10th International Conference on Operations Research

La Habana (Cuba), March 6 - 9, 2012

Multi–temperature hydrodynamic equations from kinetic theory for rarefied gas mixtures

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(joint work with G. Martalò, G. Spiga)

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Summary

- Preliminaries: physical setting and some bibliography

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- Rescaled kinetic equations for polyatomic gases and derivation of multi–temperature Euler closure

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- Rescaled kinetic equations for polyatomic gases and derivation of multi–temperature Euler closure
- Explicit exchange rates for simple collision models and analysis of the hydrodynamic system

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set of integro–differential equations of Boltzmann type for the distribution functions $f_s(\mathbf{x}, \mathbf{v}, t)$, $s = 1, \ldots, Q$

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{Q} I_{sr}[f_s, f_r]$$

$I_{sr}[f_s, f_r]$: Boltzmann collision operator describing the effects of binary collisions involving particles of gases A_s and A_r

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- Elastic collisions preserve number densities of single species, global momentum and global kinetic energy
- More complex situations like polyatomic gases or chemically reacting mixtures may involve exchange of internal or chemical energy (with conservation of total energy)

Some bibliography on the kinetic approach

- Kinetic models of Boltzmann type, possibly accounting for internal energy levels and/or dissociation and recombination processes

  [Chapman, Cowling (1970), Groppi, Spiga (1999), Giovangigli (1999), Groppi, Rossani, Spiga (2000), Polewczak (2001), Desvillettes, Monaco, Salvarani (2005), ...]

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- Kinetic models of BGK type including chemical reactions

  [Andries, Aoki, Perthame (2002), Monaco, Pandolfi Bianchi (2004), Groppi, Spiga (2004), Kremer, Pandolfi Bianchi, Soares (2006), Asinari (2008), Bisi, Cáceres, Spiga (2010), ...]

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- Hydrodynamic closures in elastically dominated regimes

  [<u>Review</u>: Bisi, Groppi, Spiga (2005), ...]

- Mixtures diffusing in a background medium: hydrodynamic equations of reaction–diffusion type

  [De Masi, Ferrari, Lebowitz (1986), De Masi, Presutti (1991), Spigler, Zanette (1993), Bisi, Desvillettes (2006), Bisi, Spiga (2006), ...]

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Remark

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Aim of our work

We present a formal derivation, starting from suitably rescaled kinetic equations, of an hydrodynamic description involving temperatures and velocities of single gases

References on multi–temperature hydrodynamics

- In the description of several physical problems, like plasmas, aerothermodynamics, thermally non–equilibrium conditions

  [Park (1990), Bose (2003), Kustova, Nagnibeda (2006), ...]

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  Here hydrodynamic variables are mass densities, global velocity, and a unique translational temperature for the mixture plus an internal (vibrational) temperature for each species

Kinetic model for polyatomic gases

[Groppi, Spiga (1999), Desvillettes, Monaco, Salvarani (2005)]

- Each species A_s, $s = 1, \ldots, Q$, is endowed with a structure of $N > 1$ discrete energy levels

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- The QN different components are ordered in such a way that the s–th gas may be regarded as the equivalence class of the indices $i \equiv s$ modulo Q
- If A_i, $1 \leq i \leq QN$, denotes the general component, and E_i the corresponding energy of its state, the general binary interaction is written as

$$A_i + A_j \rightleftharpoons A_h + A_k \qquad\qquad i \equiv h \qquad\qquad j \equiv k$$

The net increase of internal energy $\Delta E_{ij}^{hk} = E_h + E_k - E_i - E_j$ must be compensated by an opposite variation of the kinetic energies

Kinetic equations for functions $f_i(\mathbf{x},\mathbf{v},t)$, $i=1,\ldots,NQ$

$$\frac{\partial f_i}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_i \quad = \sum_{(j,h,k)\in D_i} \iint K_i^{ijhk}[\underline{f}](\mathbf{v},\mathbf{w},\hat{\mathbf{n}}')\,d\mathbf{w}\,d\hat{\mathbf{n}}',$$

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$$K_i^{ijhk}[\underline{f}](\mathbf{v},\mathbf{w},\hat{\mathbf{n}}') = \Theta(g^2-\delta_{ij}^{hk})B_{ij}^{hk}(g,\hat{\mathbf{n}}\cdot\hat{\mathbf{n}}') \cdot \left[\left(\frac{\mu_{ij}}{\mu_{hk}}\right)^3 f_h\left(\mathbf{v}_{ij}^{hk}\right) f_k\left(\mathbf{w}_{ij}^{hk}\right) - f_i(\mathbf{v})f_j(\mathbf{w})\right]$$

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with

- $\mathbf{g} = \mathbf{v} - \mathbf{w} = g\,\hat{\mathbf{n}}$ relative velocity
- B_{ij}^{hk} collision kernel (relative speed times cross section)
- μ_{ij} reduced mass
- Θ unit step function introduces a threshold for the collision
  if $\delta_{ij}^{hk} = 2\,\Delta E_{ij}^{hk} / \mu_{ij} > 0$
- $\mathbf{v}_{ij}^{hk}$, $\mathbf{w}_{ij}^{hk}$ post–collision velocities

