A BGK model for mixtures of monoatomic and polyatomic gases

Marzia Bisi *(Parma)*

(joint work with Romina Travaglini (Parma))

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Kinetic BGK approximation

BGK model for a single gas *(Bhatnagar, Gross, Krook, Phys. Rev. (1954))*

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \nu (\mathcal{M} - f)$$

where $\mathcal{M}$ is a local Maxwellian

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- Inert mixtures
  - *Andries, Aoki, Perthame, J. Stat. Phys. (2002)*
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- Reactive mixtures
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- Polyatomic gases
  - *Brull, Schneider, Contin. Mech. Thermodyn. (2009)*
  - *Bisi, Cáceres, Commun. Math. Sci. (2016)*
  - *Pirner, J. Stat. Phys. (2018)*
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- General structure of BGK relaxation models for gas mixtures

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- BGK model for a mixture of monoatomic and polyatomic gases

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- BGK model for a mixture of monoatomic and polyatomic gases

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- Macroscopic equations and some preliminary numerical tests

Boltzmann and BGK equations for gas mixtures

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Boltzmann equations

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{k=1}^{A} Q_{ik}(f_i, f_k)$$

with $$Q_{ik}(f_i, f_k) = \int_{\mathbb{R}^3 \times S^2} d\mathbf{w}\, d\omega\, g_{ik}(|\mathbf{y}|, \hat{\mathbf{y}}\cdot\omega)\Big[f_i(\mathbf{v}')\, f_k(\mathbf{w}') - f_i(\mathbf{v})\, f_k(\mathbf{w}) \Big]$$

Cross sections $g_{ik}(|\mathbf{y}|, \mu)$, $\mu \in [-1, 1]$ depend on reduced masses and on the intermolecular potential

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BGK approximation

Boltzmann collision operators are replaced by relaxation–type operators

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{k=1}^{A} \nu_{ik} (n_{ik} \mathcal{M}_{ik} - f_i)$$

Two classes of BGK models

1. Model with a sum of (binary) relaxation operators for each species

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{k=1}^{A} \nu_{ik} \left[n_{ik}\, M\left(\mathbf{v}; \mathbf{u}_{ik}, \frac{T_{ik}}{m_i} \right) - f_i \right] \qquad i = 1, \ldots, A$$

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2. Model with a single relaxation operator for each species

$$\frac{\partial f_i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \nu_i \left[\tilde{n}_i \, M\left(\mathbf{v}; \tilde{\mathbf{u}}_i, \frac{\tilde{T}_i}{m_i} \right) - f_i \right] \qquad i = 1, \ldots, A$$

as in *Andries, Aoki, Perthame (2002)*; for each species i, one assumes $n_{ik} = \tilde{n}_i$, $\mathbf{u}_{ik} = \tilde{\mathbf{u}}_i$ and $T_{ik} = \tilde{T}_i$ (for any k)

Remarks

- Models with sums of BGK operators allow to reproduce more details of the original Boltzmann equations, as single species exchange rates of momentum end energies (see *Bobylev, Bisi, Groppi, Spiga, Potapenko, Kinet. Relat. Models (2018)*)

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- For inert or reactive mixtures of polyatomic gases, with discrete or continuous internal energy, BGK models with a single relaxation operator for each species are available *(Bisi, Cáceres, Commun. Math. Sci. (2016), Bisi, Monaco, Soares, J. Phys. A - Math. Theor. (2018))*. This kind of models is more manageable, since it involves a lower number of free parameters

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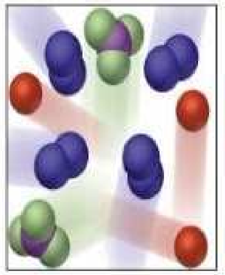
- We generalize this way of modelling to a mixture of monoatomic and polyatomic particles

Mixture of monoatomic and polyatomic species

- We consider a mixture of A monoatomic gases and B polyatomic gases
- Each polyatomic gas has a proper number L^i of discrete internal energy levels



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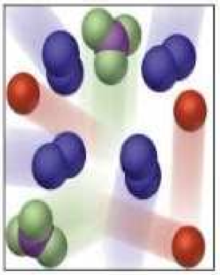

