g}_i^{r_j} = \rho_i g_i + \left(\frac{T_i}{T_{r_j}} - 1\right) \rho_i \mathfrak{U}_i^{\mathrm{F}}, \quad i, j \in \mathrm{S}$

$\Rightarrow$ The 2nd law of thermodynamics is satisfied

$$\mathrm{d}_t(\rho s) = \Upsilon_{\mathrm{th}} + \textstyle\sum_{j \in \mathrm{S}} \Upsilon_{\mathrm{ch}}^{r_j}, \quad \Upsilon_{\mathrm{th}} \geq 0, \quad \Upsilon_{\mathrm{ch}}^{r_j} \geq 0,\ j \in \mathrm{S}$$

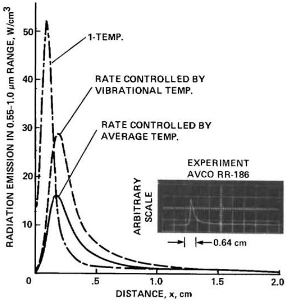
- The full thermodynamic equilibrium state of the system under well-defined and natural constraints is studied by following Giovangigli and Massot (M3AS 1998)
- The system asymptotically converges toward a unique thermal and chemical equilibrium

Outline

Motivation: developing high-fidelity nonequilibrium models

⇒ Understanding thermo-chemical nonequilibrium effects is important

- For an accurate prediction of the radiative heat flux for reentries at v>10km/s (Moon and Mars returns)
- For a correct interpretation of experimental measurements
  - In flight
  - In ground wind-tunnels



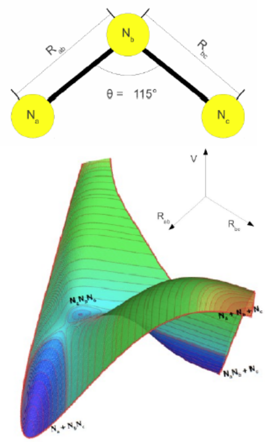
Calculated and measured intensity $N_2(1+)$ system

⇒ Standard nonequilibrium models for hypersonic flows were mainly developed in the 1980's (correlation based)

- *e.g.* dissociation model of Park
- Multitemperature model: $T = T_r, T_v = T_e = T_{ele}$
- Average temperature $\sqrt{T\ T_v}$ for fictitious Arrhenius rate coefficient

Microscopic approach to derive macroscopic nonequilibrium models...

- **e.g. NASA ARC database for nitrogen chemistry:**
  - 9390 (v,J) rovibrational energy levels for $\mathrm{N_2}$
  - 50×10^6 reaction mechanism for $\mathbf{N_2} + \mathbf{N}$ system
    - $\mathrm{N_2(v, J) + N \leftrightarrow N + N + N}$
    - $\mathrm{N_2(v, J) \leftrightarrow N + N}$
    - $\mathrm{N_2(v, J) + N \leftrightarrow N_2(v', J') + N}$
- Papers AIAA 2008-1208, 2008-1209, 2009-1569, 2010-4517, RTO-VKI LS 2008



$\mathrm{N_3}$ Potential Energy Surface

NASA Ames Research Center

Detailed chemical mechanism coupled with a flow solver

- Full master eq. of conservation of mass for the 9390 rovibrational energy levels $i = (v, J)$ for N_2, and for N atoms coupled with eqs. of conservation of momentum and total energy

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\rho_i \\ \rho_{\mathrm{N}} \\ \rho u \\ \rho E\end{pmatrix} + \frac{\mathrm{d}}{\mathrm{d}x}\begin{pmatrix}\rho_i u \\ \rho_{\mathrm{N}} u \\ \rho u^2 + p \\ \rho u H\end{pmatrix} = \begin{pmatrix}M_{\mathrm{N}_2}\omega_i \\ M_{\mathrm{N}}\omega_{\mathrm{N}} \\ 0 \\ 0\end{pmatrix}$$

... but computationally too expensive for 3D CFD applications

$\Rightarrow$ reduction of the chemical mechanism by lumping the energy levels i:

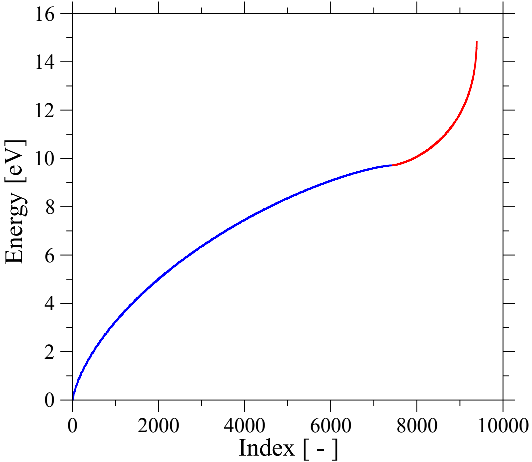
- *e.g.* vibrational state-to-state models (AIAA 2009-3837, 2010-4335)

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_v + \frac{\mathrm{d}}{\mathrm{d}x}(\rho_v u) = M_{\mathrm{N}_2}\omega_v$$

- The energy levels are lumped for each v assuming a rotational energy population following a Maxwell-Boltzmann distribution at T **[Guy, Bourdon, Perrin, 2013]**

Coarse-grain Model [M., Panesi, Bourdon, Jaffe, 2011]

- Novel lumping scheme obtained by sorting the levels by energy and grouping in a bin all levels with similar energies



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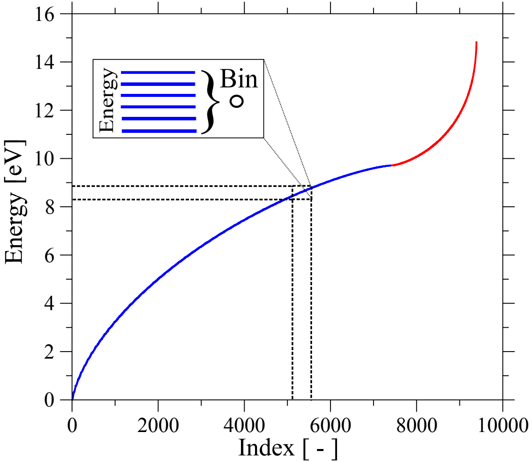

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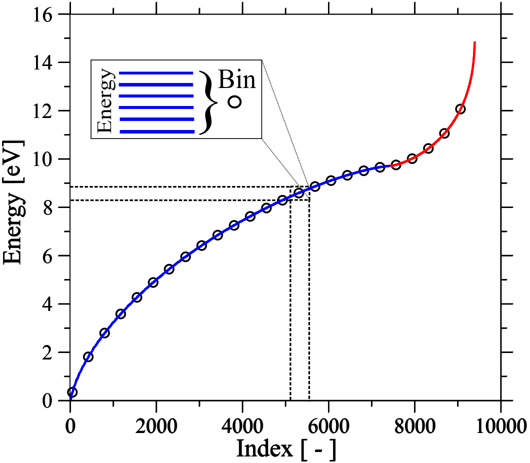


