A Boltzmann–BGK model for gas mixtures and its hydrodynamic limits

Marzia Bisi

University of Parma, Italy

Joint work with M. Groppi, G. Martalò
and the PhD students E. Lucchin, A. Macaluso

Workshop "Analysis, modeling and numerical methods for kinetic and related models"

Bordeaux (France), November 14–15, 2023

Summary of the talk

- Boltzmann description for gas mixtures

Summary of the talk

- Boltzmann description for gas mixtures
- BGK–type model for inert mixtures of monatomic gases mimicking the structure of the Boltzmann collision operator for gas mixtures [Bobylev, Bisi, Groppi, Spiga, Potapenko (KRM 2018)]

Summary of the talk

- Boltzmann description for gas mixtures
- BGK–type model for inert mixtures of monatomic gases mimicking the structure of the Boltzmann collision operator for gas mixtures [Bobylev, Bisi, Groppi, Spiga, Potapenko (KRM 2018)]
- Mixed Boltzmann–BGK model for gas mixtures, where each kind of binary interactions may be modelled by a Boltzmann or by a BGK operator

Summary of the talk

- Boltzmann description for gas mixtures
- BGK–type model for inert mixtures of monatomic gases mimicking the structure of the Boltzmann collision operator for gas mixtures [Bobylev, Bisi, Groppi, Spiga, Potapenko (KRM 2018)]
- Mixed Boltzmann–BGK model for gas mixtures, where each kind of binary interactions may be modelled by a Boltzmann or by a BGK operator

Motivation

We aim at preserving wherever possible the detailed description of interactions provided by Boltzmann operators, and at the same time we would like an analytically and numerically manageable kinetic model for gas mixtures

Particular option *(that will be mainly investigated)*

- Boltzmann operators for intra–species collisions and BGK operators for inter–species collisions

Particular option *(that will be mainly investigated)*

- Boltzmann operators for intra–species collisions and BGK operators for inter–species collisions
- Hydrodynamic limits
  - collision dominated regime;
  - dominant intra–species collisions.

BGK models for inert or reactive gas mixtures

- Inert mixtures
  - *McCormack, Phys. Fluids (1973)*
  - *Andries, Aoki, Perthame, J. Stat. Phys. (2002)*
  - *Klingenberg, Pirner, Puppo, Kinet. Relat. Models (2017)*
  - *Haack, Hauck, Murillo, J. Stat. Phys. (2017)*
  - *Todorova, Steijl, Europ. J. Mech.-B/Fluids (2019)*
  - *Haack, Hauck, Klingenberg, Pirner, Warnecke, J. Stat. Phys. (2021)*

BGK models for inert or reactive gas mixtures

- Inert mixtures
  - *McCormack, Phys. Fluids (1973)*
  - *Andries, Aoki, Perthame, J. Stat. Phys. (2002)*
  - *Klingenberg, Pirner, Puppo, Kinet. Relat. Models (2017)*
  - *Haack, Hauck, Murillo, J. Stat. Phys. (2017)*
  - *Todorova, Steijl, Europ. J. Mech.-B/Fluids (2019)*
  - *Haack, Hauck, Klingenberg, Pirner, Warnecke, J. Stat. Phys. (2021)*
- Reactive mixtures
  - *Groppi, Spiga, Phys. Fluids (2004)*
  - *Kremer, Pandolfi Bianchi, Soares, Phys. Fluids (2006)*
  - *Bisi, Groppi, Spiga, Phys. Rev. E (2010)*
  - *Brull, Schneider, Commun. Math. Sci. (2014)*

BGK models for inert or reactive gas mixtures

- Inert mixtures
  - *McCormack, Phys. Fluids (1973)*
  - *Andries, Aoki, Perthame, J. Stat. Phys. (2002)*
  - *Klingenberg, Pirner, Puppo, Kinet. Relat. Models (2017)*
  - *Haack, Hauck, Murillo, J. Stat. Phys. (2017)*
  - *Todorova, Steijl, Europ. J. Mech.-B/Fluids (2019)*
  - *Haack, Hauck, Klingenberg, Pirner, Warnecke, J. Stat. Phys. (2021)*
- Reactive mixtures
  - *Groppi, Spiga, Phys. Fluids (2004)*
  - *Kremer, Pandolfi Bianchi, Soares, Phys. Fluids (2006)*
  - *Bisi, Groppi, Spiga, Phys. Rev. E (2010)*
  - *Brull, Schneider, Commun. Math. Sci. (2014)*
- Polyatomic gases
  - *Andries, Le Tallec, Perlat, Perthame, Eur. J. Mech. B (2000)*
  - *Brull, Schneider, Contin. Mech. Thermodyn. (2009)*
  - *Bisi, Cáceres, Commun. Math. Sci. (2016)*
  - *Pirner, J. Stat. Phys. (2018)*
  - *Bisi, Travaglini, Physica A (2020)*
  - *Brull, Commun. Math. Sci. (2021)*

We consider an inert mixture of N species ($s = 1, \dots, N$)

Boltzmann equations

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \mathcal{Q}_{sr}(f_s, f_r)$$

with $$\mathcal{Q}_{sr}(f_s, f_r) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} g_{sr}(|\mathbf{y}|, \hat{\mathbf{y}} \cdot \omega) \Big[f_s(\mathbf{v}')\, f_r(\mathbf{v}'_*) - f_s(\mathbf{v})\, f_r(\mathbf{v}_*) \Big] d\mathbf{v}_*\, d\omega$$

- $\mathbf{v}'$, $\mathbf{v}'_*$ are post–collision velocities
- $\mathbf{y} = \mathbf{v} - \mathbf{v}_*$ is the relative velocity
- Cross sections $g_{sr}(|\mathbf{y}|, \mu)$, $\mu \in [-1, 1]$ depend on reduced masses and on the intermolecular potential

BBGSP model for inert gas mixtures

(Bobylev, Bisi, Groppi, Spiga, Potapenko (KRM 2018))

We want to preserve the structure of Boltzmann collision operator (sum of binary interaction operators)

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \widetilde{\mathcal{Q}}_{sr}$$

$$\text{with} \qquad \widetilde{\mathcal{Q}}_{sr} = \nu_{sr} \left(n_s \, \mathcal{M}_{sr} - f_s \right)$$

BBGSP model for inert gas mixtures

(Bobylev, Bisi, Groppi, Spiga, Potapenko (KRM 2018))

We want to preserve the structure of Boltzmann collision operator (sum of binary interaction operators)

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \widetilde{\mathcal{Q}}_{sr}$$

$$\text{with} \qquad \widetilde{\mathcal{Q}}_{sr} = \nu_{sr} \big(n_s \, \mathcal{M}_{sr} - f_s \big)$$

Maxwellian attractors

$$\mathcal{M}_{sr} = M\left(\mathbf{v}; \mathbf{u}_{sr}, \frac{T_{sr}}{m_s}\right) = \left(\frac{m_s}{2\pi \, T_{sr}}\right)^{3/2} \exp\left[-\frac{m_s |\mathbf{v} - \mathbf{u}_{sr}|^2}{2 \, T_{sr}}\right]$$

BBGSP model for inert gas mixtures

(Bobylev, Bisi, Groppi, Spiga, Potapenko (KRM 2018))

We want to preserve the structure of Boltzmann collision operator (sum of binary interaction operators)

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \widetilde{\mathcal{Q}}_{sr}$$

$$\text{with} \qquad \widetilde{\mathcal{Q}}_{sr} = \nu_{sr} \big(n_s \, \mathcal{M}_{sr} - f_s \big)$$

