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A general Boltzmann-BGK model for gas mixtures: hydrodynamic limits and convergence results

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Abstract

This thesis, in the frame of kinetic theory of gas mixtures, develops a general framework which integrates the Boltzmann and the BGK descriptions of the collision operators within one model, with the aim of combining the accuracy of the Boltzmann integral with the greater analytical and computational tractability of the BGK operator. Hence, the proposed model allows for each binary interaction to be described by either operators. After having proved the consistency properties, namely the correct conservation laws, uniqueness of equilibrium distribution and H-theorem, the dimensionless form of the model is introduced, enabling the analysis of different hydrodynamic regimes. In the classical collision dominated regime, in which all collisions are equally dominant in the evolution, we consider a Chapman-Enskog expansion in terms of a suitable Knudsen number and derive Euler and Navier-Stokes equations in the hydrodynamic limit. In order to provide a closure for the Navier-Stokes equations, we derive explicit first-order corrections for the species velocities, while the complexity of the Boltzmann linearized operator prevents a closed-form computation of the first order corrections of the pressure tensor and heat flux. Nevertheless, the computations involve linear systems which admit unique solutions, ensuring a constructive closure of the Navier–Stokes equations. Since in real mixtures the number of species is typically small, the coefficient matrix can easily be inverted using standard numerical tools. We then analyze binary mixtures in which intra-species collisions are described by Boltzmann operators and inter-species ones by BGK terms, focusing on two relevant hydrodynamic regimes. In the first one, both intra-species interactions play a dominant role, allowing to obtain the Navier-Stokes equations for macroscopic fields of both species, with source terms on the right-hand side, representative of the slow collisional dynamics. In the second one, the dominant role is played by the intra-species interactions of the heavier species only, allowing for fluid equations of Navier-Stokes type for such species, while the lightest one retains a kinetic description. Finally, exponential convergence of the species distribution functions towards the species Maxwellian distribution is proved, with explicit dependence of the convergence rate on the collision frequencies and mixture parameters.

Contents

Introduction

The kinetic theory approach to gas mixtures has received increasing attention in recent decades, and the Boltzmann description has been extended to model more complex systems, including chemically reacting mixtures [46] and polyatomic constituents [27]. For inert mixtures of monatomic species, the classical Boltzmann description is well established, but the analytical investigation of its mathematical properties remains challenging. Despite several advances, both in rigorous results and in the construction of efficient numerical schemes, the Boltzmann system for mixtures is still notoriously difficult to handle because of its nonlinear and multidimensional integral structure. To overcome these difficulties, several simplified models have been proposed, most notably of the BGK type, generalizing the relaxation model proposed by Bhatnagar-Groos-Krook in [3] for a single gas.
A first mathematically rigorous BGK model for gas mixtures was proposed in [1], employing for each species a global relaxation operator towards an auxiliary attracting Maxwellian that accounts for all interactions with all the constituents. Despite its simplicity, this model has been effective and has inspired various generalizations, also to reactive mixtures [29], even of monatomic and polyatomic gases [12]. In a recent paper [13], the analogies and differences among existing BGK models for inert mixtures were discussed, and a new BGK approximation was developed. In this model, the collision operators are expressed as appropriate sums of binary relaxation terms, each reproducing the exchange rates of momentum and energy corresponding to the binary Boltzmann operator. This correspondence between BGK and Boltzmann exchange rates is exact for Maxwell molecule interactions, while a suitable approximation enables the determination of consistent auxiliary parameters, defining the Maxwellian attractors of the BGK operators, even for more general intermolecular potentials. This approach thus extends the applicability of the BGK approximation. However, the important features that make BGK-type models more tractable than the Boltzmann ones also limit their accuracy, and this trade-off between computational manageability and accuracy of the description is what has motivated the construction of a hybrid kinetic model.
Specifically, in this thesis we aim at combining in one model the BGK and the Boltzmann descriptions, therefore we propose a mixed Boltzmann–BGK model for inert mixtures of monatomic gases, where some kinds of interactions are described by means of classical bi-species Boltzmann operators, and the others