Collision equilibria

$$\mathcal{M}_i(\mathbf{v}) = n_i \left(\frac{m_s}{2\pi KT}\right)^{3/2} \exp\left[-\frac{m_s}{2KT}(\mathbf{v}-\mathbf{u})^2\right] \;\; \forall i \equiv s,\ \forall s = 1,\ldots,Q$$

where

$$n_i = \psi_i(E_i, T)\, N_s \qquad\qquad \psi_i(E_i,T) = \frac{\exp\left(-\frac{E_i - E_s}{KT}\right)}{\sum_{i\equiv s} \exp\left(-\frac{E_i - E_s}{KT}\right)} = \frac{\exp\left(-\frac{E_i - E_s}{KT}\right)}{Z_s(T)}$$

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H–functional

$$H = \sum_{s=1}^{Q} \sum_{i\equiv s} \int f_i \log f_i \, d\mathbf{v}$$

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$Q+4$ independent **conservation laws**:

$N_s = \sum_{i\equiv s} n_i \,, \quad s = 1, \dots, Q,$ number densities of single species

$\mathbf{u}$ global momentum

$\frac{3}{2} NKT + \sum_{i=1}^{QN} E_i n_i$ total (kinetic + internal) energy

Rescaled kinetic model

Among all possible interactions

$$A_i + A_j \rightleftharpoons A_h + A_k \qquad\qquad i \equiv h \qquad\quad j \equiv k$$

we assume the mean free path for collisions between components of the same species much shorter than for collisions between components of different species:

$$\text{FAST}: \qquad i \equiv j \equiv h \equiv k$$

$$\text{SLOW}: \qquad i \not\equiv j \qquad\quad i \equiv h \qquad\quad j \equiv k$$

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Scaled kinetic equations

$$\boxed{\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \frac{1}{\epsilon} I_i^{FA} + I_i^{SL}}$$

Investigation of the leading operators I_i^{FA}

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Dominant collision equilibria

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$$\forall i \equiv s\,, \quad \forall s = 1, \ldots, Q,$$

with free parameters N_s, $\mathbf{u}_s$, T_s

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$\Rightarrow$ $5Q$ collision invariants corresponding to preservation of number density, momentum, and kinetic energy within each species

$\Rightarrow$ $5Q$ macroscopic “conservation” (for the fast operator) equations, that we aim at closing at Euler accuracy

$$\frac{\partial N_s}{\partial t} + \nabla_{\mathbf{x}} \cdot \left(N_s \mathbf{u}_s\right) = 0$$

$$\frac{\partial}{\partial t}(\rho_s \mathbf{u}_s) + \nabla_{\mathbf{x}} \cdot \sum_{i \equiv s} \left(\rho_i \mathbf{u}_i \otimes \mathbf{u}_i + \mathbf{P}_i\right) = \mathbf{R}_s$$

$$\frac{\partial}{\partial t}\left[\sum_{i \equiv s}\left(\frac{1}{2}\rho_i u_i^2 + \frac{3}{2} n_i K T_i + E_i n_i\right)\right] + \nabla_{\mathbf{x}} \cdot \left\{\sum_{i \equiv s}\left[\left(\frac{1}{2}\rho_i u_i^2 + \frac{3}{2} n_i K T_i + E_i n_i\right)\mathbf{u}_i + \mathbf{P}_i \cdot \mathbf{u}_i + \mathbf{q}_i\right]\right\} = S_s$$

where $\mathbf{R}_s$ and S_s are collision contributions due to the slow interactions

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$$\left.\left.\left. + \frac{3}{2} n_i K T_i + E_i n_i\right)\mathbf{u}_i + \mathbf{P}_i \cdot \mathbf{u}_i + \mathbf{q}_i\right]\right\} = S_s$$

where $\mathbf{R}_s$ and S_s are collision contributions due to the slow interactions

They are provided by weak forms of the Boltzmann operators corresponding to the test functions $\varphi_i(\mathbf{v}) = m_i \mathbf{v}$ and $\varphi_i(\mathbf{v}) = \frac{1}{2} m_i v^2 + E_i$

$$\mathbf{R}_s = \sum_{r \neq s} \sum_{i,h \equiv s} \sum_{j,k \equiv r} \iiint m_s \left(\mathbf{v}_{ij}^{hk} - \mathbf{v} \right) B_{ij}^{hk}(g, \hat{\mathbf{n}} \cdot \hat{\mathbf{n}}') \Theta(g^2 - \delta_{ij}^{hk}) f_i(\mathbf{v}) f_j(\mathbf{w}) d\mathbf{v} d\mathbf{w} d\hat{\mathbf{n}}'$$

$$S_s = \sum_{r \neq s} \sum_{i,h \equiv s} \sum_{j,k \equiv r} \iiint \left\{ \frac{1}{2} m_s \left[(v_{ij}^{hk})^2 - v^2 \right] + E_h - E_i \right\}$$

$$\times B_{ij}^{hk}(g, \hat{\mathbf{n}} \cdot \hat{\mathbf{n}}') \Theta(g^2 - \delta_{ij}^{hk}) f_i(\mathbf{v}) f_j(\mathbf{w}) \, d\mathbf{v} \, d\mathbf{w} \, d\hat{\mathbf{n}}'$$