- Monoatomic gases G^i, with $i = 1, \dots, A$:
  they are described by distributions f^i, and densities n^i, velocities $\mathbf{u}^i$, temperatures T^i are provided by

$$n^i = \int_{\mathbb{R}^3} f^i(\mathbf{v})\, d\mathbf{v}\,, \qquad \mathbf{u}^i = \frac{1}{n^i} \int_{\mathbb{R}^3} \mathbf{v}\, f^i(\mathbf{v})\, d\mathbf{v}\,, \qquad T^i = \frac{m^i}{3\, n^i} \int_{\mathbb{R}^3} |\mathbf{v}-\mathbf{u}^i|^2 f^i(\mathbf{v})\, d\mathbf{v}$$

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$$n^i = \sum_{j=1}^{L^i} n^i_j\,, \qquad \mathbf{u}^i = \frac{1}{n^i}\sum_{j=1}^{L^i} n^i_j\,\mathbf{u}^i_j\,, \qquad n^i\,T^i = \sum_{j=1}^{L^i} n^i_j\,T^i_j + \frac{1}{3}\,m^i \sum_{j=1}^{L^i} n^i_j\left(|\mathbf{u}^i_j|^2 - |\mathbf{u}^i|^2\right)$$

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- We have to manage a set of $A + L^{A+1} + \cdots + L^{A+B}$ equations for distributions $\underline{\mathbf{f}} = (f^1, \dots, f^{A+B}_{L^{A+B}})$

- **Possible collisions**

Monoatomic-Monoatomic	Polyatomic-Polyatomic	Polyatomic-Monoatomic
$G^i + G^h \longrightarrow G^i + G^h$	$C^i_j + C^h_k \longrightarrow C^i_l + C^h_m$	$G^i + C^h_j \longrightarrow G^i + C^h_k$
$1 \leq i, h \leq A$	$A + 1 \leq i, h \leq A + B$	$1 \leq i \leq A\,, \quad A + 1 \leq h \leq A + B$

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- **Preservation of global momentum and energy**

$$m^i\,\mathbf{v} + m^h\,\mathbf{w} = m^i\,\mathbf{v}' + m^h\,\mathbf{w}'$$

$$\frac{1}{2}\,m^i\,|\mathbf{v}|^2 + E^i_j + \frac{1}{2}\,m^h\,|\mathbf{w}|^2 + E^h_k = \frac{1}{2}\,m^i\,|\mathbf{v}'|^2 + E^i_l + \frac{1}{2}\,m^h\,|\mathbf{w}'|^2 + E^h_m$$

where internal energies may be equal to zero if one or both gases are monoatomic

Collision equilibria

Maxwellian distributions $\underline{\mathbf{f}}_M$ sharing a common velocity and temperature:

- for monoatomic gases

$$f_M^i(\mathbf{v}) = n^i\, M^i\left(\mathbf{v}; \mathbf{u}, \frac{T}{m^i}\right), \qquad\qquad i = 1, \ldots, A$$

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with

$$n^i_j = n^i\, \exp\left(-\frac{E^i_j - E^i_1}{T}\right)\Bigg/\left[\sum_{k=1}^{L^i}\exp\left(-\frac{E^i_k - E^i_1}{T}\right)\right]$$

Since internal energies are increasing with their subindex, in any equilibrium configuration we have $n^i_j > n^i_k$*, for any* $j < k$

BGK model *by Bisi, Travaglini (2019)*

We take a single relaxation operator for each component

$$
\begin{cases}
\dfrac{\partial f^i}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f^i = \nu^i (\mathcal{M}^i - f^i)\,, & i = 1, \ldots, A \\
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with Maxwellian attractors

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$\Rightarrow \quad \tilde{n}^i, \tilde{\mathbf{u}}, \tilde{T}$ are $A + B + 4$ disposable free parameters

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- number densities of monoatomic species

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- total energy

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$\Rightarrow$ These are $A + B + 4$ constraints for our $A + B + 4$ free parameters

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$$\tilde{\mathbf{u}} = \left(\sum_{i=1}^{A} \nu^i \, m^i \, n^i \, \mathbf{u}^i + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i \, m^i \, n_j^i \, \mathbf{u}_j^i \right) \Bigg/ \left(\sum_{i=1}^{A} \nu^i \, m^i \, n^i + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i \, m^i \, n_j^i \right)$$