by means of the binary BGK operators introduced in [13]. It is well–known indeed that the numerical methods for multi–species Boltzmann equations are computationally expensive, as we can see in [31]. On the other hand, BGK approximations are not capable to reproduce peculiar nonlinear effects, especially in the evolution of high order moments in mixtures with heavy and light components [30]. Considering pros and cons of Boltzmann and BGK approaches, we would like to preserve as much as possible the details of collision parameters and intermolecular potentials as in the Boltzmann description, but keeping the kinetic model manageable from the analytical and the numerical points of view. For this reason, we try to replace some of the integral Boltzmann operators by their simpler BGK approximation, which takes into account the collision process only through the Maxwellian attractor and the collision frequency. Among the many BGK models available for inert mixtures, we use the one of Ref. [13], since it has the same structure as the Boltzmann model and simply replaces each bi–species Boltzmann operator by a proper relaxation term. In addition, contrary to other BGK approaches, this model allows to relate its parameters to each binary interaction potential, preserving a more physically realistic description of the collisions. Thus, it seemed us well suited as a starting point to construct a hybrid kinetic model where only some bi–species interactions are described by relaxation–type operators. It is remarkable that such structure of the mixed kinetic model, mimicking the one of the Boltzmann system, is particularly suitable to describe mixtures of gases with disparate masses, in which the role played by collisions of heavier particles can be put in the right light.
The thesis is organized as follows. In the first chapter we present the distribution function, its moments and the full Boltzmann description of a gas mixture, along with the properties of the collisional operator, the momentum and kinetic energy exchange between generic species s and r, the weak form of the Boltzmann equation and the equilibrium distribution. Then we introduce the BGK model presented in [13] and, by imposing that the exchange of momentum and kinetic energy occurring between species s and r is the same when collisions are described by either the Boltzmann or the BGK operator, we fix the fictitious parameters involved in the auxiliary Maxwellian $\mathcal{M}_{sr}$ of the BGK operator.
In the second chapter we introduce our generalized Boltzmann-BGK model. Specifically, for any pair of species (s, r) with $s, r = 1, \ldots, N$, the relative collision may be described by a Boltzmann or a BGK operator: we fix a set of coefficients $\chi_{sr} \in \{0, 1\}$, with the reasonable symmetry assumption $\chi_{sr} = \chi_{rs}$, such that if $\chi_{sr} = 1$ the (s, r) interactions are modeled by the Boltzmann operator, while if $\chi_{sr} = 0$ by a BGK one. The option $\chi_{sr} = 1$, $\forall(s, r)$ reproduces the full Boltzmann model, while the option $\chi_{sr} = 0$ yields the BGK model built up in [13]. The construction of the mixed kinetic model and its main properties have been published in Ref. [5]. We prove the consistency properties of the model, including the H-theorem, for any choices of coefficients χ_{sr}.
The general structure of this hybrid kinetic model allows, in particular, modeling the more significant part of the collision operator by Boltzmann terms (for instance the dominant interactions, or the ones giving rise to specific features of the considered physical problem), and the other ones by means of simpler

relaxation terms. For instance, in plasmas the physically admissible scalings are strongly affected by the very large mass ratio between ions and electrons, so that the ions–ions interactions play the dominant role (and should be properly described by Boltzmann operators), whereas ions are almost no affected by electrons [32]. Analogously, when a gaseous mixture is assumed diffusing in a much denser host medium [10], Boltzmann description could be used only for the dominant interactions with the background, leaving other intra- and inter–species interactions modeled by BGK terms.

After establishing the consistency properties, we derive the dimensionless form of the model equations. The presence of a collision operator for each gaseous component allows for the study of different hydrodynamic regimes, while also enabling the derivation of evolution equations for the main macroscopic fields. A suitable coefficient appears in front of each collision operator, allowing the selection of the desired regime.