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They correctly reproduce the overall conservations of momentum and energy

$$\sum_{s=1}^{Q} \mathbf{R}_s = \mathbf{0} \qquad \sum_{s=1}^{Q} S_s = 0$$

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$$\sum_{s=1}^{Q} \mathbf{R}_s = \mathbf{0} \qquad\qquad \sum_{s=1}^{Q} S_s = 0$$

The zero–order closure is achieved by substituting into macroscopic equations the fast collision equilibrium $f_i^M(N_s, \mathbf{u}_s, T_s)$ for the actual distribution functions

Fluid–dynamic Euler equations

$$\frac{\partial N_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (N_s \mathbf{u}_s) = 0$$

$$\frac{\partial}{\partial t} (\rho_s \mathbf{u}_s) + \nabla_{\mathbf{x}} \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla_{\mathbf{x}} (N_s K T_s) = \hat{\mathbf{R}}_s$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_s u_s^2 + \frac{3}{2} N_s K T_s + N_s \bar{E}_s (T_s) \right) +$$

$$+ \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho_s u_s^2 + \frac{5}{2} N_s K T_s + N_s \bar{E}_s (T_s) \right) \mathbf{u}_s \right] = \hat{S}_s$$

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where

$$\bar{E}_s (T_s) = \frac{1}{Z_s (T_s)} \sum_{i \equiv s} E_i \exp \left(-\frac{E_i - E_s}{K T_s} \right)$$

and $\hat{\mathbf{R}}_s$, $\hat{S}_s$ have become known functions of the $5Q$ unknown fields N_s, $\mathbf{u}_s$, T_s

Evaluation of collision contributions:
crucial steps and difficulties

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1) The product of two Maxwellians at different velocities and temperatures may be cast as

$$f_i^M(\mathbf{v}) f_j^M(\mathbf{w}) = \frac{N_s}{Z_s\left(T_s\right)} \frac{N_r}{Z_r\left(T_r\right)} \left(\frac{m_s}{2\pi K T_s}\right)^{\frac{3}{2}} \left(\frac{m_r}{2\pi K T_r}\right)^{\frac{3}{2}} \exp\left(-\frac{E_i - E_s}{K T_s} - \frac{E_j - E_r}{K T_r}\right) \exp\left[-\alpha_{sr}\left(\mathbf{G}_{sr} + \gamma_{sr}\mathbf{g} - \boldsymbol{\delta}_{sr}\right)^2\right] \exp\left\{-\beta_{sr}\left[\mathbf{g} - \left(\mathbf{u}_s - \mathbf{u}_r\right)\right]^2\right\}$$

where

$$\mathbf{G}_{sr} = \frac{m_s}{m_s + m_r}\mathbf{v} + \frac{m_r}{m_s + m_r}\mathbf{w} \qquad \mathbf{g} = \mathbf{v} - \mathbf{w}$$

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where

$$\mathbf{G}_{sr} = \frac{m_s}{m_s + m_r}\mathbf{v} + \frac{m_r}{m_s + m_r}\mathbf{w} \qquad \mathbf{g} = \mathbf{v} - \mathbf{w}$$

$$\alpha_{sr} = \frac{m_s}{2KT_s} + \frac{m_r}{2KT_r} \qquad \beta_{sr} = \left(\frac{2KT_s}{m_s} + \frac{2KT_r}{m_r}\right)^{-1}$$

$$\gamma_{sr} = \frac{\mu_{sr}}{\alpha_{sr}}\left(\frac{1}{2KT_s} - \frac{1}{2KT_r}\right) \qquad \boldsymbol{\delta}_{sr} = \frac{1}{\alpha_{sr}}\left(\frac{m_s}{2KT_s}\mathbf{u}_s + \frac{m_r}{2KT_r}\mathbf{u}_r\right)$$

2) Angular integrations may be cast in terms of suitably averages of the collision kernel:

$$\bar{B}_{ij}^{hk}(g) = B_{ij}^{hk(0)}(g) - \left(1 - \frac{\delta_{ij}^{hk}}{g^2}\right)^{\frac{1}{2}} B_{ij}^{hk(1)}(g)\,.$$

where

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3) Integrations over $\mathbf{G}_{sr}$ may be explicitly performed, and it can be checked that