Simulation of internal energy excitation and dissociation processes behind a strong shockwave in N_2 flow

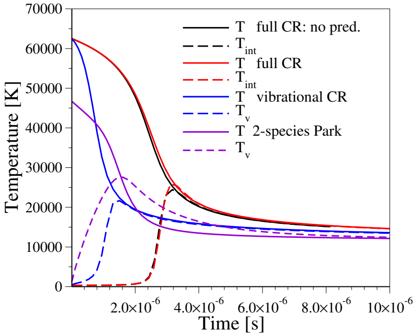
- The post-shock conditions are obtained from the Rankine-Hugoniot jump relations
- The 1D Euler eqs. for collisional model comprises
  - Mass conservation eqs. for N
  - Mass conservation eqs. for the 9390 rovibrational levels of N_2
  - Momentum conservation eq.
  - Total energy conservation eq.
- Free stream (1), post-shock (2), and LTE (3) conditions

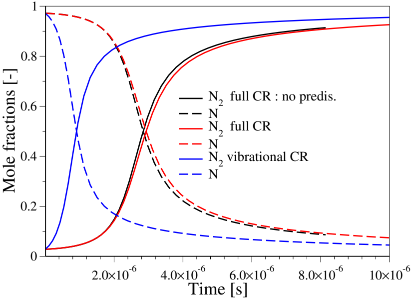
	1	2	3
T [K]	300	62,546	11,351
p [Pa]	13	10,792	13,363
u [km/s]	10	2.51	0.72
x_{N}	0.028	0.028	1

Temperature and composition profiles

[Panesi, Munafo, M., Jaffe 2013]

Temperatures T, T_v ($v = 1$), T_{int} ($v = 0, J = 10$)



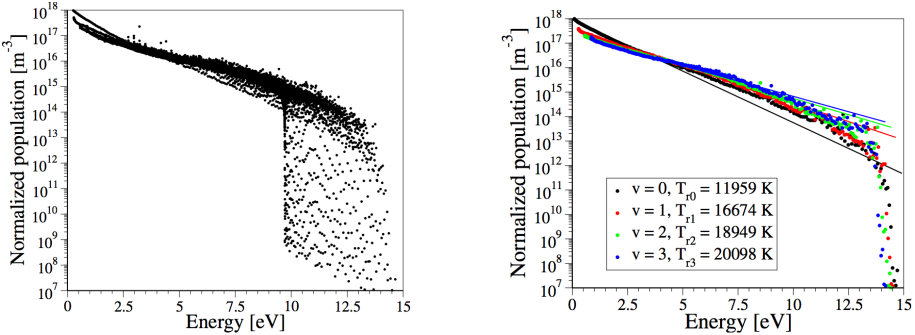


Free stream: $T_1 = 300$ K, $p_1 = 13$ Pa, $u_1 = 10$ km/s, $x_{\mathrm{N}1} \sim 2.8\%$, $10^{-5}\ \mathrm{s} \leftrightarrow 2.5\ \mathrm{cm}$

⇒ Thermalization and dissociation occur after a larger distance for the full collisional model

Rovibrational energy population of N_2

$n(v, J)$ in function of $E(v, J)$ at $t = 2.6 \times 10^{-6}$s (7mm)



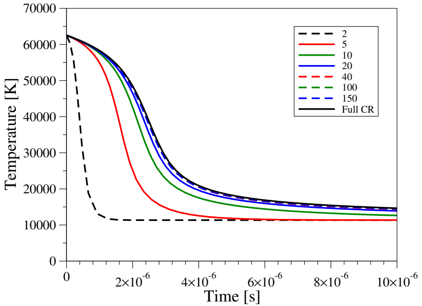
A rotational temperature $T_r(v)$ is introduced for each vibrational energy level v:

$$\frac{\sum_{J=0}^{J_{max(v)}} n(v,J)\Delta E(v,J)}{\sum_{J=0}^{J_{max(v)}} n(v,J)} = \frac{\sum_{J=0}^{J_{max(v)}} g_J \Delta E(v,J) \exp\left(\frac{-\Delta E(v,J)}{k T_r(v)}\right)}{\sum_{J=0}^{J_{max(v)}} g_J \exp\left(\frac{-\Delta E(v,J)}{k T_r(v)}\right)}$$

$\Rightarrow$ The assumption of equilibrium between the rotational and translational modes is questionable...

Coarse graining model for 3D CFD applications

- Coarse-graining model: lumping the energy levels into bins as a function of their global energy



Without predissociation reactions

Free stream: $T_1 = 300$ K, $p_1 = 13$ Pa, $u_1 = 10$ km/s, $x_{\mathrm{N1}} \sim 2.8\%$, $10^{-5}\ \mathrm{s} \leftrightarrow 2.5\ \mathrm{cm}$

$\Rightarrow$ The uniform distribution allows to describe accurately the internal energy relaxation and dissociation processes for $\sim$20 bins

[Munafo, Panesi, Jaffe, M. 2014]

Internal energy excitation in molecular gases

Wang-Chang-Uhlenbeck quasi-classical description

- The gas is composed of identical particles with internal degrees of freedom
- The particles may have only certain discrete internal energy levels
- These levels are labelled with an index i, with the set of indices I
- Quantity $E_i^\star$ stands for the energy of level $i \in \mathrm{I}$, and a_i, its degeneracy[a]

[a] Dimensional quantities are denoted by the superscript *

$$(i,j) \rightleftharpoons (i',j'), \quad i,j,i',j' \in \mathrm{I}, \quad (i',j')$$

- (i,j) and (i',j') are ordered pairs of energy levels
- with the net internal energy $E_{ij}^{i'j'\star} = E_{i'}^\star + E_{j'}^\star - E_i^\star - E_j^\star$

Collision zoology according to Ferziger and Kaper

- Elastic collisions

$$(i,j) \rightleftharpoons (i,j), \quad i,j \in \mathrm{I}$$

$\Rightarrow$ Both kinetic and internal energies are conserved: $E_{ij}^{i'j'\star} = 0$

- Inelastic collisions

$$(i,j) \rightleftharpoons (i',j'), \quad i,j,i',j' \in \mathrm{I}, \quad (i',j') \neq (i,j)$$

  - General case: $E_{ij}^{i'j'\star} \neq 0$
  - Resonant collisions: $E_{ij}^{i'j'\star} = 0$
    - *e.g.* exchange collision: $(i,j) \rightleftharpoons (j,i), \quad i,j \in \mathrm{I}, \ i \neq j$
  - Quasi-resonant collisions: $E_{ij}^{i'j'\star} \sim 0$

Boltzmann equation

- The temporal evolution of $f_i^\star(t^\star, \mathbf{x}^\star, \mathbf{c}_i^\star)$ is governed by