In chapter 3, we focus on the classical collision dominated regime, which is particularly useful when the system is close to local equilibrium and collisions occur much more frequently than macroscopic variations. Using Chapman-Enskog expansion, we derive the Euler equations and we adopt the same approach as in [9] to obtain a closure for the Navier–Stokes equations. We first derive an explicit expression for the first-order approximation of the species velocities. As regards the first-order approximation of the pressure tensor and of the heat-flux vector, the algebraic complexity of the moment equations, due to the simultaneous presence of the Boltzmann linearized operators and of the first order approximation of the BGK terms, prevents their explicit computations; nonetheless, we rigorously establish the existence and uniqueness of solutions to the associated linear systems, proving diagonal dominance of the system matrix and thus providing a constructive closure of the Navier–Stokes equations. However, in real mixtures the number of species N is typically not very large, and the variables involved reduce to strictly positive real numbers. In such cases, the coefficient matrix can be inverted straightforwardly using standard mathematical software.

In chapter 4, we investigate the case in which intra-species collisions are described by the the Boltzmann operators and inter-species ones are treated by the BGK formulation. Exploiting the simpler computations involved, in this case it is possible to provide an explicit expression for any of the additional unknowns of the Navier-Stokes system, and therefore to derive explicitly the transport coefficients, which will still depend on the collision frequencies of binary Boltzmann and BGK operators.

In the last part of the thesis, still pertaining to the case where intra-species collisions are described through the Boltzmann integral and inter-species ones through the BGK operator, the analysis is focused on binary mixtures. In particular, in Chapter 5 we first consider a mixture where one species is much heavier than the other, and investigate the asymptotic limit in the regime dominated by the intra-species collision, obtaining multi-velocities and multi-temperatures Navier-Stokes equations, with source terms accounting for the slow collisional dynamics. In the second part of the same chapter, we analyze a regime where the dominant role is played only by intra-species collisions of the heaviest con-

stituent. This more realistic situation has not yet been deeply investigated in literature and leads to a fluid-kinetic system, composed by macroscopic equations for the heaviest component, coupled with a kinetic equation for the light one, according with the multiscale feature of the dynamics.
In the last Chapter, in the space-homogeneous case, we focus on the estimate of the convergence rate of the kinetic solutions towards the species Maxwellian distributions. We begin by proving the exponential decay rate of the velocities and the temperatures. We then introduce some analytical lemmas that allow us to establish a rigorous proof of exponential convergence of the kinetic solutions towards the local species Maxwellians, showing that any initial distribution relaxes at an explicit rate, depending on collision frequencies and mixture parameters.
Finally, we present some concluding remarks and in Appendix we collect several useful formulas and calculation details of results presented in the thesis.

Chapter 1

Boltzmann and BGK models for gas mixtures

1.1 The distribution function and its moments

In this chapter we report some preliminaries on kinetic theory for rarefied gases, that is at the basis of our research work. Further details may be found in classical books [18, 20, 25, 34]. Since gases involved in physical problems are usually composed of particles of different constituents, in this thesis we consider an inert mixture of N rarefied monatomic gases. Generalizations of kinetic models to polyatomic particles (with translational and rotational degrees of freedom) are available in [23, 27, 47].

We begin with some basic notions and results from the kinetic theory of gas mixtures, [18].
Each species is characterized by its molecular mass

$$m_s, \quad s = 1, \dots, N.$$

The molecules are regarded as point particles that possess only translational degrees of freedom, which can be identified with the spatial coordinates of its center of mass, collected in the vector $\boldsymbol{x} \in \mathbb{R}^3$.
Furthermore, the kinetic state of each molecule is identified with its velocity vector $\boldsymbol{v} \in \mathbb{R}^3$.

The evolution of the mixture is described through the distribution functions vector

$$\boldsymbol{f} = (f_1, \dots, f_N)^T ,$$

in which $f_s = f_s(\boldsymbol{v}, \boldsymbol{x}, t)$, where $t \in \mathbb{R}^+$ is obviously representative for the time.