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$\Rightarrow$ This allows to push further analytical manipulations in polar coordinates, leaving only a one–dimensional integral with respect to $g = |\mathbf{g}|$

$$
\hat{\mathbf{R}}_{sr} = -\frac{\mu_{sr}}{2\sqrt{\pi}} \, \frac{1}{\beta_{sr}^{3/2} |\mathbf{u}_s - \mathbf{u}_r|^2} \, \frac{N_s}{Z_s\left(T_s\right)} \frac{N_r}{Z_r\left(T_r\right)}
$$

$$
\times \sum_{i,h\equiv s} \sum_{j,k\equiv r} \exp\left(-\frac{E_i - E_s}{KT_s} - \frac{E_j - E_r}{KT_r} \right) X_{ij}^{hk}(|\mathbf{u}_s - \mathbf{u}_r|, \beta_{sr}) \, \frac{\mathbf{u}_s - \mathbf{u}_r}{|\mathbf{u}_s - \mathbf{u}_r|}
$$

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where, setting $\Delta_{sr} = \beta_{sr}^{1/2} |\mathbf{u}_s - \mathbf{u}_r|$,

$$X_{ij}^{hk}(|\mathbf{u}_s - \mathbf{u}_r|, \beta_{sr}) = \int_0^\infty \Theta\left(x^2 - \beta_{sr}\delta_{ij}^{hk}\right) \bar{B}_{ij}^{hk}(\beta_{sr}^{-1/2} x)$$

$$\times \left\{(2\Delta_{sr} x - 1)\exp\left[-(x - \Delta_{sr})^2\right] + (2\Delta_{sr} x + 1)\exp\left[-(x + \Delta_{sr})^2\right]\right\} x\,dx$$

$$\hat{\mathbf{R}}_{sr} = -\frac{\mu_{sr}}{2\sqrt{\pi}}\,\frac{1}{\beta_{sr}^{3/2}|\mathbf{u}_s-\mathbf{u}_r|^2}\,\frac{N_s}{Z_s\left(T_s\right)}\frac{N_r}{Z_r\left(T_r\right)}$$

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$$Y_{ij}^{hk} = \int_0^\infty \Theta\left(x^2-\beta_{sr}\delta_{ij}^{hk}\right)\Big\{\mu_{sr}\gamma_{sr}\beta_{sr}^{-1}x^3\bar{B}_{ij}^{hk}\left(\beta_{sr}^{-1/2}x\right)$$

$$+\left[\varepsilon_{sr}\left(E_h-E_i\right)-\varepsilon_{rs}\left(E_k-E_j\right)\right]xB_{ij}^{hk(0)}\left(\beta_{sr}^{-1/2}x\right)\Big\}$$

$$\times\left\{\exp\left[-\left(x-\Delta_{sr}\right)^2\right]-\exp\left[-\left(x+\Delta_{sr}\right)^2\right]\right\}dx$$

Exchange rates for simple models

Maxwell molecule frame

If for a given collision $(i,j) \to (h,k)$ we assume B_{ij}^{hk} depending only on $\hat{\mathbf{n}} \cdot \hat{\mathbf{n}}' \Rightarrow \bar{B}_{ij}^{hk}(g) = B_{ij}^{hk(0)}(g) = \kappa_{ij}^{hk} = \mathrm{constant}$

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We get $$X_{ij}^{hk} = 2\sqrt{\pi}\kappa_{ij}^{hk}\Delta_{sr}^3 \qquad \text{for} \qquad \delta_{ij}^{hk} \le 0$$

$$\begin{aligned} X_{ij}^{hk} &= 2\sqrt{\pi}\kappa_{ij}^{hk}\left\{\Delta_{sr}^3\mathcal{F}_1(\beta_{sr},\Delta_{sr}) - \left(\Delta_{sr}^2 - \tfrac{1}{2}\right)\mathcal{F}_2(\beta_{sr},\Delta_{sr})\right. \\ &\left. +\Delta_{sr}\sqrt{\beta_{sr}\,\delta_{ij}^{hk}}\,\mathcal{F}_3(\beta_{sr},\Delta_{sr})\right\} \qquad \text{for} \qquad \delta_{ij}^{hk} > 0 \end{aligned}$$

(with $\mathcal{F}_1$, $\mathcal{F}_2$, $\mathcal{F}_3$ suitable combinations of exponentials and error functions)

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(with $\mathcal{F}_1$, $\mathcal{F}_2$, $\mathcal{F}_3$ suitable combinations of exponentials and error functions)

Remark: Unfortunately, this does not make explicit the whole exchange rate $\hat{\mathbf{R}}_s$, since the sums in $\hat{\mathbf{R}}_s$ involve also its "reciprocal" X_{hk}^{ij}, for which the collision kernel is not Maxwellian anymore:

$$\bar{B}_{hk}^{ij}(g) = \kappa_{ij}^{hk}\left(1 + \frac{\delta_{ij}^{hk}}{g^2}\right)^{1/2}$$