Maxwellian attractors

$$\mathcal{M}_{sr} = M\left(\mathbf{v}; \mathbf{u}_{sr}, \frac{T_{sr}}{m_s}\right) = \left(\frac{m_s}{2\pi \, T_{sr}} \right)^{3/2} \exp\left[- \frac{m_s |\mathbf{v} - \mathbf{u}_{sr}|^2}{2 \, T_{sr}} \right]$$

$\Rightarrow$ $5\,N^2$ free parameters $\left\{ \nu_{sr}, \; \mathbf{u}_{sr}, \; T_{sr}; \; s, r = 1, \ldots, N \right\}$ to be combined with only (N+4) conservation laws

[For this reason many consistent BGK models are available for gas mixtures]

Construction of auxiliary parameters of BBGSP model

- Collisions of identical particles are described by the usual BGK model: $\mathbf{u}_{ss} = \mathbf{u}_s \,, \qquad T_{ss} = T_s \,, \qquad s = 1, \dots, N$

Construction of auxiliary parameters of BBGSP model

- Collisions of identical particles are described by the usual BGK model: $\mathbf{u}_{ss} = \mathbf{u}_s\,, \qquad T_{ss} = T_s\,, \qquad s = 1, \dots, N$

- We impose that each bi-species BGK operator $\widetilde{\mathcal{Q}}_{sr}$ prescribes the same exchange rates (of momentum and energy) of the corresponding binary Boltzmann operator $\mathcal{Q}_{sr}$

$$\langle\ \mathcal{Q}_{sr} - \widetilde{\mathcal{Q}}_{sr}, \mathbf{v}\rangle = \mathbf{0}\,, \qquad \langle\ \mathcal{Q}_{sr} - \widetilde{\mathcal{Q}}_{sr}, |\mathbf{v}|^2\rangle = 0$$

$$\left(\text{where} \quad \langle g, h\rangle = \int_{\mathbb{R}^3} g(\mathbf{v})h(\mathbf{v})\, d\mathbf{v}\right)$$

- Collisions of identical particles are described by the usual BGK model: $\mathbf{u}_{ss} = \mathbf{u}_s\,, \qquad T_{ss} = T_s\,, \qquad s = 1, \ldots, N$

- We impose that each bi-species BGK operator $\widetilde{\mathcal{Q}}_{sr}$ prescribes the same exchange rates (of momentum and energy) of the corresponding binary Boltzmann operator $\mathcal{Q}_{sr}$

$$\langle\, \mathcal{Q}_{sr} - \widetilde{\mathcal{Q}}_{sr}, \mathbf{v} \rangle = \mathbf{0}\,, \qquad \langle\, \mathcal{Q}_{sr} - \widetilde{\mathcal{Q}}_{sr}, |\mathbf{v}|^2 \rangle = 0$$

$$\left(\text{where} \quad \langle g, h \rangle = \int_{\mathbb{R}^3} g(\mathbf{v}) h(\mathbf{v})\, d\mathbf{v}\right)$$

  - Moments of BGK operators may be easily computed, leading to

$$\nu_{sr}\, n_s \left(\mathbf{u}_{sr} - \mathbf{u}_s\right) = \langle \mathcal{Q}_{sr}, \mathbf{v} \rangle, \qquad \nu_{sr}\, n_s \left(3\,\frac{T_{sr} - T_s}{m_s} + |\mathbf{u}_{sr}|^2 - |\mathbf{u}_s|^2\right) = \langle \mathcal{Q}_{sr}, |\mathbf{v}|^2 \rangle$$

- Moments of Boltzmann operators $\mathcal{Q}_{sr}$ involve

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f_s(\mathbf{v})\, f_r(\mathbf{v}_*)\, \widehat{g}_{sr}(|\mathbf{v}-\mathbf{v}_*|)\, \psi(\mathbf{v},\mathbf{v}_*)\, d\mathbf{v}\, d\mathbf{v}_*$$

$$\text{where} \quad \widehat{g}_{sr}(|\mathbf{y}|) = 2\,\pi \int_{-1}^{1} (1-\mu)\, g_{sr}(|\mathbf{y}|,\mu)\, d\mu$$

- Moments of Boltzmann operators $\mathcal{Q}_{sr}$ involve

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f_s(\mathbf{v})\, f_r(\mathbf{v}_*)\, \widehat{g}_{sr}(|\mathbf{v}-\mathbf{v}_*|)\, \psi(\mathbf{v},\mathbf{v}_*)\, d\mathbf{v}\, d\mathbf{v}_*$$

$$\text{where} \quad \widehat{g}_{sr}(|\mathbf{y}|) = 2\,\pi \int_{-1}^{1} (1-\mu)\, g_{sr}(|\mathbf{y}|,\mu)\, d\mu$$

For Maxwell molecules the collision kernel g_{sr} is independent of $|\mathbf{y}|$

$\Rightarrow \quad \widehat{g}_{sr} = \lambda_{sr} = \mathrm{const}$

- Moments of Boltzmann operators $\mathcal{Q}_{sr}$ involve

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f_s(\mathbf{v})\, f_r(\mathbf{v}_*)\, \widehat{g}_{sr}(|\mathbf{v}-\mathbf{v}_*|)\, \psi(\mathbf{v},\mathbf{v}_*)\, d\mathbf{v}\, d\mathbf{v}_*$$

$$\text{where} \quad \widehat{g}_{sr}(|\mathbf{y}|) = 2\,\pi \int_{-1}^{1} (1-\mu)\, g_{sr}(|\mathbf{y}|,\mu)\, d\mu$$

For Maxwell molecules the collision kernel g_{sr} is independent of $|\mathbf{y}|$

$$\Rightarrow \quad \widehat{g}_{sr} = \lambda_{sr} = \text{const}$$

For general intermolecular potentials we approximate $\widehat{g}_{sr}(|\mathbf{v}-\mathbf{v}_*|)$ by its value in some typical point

$$z_{sr} = \left(\overline{|\mathbf{v}-\mathbf{v}_*|^2}\right)^{\frac{1}{2}} = \left(\frac{1}{n_s\, n_r}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\mathbf{v})\, f_r(\mathbf{v}_*)\, |\mathbf{v}-\mathbf{v}_*|^2\, d\mathbf{v}\, d\mathbf{v}_*\right)^{\frac{1}{2}} = \left[3\left(\frac{T_s}{m_s}+\frac{T_r}{m_r}\right) + |\mathbf{u}_s-\mathbf{u}_r|^2\right]^{\frac{1}{2}}$$

and consequently $\widehat{g}_{sr}(|\mathbf{y}|) \simeq \widehat{g}_{sr}(z_{sr}) := \lambda_{sr}$

- Moments of Boltzmann operators $\mathcal{Q}_{sr}$ involve

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f_s(\mathbf{v})\, f_r(\mathbf{v}_*)\, \widehat{g}_{sr}(|\mathbf{v}-\mathbf{v}_*|)\, \psi(\mathbf{v},\mathbf{v}_*)\, d\mathbf{v}\, d\mathbf{v}_*$$

$$\text{where} \quad \widehat{g}_{sr}(|\mathbf{y}|) = 2\,\pi \int_{-1}^{1} (1-\mu)\, g_{sr}(|\mathbf{y}|,\mu)\, d\mu$$

For Maxwell molecules the collision kernel g_{sr} is independent of $|\mathbf{y}|$