Remark. *For simplicity, for any vector $\boldsymbol{a} \in \mathbb{R}^3$, we denote the square of its norm $|\boldsymbol{a}|^2$, by a^2 or by $(\boldsymbol{a})^2$.*

We are now going to introduce the macroscopic and measurable quantities of each species and of the whole mixture, as suitable moments of the distribution function f_s.
For every species we define its **number density** n_s, **mass velocity** $\boldsymbol{u}_s$ and **kinetic temperature** T_s (in which the Boltzmann constant K_B is incorporated for convenience) as follows

$$n_s = \int_{\mathbb{R}^3} f_s(\boldsymbol{v}) d\boldsymbol{v} \,, \quad \boldsymbol{u}_s = \frac{1}{n_s} \int_{\mathbb{R}^3} \boldsymbol{v} f_s(\boldsymbol{v}) d\boldsymbol{v} \,, \quad T_s = \frac{m_s}{3n_s} \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u}_s)^2 f_s(\boldsymbol{v}) d\boldsymbol{v} \,.$$

For the whole mixture, we define the **number density** n

$$n := \sum_{s=1}^{N} n_s \,,$$

the **average mass velocity** $\boldsymbol{u}$

$$\boldsymbol{u} := \frac{1}{\rho} \sum_{s=1}^{N} \rho_s \boldsymbol{u}_s \,,$$

where $\rho_s := m_s n_s$ represents the **mass density** of each species and the **global mass density** ρ is given by

$$\rho := \sum_{s=1}^{N} \rho_s \quad .$$

Pertaining to the **global temperature** T (in which we incorporate once again the Boltzmann constant K_B), we require it to represent a measure of the mixture thermal agitation. We define indeed the global kinetic energy density, obtained as the sum of the species-specific kinetic energy densities, to be equal to

$$\frac{1}{2}\rho u^2 + \frac{3}{2} n T \,,$$

and, specifically, we have

$$\begin{aligned}
&\frac{1}{2} \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} v^2 f_s(\boldsymbol{v}) d\boldsymbol{v} \\
&= \frac{1}{2} u^2 \sum_{s=1}^{N} m_s n_s + \boldsymbol{u} \cdot \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u}) f_s(\boldsymbol{v}) d\boldsymbol{v} + \frac{1}{2} \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u})^2 f_s(\boldsymbol{v}) d\boldsymbol{v} \\
&= \frac{1}{2} \rho u^2 + \boldsymbol{u} \cdot \sum_{s=1}^{N} (m_s n_s \boldsymbol{u}_s - m_s n_s \boldsymbol{u}) + \sum_{s=1}^{N} \frac{1}{2} m_s \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u})^2 f_s(\boldsymbol{v}) d\boldsymbol{v} \\
&= \frac{1}{2} \rho u^2 + \frac{1}{2} \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u})^2 f_s(\boldsymbol{v}) d\boldsymbol{v} \quad .
\end{aligned}$$

Introducing the **peculiar velocity** $\boldsymbol{c} := \boldsymbol{v} - \boldsymbol{u}$, the global temperature turns out to be

$$nT = \frac{1}{3}\sum_{s=1}^{N}\int_{\mathbb{R}^3} c^2 f_s(\boldsymbol{v})d\boldsymbol{v} \ ,$$

that can be reformulated as follows

$$\begin{aligned}
nT &= \frac{1}{3}\sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} \big[\,(\boldsymbol{v}-\boldsymbol{u}_s)+(\boldsymbol{u}_s-\boldsymbol{u})\,\big]^2 f_s(\boldsymbol{v})d\boldsymbol{v} \\
&= \frac{1}{3}\sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} (\boldsymbol{v}-\boldsymbol{u}_s)^2 f_s(\boldsymbol{v})d\boldsymbol{v} + \frac{2}{3}\sum_{s=1}^{N} m_s\,(\boldsymbol{u}_s-\boldsymbol{u})\cdot \underbrace{\int_{\mathbb{R}^3}(\boldsymbol{v}-\boldsymbol{u}_s)\,f_s(\boldsymbol{v})d\boldsymbol{v}}_{=n_s\boldsymbol{u}_s - n_s\boldsymbol{u}_s = 0} \\
&+ \frac{1}{3}\sum_{s=1}^{N} m_s\,(\boldsymbol{u}_s-\boldsymbol{u})^2 \int_{\mathbb{R}^3} f_s(\boldsymbol{v})d\boldsymbol{v} = \sum_{s=1}^{N} n_s T_s + \frac{1}{3}\sum_{s=1}^{N}\rho_s\,(\boldsymbol{u}_s-\boldsymbol{u})^2 \\
&\Longrightarrow\ nT = \sum_{s=1}^{N} n_s T_s + \frac{1}{3}\sum_{s=1}^{N}\rho_s\,(\boldsymbol{u}_s-\boldsymbol{u})^2 \qquad (1.1)
\end{aligned}$$