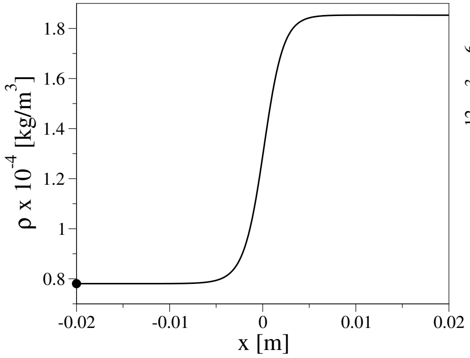
$$\partial_{t^\star} f_i^\star + \mathbf{c}_i^\star \cdot \boldsymbol{\partial}_{\mathbf{x}^\star} f_i^\star = \mathcal{J}_i^\star(f^\star), \quad i \in \mathsf{I}$$

with the partial collision operators

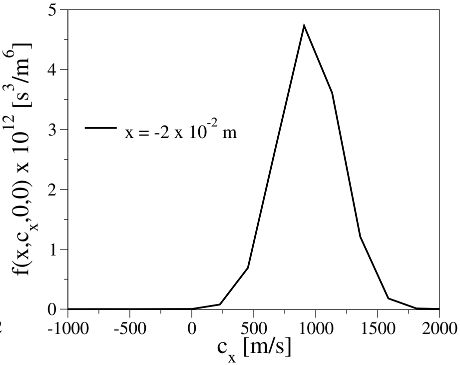
$$\mathcal{J}_{ij}^{i'j'\star}(f_i^\star, f_j^\star) = \int \left(f_{i'}^\star f_{j'}^\star \frac{a_i a_j}{a_{i'} a_{j'}} - f_i^\star f_j^\star \right) W_{ij}^{i'j'\star} \mathrm{d}\mathbf{c}_j^\star \mathrm{d}\mathbf{c}_{i'}^\star \mathrm{d}\mathbf{c}_{j'}^\star$$

- Development of a deterministic Boltzmann solver
  - [Bobylev and Rjasanov (1997,1999), Pareschi and Russo (2000), Gamba and Tharkabhushanam (2009,2010)]
  - [Munafo, Haack, Gamba, M., 2013]
- Difficulty: multi-species gas and inelastic collisions

Statistical description



Density



Velocity distribution function

Velocity distribution function for 1D shockwave (Mach 3) in a multi-energy level gas at different positions $x \in [-2\mathrm{cm}, +2\mathrm{cm}]$

[Munafo, Haack, Gamba, M., 2013]

- $n_i = \int f_i d\mathbf{c}_i$
- Dimensions: $[f_i] = [n_i] \, / \, [c_i]^3 = \mathrm{m}^{-3}/(\mathrm{m/s})^3 = \mathrm{s}^3/\mathrm{m}^6$

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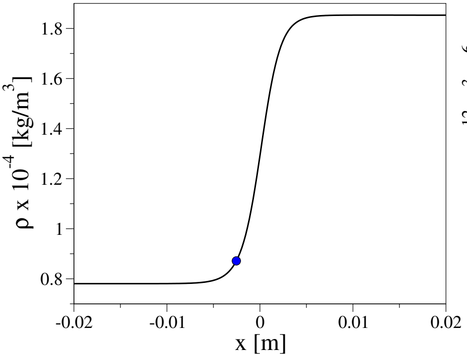

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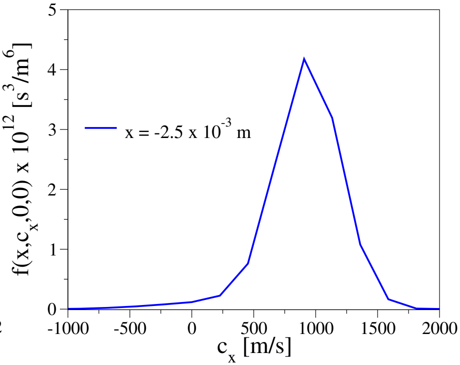

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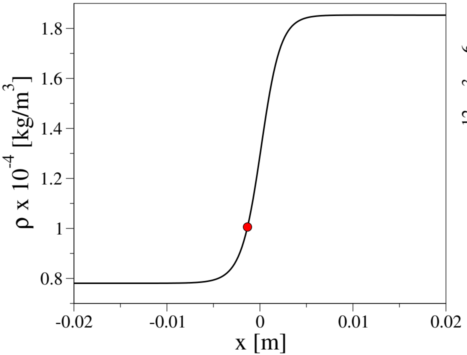

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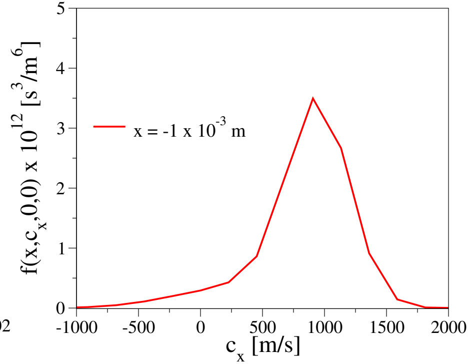

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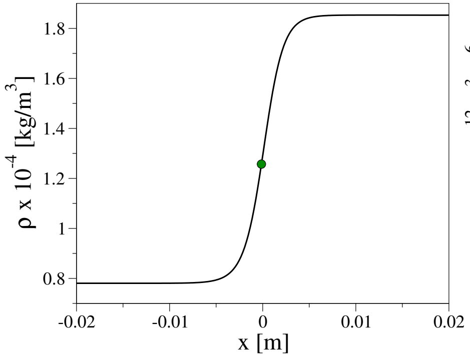

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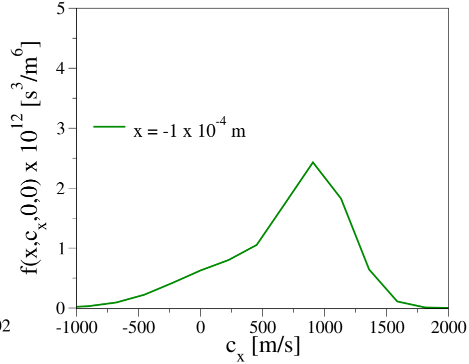

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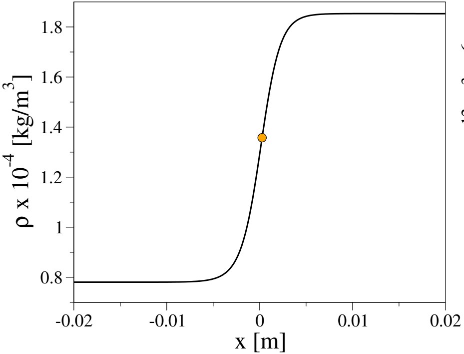
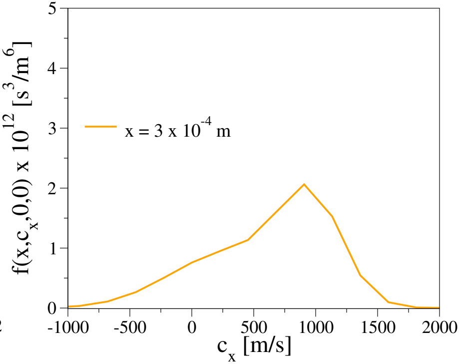