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$$\tilde{\mathbf{u}} = \left(\sum_{i=1}^{A} \nu^i\, m^i\, n^i\, \mathbf{u}^i + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i\, m^i\, n_j^i\, \mathbf{u}_j^i\right) \Big/ \left(\sum_{i=1}^{A} \nu^i\, m^i\, n^i + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i\, m^i\, n_j^i\right)$$

and a transcendental equation for auxiliary temperature

$\mathcal{F}(\tilde{T}) = \Lambda$ where Λ is an explicit function of the actual macroscopic fields and

$$\mathcal{F}(\tilde{T}) = \frac{3}{2}\,\tilde{T}\left(\sum_{i=1}^{A} \nu^i\, n^i + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i\, n_j^i\right) + \sum_{i=A+1}^{A+B}\left(\sum_{j=1}^{L^i} \nu_j^i\, n_j^i\right) \frac{\sum_{k=1}^{L^i} \nu_k^i\, E_k^i \exp\left(-\frac{E_k^i - E_1^i}{\tilde{T}}\right)}{\sum_{h=1}^{L^i} \nu_h^i \exp\left(-\frac{E_h^i - E_1^i}{\tilde{T}}\right)}$$

Such conditions provide

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$\mathcal{F}(\tilde{T})$ is strictly monotone and it varies from

$\lim_{\tilde{T}\to 0} \mathcal{F}(\tilde{T}) = \sum_{i=A+1}^{A+B} \left(\sum_{j=1}^{L^i} \nu^i_j n^i_j\right) E^i_1 \leq \Lambda$ *to* $\lim_{\tilde{T}\to +\infty} \mathcal{F}(\tilde{T}) = +\infty$

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$\Rightarrow$ *$\mathcal{F}(\tilde{T}) = \Lambda$ admits a unique solution for any values of masses, energies, collision frequencies, and species fields*

H–theorem

In space homogeneous conditions,

$$H[\underline{\mathbf{f}}] = \sum_{i=1}^{A} \int_{\mathbb{R}^3} f^i \log(f^i)\, d\mathbf{v} + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \int_{\mathbb{R}^3} f_j^i \log(f_j^i)\, d\mathbf{v}$$

is a Lyapunov functional for the present BGK model:

$\forall \underline{\mathbf{f}} \neq \underline{\mathbf{f}}_M, \quad H'[\underline{\mathbf{f}}] < 0$ and $H[\underline{\mathbf{f}}] > H[\underline{\mathbf{f}}_M]$

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Sketch of the proof of the entropy dissipation

$$H'[\underline{\mathbf{f}}] = \sum_{i=1}^{A} \nu^i \int_{\mathbb{R}^3} (\mathcal{M}^i - f^i) \log(f^i)\, d\mathbf{v} + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu^i_j \int_{\mathbb{R}^3} (\mathcal{M}^i_j - f^i_j) \log(f^i_j)\, d\mathbf{v}$$

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We can check that

$$\sum_{i=1}^{A} \nu^i \int_{\mathbb{R}^3} (\mathcal{M}^i - f^i) \log(\mathcal{M}^i)\, d\mathbf{v} + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu^i_j \int_{\mathbb{R}^3} (\mathcal{M}^i_j - f^i_j) \log(\mathcal{M}^i_j)\, d\mathbf{v} = 0\,, \qquad (*)$$

hence, by usual convexity arguments, $\forall \underline{\mathbf{f}} \neq \underline{\mathbf{f}}_M$,

$$H'[\underline{\mathbf{f}}] = -\sum_{i=1}^{A} \nu^i \int_{\mathbb{R}^3} (f^i - \mathcal{M}^i) \log\left(\frac{f^i}{\mathcal{M}^i}\right) d\mathbf{v} - \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu^i_j \int_{\mathbb{R}^3} (f^i_j - \mathcal{M}^i_j) \log\left(\frac{f^i_j}{\mathcal{M}^i_j}\right) d\mathbf{v} < 0$$

Proof of (∗):

$$\sum_{i=1}^{A} \nu^i \int_{\mathbb{R}^3} (\mathcal{M}^i - f^i) \log(\mathcal{M}^i)\, d\mathbf{v} + \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i \int_{\mathbb{R}^3} (\mathcal{M}_j^i - f_j^i) \log(\mathcal{M}_j^i)\, d\mathbf{v} =$$