$\Rightarrow \quad \widehat{g}_{sr} = \lambda_{sr} = \mathrm{const}$

For general intermolecular potentials we approximate $\widehat{g}_{sr}(|\mathbf{v}-\mathbf{v}_*|)$ by its value in some typical point

$$z_{sr} = \left(\overline{|\mathbf{v}-\mathbf{v}_*|^2}\right)^{\frac{1}{2}} = \left(\frac{1}{n_s\, n_r}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\mathbf{v})\, f_r(\mathbf{v}_*)\, |\mathbf{v}-\mathbf{v}_*|^2\, d\mathbf{v}\, d\mathbf{v}_*\right)^{\frac{1}{2}} = \left[3\left(\frac{T_s}{m_s}+\frac{T_r}{m_r}\right) + |\mathbf{u}_s-\mathbf{u}_r|^2\right]^{\frac{1}{2}}$$

and consequently $\widehat{g}_{sr}(|\mathbf{y}|) \simeq \widehat{g}_{sr}(z_{sr}) := \lambda_{sr}$

$\Rightarrow$ We get explicit expressions for the exchange rates of the bi-species Boltzmann integrals even for general interaction potentials

From these explicit expressions it is possible to define uniquely the parameters $\mathbf{u}_{sr}$, T_{sr} as

$$\boxed{\begin{aligned} \mathbf{u}_{sr} &= (1 - a_{sr})\,\mathbf{u}_s + a_{sr}\,\mathbf{u}_r \\ T_{sr} &= (1 - b_{sr})\,T_s + b_{sr}\,T_r + \gamma_{sr}\,|\mathbf{u}_s - \mathbf{u}_r|^2 \end{aligned}}$$

where

$$a_{sr} = \frac{\lambda_{sr}\, n_r\, m_r}{\nu_{sr}(m_r + m_r)}, \qquad b_{sr} = \frac{2\, a_{sr}\, m_s}{m_s + m_r}, \qquad \gamma_{sr} = \frac{m_s\, a_{sr}}{3}\left(\frac{2\, m_r}{m_s + m_r} - a_{sr}\right)$$

From these explicit expressions it is possible to define uniquely the parameters $\mathbf{u}_{sr}$, T_{sr} as

$$\boxed{\begin{aligned} \mathbf{u}_{sr} &= (1 - a_{sr})\,\mathbf{u}_s + a_{sr}\,\mathbf{u}_r \\ T_{sr} &= (1 - b_{sr})\,T_s + b_{sr}\,T_r + \gamma_{sr}\,|\mathbf{u}_s - \mathbf{u}_r|^2 \end{aligned}}$$

where

$$a_{sr} = \frac{\lambda_{sr}\, n_r\, m_r}{\nu_{sr}(m_r + m_r)}\,, \qquad b_{sr} = \frac{2\, a_{sr}\, m_s}{m_s + m_r}\,, \qquad \gamma_{sr} = \frac{m_s\, a_{sr}}{3}\left(\frac{2\, m_r}{m_s + m_r} - a_{sr}\right)$$

The effects of the intermolecular potentials are included in coefficients λ_{sr}, and possibly in collision frequencies ν_{sr} (free parameters)

Main properties

Theorem

The BBGSP model preserves positivity of solutions f_s and of corresponding temperatures T_s, $s = 1, \dots, N$, provided that collision frequencies satisfy the conditions

$$\nu_{sr} \geq \frac{1}{2}\lambda_{sr}\, n_r$$

The BGK model satisfies all the main properties of Boltzmann equations:

- *conservation laws (for mass, momentum and energy);*
- *H–theorem;*
- *uniqueness of equilibrium solution* $f_s^{eq} = n_s\, M\left(\mathbf{v}; \mathbf{u}, \dfrac{T}{m_s}\right)$

Collision frequencies

Various strategies are available in order to fix collision frequencies ν_{sr} of a BGK model for mixtures:

- imposing preservation even of Boltzmann exchange rates of viscous stress;
- imposing that average loss terms of Boltzmann equations equal the BGK ones;

  ...

Collision frequencies

Various strategies are available in order to fix collision frequencies ν_{sr} of a BGK model for mixtures:

- imposing preservation even of Boltzmann exchange rates of viscous stress;
- imposing that average loss terms of Boltzmann equations equal the BGK ones;
- ...

Hydrodynamic limits

The structure of BBGSP model allows to investigate its hydrodynamic limit not only in the classical collision dominated regime:

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \frac{1}{\varepsilon} \sum_{r=1}^{N} \nu_{sr} \left(n_s \mathcal{M}_{sr} - f_s \right)$$

but also in situations where only intra–species collisions are dominant

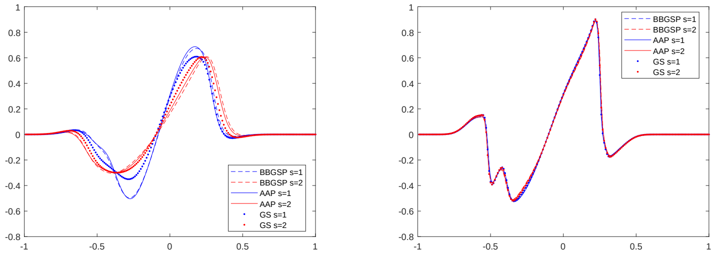
$\Rightarrow$ In both regimes, Navier–Stokes equations have been derived owing to a Chapman–Enskog asymptotic procedure

(Bisi, Groppi, Martalò, J. Phys. A 2021)

Numerical comparison with other BGK models

(Cho, Boscarino, Groppi, Russo, KRM 2021)

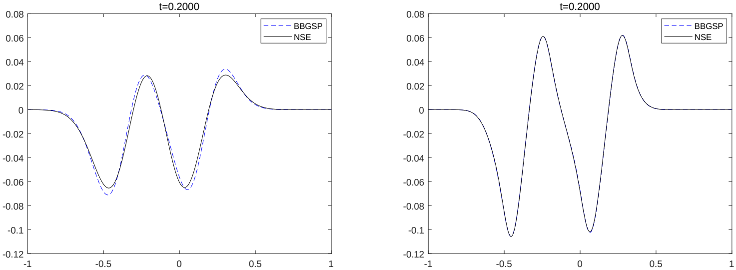
Numerical approximation: conservative semi-Lagrangian methods with high order Diagonally Implicit Runge Kutta or Backward Difference Formula methods for time discretization (asymptotic preserving (AP) schemes)



(a) $\varepsilon = 10^{-2}$ (b) $\varepsilon = 10^{-3}$

Figure: Comparison of species velocities u_s from three BGK models: Andries, Aoki, Perthame 2002 (solid line), Bisi, Groppi, Spiga 2010 ('$\cdot\cdot\cdot$'), BBGSP ('$- - -$')

Comparison between BBGSP model and Navier–Stokes equations



(a) $\varepsilon = 10^{-2}$ (b) $\varepsilon = 10^{-3}$

Figure: Comparison of global velocity u from BBGSP and NS equations

Mixed Boltzmann–BGK model

- **Boltzmann model**
  - integro-differential Boltzmann equations for distribution functions
  - collision operators as sum of binary terms
  - detailed description of the interactions between any pair of components
  - high computational cost for integral operators

- **BGK models**
  - simpler linear relaxation operators
  - more manageable numerics and hydrodynamic limits
  - not unique model for mixtures
  - no detail at microscopic level

- **Aim of the mixed model**:
  to combine the positive features of the two descriptions

General form of the Boltzmann–BGK model

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \left[\chi_{sr}\, \mathcal{Q}_{sr}(f_s, f_r) + (1 - \chi_{sr})\, \widetilde{\mathcal{Q}}_{sr}(f_s) \right], \quad s = 1, \ldots, N$$

where

- $\mathcal{Q}_{sr}(f_s, f_r)$ is the usual bi–species Boltzmann operator;
- $\widetilde{\mathcal{Q}}_{sr}(f_s)$ is the BGK operator constructed above *(BBGSP model, 2018)*;
- $\chi_{sr} \in \{0, 1\}$ are such that $\chi_{sr} = \chi_{rs}$, $\forall s, r = 1, \ldots, N$