Density



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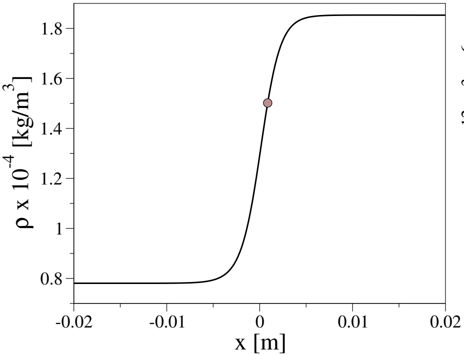

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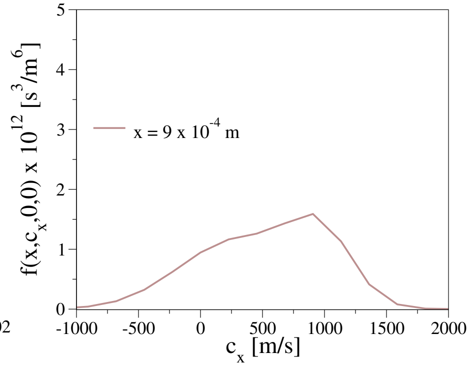

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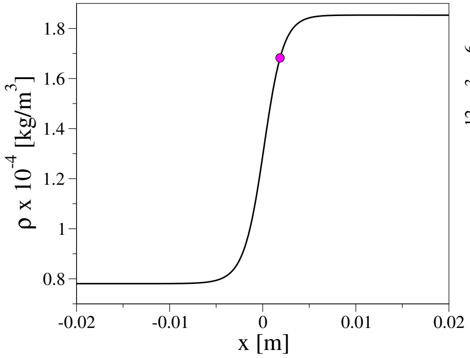

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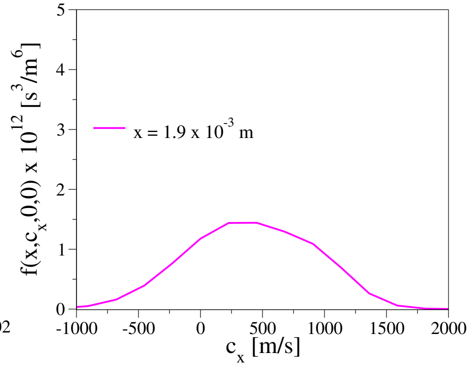

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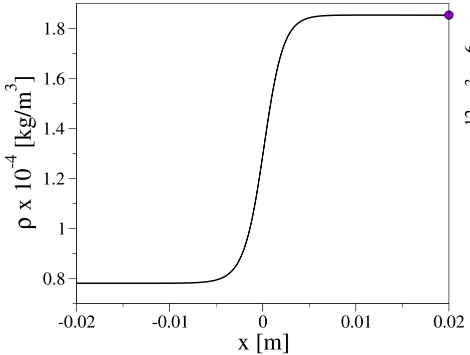

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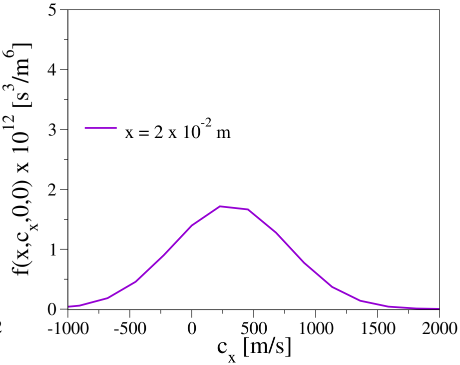

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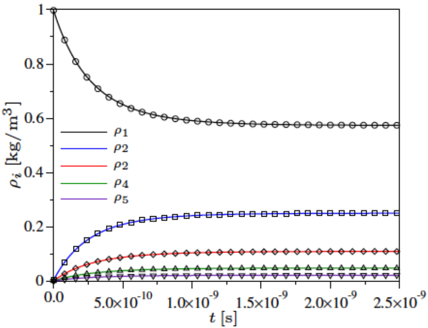
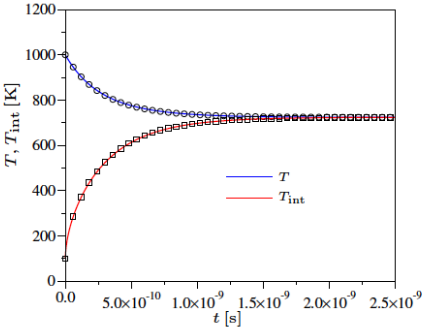
Relaxation towards equilibrium of a multi-energy level gas

- Translational and internal degrees of freedom initially in equilibrium at their own temperature
  - $\rho = 1\mathrm{kg/m^3}$, $T = 1000\,\mathrm{K}$, $T_{\mathrm{int}} = 100\,\mathrm{K}$
  - 5 levels, Anderson cross-section model
- Unbroken lines: Spectral Boltzmann Solver [Munafo, Haack, Gamba, M., 2013], symbols: DSMC [Torres, M. 2013]



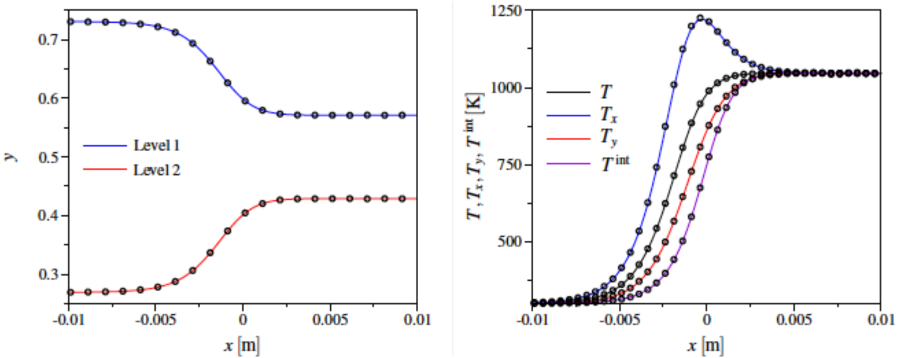
Species densities ($N_v = 16$)



Translational and internal temperatures ($N_v = 16$)