Monoatomic gases

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Hard spheres

$$\left(\bar{B}_{sr}^{sr}(g) = \eta_{sr}^{sr} g, \qquad \Delta_{sr} = \beta_{sr}^{1/2} |\mathbf{u}_s - \mathbf{u}_r|\right)$$

$$\hat{\mathbf{R}}_{sr} = -\frac{\eta_{sr}^{sr}\mu_{sr}N_sN_r}{\sqrt{\pi}\beta_{sr}^{1/2}} (\mathbf{u}_s - \mathbf{u}_r) \left[\frac{4\Delta_{sr}^4 + 4\Delta_{sr}^2 - 1}{4\Delta_{sr}^3} \sqrt{\pi}\, \mathrm{erf}(\Delta_{sr}) + \frac{2\Delta_{sr}^2 + 1}{2\Delta_{sr}^2} \exp(-\Delta_{sr}^2) \right]$$

$$\begin{aligned} \hat{S}_{sr} = -\mu_{sr} N_s N_r \eta_{sr}^{sr} \beta_{sr}^{-1/2} \Bigg\{ & \frac{1}{\alpha_{sr}} \left[\left(\Delta_{sr}^2 + 1 - \frac{1}{4\Delta_{sr}^2} \right) \frac{\mathrm{erf}(\Delta_{sr})}{\Delta_{sr}} \right. \\ & \left. + \left(1 + \frac{1}{2\Delta_{sr}^2} \right) \frac{e^{-\Delta_{sr}^2}}{\sqrt{\pi}} \right] \left(\frac{m_s}{2KT_s}\mathbf{u}_s + \frac{m_r}{2KT_r}\mathbf{u}_r \right) \cdot (\mathbf{u}_s - \mathbf{u}_r) + \frac{2K(T_s - T_r)}{m_s + m_r} \\ & \times \left[\left(\Delta_{sr}^4 + 3\Delta_{sr}^2 + \frac{3}{4} \right) \frac{\mathrm{erf}(\Delta_{sr})}{\Delta_{sr}} + \left(\Delta_{sr}^2 + \frac{5}{2} \right) \frac{e^{-\Delta_{sr}^2}}{\sqrt{\pi}} \right] \Bigg\} \end{aligned}$$

Chemically reacting mixture

Assumptions:

- Mixture of 4 gases that, besides elastic collisions, are subject to a bimolecular and reversible chemical reaction

$$A_1 + A_2 \rightleftharpoons A_3 + A_4$$

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In equations for number densities, suitable reactive contributions appear:

$$Q_s^{\text{ch}} = \lambda_s \, B_{\text{ch}}^0 \left[\left(\frac{\mu_{12}}{\mu_{34}} \right)^{3/2} N_3 N_4 - N_1 N_2 \right], \qquad \lambda_1 = \lambda_2 = -\lambda_3 = -\lambda_4 = 1$$

(Analogous chemical contributions in equations for $\mathbf{u}_s$ and T_s)

Remark

In space homogeneous conditions, seven independent first integrals are in order:

$$
\begin{aligned}
& N_s + N_r = N_s^0 + N_r^0 \qquad\qquad (s,r) = (1,3),\ (1,4),\ (2,4) \\
& \mathbf{u} = \frac{1}{\rho^0} \sum_{s=1}^{4} \rho_s \mathbf{u}_s = \mathbf{u}^0 \\
& T = \frac{1}{3KN^0} \sum_{s=1}^{4} \rho_s u_s^2 + \frac{1}{N^0} \sum_{s=1}^{4} N_s T_s = T^0
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\end{aligned}
\tag{2}
$$

$\Rightarrow$ The evolution actually takes place in a 13–dimensional subspace, once initial conditions are given, and independent variables may be chosen, for instance, as

$$
N_1,\ \ \mathbf{u}_2,\ \ \mathbf{u}_3,\ \ \mathbf{u}_4,\ \ T_2,\ T_3,\ \ T_4
$$

Collision equilibria

The “collision” operator in the Euler equations vanishes at the “physical” equilibrium

$$\mathbf{u}_1 = \mathbf{u}_2 = \mathbf{u}_3 = \mathbf{u}_4 (= \mathbf{u}) \qquad\qquad T_1 = T_2 = T_3 = T_4 (= T)$$

$$\frac{N_1 N_2}{N_3 N_4} = \left(\frac{\mu_{12}}{\mu_{34}}\right)^{\frac{3}{2}} \equiv \xi$$

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and then one gets for densities a quadratic equation with only one admissible (positive) solution

$$N_1^* = \frac{1}{2(1-\xi)} \Big\{ \Big[\big(\xi (2N_1^0 + N_3^0 + N_4^0) - (N_1^0 - N_2^0) \big)^2 + 4\xi(1-\xi)(N_1^0 + N_3^0) \times (N_1^0 + N_4^0) \Big]^{1/2} - \big[\xi (2N_1^0 + N_3^0 + N_4^0) - (N_1^0 - N_2^0) \big] \Big\}$$