General form of the Boltzmann–BGK model

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \left[\chi_{sr} \, \mathcal{Q}_{sr}(f_s, f_r) + (1 - \chi_{sr}) \, \widetilde{\mathcal{Q}}_{sr}(f_s) \right], \quad s = 1, \ldots, N$$

where

- $\mathcal{Q}_{sr}(f_s, f_r)$ is the usual bi–species Boltzmann operator;
- $\widetilde{\mathcal{Q}}_{sr}(f_s)$ is the BGK operator constructed above *(BBGSP model, 2018)*;
- $\chi_{sr} \in \{0, 1\}$ are such that $\chi_{sr} = \chi_{rs}$, $\forall s, r = 1, \ldots, N$

- Interactions between any pair of species (s, r) may be modelled by a Boltzmann or by a BGK operator
- The option $\chi_{sr} = 1, \ \forall (s, r)$ provides the full Boltzmann model
- The option $\chi_{sr} = 0, \ \forall (s, r)$ provides the BBGSP relaxation model

General form of the Boltzmann–BGK model

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \left[\chi_{sr}\, \mathcal{Q}_{sr}(f_s, f_r) + (1 - \chi_{sr})\, \widetilde{\mathcal{Q}}_{sr}(f_s) \right], \quad s = 1, \dots, N$$

where

- $\mathcal{Q}_{sr}(f_s, f_r)$ is the usual bi–species Boltzmann operator;
- $\widetilde{\mathcal{Q}}_{sr}(f_s)$ is the BGK operator constructed above *(BBGSP model, 2018)*;
- $\chi_{sr} \in \{0, 1\}$ are such that $\chi_{sr} = \chi_{rs}$, $\forall s, r = 1, \dots, N$

- Interactions between any pair of species (s, r) may be modelled by a Boltzmann or by a BGK operator
- The option $\chi_{sr} = 1,\ \forall (s, r)$ provides the full Boltzmann model
- The option $\chi_{sr} = 0,\ \forall (s, r)$ provides the BBGSP relaxation model

Particular option *(that will be mainly shown)*

$$\chi_{ss} = 1, \quad \forall s \qquad \text{and} \qquad \chi_{sr} = 0, \quad \forall r \neq s$$

$\Rightarrow$ Boltzmann operators for intra–species collisions and BGK operators for inter–species interactions

Boltzmann/BGK model for intra–species / inter–species interactions

- Intra–species collisions between molecules of the same component are modelled by Boltzmann operators
- Inter–species collisions between molecules of different constituents are described by BGK operators

- Intra–species collisions between molecules of the same component are modelled by Boltzmann operators
- Inter–species collisions between molecules of different constituents are described by BGK operators

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \widehat{\mathcal{Q}}_s = \underbrace{\mathcal{Q}_{ss}}_{Boltzmann} + \sum_{\substack{r=1 \\ r \neq s}}^{N} \underbrace{\widetilde{\mathcal{Q}}_{sr}}_{BGK} \quad , \quad s = 1, \ldots, N$$

with BGK operators of the BBGSP model

- Intra–species collisions between molecules of the same component are modelled by Boltzmann operators
- Inter–species collisions between molecules of different constituents are described by BGK operators

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \widehat{\mathcal{Q}}_s = \underbrace{\mathcal{Q}_{ss}}_{Boltzmann} + \sum_{\substack{r=1 \\ r \neq s}}^{N} \underbrace{\widetilde{\mathcal{Q}}_{sr}}_{BGK} \quad , \qquad s = 1, \dots, N$$

with BGK operators of the BBGSP model

$$\widetilde{\mathcal{Q}}_{sr} = \nu_{sr} \left(n_s \mathcal{M}_{sr} - f_s \right), \qquad \text{where } \mathcal{M}_{sr} = \mathcal{M}_{sr}(\mathbf{v}; \mathbf{u}_{sr}, \tfrac{T_{sr}}{m_s}) \text{ with}$$

$$\begin{aligned} \mathbf{u}_{sr} &= (1 - a_{sr})\mathbf{u}_s + a_{sr}\mathbf{u}_r \\ T_{sr} &= (1 - b_{sr}) T_s + b_{sr} T_r + \gamma_{sr} \left| \mathbf{u}_s - \mathbf{u}_r \right|^2 \end{aligned}$$

where $s \neq r$ and

$$a_{sr} = \frac{\lambda_{sr} n_r m_r}{\nu_{sr}(m_s + m_r)}, \qquad b_{sr} = \frac{2 a_{sr} m_s}{m_s + m_r}, \qquad \gamma_{sr} = \frac{m_s a_{sr}}{3} \left(\frac{2 m_r}{m_s + m_r} - a_{sr} \right)$$

with λ_{sr} related to the interaction potential

Consistency of the mixed kinetic model

We have to prove

1. Conservation of mass, momentum and energy

$$< \widehat{\mathcal{Q}}_s, 1 >= 0 \quad , \quad s = 1, \ldots, N$$

$$\sum_{s=1}^{N} m_s < \widehat{\mathcal{Q}}_s, \mathbf{v} >= \mathbf{0} \quad , \quad \sum_{s=1}^{N} m_s < \widehat{\mathcal{Q}}_s, |\mathbf{v}|^2 >= 0$$

Consistency of the mixed kinetic model

We have to prove

1. Conservation of mass, momentum and energy

$$< \widehat{\mathcal{Q}}_s, 1 >= 0 \quad , \quad s = 1, \dots, N$$

$$\sum_{s=1}^{N} m_s < \widehat{\mathcal{Q}}_s, \mathbf{v} >= \mathbf{0} \quad , \quad \sum_{s=1}^{N} m_s < \widehat{\mathcal{Q}}_s, |\mathbf{v}|^2 >= 0$$

2. H–theorem (space homogeneous case)

$$\mathcal{H} = \sum_{s=1}^{N} < f_s, \log f_s > \text{ is a Lyapunov functional}$$

Consistency of the mixed kinetic model

We have to prove

1. Conservation of mass, momentum and energy

$$< \widehat{\mathcal{Q}}_s, 1 >= 0 \quad , \quad s = 1, \dots, N$$

$$\sum_{s=1}^{N} m_s < \widehat{\mathcal{Q}}_s, \mathbf{v} >= \mathbf{0} \quad , \quad \sum_{s=1}^{N} m_s < \widehat{\mathcal{Q}}_s, |\mathbf{v}|^2 >= 0$$

2. H–theorem (space homogeneous case)

$$\mathcal{H} = \sum_{s=1}^{N} < f_s, \log f_s > \ \text{ is a Lyapunov functional}$$

3. Equilibrium distributions

$$\widehat{\mathcal{Q}}_s = 0\,, \quad s = 1, \dots, N \iff f_s = n_s \left(\frac{m_s}{2\pi T} \right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T} |\mathbf{v} - \mathbf{u}|^2 \right]$$