Flow across a normal shockwave for multi-energy level gas

- Free stream conditions
  - $\rho_\infty = 10^{-4}\mathrm{kg/m^3}$, $T_\infty = 300\,\mathrm{K}$, $v_\infty = 954\,\mathrm{m/s}$
  - 2 levels, Anderson cross-section model
- Unbroken lines: Spectral Boltzmann Solver [Munafo, Haack, Gamba, M., 2013], symbols: DSMC [Torres, M. 2013]



Outline

Translational thermal nonequilibrium and electromagnetic field influence in multicomponent plasma flows

- Plasma composed of **electrons** (index $\mathfrak{e}$), and **heavy particles**, atoms and molecules, neutral or ionized (set of indices H); the full mixture of species is denoted by the set $\mathrm{S} = \{\mathfrak{e}\} \cup \mathrm{H}$

- Scaling parameter: $\varepsilon = (m_{\mathfrak{e}}^0 / m_{\mathfrak{h}}^0)^{1/2} \ll 1$
  1. Classical mechanics description provided that
     $$\frac{1}{(\mathbf{n}^0)^{1/3}} \gg \frac{(\mathbf{m}_{\mathfrak{h}}^0 \, \mathrm{k_B} \mathbf{T}^0)^{1/2}}{\mathrm{h_P}} \quad \text{and} \quad \frac{\mathrm{k_B} T^0}{m_{\mathfrak{e}}^0} \ll c^2$$
  2. Binary charged interactions with screening of the Coulomb potential
     $$\boldsymbol{\Lambda} \simeq \mathbf{n}_{\mathfrak{e}}^0 \tfrac{4}{3} \pi \lambda_{\mathrm{Debye}}^3 \gg \mathbf{1}$$
  3. Reference electrical and thermal energies of the system are of the same order
     $$\mathbf{q}^0 \mathbf{E}^0 \mathbf{L}^0 \simeq \mathrm{k_B} \mathbf{T}^0$$
  4. Magnetic field influence determined by the Hall parameter magnitude **b**
     $$\beta_{\mathfrak{e}} = \frac{\mathbf{q}^0 \mathbf{B}^0}{\mathbf{m}_{\mathfrak{e}}^0} \mathbf{t}_{\mathfrak{e}}^0 = \varepsilon^{1-\mathbf{b}} \qquad (b < 0,\ b = 0,\ b = 1)$$
  5. Continuum description for compressible flows: $\mathcal{O}(M_{\mathfrak{h}}) \gg \varepsilon$
     $$\mathbf{Kn}\ \mathbf{M}_{\mathfrak{h}} \simeq \varepsilon$$

Dimensional analysis of the Boltzmann eq. [Petit, Darrozes 1975]

- 2 thermal speeds

$$V_{\mathfrak{e}}^0 = \sqrt{\frac{\mathrm{k_B}\, T^0}{m_{\mathfrak{e}}^0}}, \qquad V_{\mathfrak{h}}^0 = \sqrt{\frac{\mathrm{k_B}\, T^0}{m_{\mathfrak{h}}^0}} = \varepsilon\, V_{\mathfrak{e}}^0, \qquad \varepsilon = \sqrt{\frac{m_{\mathfrak{e}}^0}{m_{\mathfrak{h}}^0}}$$

- 2 kinetic temporal scales

$$t_{\mathfrak{e}}^0 = \frac{l^0}{V_{\mathfrak{e}}^0}, \qquad t_{\mathfrak{h}}^0 = \frac{l^0}{V_{\mathfrak{h}}^0} = \frac{t_{\mathfrak{e}}^0}{\varepsilon} \quad \text{with} \quad l^0 = \frac{1}{n^0 \sigma^0}$$

- 1 macroscopic temporal scale

$$t^0 = \frac{L^0}{v^0} = \frac{L^0}{l^0}\frac{l^0}{V_{\mathfrak{h}}^0}\frac{V_{\mathfrak{h}}^0}{v^0} = \frac{1}{Kn}\, t_{\mathfrak{h}}^0 \frac{1}{M_{\mathfrak{h}}} = \frac{t_{\mathfrak{h}}^0}{\varepsilon}$$

Change of variable: heavy-particle velocity frame [M3AS 2009]

- The peculiar velocities are given by the relations

$$\mathbf{C}_{\mathfrak{e}} = \mathbf{c}_{\mathfrak{e}} - \varepsilon M_{\mathfrak{h}} \mathbf{v}_{\mathfrak{h}}, \qquad \mathbf{C}_i = \mathbf{c}_i - M_{\mathfrak{h}} \mathbf{v}_{\mathfrak{h}}, \quad i \in \mathrm{H}$$

$\Rightarrow$ The heavy-particle diffusion flux vanishes

$$\sum_{j \in \mathrm{H}} \int m_j \mathbf{C}_j f_j \, \mathrm{d}\mathbf{C}_j = 0$$

- The choice of the heavy-particle velocity frame $\mathbf{v}_{\mathfrak{h}}$ is natural for plasmas. In this frame:
  - Heavy particles thermalize
  - All particles diffuse

Boltzmann equation: nondimensional form and scaling

- Electrons: $\mathfrak{e}$

$$\partial_t f_{\mathfrak{e}} + \frac{1}{\varepsilon M_{\mathfrak{h}}}(\mathbf{C}_{\mathfrak{e}} + \varepsilon M_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}})\cdot\partial_{\mathbf{x}} f_{\mathfrak{e}} + \frac{\varepsilon^{-b}}{M_{\mathfrak{h}} Kn} q_e \left[(\mathbf{C}_{\mathfrak{e}} + \varepsilon M_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}})\wedge\mathbf{B}\right]\cdot\partial_{\mathbf{C}_{\mathfrak{e}}} f_{\mathfrak{e}}$$
$$+\left(\frac{1}{\varepsilon M_{\mathfrak{h}}} q_e \mathbf{E} - \varepsilon M_{\mathfrak{h}} \frac{\mathrm{D}\mathbf{v}_{\mathfrak{h}}}{\mathrm{D}t}\right)\cdot\partial_{\mathbf{C}_{\mathfrak{e}}} f_{\mathfrak{e}} - (\partial_{\mathbf{C}_{\mathfrak{e}}} f_{\mathfrak{e}} \otimes \mathbf{C}_{\mathfrak{e}}):\partial_{\mathbf{x}}\mathbf{v}_{\mathfrak{h}} = \frac{1}{\varepsilon M_{\mathfrak{h}} Kn}\mathcal{J}_{\mathfrak{e}}$$

- Heavy particles: $i \in \mathrm{H}$

$$\partial_t f_i + \frac{1}{M_{\mathfrak{h}}}(\mathbf{C}_i + M_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}})\cdot\partial_{\mathbf{x}} f_i + \frac{\varepsilon^{2-b}}{M_{\mathfrak{h}} Kn} \frac{q_i}{m_i}\left[(\mathbf{C}_i + M_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}})\wedge\mathbf{B}\right]\cdot\partial_{\mathbf{C}_i} f_i$$
$$+\left(\frac{1}{M_{\mathfrak{h}}}\frac{q_i}{m_i}\mathbf{E} - M_{\mathfrak{h}}\frac{\mathrm{D}\mathbf{v}_{\mathfrak{h}}}{\mathrm{D}t}\right)\cdot\partial_{\mathbf{C}_i} f_i - (\partial_{\mathbf{C}_i} f_i \otimes \mathbf{C}_i):\partial_{\mathbf{x}}\mathbf{v}_{\mathfrak{h}} = \frac{1}{M_{\mathfrak{h}} Kn}\mathcal{J}_i$$