The overall thermal agitation of the mixture arises both from the thermal motion of each species individually and from the motion of each species relative to the mixture. For this reason, the temperature of the mixture is always greater—often significantly greater—than the weighted average of the temperatures of its constituent species. Similarly, the scalar pressure of the mixture, $p = nT$, exceeds the sum of the partial scalar pressures, $p_s = n_s T_s$, with equality occurring only when all diffusion velocities $\boldsymbol{u}_s - \boldsymbol{u}$ vanish.
Let us examine the components of the pressure tensor $\underline{\boldsymbol{P}}$, considered as the total flux of momentum relative to a surface moving with the macroscopic velocity $\boldsymbol{u}$ of the gas

$$P_{ij} = \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3}(v_i-u_i)v_j f_s(\boldsymbol{v})d\boldsymbol{v} = \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} c_i c_j f_s(\boldsymbol{v})d\boldsymbol{v}\,. \qquad (1.2)$$

Defining the component of the pressure tensor for single species P^s_{ij} as

$$P^s_{ij} = \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} c^s_i c^s_j f_s(\boldsymbol{v})d\boldsymbol{v}\,,$$

where $c^s_i = v_i - u^s_i$, the following relation between the pressure tensor of the mixture and of the single species holds

$$P_{ij} = \sum_{s=1}^{N} P^s_{ij} + \sum_{s=1}^{N}\rho_s(u^s_i - u_i)(u^s_j - u_j).$$

In fact, $\underline{\boldsymbol{P}}$ is not only obtained by adding the tensors corresponding to the individual species; an additional contribution, which (as for the temperatures)

arises from the diffusion velocities, must be included.
In the case of a single gas we have $nT = \frac{1}{3}Tr(\underline{\boldsymbol{P}})$ and this continues to hold for a mixture as well

$$\frac{1}{3}Tr(\underline{\boldsymbol{P}}) = \sum_{s=1}^{N} n_s T_s + \frac{1}{3}\sum_{s=1}^{N} \rho_s(\boldsymbol{u}_s - \boldsymbol{u})^2 = nT\,.$$

Furthermore, the following decomposition

$$\underline{\boldsymbol{P}} = nT\underline{\boldsymbol{I}} + \underline{\boldsymbol{\Pi}}\,,$$

where $\underline{\boldsymbol{\Pi}}$ is the traceless viscous stress tensor, remains valid in the case of a mixture.
Finally, we define the heat flux $\boldsymbol{q}$ of the mixture and of the individual species. We have

$$q_i = \frac{1}{2}\sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} c^2 c_i f_s(\boldsymbol{v}) d\boldsymbol{v}\,,$$

and

$$q_i^s = \frac{1}{2} m_s \int_{\mathbb{R}^3} c_s^2 c_i^s f_s(\boldsymbol{v}) d\boldsymbol{v}\,.$$

Proceeding as before, it is not difficult to show that

$$q_i = \sum_{s=1}^{N} q_i^s + \sum_{s=1}^{N} P_{ij}^s(u_j^s - u_j) + \frac{3}{2}\sum_{s=1}^{N} n_s T_s(u_i^s - u_i) + \frac{1}{2}\sum_{s=1}^{N} \rho_s(u_i^s - u_i)(\boldsymbol{u}_s - \boldsymbol{u})^2, \tag{1.3}$$

where diffusion velocities continue to play a crucial role.