Conservation of mass, momentum and energy

- Mass conservation easily follows from

$$< \mathcal{Q}_{ss}, 1 >=< \widetilde{\mathcal{Q}}_{sr}, 1 >= 0$$

Conservation of mass, momentum and energy

- Mass conservation easily follows from

$$< \mathcal{Q}_{ss}, 1 >=< \widetilde{\mathcal{Q}}_{sr}, 1 >= 0$$

- For momentum and energy conservation

$$\sum_{s=1}^{N} < \mathcal{Q}_{ss}, \begin{pmatrix} m_s \mathbf{v} \\ m_s |\mathbf{v}|^2 \end{pmatrix} > + \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \begin{pmatrix} m_s \mathbf{v} \\ m_s |\mathbf{v}|^2 \end{pmatrix} >= \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$$

we observe that

- $m_s \mathbf{v}$ and $m_s |\mathbf{v}|^2$ are collision invariants for single–species Boltzmann operators;
- it holds

$$< \widetilde{\mathcal{Q}}_{sr}, \begin{pmatrix} m_s \mathbf{v} \\ m_s |\mathbf{v}|^2 \end{pmatrix} >= - < \widetilde{\mathcal{Q}}_{rs}, \begin{pmatrix} m_r \mathbf{v} \\ m_r |\mathbf{v}|^2 \end{pmatrix} >$$

H-theorem

$$\mathcal{H} = \sum_{s=1}^{N} < f_s, \log f_s > \qquad \Rightarrow \qquad \frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > \leq 0$$

H-theorem

$$\mathcal{H} = \sum_{s=1}^{N} < f_s, \log f_s > \qquad \Rightarrow \qquad \frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > \leq 0$$

Proof.

$$\sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > = \sum_{s=1}^{N} \underbrace{< \mathcal{Q}_{ss}, \log f_s >}_{\leq 0} + \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s >$$

$$\mathcal{H} = \sum_{s=1}^{N} < f_s, \log f_s > \qquad \Rightarrow \qquad \frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > \leq 0$$

Proof.

$$\sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > = \sum_{s=1}^{N} \underbrace{< \mathcal{Q}_{ss}, \log f_s >}_{\leq 0} + \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s >$$

where

$$\sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s > = \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} < n_s \mathcal{M}_{sr} - f_s, \log f_s >$$

H-theorem

$$\mathcal{H} = \sum_{s=1}^{N} < f_s, \log f_s > \qquad \Rightarrow \qquad \frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > \leq 0$$

Proof.

$$\sum_{s=1}^{N} < \widehat{\mathcal{Q}}_s, \log f_s > = \sum_{s=1}^{N} \underbrace{< \mathcal{Q}_{ss}, \log f_s >}_{\leq 0} + \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s >$$

where

$$\sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s > = \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} < n_s \mathcal{M}_{sr} - f_s, \log f_s >$$

by using $(y - x) \log x \leq y(\log y - 1) - x(\log x - 1)$

$$\leq \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} \left[< n_s \mathcal{M}_{sr}, \log(n_s \mathcal{M}_{sr}) > - < f_s, \log f_s > - \underbrace{< n_s \mathcal{M}_{sr} - f_s, 1 >}_{= n_s - n_s = 0} \right]$$

by recalling that $< f_s, \log f_s >$ takes its minimum at $f_s = n_s \, \mathcal{M}_s$

where $\mathcal{M}_s$ is the Maxwellian having the same moments of f_s

$$\leq \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} \left[< n_s \mathcal{M}_{sr}, \log(n_s \mathcal{M}_{sr}) > - < n_s \mathcal{M}_s, \log(n_s \mathcal{M}_s) > \right]$$

by recalling that $< f_s, \log f_s >$ takes its minimum at $f_s = n_s \mathcal{M}_s$ where $\mathcal{M}_s$ is the Maxwellian having the same moments of f_s

$$\leq \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} \left[< n_s \mathcal{M}_{sr}, \log(n_s \mathcal{M}_{sr}) > - < n_s \mathcal{M}_s, \log(n_s \mathcal{M}_s) > \right]$$

by computing the logarithm of Maxwellian distributions

$$= -\frac{3}{2} \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} n_s \nu_{sr} \left(\log T_{sr} - \log T_s \right)$$

by recalling that $< f_s, \log f_s >$ takes its minimum at $f_s = n_s\, \mathcal{M}_s$
where $\mathcal{M}_s$ is the Maxwellian having the same moments of f_s

$$\leq \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r\neq s}}^{N} \nu_{sr} \left[< n_s \mathcal{M}_{sr}, \log(n_s \mathcal{M}_{sr}) > - < n_s \mathcal{M}_s, \log(n_s \mathcal{M}_s) >\right]$$

by computing the logarithm of Maxwellian distributions

$$= -\frac{3}{2} \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r\neq s}}^{N} n_s \nu_{sr} \left(\log T_{sr} - \log T_s\right) \leq 0$$

by recalling the expressions of the and auxiliary temperatures

$T_{sr} \geq (1 - b_{sr})\, T_s + b_{sr}\, T_r$,

and symmetry properties of coefficients $(n_s \nu_{sr} b_{sr} = n_r \nu_{rs} b_{rs})$

□

Equilibrium distributions

$$\widehat{\mathcal{Q}}_s = 0, \quad s = 1, \ldots, N \iff f_s = n_s \left(\frac{m_s}{2\pi T} \right)^{\frac{3}{2}} \exp \left[-\frac{m_s}{2T} |\mathbf{v} - \mathbf{u}|^2 \right]$$

Equilibrium distributions

$$\widehat{\mathcal{Q}}_s = 0, \quad s = 1, \ldots, N \iff f_s = n_s \left(\frac{m_s}{2\pi T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T}\left|\mathbf{v} - \mathbf{u}\right|^2\right]$$

$\Longleftarrow$ Trivial

Equilibrium distributions

$$\widehat{\mathcal{Q}}_s = 0, \quad s = 1, \ldots, N \iff f_s = n_s \left(\frac{m_s}{2\pi T} \right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T} |\mathbf{v} - \mathbf{u}|^2 \right]$$

$\Longleftarrow$ Trivial

$\Longrightarrow$ The H–theorem provides

$$\frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} \underbrace{< \mathcal{Q}_{ss}, \log f_s >}_{\leq 0} + \underbrace{\sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s >}_{\leq 0}$$

Equilibrium distributions

$$\widehat{\mathcal{Q}}_s = 0, \quad s = 1, \ldots, N \iff f_s = n_s \left(\frac{m_s}{2\pi T} \right)^{\frac{3}{2}} \exp \left[-\frac{m_s}{2T} |\mathbf{v} - \mathbf{u}|^2 \right]$$

$\Longleftarrow$ Trivial

$\Longrightarrow$ The H–theorem provides

$$\frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} \underbrace{< \mathcal{Q}_{ss}, \log f_s >}_{\leq 0} + \underbrace{\sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s >}_{\leq 0}$$

$\Rightarrow$ From Boltzmann operators, equilibria are local Maxwellians.

Equilibrium distributions

$$\widehat{\mathcal{Q}}_s = 0, \quad s = 1, \ldots, N \iff f_s = n_s \left(\frac{m_s}{2\pi T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T}|\mathbf{v}-\mathbf{u}|^2\right]$$

$\Longleftarrow$ Trivial

$\Longrightarrow$ The H–theorem provides

$$\frac{\partial \mathcal{H}}{\partial t} = \sum_{s=1}^{N} \underbrace{< \mathcal{Q}_{ss}, \log f_s >}_{\leq 0} + \underbrace{\sum_{s=1}^{N} \sum_{\substack{r=1 \\ r\neq s}}^{N} < \widetilde{\mathcal{Q}}_{sr}, \log f_s >}_{\leq 0}$$

$\Rightarrow$ From Boltzmann operators, equilibria are local Maxwellians.