$\Rightarrow$ The multiscale analysis $(\varepsilon, Kn, \beta_{\mathfrak{e}})$ occurs at three levels

- in the kinetic eqs.
- in the crossed collision operators
- in the collisional invariants

Boltzmann equation: nondimensional form and scaling

- Collision operators:

$$\mathcal{J}_{\mathfrak{e}} = \mathcal{J}_{\mathfrak{e}\mathfrak{e}}(f_{\mathfrak{e}}, f_{\mathfrak{e}}) + \sum_{j \in \mathrm{H}} \mathcal{J}_{\mathfrak{e}j}(f_{\mathfrak{e}}, f_j)$$

$$\mathcal{J}_i = \frac{1}{\varepsilon}\mathcal{J}_{i\mathfrak{e}}(f_i, f_{\mathfrak{e}}) + \sum_{j \in \mathrm{H}} \mathcal{J}_{ij}(f_i, f_j), \quad i \in \mathrm{H}$$

- $\mathcal{J}_{\mathfrak{e}\mathfrak{e}}$ and $\mathcal{J}_{ij}$, $i, j \in \mathrm{H}$, are dealt with as usual
- $\mathcal{J}_{\mathfrak{e}i}$ and $\mathcal{J}_{i\mathfrak{e}}$, $i \in \mathrm{H}$, depend on ε

Theorem (Degond, Lucquin 1996, Graille, M., Massot 2009)

The crossed collision operators can be expanded in the form:

$$\begin{aligned}
\mathcal{J}_{\mathfrak{e}i}(f_{\mathfrak{e}}, f_i) &= \mathcal{J}^0_{\mathfrak{e}i}(f_{\mathfrak{e}}, f_i)(\mathbf{c}_{\mathfrak{e}}) + \varepsilon\mathcal{J}^1_{\mathfrak{e}i}(f_{\mathfrak{e}}, f_i)(\mathbf{c}_{\mathfrak{e}}) + \varepsilon^2\mathcal{J}^2_{\mathfrak{e}i}(f_{\mathfrak{e}}, f_i)(\mathbf{c}_{\mathfrak{e}}) \\
&\quad + \varepsilon^3\mathcal{J}^3_{\mathfrak{e}i}(f_{\mathfrak{e}}, f_i)(\mathbf{C}_{\mathfrak{e}}) + \mathcal{O}(\varepsilon^4) \\
\mathcal{J}_{i\mathfrak{e}}(f_i, f_{\mathfrak{e}}) &= \varepsilon\mathcal{J}^1_{i\mathfrak{e}}(f_i, f_{\mathfrak{e}})(\mathbf{c}_i) + \varepsilon^2\mathcal{J}^2_{i\mathfrak{e}}(f_i, f_{\mathfrak{e}})(\mathbf{c}_i) + \varepsilon^3\mathcal{J}^3_{i\mathfrak{e}}(f_i, f_{\mathfrak{e}})(\mathbf{C}_i) + \mathcal{O}(\varepsilon^4)
\end{aligned}$$

where $i \in \mathrm{H}$

Generalized Chapman-Enskog method [Graille, M., Massot 2009]

$$Kn = \frac{\varepsilon}{M_{\mathfrak{h}}} \Rightarrow \quad \begin{aligned} f_{\mathfrak{e}} &= f_{\mathfrak{e}}^0(1 + \varepsilon\hat{\phi}_{\mathfrak{e}} + \varepsilon^2\hat{\phi}_{\mathfrak{e}}^{(2)}) + \mathcal{O}(\varepsilon^3) \\ f_i &= \hat{f}_i^0(1 + \varepsilon\hat{\phi}_i) + \mathcal{O}(\varepsilon^2), \qquad i \in \mathrm{H} \end{aligned}$$

Order	Time	Heavy particles	Electrons
ε^{-2}	$t_{\mathfrak{e}}$	–	Eq. for $f_{\mathfrak{e}}^0$ Thermalization ($T_{\mathfrak{e}}$)
ε^{-1}	t_h^0	Eq. for f_i^0, $i \in \mathrm{H}$ Thermalization ($T_{\mathfrak{h}}$)	Eq. for $\phi_{\mathfrak{e}}$ Electron momentum relation
ε^0	t^0	Eq. for ϕ_i, $i \in \mathrm{H}$ Euler eqs.	Eq. for $\phi_{\mathfrak{e}}^{(2)}$ Zero-order drift-diffusion eqs.
ε	$\frac{t^0}{\varepsilon}$	Navier-Stokes eqs.	1^{st}-order drift-diffusion eqs.

Collisional invariants

- Electron and heavy-particle linearized collision operators

$$\mathcal{F}_{\mathfrak{e}}(\phi_{\mathfrak{e}}) = -\int f^0_{\mathfrak{e}1}\left(\phi'_{\mathfrak{e}} + \phi'_{\mathfrak{e}1} - \phi_{\mathfrak{e}} - \phi_{\mathfrak{e}1}\right)|\mathbf{C}_{\mathfrak{e}} - \mathbf{C}_{\mathfrak{e}1}|\sigma_{\mathfrak{e}\mathfrak{e}1}\, \mathrm{d}\boldsymbol{\omega}\mathrm{d}\mathbf{C}_{\mathfrak{e}1}$$

$$-\sum_{j\in\mathrm{H}} n_j \int \sigma_{\mathfrak{e}j}\left(|\mathbf{C}_{\mathfrak{e}}|^2, \boldsymbol{\omega}\cdot\frac{\mathbf{C}_{\mathfrak{e}}}{|\mathbf{C}_{\mathfrak{e}}|}\right)|\mathbf{C}_{\mathfrak{e}}|\left(\phi_{\mathfrak{e}}(|\mathbf{C}_{\mathfrak{e}}|\boldsymbol{\omega}) - \phi_{\mathfrak{e}}(\mathbf{C}_{\mathfrak{e}})\right)\mathrm{d}\boldsymbol{\omega}$$

$$\mathcal{F}_{\mathfrak{h}}(\phi) = -[\sum_{j\in\mathrm{H}} \int f^0_j \left(\phi'_i + \phi'_j - \phi_i - \phi_j\right)|\mathbf{C}_i - \mathbf{C}_j|\sigma_{ij}\mathrm{d}\boldsymbol{\omega}\mathrm{d}\mathbf{C}_j]_{i\in\mathrm{H}}$$