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- *$\underset{\sim}{\bar{\mathbf{A}}}$, $\underset{\sim}{\hat{\mathbf{A}}}$ (and then $\underset{\sim}{\mathbf{A}}$) are symmetric and singular (sums of rows/columns equal to zero)*
- *The sub–matrices of $\underset{\sim}{\bar{\mathbf{A}}}$, $\underset{\sim}{\hat{\mathbf{A}}}$ made by the first 3 rows and columns are non–singular and negative definite*

$\Rightarrow$ the system admits ∞^1 solutions, corresponding to all equal velocities

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- Analogously for temperatures equations

Entropy dissipation

We consider the restriction of the classical reactive H–functional to the finite dimensional subspace of distribution functions defined by the fast collision equilibria $f_s^M(N_s, \mathbf{u}_s, T_s)$

$$\hat{H} = \sum_{s=1}^{4} N_s \left[\log\left(\frac{N_s}{m_s^3}\right) + \frac{3}{2}\log\left(\frac{m_s}{2\pi K T_s}\right)\right]$$

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It is possible to prove that it attains its minimum at the unique admissible equilibrium point and, in the space independent case, formal derivation yields

$$\partial_t \hat{H} = \sum_{s=1}^{4} (\partial_t N_s) \left[\log\left(\frac{N_s}{m_s^3}\right) + \frac{3}{2}\log\left(\frac{m_s}{2\pi K T_s}\right)\right] - \frac{3}{2}\sum_{s=1}^{4} N_s \frac{\partial_t T_s}{T_s} \leq 0$$

Numerical examples

Reference case

Initial data and averaged collision frequencies

$$N_1^0 = 2\,, \quad N_2^0 = 4\,, \quad N_3^0 = 3\,, \quad N_4^0 = 1$$

$$\mathbf{u}_1^0 = (2,2,2)\ , \quad \mathbf{u}_2^0 = (4,4,4)\ , \quad \mathbf{u}_3^0 = (1,1,1)\ , \quad \mathbf{u}_4^0 = (3,3,3)$$

$$T_1^0 = 2\,, \quad T_2^0 = 3\,, \quad T_3^0 = 4\,, \quad T_4^0 = 1$$

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Particle masses

$$m_1 = 1.2\,, \quad m_2 = 0.8\,, \quad m_3 = 0.95\,, \quad m_4 = 1.05$$

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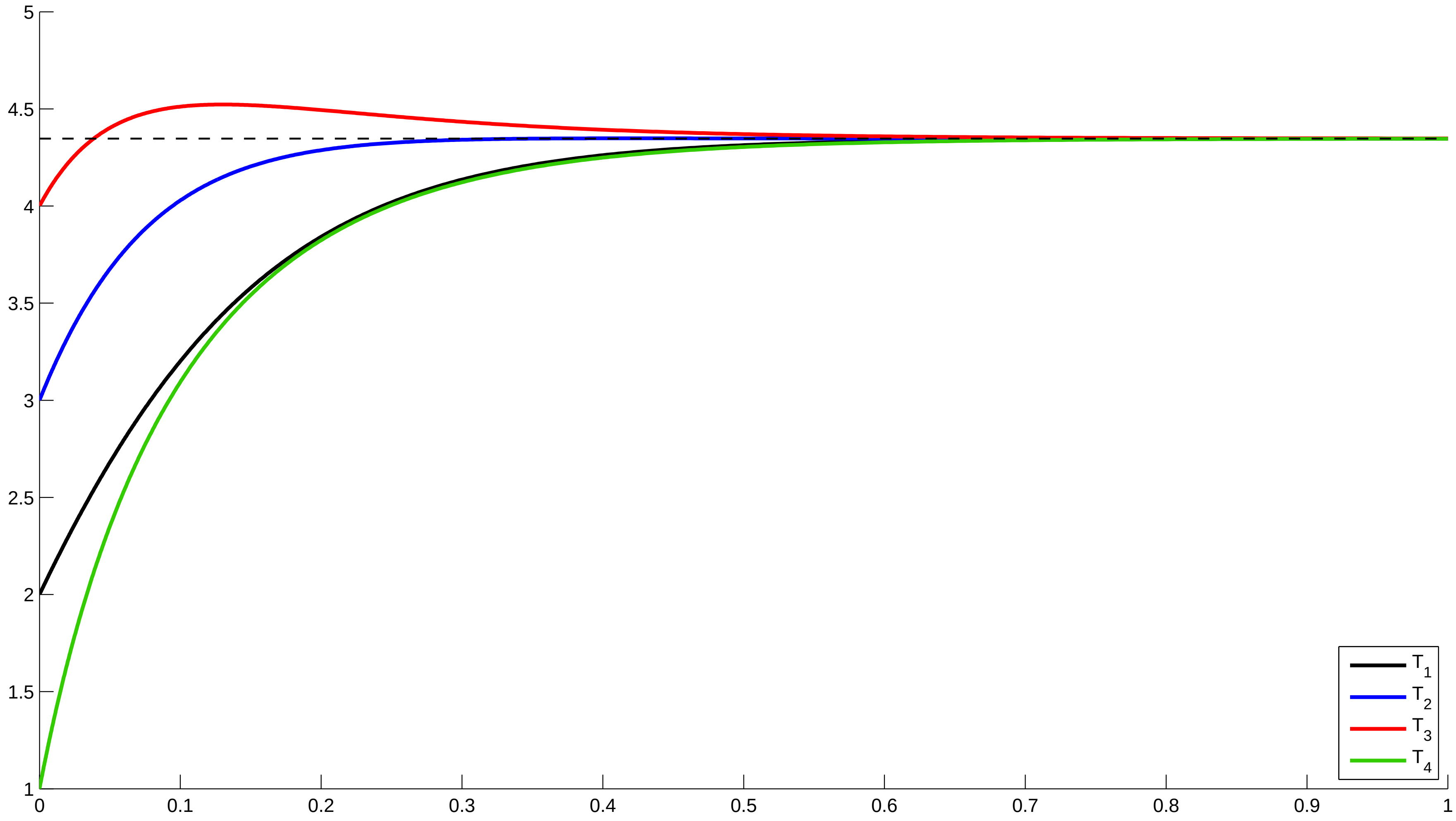
Equilibrium values and relaxation rates are strongly depending on