Passing to the weak form

$$\widehat{\mathcal{Q}}_s = 0 \quad \Rightarrow \quad < \mathcal{Q}_{ss}, \begin{pmatrix} m_s \mathbf{v} \\ m_s|\mathbf{v}|^2 \end{pmatrix} > + \sum_{r\neq s} < \widetilde{\mathcal{Q}}_{sr}, \begin{pmatrix} m_s \mathbf{v} \\ m_s|\mathbf{v}|^2 \end{pmatrix} > = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$$

and computing explicitly, we obtain

$$\sum_{r\neq s} \lambda_{sr} \frac{m_s m_r}{m_s + m_r} n_s n_r (\mathbf{u}_s - \mathbf{u}_r) = \mathbf{0} \quad \Longrightarrow \quad \mathbf{u}_1 = \mathbf{u}_2 = \ldots = \mathbf{u}_N$$

$$\sum_{r\neq s} 2\lambda_{sr} \frac{m_s m_r}{(m_s + m_r)^2} n_s n_r (T_s - T_r) = 0 \quad \Longrightarrow \quad T_1 = T_2 = \ldots = T_N$$

General mixed Boltzmann–BGK model

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \left[\chi_{sr}\, \mathcal{Q}_{sr}(f_s, f_r) + (1 - \chi_{sr})\, \widetilde{\mathcal{Q}}_{sr}(f_s) \right], \qquad {}^{s=1,\dots,N}_{\chi_{sr} \in \{0,1\}}$$

By similar arguments as above, it is possible to prove

- conservations of mass, momentum and energy;
- H-theorem;
- uniqueness of equilibrium solutions.

General mixed Boltzmann–BGK model

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \sum_{r=1}^{N} \left[\chi_{sr}\, \mathcal{Q}_{sr}(f_s, f_r) + (1 - \chi_{sr})\, \widetilde{\mathcal{Q}}_{sr}(f_s) \right], \qquad \begin{array}{c} s=1,\dots,N \\ \chi_{sr} \in \{0,1\} \end{array}$$

By similar arguments as above, it is possible to prove

- conservations of mass, momentum and energy;
- H-theorem;
- uniqueness of equilibrium solutions.

The proof of the entropy dissipation is based on

$$\begin{aligned} \frac{\partial \mathcal{H}}{\partial t} = & \sum_{s=1}^{N} \chi_{ss} \underbrace{< \mathcal{Q}_{ss}(f_s, f_s), \log f_s >}_{\leq 0} + \sum_{s=1}^{N} (1 - \chi_{ss}) \underbrace{< \widetilde{\mathcal{Q}}_{ss}(f_s), \log f_s >}_{\leq 0} \\ & + \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r>s}}^{N} \chi_{sr} \Big(\underbrace{< \mathcal{Q}_{sr}(f_s, f_r), \log f_s > + < \mathcal{Q}_{rs}(f_r, f_s), \log f_r >}_{\leq 0} \Big) \\ & + \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r>s}}^{N} (1 - \chi_{sr}) \Big(\underbrace{< \widetilde{\mathcal{Q}}_{sr}(f_s), \log f_s > + < \widetilde{\mathcal{Q}}_{rs}(f_r), \log f_r >}_{\leq 0} \Big) \end{aligned}$$

Hydrodynamic limits

of Boltzmann/BGK model for intra–species / inter–species interactions

By a proper scaling, we introduce the non-dimensional equations

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \frac{1}{\varepsilon} \mathcal{Q}_{ss} + \frac{\alpha}{\varepsilon} \sum_{\substack{r=1 \\ r \neq s}}^{N} \widetilde{\mathcal{Q}}_{sr} \quad , \quad s = 1, \ldots, N$$

where

- ε is the Knudsen number (small parameter)
- α is a proper constant allowing to analyze different regimes *(related to collision frequencies ν_{sr} of BGK operators)*

Hydrodynamic limits

of Boltzmann/BGK model for intra–species / inter–species interactions

By a proper scaling, we introduce the non-dimensional equations

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \frac{1}{\varepsilon} \mathcal{Q}_{ss} + \frac{\alpha}{\varepsilon} \sum_{\substack{r=1 \\ r \neq s}}^{N} \widetilde{\mathcal{Q}}_{sr} \quad , \quad s = 1, \ldots, N$$

where

- ε is the Knudsen number (small parameter)
- α is a proper constant allowing to analyze different regimes *(related to collision frequencies ν_{sr} of BGK operators)*

We consider two different hydrodynamic regimes:

1. all collisions are dominant $\Longrightarrow \alpha = 1$
2. only intra–species collisions are dominant $\Longrightarrow \alpha = \varepsilon$

Hydrodynamic limits

of Boltzmann/BGK model for intra–species / inter–species interactions

By a proper scaling, we introduce the non-dimensional equations

$$\frac{\partial f_s}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s = \frac{1}{\varepsilon} \mathcal{Q}_{ss} + \frac{\alpha}{\varepsilon} \sum_{\substack{r=1 \\ r \neq s}}^{N} \widetilde{\mathcal{Q}}_{sr} \quad , \quad s = 1, \dots, N$$

where

- ε is the Knudsen number (small parameter)
- α is a proper constant allowing to analyze different regimes *(related to collision frequencies ν_{sr} of BGK operators)*

We consider two different hydrodynamic regimes:

1. all collisions are dominant $\Longrightarrow \alpha = 1$
2. only intra–species collisions are dominant $\Longrightarrow \alpha = \varepsilon$

We expand distribution functions in powers of ε as $f_s = f_s^{(0)} + \varepsilon f_s^{(1)}$

Euler equations

$\alpha = 1$: collision dominated regime

At the zero-th order of approximation, we have

$$f_s \simeq n_s \left(\frac{m_s}{2\pi T}\right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T}|\mathbf{v}-\mathbf{u}|^2\right]$$

and the evolution is governed by classical Euler equations

Euler equations

$\alpha = 1$: collision dominated regime

At the zero-th order of approximation, we have

$$f_s \simeq n_s \left(\frac{m_s}{2\pi T} \right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T} |\mathbf{v} - \mathbf{u}|^2 \right]$$

and the evolution is governed by classical Euler equations

$\alpha = \varepsilon$: intra–species dominant collisions

At the zero-th order of approximation, we have

$$f_s \simeq n_s \left(\frac{m_s}{2\pi T_s} \right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T_s} |\mathbf{v} - \mathbf{u}_s|^2 \right]$$

and we obtain macroscopic multi-velocity and multi-temperature equations, with production terms due to inter–species interactions

Euler equations in the regime with intra–species dominant collisions

$$\frac{\partial n_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_s \, \mathbf{u}_s) = 0 \,, \qquad s = 1, \ldots, N$$

$$\frac{\partial}{\partial t}(\rho_s \mathbf{u}_s) + \nabla_{\mathbf{x}} \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla_{\mathbf{x}}(n_s \, T_s) = \sum_{\substack{r=1 \\ r \neq s}}^{N} \mathbf{R}_{sr} \,,$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \, \rho_s |\mathbf{u}_s|^2 + \frac{3}{2} \, n_s \, T_s \right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2} \, \rho_s |\mathbf{u}_s|^2 + \frac{5}{2} \, n_s \, T_s \right) \mathbf{u}_s \right] = \sum_{\substack{r=1 \\ r \neq s}}^{N} \mathbf{S}_{sr}$$