- Collisional invariants

$$\hat{\psi}^1_{\mathfrak{e}} = 1 \qquad \hat{\psi}^l_{\mathfrak{h}} = \left(m_i\delta_{il}\right)_{i\in\mathrm{H}}, \quad l\in\mathrm{H}$$

$$\hat{\psi}^2_{\mathfrak{e}} = \tfrac{1}{2}\mathbf{C}_{\mathfrak{e}}\cdot\mathbf{C}_{\mathfrak{e}} \qquad \hat{\psi}^{n^{\mathrm{H}}+\nu}_{\mathfrak{h}} = \left(m_i C_{i\nu}\right)_{i\in\mathrm{H}}, \quad \nu\in\{1,2,3\}$$

$$\hat{\psi}^{n^{\mathrm{H}}+4}_{\mathfrak{h}} = \left(\tfrac{1}{2}m_i\mathbf{C}_i\cdot\mathbf{C}_i\right)_{i\in\mathrm{H}}$$

- Properties

$$\langle\!\langle \mathcal{F}_{\mathfrak{e}}(\phi_{\mathfrak{e}}), \hat{\psi}^l_{\mathfrak{e}}\rangle\!\rangle_{\mathfrak{e}} = 0, \quad l \in \{1,2\}$$

$$\langle\!\langle \mathcal{F}_{\mathfrak{h}}(\phi_{\mathfrak{h}}), \hat{\psi}^l_{\mathfrak{h}}\rangle\!\rangle_{\mathfrak{h}} = 0, \quad l \in \{1,\dots,n^{\mathrm{H}}+4\}$$

Electron momentum relation

- The projection of the Boltzmann eq. at order ε^{-1} on the collisional invariants $\hat{\psi}_{\mathfrak{e}}^{l}$, $l \in \{1, 2\}$, is trivial
- Momentum is not included in the electron collisional invariants since

$$\langle\!\langle \mathcal{F}_{\mathfrak{e}}(\phi_{\mathfrak{e}}), \mathbf{C}_{\mathfrak{e}} \rangle\!\rangle_{\mathfrak{e}} \neq 0$$

  - At order ε^{-1}, the zero-order momentum transferred from electrons to heavy particles reads

$$\sum_{j \in \mathrm{H}} \langle\!\langle \mathcal{J}_{\mathfrak{e}j}^{0}(f_{\mathfrak{e}}^{0}\phi_{\mathfrak{e}}, \hat{f}_{j}^{0}), \mathbf{C}_{\mathfrak{e}} \rangle\!\rangle_{\mathfrak{e}} = \frac{1}{M_{\mathfrak{h}}} \partial_{\mathbf{x}} p_{\mathfrak{e}} - \frac{n_{\mathfrak{e}} q_{e}}{M_{\mathfrak{h}}} \mathbf{E}$$

  - A 1^{st}order electron momentum is also derived at order ε^{0}

[M., Graille, Massot, AIAA 2008]
[M., Graille, Massot, NASA/TM-214578 2008]
[Graille, M., Massot, M3AS 2009]

1^{st} order drift-diffusion and Navier-Stokes eqs.

- 1^{st} and 2^{nd} order transport fluxes for the electrons

$$\begin{aligned}\partial_t\rho_{\mathfrak{e}}+\boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_{\mathfrak{e}}\mathbf{v}_{\mathfrak{h}}) &= -\frac{1}{M_{\mathfrak{h}}}\boldsymbol{\partial}_{\mathbf{x}}\cdot[\rho_{\mathfrak{e}}(\mathbf{V}_{\mathfrak{e}}+\varepsilon\mathbf{V}_{\mathfrak{e}}^2)]\\ \partial_t(\rho_{\mathfrak{e}}e_{\mathfrak{e}})+\boldsymbol{\partial}_{\mathbf{x}}\cdot\left(\rho_{\mathfrak{e}}e_{\mathfrak{e}}\mathbf{v}_{\mathfrak{h}}\right)+p_{\mathfrak{e}}\boldsymbol{\partial}_{\mathbf{x}}\cdot\mathbf{v}_{\mathfrak{h}} &= -\frac{1}{M_{\mathfrak{h}}}\boldsymbol{\partial}_{\mathbf{x}}\cdot\left(\mathbf{q}_{\mathfrak{e}}+\varepsilon\mathbf{q}_{\mathfrak{e}}^2\right)+\frac{1}{M_{\mathfrak{h}}}\left(\mathbf{J}_{\mathfrak{e}}+\varepsilon\mathbf{J}_{\mathfrak{e}}^2\right)\cdot\mathbf{E}'+\delta_{b0}\varepsilon M_{\mathfrak{h}}\mathbf{J}_{\mathfrak{e}}\cdot\mathbf{v}_{\mathfrak{h}}\wedge\mathbf{B}\\ &\quad+\Delta E_{\mathfrak{e}}^0+\varepsilon\Delta E_{\mathfrak{e}}^1\end{aligned}$$

- 1^{st} order transport fluxes for the heavy particles

$$\begin{aligned}\partial_t\rho_i+\boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_i\mathbf{v}_{\mathfrak{h}}) &= -\frac{\varepsilon}{M_{\mathfrak{h}}}\boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_i\mathbf{V}_i),\quad i\in\mathrm{H}\\ \partial_t(\rho_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}})+\boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}}\otimes\mathbf{v}_{\mathfrak{h}}+\frac{1}{M_{\mathfrak{h}}^2}p\mathbb{I}) &= -\frac{\varepsilon}{M_{\mathfrak{h}}^2}\boldsymbol{\partial}_{\mathbf{x}}\cdot\boldsymbol{\Pi}_{\mathfrak{h}}+\frac{1}{M_{\mathfrak{h}}^2}nq\mathbf{E}+(\delta_{b0}\mathbf{I}_0+\delta_{b1}\mathbf{I})\wedge\mathbf{B}\\ \partial_t(\rho_{\mathfrak{h}}e_{\mathfrak{h}})+\boldsymbol{\partial}_{\mathbf{x}}\cdot(\rho_{\mathfrak{h}}e_{\mathfrak{h}}\mathbf{v}_{\mathfrak{h}})+p_{\mathfrak{h}}\boldsymbol{\partial}_{\mathbf{x}}\cdot\mathbf{v}_{\mathfrak{h}} &= -\varepsilon\boldsymbol{\Pi}_{\mathfrak{h}}:\boldsymbol{\partial}_{\mathbf{x}}\mathbf{v}_{\mathfrak{h}}-\frac{\varepsilon}{M_{\mathfrak{h}}}\boldsymbol{\partial}_{\mathbf{x}}\cdot\mathbf{q}_{\mathfrak{h}}+\frac{\varepsilon}{M_{\mathfrak{h}}}\mathbf{J}_{\mathfrak{h}}\cdot\mathbf{E}'+\Delta E_{\mathfrak{h}}^0+\varepsilon\Delta E_{\mathfrak{h}}^1\end{aligned}$$