$$\xi \equiv \left(\frac{\mu_{12}}{\mu_{34}}\right)^{\frac{3}{2}} = 0.94$$

Temperatures evolution

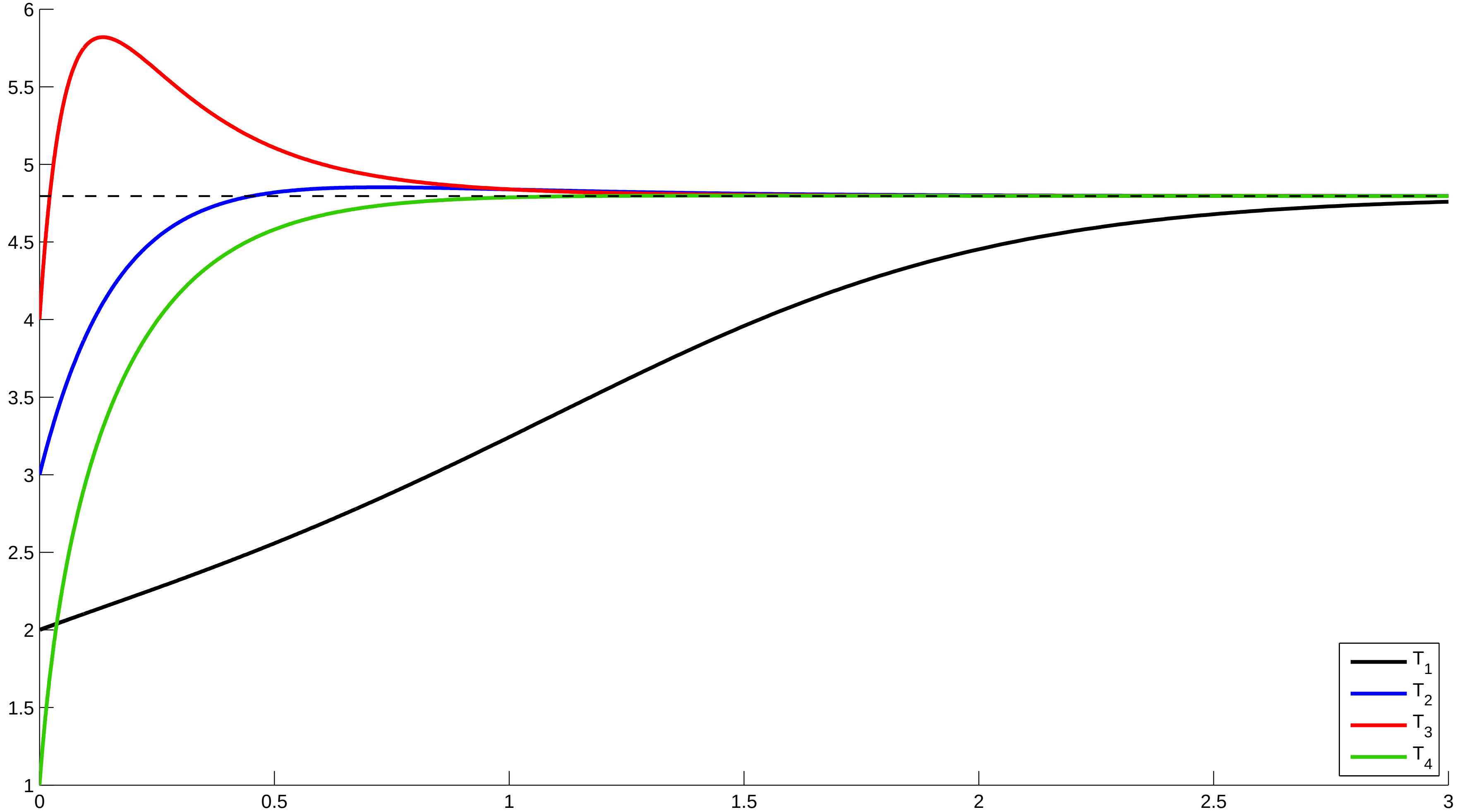


Ex. 2

$$m_1 = 0.02\,, \quad m_2 = 1.98\,, \quad m_3 = 0.95\,, \quad m_4 = 1.05$$

$$\Rightarrow \qquad \xi \equiv \left(\frac{\mu_{12}}{\mu_{34}}\right)^{\frac{3}{2}} = 0.0079$$