Euler equations in the regime with intra–species dominant collisions

$$\frac{\partial n_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_s\, \mathbf{u}_s) = 0\,, \qquad\qquad s = 1, \dots, N$$

$$\frac{\partial}{\partial t}(\rho_s \mathbf{u}_s) + \nabla_{\mathbf{x}} \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla_{\mathbf{x}}(n_s\, T_s) = \sum_{\substack{r=1 \\ r\neq s}}^{N} \mathbf{R}_{sr},$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\,\rho_s |\mathbf{u}_s|^2 + \frac{3}{2}\, n_s\, T_s\right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2}\,\rho_s |\mathbf{u}_s|^2 + \frac{5}{2}\, n_s\, T_s\right)\mathbf{u}_s\right] = \sum_{\substack{r=1 \\ r\neq s}}^{N} \mathbf{S}_{sr}$$

with collision contributions (coming from slow BGK operators)

$$\mathbf{R}_{sr} = -\,\lambda_{sr}\, \frac{m_s\, m_r}{m_s + m_r}\, n_s n_r\, (\mathbf{u}_s - \mathbf{u}_r)$$

$$\mathbf{S}_{sr} = -\,\lambda_{sr}\, \frac{m_s\, m_r}{(m_s + m_r)^2}\, n_s\, n_r \Big[(m_s\, \mathbf{u}_s + m_r\, \mathbf{u}_r) \cdot (\mathbf{u}_s - \mathbf{u}_r) + 3\,(T_s - T_r) \Big]$$

In progress: **Collision dominated regime** $\alpha = 1$

First order distribution:

$$f_s^{(1)} = \frac{1}{\sum_{\substack{r=1\\ r\neq s}}^N \nu_{sr}^{(0)}} \left[n_s \sum_{\substack{r=1\\ r\neq s}}^N \nu_{sr}^{(0)} \mathcal{M}_{sr}^{(1)} + L(f_s^{(1)}) - \left(\frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)} \right) \right]$$

In progress: **Collision dominated regime** $\alpha = 1$

First order distribution:

$$f_s^{(1)} = \frac{1}{\sum_{\substack{r=1 \\ r\neq s}}^N \nu_{sr}^{(0)}} \left[n_s \sum_{\substack{r=1 \\ r\neq s}}^N \nu_{sr}^{(0)} \mathcal{M}_{sr}^{(1)} + L(f_s^{(1)}) - \left(\frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)} \right) \right]$$

where

- $\mathcal{M}_{sr}^{(1)} = \dfrac{\partial}{\partial \varepsilon} \mathcal{M}_{sr} \left(\mathbf{v}; \mathbf{u} + \varepsilon\, u_{sr}^{(1)}, \dfrac{T + \varepsilon\, T_{sr}^{(1)}}{m_s} \right) \Big|_{\varepsilon=0}$
- $\dfrac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)}$ may be computed owing to Euler equations
- $L(f_s^{(1)}) = \mathcal{Q}_{ss}(f_s^{(0)}, f_s^{(1)}) + \mathcal{Q}_{ss}(f_s^{(1)}, f_s^{(0)})$
  is the linearized Boltzmann operator

In progress: **Collision dominated regime** $\alpha = 1$

First order distribution:

$$f_s^{(1)} = \frac{1}{\sum_{\substack{r=1\\ r\neq s}}^N \nu_{sr}^{(0)}} \left[n_s \sum_{\substack{r=1\\ r\neq s}}^N \nu_{sr}^{(0)} \mathcal{M}_{sr}^{(1)} + L(f_s^{(1)}) - \left(\frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)} \right) \right]$$

where

- $\mathcal{M}_{sr}^{(1)} = \frac{\partial}{\partial \varepsilon} \mathcal{M}_{sr} \left(\mathbf{v}; \mathbf{u} + \varepsilon\, u_{sr}^{(1)}, \frac{T + \varepsilon\, T_{sr}^{(1)}}{m_s} \right) \Big|_{\varepsilon=0}$
- $\frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)}$ may be computed owing to Euler equations
- $L(f_s^{(1)}) = \mathcal{Q}_{ss}(f_s^{(0)}, f_s^{(1)}) + \mathcal{Q}_{ss}(f_s^{(1)}, f_s^{(0)})$
  is the linearized Boltzmann operator

$\Rightarrow$ We have to solve an equation of the form $\widetilde{L}_s[f_s^{(1)}] = \Phi_s$

Solvability of $\widetilde{L}_s[f_s^{(1)}] = \Phi_s,$ where $\widetilde{L}_s = \dfrac{1}{\sum_{\substack{r=1 \\ r\neq s}}^{N} \nu_{sr}^{(0)}} L_s - Id$

(in collaboration with N. Bernhoff (Karlstad))

Solvability of $\widetilde{L}_s[f_s^{(1)}] = \Phi_s,$ where $\widetilde{L}_s = \dfrac{1}{\sum_{\substack{r=1\\ r\neq s}}^N \nu_{sr}^{(0)}} L_s - Id$

(in collaboration with N. Bernhoff (Karlstad))

- Under the Grad's assumption on the collision kernel g_{ss} (which is fulfilled by hard spheres and cut-off inverse power-law potentials)

  $\widetilde{L}_s$ is a coercive self-adjoint Fredholm operator

  on the real Hilbert space $L^2(\mathbb{R}^3; f_s^{(0)}\, d\mathbf{v})$ with inner product $\langle \cdot, \cdot \rangle_{f_s^{(0)}}$ and $Ker(\widetilde{L}_s) = \{0\}$
- $\widetilde{L}_s$ is invertible, with inverse operator $\widetilde{L}_s^{-1}$ such that $\| \widetilde{L}_s^{-1} \|_{f_s^{(0)}} \leq 1$

Solvability of $\widetilde{L_s}[f_s^{(1)}] = \Phi_s,$ where $\widetilde{L_s} = \dfrac{1}{\sum_{\substack{r=1\\r\neq s}}^{N} \nu_{sr}^{(0)}} L_s - Id$

(in collaboration with N. Bernhoff (Karlstad))

- Under the Grad's assumption on the collision kernel g_{ss} (which is fulfilled by hard spheres and cut-off inverse power-law potentials)

  $\widetilde{L_s}$ is a coercive self-adjoint Fredholm operator

  on the real Hilbert space $L^2(\mathbb{R}^3; f_s^{(0)}\, d\mathbf{v})$ with inner product $\langle \cdot, \cdot \rangle_{f_s^{(0)}}$ and $Ker(\widetilde{L_s}) = \{0\}$
- $\widetilde{L_s}$ is invertible, with inverse operator $\widetilde{L_s}^{-1}$ such that $\|\widetilde{L_s}^{-1}\|_{f_s^{(0)}} \leq 1$

$\Rightarrow$ $f_s^{(1)}$ exists, is unique but cannot be made explicit;
however, its moments needed in the Navier–Stokes approximation may be recovered by suitable computations
(in progress by the PhD student E. Lucchin (Parma))

Regime with dominant intra–species collisions $\alpha = \varepsilon$

$$L(f_s^{(1)}) = \frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)} - \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr}^{(0)} \left(n_s \, \mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right)$$

where $L(f_s^{(1)})$ is classical linearized Boltzmann operator

Regime with dominant intra–species collisions $\alpha = \varepsilon$

$$L(f_s^{(1)}) = \frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)} - \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr}^{(0)} \left(n_s \, \mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right)$$

where $L(f_s^{(1)})$ is classical linearized Boltzmann operator

$\Rightarrow$ We obtain the **Navier–Stokes equations**

$$\frac{\partial n_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_s \mathbf{u}_s) = 0 \,, \qquad s = 1, \ldots, N$$

$$\frac{\partial}{\partial t}(\rho_s \mathbf{u}_s) + \nabla_{\mathbf{x}} \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla_{\mathbf{x}}(n_s T_s) + \varepsilon \nabla_{\mathbf{x}} \cdot \mathbf{P}_s^{(1)} = \sum_{\substack{r=1 \\ r \neq s}}^{N} \mathbf{R}_{sr}$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho u_s^2 + \frac{3}{2} n_s T_s \right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho_s u_s^2 + \frac{5}{2} n_s T_s \right) \mathbf{u}_s \right]$$

$$+ \varepsilon \nabla_{\mathbf{x}} \cdot \left[\mathbf{P}_s^{(1)} \cdot \mathbf{u}_s + \mathbf{q}_s^{(1)} \right] = \sum_{\substack{r=1 \\ r \neq s}}^{N} \mathbf{S}_{sr}$$