  - with 1^{st} order energy exchange terms

$$\begin{aligned}\Delta E_{\mathfrak{h}}^1+\Delta E_{\mathfrak{e}}^1 &= 0\\ \Delta E_{\mathfrak{h}}^1 &= \sum_{j\in\mathrm{H}} n_j\mathbf{V}_j\cdot\mathbf{F}_{j\mathfrak{e}}\end{aligned}$$

  - and average electron force acting on the heavy particles

$$\mathbf{F}_{i\mathfrak{e}}=\int Q_{i\mathfrak{e}}^{(1)}(|\mathbf{C}_{\mathfrak{e}}|^2)\,|\mathbf{C}_{\mathfrak{e}}|\mathbf{C}_{\mathfrak{e}}\,f_{\mathfrak{e}}^0\phi_{\mathfrak{e}}\,\mathrm{d}\mathbf{C}_{\mathfrak{e}},\quad i\in\mathrm{H}$$

Kolesnikov effect [Graille, M., Massot 2008]

- The second-order electron diffusion velocity and heat flux are also proportional to the heavy-particle diffusion velocities
- We refer to this coupling phenomenon as the Kolesnikov effect (1974)
- The heavy-particle diffusion velocities

$$\mathbf{V}_i = -\sum_{j\in \mathrm{H}} D_{ij}\hat{\mathbf{d}}_j - \theta_i^{\mathfrak{h}} \partial_{\mathbf{x}} \ln T_{\mathfrak{h}}, \quad i \in \mathrm{H}$$

are proportional to

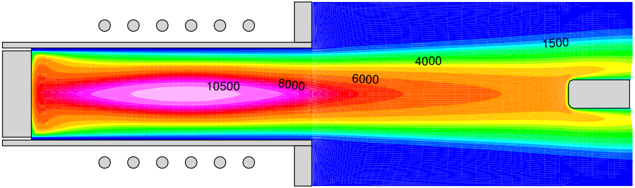
  - The diffusion driving forces $\hat{\mathbf{d}}_i = \frac{1}{p_{\mathfrak{h}}}\partial_{\mathbf{x}} p_i - \frac{n_i q_i}{p_{\mathfrak{h}}}\mathbf{E} - \frac{n_i M_{\mathfrak{h}}}{p_{\mathfrak{h}}}\mathbf{F}_{i\mathfrak{e}}$
  - The heavy-particle temperature gradient (Soret effect)

- The average electron force $\mathbf{F}_{i\mathfrak{e}}$ contributes to the diffusion driving force $\hat{\mathbf{d}}_i$
  - The average electron force acting on the heavy particles is expressed in terms of the electron driving force and temperature gradient

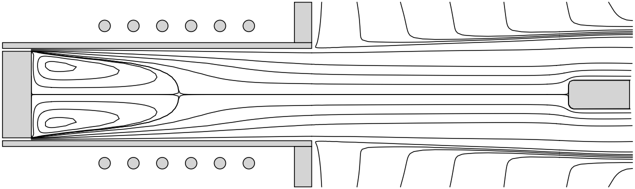
$$\mathbf{F}_{i\mathfrak{e}} = -\frac{p_{\mathfrak{e}}}{n_i M_{\mathfrak{h}}}\alpha_{\mathfrak{e}i}\mathbf{d}_{\mathfrak{e}} - \frac{p_{\mathfrak{e}}}{n_i M_{\mathfrak{h}}}\chi_i^{\mathfrak{e}}\partial_{\mathbf{x}} \ln T_{\mathfrak{e}}$$

LTE computation of the VKI Plasmatron facility

(p=10 000 Pa, P=120 kW, $\dot{m}$=8 g/s) [M. and Degrez 2004]



Temperature field [K]



Streamlines

Modified Grad-Zhdanov eqs. for multicomponent plasmas

Mass diffusion equations [Martin, Torrilhon, M. 2010]

$$\frac{\partial p_{\mathfrak{e}}}{\partial x_r} - n_{\mathfrak{e}} q_e E^r = -\frac{\varepsilon}{Kn} \sum_{j \in \mathrm{H}} n_j F^r_{je},$$

$$Kn \frac{\mathrm{D}(\rho_i \omega_i^r)}{\mathrm{D}t} + Kn \rho_i \Big(\omega_i^r \frac{\partial v_h^s}{\partial x_s} + \omega_i^s \frac{\partial v_h^r}{\partial x_s}\Big) + \frac{1}{M_{\mathfrak{h}}} \Big(Kn \frac{\partial \pi_i^{rs}}{\partial x_s} + \frac{\partial p_i}{\partial x_r} - n_i q_i E^r\Big)$$

$$= \frac{1}{M_{\mathfrak{h}} Kn} \sum_{j \in \mathrm{H}} \int \mathcal{J}_{ij}(f_i, f_j)\, m_i C_i^r \, d\mathbf{C_i} + \frac{\varepsilon}{M_{\mathfrak{h}} Kn} n_i F^s_{ie}, \quad i \in \mathrm{H}$$

- with the average electron force acting on the heavy particle $i \in \mathrm{H}$

$$F^s_{ie} = -\frac{1}{M_{\mathfrak{h}}} \Big[\omega_e^r \frac{I^{rs}_{1,i}}{T_e} - \frac{h_e^r}{5 p_e T_e} \Big(\frac{I^{rs}_{3,i}}{T_e} - 5 I^{rs}_{1,i}\Big)\Big]$$

$\Rightarrow$ Momentum conservation

$$\rho_{\mathfrak{h}} \frac{\mathrm{D} v_h^r}{\mathrm{D}t} + \frac{1}{M_{\mathfrak{h}}^2} \Big(Kn \frac{\partial \pi_h^{sr}}{\partial x_s} + \frac{\partial p}{\partial x_r}\Big) = 0$$

Outline

Final thoughts

- Plasmadynamical models based on multiscale CE method
  - Scaling derived from a dimensional analysis of the Boltzmann eq.
  - Collisional invariants identified in the kernel of collision operators
  - Macroscopic conservation eqs. follow from Fredholm's alternative
  - Laws of thermodynamics and law of mass action are satisfied
  - Well-posedness of the transport properties is established, provided that some conditions on the kinetic data are met
- Advantages compared to conventional models for plasma flows
  - Mathematical structure of the conservation equations well identified
  - Rigorous derivation of a set of macroscopic equations where hyperbolic and parabolic scalings are entangled [Bardos, Golse, Levermore 1991]
  - The mathematical structure of the transport matrices is readily used to build transport algorithms (direct linear solver / convergent iterative Krylov projection methods) [Ern and Giovangigli 1994, M. and Degrez 2004]
- Future work
  - CE for dissociation of molecular gases and radiation
  - New application: radar detection of meteors

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