Temperatures



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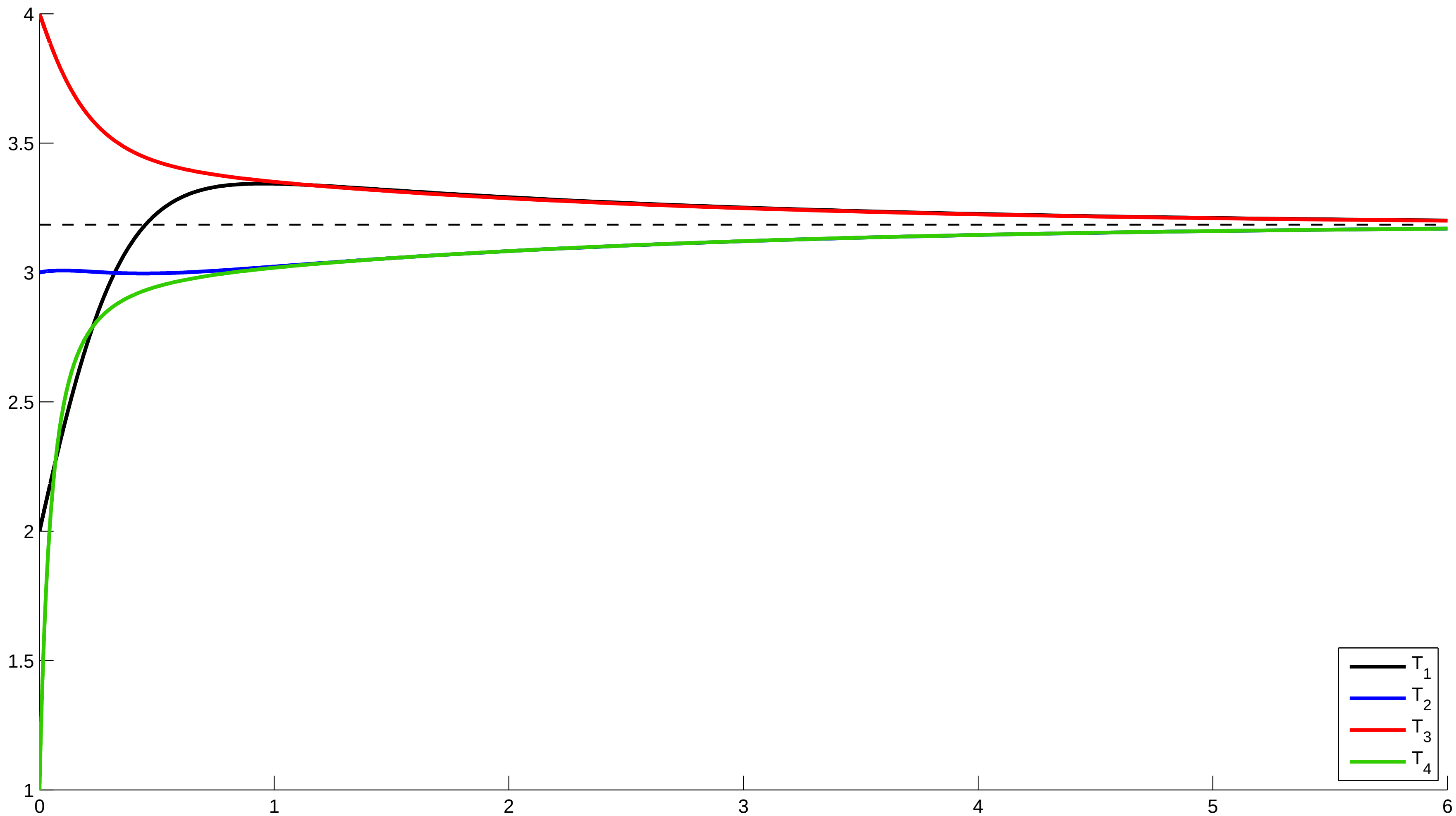
$$\Rightarrow \qquad \xi \equiv \left(\frac{\mu_{12}}{\mu_{34}}\right)^{\frac{3}{2}} = 0.26$$

Temperatures



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Thank you for your attention!