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$$= \sum_{i=1}^{A} \nu^i \int_{\mathbb{R}^3} (\mathcal{M}^i - f^i) \left[\log n^i + \frac{3}{2} m^i - \frac{3}{2} \log(2\pi \tilde{T}) - \frac{m^i}{2\tilde{T}} (|\mathbf{v}|^2 - 2\tilde{\mathbf{u}} \cdot \mathbf{v} + |\tilde{\mathbf{u}}|^2) \right] d\mathbf{v}$$

$$+ \sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i \int_{\mathbb{R}^3} (\mathcal{M}_j^i - f_j^i) \left[\log \tilde{n}_j^i + \frac{3}{2} m^i - \frac{3}{2} \log(2\pi \tilde{T}) - \frac{m^i}{2\tilde{T}} (|\mathbf{v}|^2 - 2\tilde{\mathbf{u}} \cdot \mathbf{v} + |\tilde{\mathbf{u}}|^2) \right] d\mathbf{v}$$

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Owing to conservation laws, the contribution of monoatomic species vanishes and the polyatomic one simplifies to

$$\sum_{i=A+1}^{A+B} \sum_{j=1}^{L^i} \nu_j^i (\tilde{n}_j^i - n_j^i) \left[\log \tilde{n}_j^i + \frac{E_j^i}{\tilde{T}} \right]$$

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This also vanishes since, bearing in mind the expression of $\tilde{n}_j^i$, the term

$$\log \tilde{n}_j^i + \frac{E_j^i}{\tilde{T}} = \frac{E_1^i}{\tilde{T}} + \log\left(\sum_{h=1}^{L^i} \nu_h^i\, n_h^i \right) - \log\left[\sum_{h=1}^{L^i} \nu_h^i \exp\left(- \frac{E_h^i - E_1^i}{\tilde{T}} \right) \right]$$

does not depend on the subindex j and $\sum_{j=1}^{L^i} \nu_j^i (\tilde{n}_j^i - n_j^i) = 0$ •

Macroscopic equations

From our BGK model we derive evolution equations for species densities, velocities, and temperatures

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Monoatomic gases

$$\begin{cases} \dfrac{\partial n^i}{\partial t} + \nabla_{\mathbf{x}} \cdot (n^i\, \mathbf{u}^i) = 0\,, \\ n^i \left(\dfrac{\partial \mathbf{u}^i}{\partial t} + \mathbf{u}^i \cdot \nabla_{\mathbf{x}} \mathbf{u}^i \right) + \dfrac{1}{m^i} \nabla_{\mathbf{x}} \cdot \mathbf{P}^i = \nu^i\, n^i (\tilde{\mathbf{u}} - \mathbf{u}^i)\,, \\ \dfrac{3}{2}\, n^i \left(\dfrac{\partial T^i}{\partial t} + \mathbf{u}^i \cdot \nabla_{\mathbf{x}} T^i \right) + \mathbf{P}^i : \nabla_{\mathbf{x}} \mathbf{u}^i + \nabla_{\mathbf{x}} \cdot \mathbf{q}^i \\ \qquad = \nu^i\, n^i \left[\dfrac{3}{2} (\tilde{T} - T^i) + \dfrac{1}{2}\, m^i\, |\tilde{\mathbf{u}} - \mathbf{u}^i|^2 \right], \end{cases}$$

$$i = 1, \ldots, A$$

Polyatomic components

$$\begin{cases} \dfrac{\partial n_j^i}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_j^i \, \mathbf{u}_j^i) = \nu_j^i (\tilde{n}_j^i - n_j^i) \,, \\ n_j^i \left(\dfrac{\partial \mathbf{u}_j^i}{\partial t} + \mathbf{u}_j^i \cdot \nabla_{\mathbf{x}} \mathbf{u}_j^i \right) + \dfrac{1}{m^i} \nabla_{\mathbf{x}} \cdot \mathbf{P}_j^i = \nu_j^i \, \tilde{n}_j^i (\tilde{\mathbf{u}} - \mathbf{u}_j^i) \,, \\ \dfrac{3}{2} \, n_j^i \left(\dfrac{\partial T_j^i}{\partial t} + \mathbf{u}_j^i \cdot \nabla_{\mathbf{x}} T_j^i \right) + \mathbf{P}_j^i : \nabla_{\mathbf{x}} \mathbf{u}_j^i + \nabla_{\mathbf{x}} \cdot \mathbf{q}_j^i \\ \qquad = \nu_j^i \, \tilde{n}_j^i \left[\dfrac{3}{2} \, (\tilde{T} - T_j^i) + \dfrac{1}{2} \, m^i \, |\tilde{\mathbf{u}} - \mathbf{u}_j^i|^2 \right], \end{cases}$$

$$i = A+1, \ldots, A+B, \qquad j = 1, \ldots, L^i$$

Numerical tests

- In space homogeneous conditions, macroscopic equations constitute a closed system of $4(A + L^{A+1} + \cdots + L^{A+B})$ equations (auxiliary parameters are uniquely defined by the actual ones)