Regime with dominant intra–species collisions $\alpha = \varepsilon$

$$L(f_s^{(1)}) = \frac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)} - \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr}^{(0)} \left(n_s \, \mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right)$$

where $L(f_s^{(1)})$ is classical linearized Boltzmann operator

$\Rightarrow$ We obtain the **Navier–Stokes equations**

$$\frac{\partial n_s}{\partial t} + \nabla_{\mathbf{x}} \cdot (n_s \mathbf{u}_s) = 0 \,, \qquad s = 1, \ldots, N$$

$$\frac{\partial}{\partial t}(\rho_s \mathbf{u}_s) + \nabla_{\mathbf{x}} \cdot (\rho_s \mathbf{u}_s \otimes \mathbf{u}_s) + \nabla_{\mathbf{x}}(n_s T_s) + \varepsilon \nabla_{\mathbf{x}} \cdot \mathbf{P}_s^{(1)} = \sum_{\substack{r=1 \\ r \neq s}}^{N} \mathbf{R}_{sr}$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho u_s^2 + \frac{3}{2} n_s T_s \right) + \nabla_{\mathbf{x}} \cdot \left[\left(\frac{1}{2} \rho_s u_s^2 + \frac{5}{2} n_s T_s \right) \mathbf{u}_s \right]$$

$$+ \varepsilon \nabla_{\mathbf{x}} \cdot \left[\mathbf{P}_s^{(1)} \cdot \mathbf{u}_s + \mathbf{q}_s^{(1)} \right] = \sum_{\substack{r=1 \\ r \neq s}}^{N} \mathbf{S}_{sr}$$

with $\quad \mathbf{P}_s^{(1)} = \int_{\mathbb{R}^3} m_s (\mathbf{c}_s \otimes \mathbf{c}_s) f_s^{(1)}(\mathbf{v}) d\mathbf{v} \,, \qquad \mathbf{q}_s^{(1)} = \int_{\mathbb{R}^3} \frac{1}{2} m_s \mathbf{c}_s c_s^2 f_s^{(1)}(\mathbf{v}) d\mathbf{v}$

where $\mathbf{c}_s = \mathbf{v} - \mathbf{u}_s$ is the peculiar velocity

For pressure tensor, we have

$$\mathbf{P}_s^{(1)} = -\mu_s \boldsymbol{\Upsilon}_s + \frac{4}{3 n_s \lambda_{ss}^2} \sum_{\substack{r=1 \\ r\neq s}}^{N} \nu_{sr}^{(0)} \rho_i (a_{sr}^{(0)})^2 \left[(\mathbf{u}_s - \mathbf{u}_r) \otimes (\mathbf{u}_s - \mathbf{u}_r) - \frac{1}{3} |\mathbf{u}_s - \mathbf{u}_r|^2 \mathbf{I} \right]$$

where

- $\boldsymbol{\Upsilon}_s$ is the strain rate tensor, given by

$$\Upsilon_{s,ij} = \frac{\partial u_{s,i}}{\partial x_j} + \frac{\partial u_{s,j}}{\partial x_i} - \frac{2}{3} \nabla_{\mathbf{x}} \cdot \mathbf{u}_s \delta_{ij}$$

- $\mu_s = \dfrac{4 T_s}{3 \lambda_{ss}^2}$ is the viscosity coefficient

For heat flux, we have

$$\mathbf{q}_s^{(1)} = -\Lambda_s \nabla_{\mathbf{x}} T_s + \frac{10}{\lambda_{ss}^2} \sum_{\substack{r=1 \\ r\neq s}}^{N} \alpha_{sr} \nu_{sr}^{(0)} (a_{sr}^{(0)})^2 (T_s - T_r)(\mathbf{u}_s - \mathbf{u}_r)$$

$$+ \frac{2m_s}{3\lambda_{ss}^2} \sum_{\substack{r=1 \\ r\neq s}}^{N} \nu_{sr}^{(0)} (a_{sr}^{(0)})^2 (a_{sr}^{(0)} - 5\alpha_{rs}) |\mathbf{u}_s - \mathbf{u}_r|^2 (\mathbf{u}_s - \mathbf{u}_r)$$

where

- $\Lambda_s = \dfrac{5T_s}{m_s \lambda_{ss}^2}$ is the heat conductivity coefficient

(results included in the Master thesis of A. Macaluso)

Concluding remarks

- The mixed Boltzmann-BGK model allows to combine the detailed description of the collisions with the simplicity of the relaxation operators

Concluding remarks

- The mixed Boltzmann-BGK model allows to combine the detailed description of the collisions with the simplicity of the relaxation operators
- Various scenarios can be obtained in the hydrodynamic limit; different Euler and Navier–Stokes equations can be deduced in proper collision-dominated regimes

Concluding remarks

- The mixed Boltzmann-BGK model allows to combine the detailed description of the collisions with the simplicity of the relaxation operators
- Various scenarios can be obtained in the hydrodynamic limit; different Euler and Navier–Stokes equations can be deduced in proper collision-dominated regimes
- The dynamics of mixtures of heavy and light particles (plasma physics, noble gases) can be more suitably reproduced in many applications by a multi-velocity and multi-temperature description

Concluding remarks

- The mixed Boltzmann-BGK model allows to combine the detailed description of the collisions with the simplicity of the relaxation operators
- Various scenarios can be obtained in the hydrodynamic limit; different Euler and Navier–Stokes equations can be deduced in proper collision-dominated regimes
- The dynamics of mixtures of heavy and light particles (plasma physics, noble gases) can be more suitably reproduced in many applications by a multi-velocity and multi-temperature description

Reference paper

M. Bisi, M. Groppi, E. Lucchin, G. Martalò, A mixed Boltzmann–BGK model for inert gas mixtures, *Kinetic and Related Models* (2023), in press.

Future works

- Investigation of other collision–dominated regimes, like for instance the one in which only collisions between heaviest particles are dominant

Future works

- Investigation of other collision–dominated regimes, like for instance the one in which only collisions between heaviest particles are dominant
- Numerical simulations of the kinetic model: some preliminary numerical tests have been recently performed for a binary mixture owing to an IMEX finite volume scheme on unstructured meshes *(M. Bisi, W. Boscheri, G. Dimarco, M. Groppi, G. Martalò, Appl. Math. Comput. (2022))*

Future works

- Investigation of other collision–dominated regimes, like for instance the one in which only collisions between heaviest particles are dominant
- Numerical simulations of the kinetic model: some preliminary numerical tests have been recently performed for a binary mixture owing to an IMEX finite volume scheme on unstructured meshes *(M. Bisi, W. Boscheri, G. Dimarco, M. Groppi, G. Martalò, Appl. Math. Comput. (2022))*
- Extension of the BBGSP model and of the mixed Boltzmann–BGK model to polyatomic gases and to reactive mixtures *(some work is in progress by G. Martalò, A.J. Soares, R. Travaglini)*

Thank you for your attention