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- If we assign the initial values $(n^i)_0$, $(n^i_j)_0$, $(\mathbf{u}^i)_0$, $(\mathbf{u}^i_j)_0$, $(T^i)_0$, $(T^i_j)_0$, the corresponding collision equilibrium is uniquely determined from conservation laws

$$n^i_M = (n^i)_0 \,, \qquad (n^i_j)_M = \sum_{h=1}^{L^i} (n^i_h)_0 \exp\left(-\frac{E^i_j - E^i_1}{T_M}\right) \Bigg/ \left[\sum_{k=1}^{L^i} \exp\left(-\frac{E^i_k - E^i_1}{T_M}\right)\right]$$

$$\mathbf{u}_M = \left(\sum_{i=1}^{A} m^i\,(n^i)_0\,(\mathbf{u}^i)_0 + \sum_{i=A+1}^{A+B}\sum_{j=1}^{L^i} m^i\,(n^i_j)_0\,(\mathbf{u}^i_j)_0\right) \Bigg/ \left(\sum_{i=1}^{A} m^i\,(n^i)_0 + \sum_{i=A+1}^{A+B}\sum_{j=1}^{L^i} m^i\,(n^i_j)_0\right)$$

T_M *is the unique solution of a proper transcendental equation* $\mathcal{G}(T_M) = \Gamma$

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- We consider a monoatomic gas G^1 and a polyatomic species G^2 divided into three different components

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	G^1	C_1^2	C_2^2	C_3^2
n_0	10	8	6	7
u_0	0.3	0	0.1	0.4
T_0	2	4	1	2.5

for internal energies ($E_1^2 = 5$, $E_2^2 = 6$, $E_3^2 = 9$) and for collision frequencies (depending on number densities)

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  - $(m_1, m_2) = (1, 64.97)$ *(mass ratio of Helium He / Iodine Heptafluoride IF_7)*
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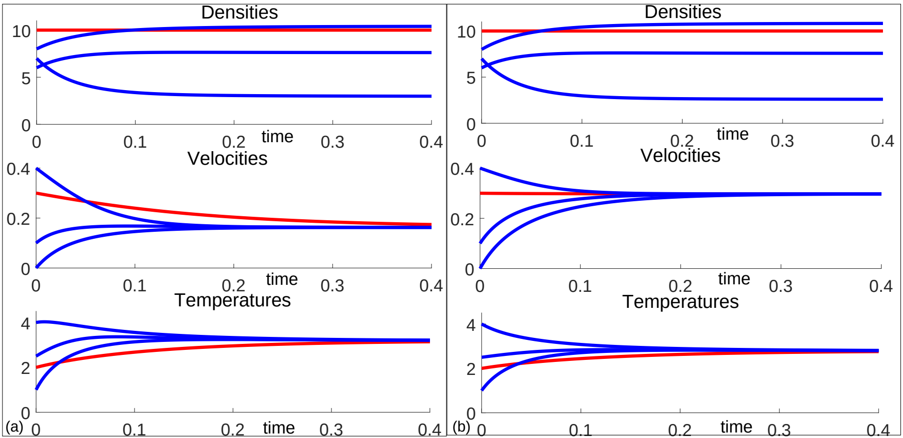
- Velocities and temperatures of the three components of G^2 tend to assume at first a common value and then they evolve together to the global equilibrium

Plots of the macroscopic fields



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The gas G^1 has has two internal energy levels and the gas G^2 has three energy levels

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Test 1.

- We take similar masses $(m_1, m_2) = (1, 1.09)$ *(mass ratio of Nitrous Oxide* N_2O / *Ozone* O_3*)*, and initial data

	C_1^1	C_2^1	C_1^2	C_2^2	C_3^2
n_0	10	9	8	6	7
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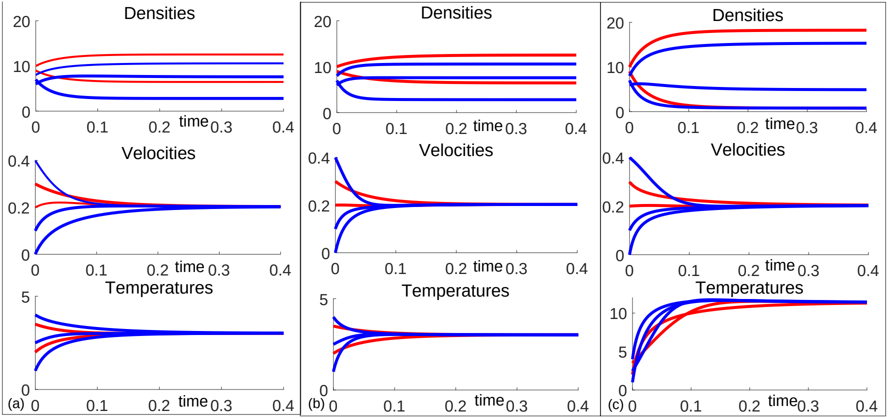
T_0	2	3.5	4	1	2.5

- We vary the values of energy levels
- When there is a big gap between energy values of the same species, there is also a big gap between equilibrium densities.
  A high gap between internal energies causes a considerably higher value for the final temperature (strongly affected by all the differences $E_j^i - E_1^i$)



Panel (a) : $E^1_1 = 38$, $E^1_2 = 40$, $E^2_1 = 35$, $E^2_2 = 36$, $E^2_3 = 39$

Panel (b) : $E^1_1 = 2$, $E^1_2 = 4$, $E^2_1 = 35$, $E^2_2 = 36$, $E^2_3 = 39$

Panel (c) : $E^1_1 = 4$, $E^1_2 = 40$, $E^2_1 = 5$, $E^2_2 = 18$, $E^2_3 = 39$

Test 2.

- We take polyatomic gases with different masses $(m_1, m_2) = (1, 38.97)$ *(mass ratio of Hydrogen* H_2 / *Arsine* AsH_3*)*, and energy levels of the same order of magnitude

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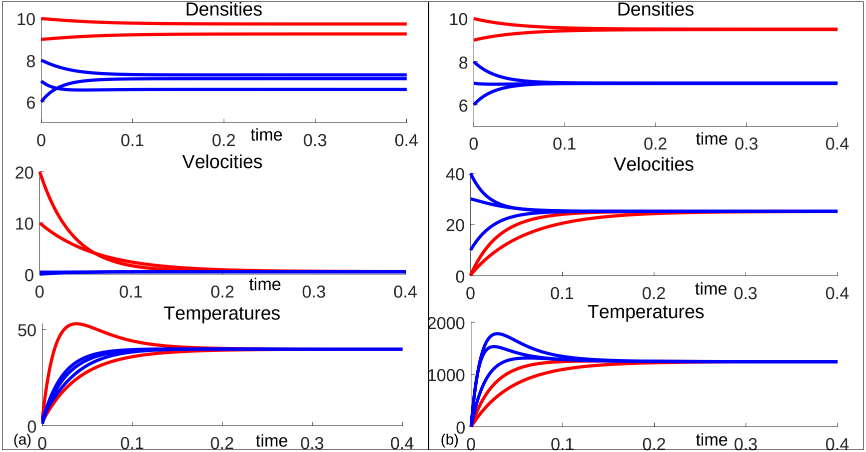
- We increase the initial velocities of the components
- The trend to equilibrium for the heavy particles is usually faster than for the light ones.
  The temperatures trend to the steady value turns out to be monotone for components of the gas with low velocities, while an evident overshooting appears in the first stage of the evolution of the faster components



Panel (a) : $(u_1^1)_0 = 10$, $(u_2^1)_0 = 20$, $(u_1^2)_0 = 0$, $(u_2^2)_0 = 0.1$, $(u_3^2)_0 = 0.4$

Panel (b) : $(u_1^1)_0 = 0.3$, $(u_2^1)_0 = 0.2$, $(u_1^2)_0 = 10$, $(u_2^2)_0 = 30$, $(u_3^2)_0 = 40$

Future works

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- BGK models for polyatomic (and reacting) gases involving sums of relaxation operators, able to separate elastic and inelastic collisions
- Kinetic models for polyatomic particles with the internal energy separated into two different components, the vibrational and the rotational ones
  (since the gap between two subsequent discrete levels is much lower for rotational energy than for vibrational energy, the rotational part could be approximated by a continuous variable, keeping the vibrational part discrete)

Thank you for your attention