1.2 Boltzmann system for a gas mixture

Assuming that no external forces are present, the dynamics of a mixture of rarefied gases is governed by a system of Boltzmann-type equations

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s = Q_s\ , \qquad s = 1, \ldots, N,$$

where the left-hand side describes the "free-flight" phase, in which the term depending on spatial gradients stands for the streaming operator, and the right-hand side is responsible for the collision contributions.
Consistently with the rarefied gas assumption, the model considers exclusively binary collisions, that is, if two molecules collide with each other, no other collision involving them can occur until such a phase has ended.
The molecules of each species collide with any other species molecule. Therefore, the collision operator Q_s is the result of the sum of the contribution due to the collision of the s-th species with each of the other N species

$$Q_s = \sum_{r=1}^{N} Q_{sr}(f_s, f_r)\,.$$

We are ready to construct the Boltzmann operator that describes the collisions between molecules of the s-th and r-th species.
We begin by introducing the collision **total mass**

$$M_{sr} := m_s + m_r,$$

the **reduced mass**

$$\mu_{sr} := \frac{m_s m_r}{m_s + m_r},$$

and the **mass fractions**

$$\alpha_{sr} = \frac{m_s}{M_{sr}}, \quad \alpha_{rs} = \frac{m_r}{M_{sr}},$$

with obviously $\alpha_{sr} + \alpha_{rs} = 1$.

Remark. *Let $\boldsymbol{v}, \boldsymbol{w}$ be the pre-collision velocities of species s and r. Post-collision velocities are indicated by an apex $'$, $\boldsymbol{v}'_{sr}, \boldsymbol{w}'_{sr}$.*

Bearing in mind that having assumed collisions to be elastic, the momentum and the kinetic energy are preserved in each of them, and it holds

$$\begin{cases} m_s \boldsymbol{v} + m_r \boldsymbol{w} = m_s \boldsymbol{v}'_{sr} + m_r \boldsymbol{w}'_{sr} \\ m_s v^2 + m_r w^2 = m_s v'^2_{sr} + m_r w'^2_{sr} \,. \end{cases} \tag{1.4}$$

Being $\boldsymbol{Y}$ the **velocity of the center of mass**, $\boldsymbol{Y} = \alpha_{sr}\boldsymbol{v} + \alpha_{rs}\boldsymbol{w}$, and $\boldsymbol{y}$ the **relative velocity of the colliding molecules**, $\boldsymbol{y} = \boldsymbol{v} - \boldsymbol{w}$, we reformulate system (1.4) as follows

$$\begin{cases} (m_s + m_r)\, \boldsymbol{Y} = (m_s + m_r)\, \boldsymbol{Y}' \\ (m_s + m_r)\, Y^2 + \mu_{sr} y^2 = (m_s + m_r)\, Y'^2 + \mu_{sr} y'^2 \,, \end{cases}$$

from which we obtain

$$\boldsymbol{Y}' = \boldsymbol{Y} \quad \text{and} \quad \boldsymbol{y}' = |\boldsymbol{y}|\omega, \quad \omega \in \mathbb{S}^2,$$

where ω is the **unit vector of the post-collisional relative velocity**.
Combining the above equalities, velocities $\boldsymbol{v}$, $\boldsymbol{w}$ can be expressed in terms of $\boldsymbol{Y}$ and $\boldsymbol{y}$

$$\begin{cases} \boldsymbol{v} = \boldsymbol{Y} + \alpha_{rs}\boldsymbol{y} \\ \boldsymbol{w} = \boldsymbol{Y} - \alpha_{sr}\boldsymbol{y} \,, \end{cases}$$

and making use of momentum and energy conservations, we can reformulate post-collisional velocities as functions of the incoming velocities

$$\begin{cases} \boldsymbol{v}'_{sr} = \alpha_{sr}\boldsymbol{v} + \alpha_{rs}\left(\boldsymbol{w} + |\boldsymbol{y}|\omega\right) \\ \boldsymbol{w}'_{sr} = \alpha_{rs}\boldsymbol{w} + \alpha_{sr}\left(\boldsymbol{v} - |\boldsymbol{y}|\omega\right) \,. \end{cases} \tag{1.5}$$

We are now ready to formulate the Boltzmann collision operator $Q_{sr}(f_s, f_r)$ that will be the result of the difference between a **scattering in** term Q^+_{sr} and a **scattering out** one Q^-_{sr}, i.e.

$$Q_{sr} = Q^+_{sr} - Q^-_{sr} \ . \tag{1.6}$$

Let $g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega)$ be the collision kernel function that provides the interaction between the $s-$ and $r-$ species molecules, in which $\hat{\boldsymbol{y}}$ is the unit vector of relative velocity. It is obviously symmetric with respect to their indices, i.e. $g_{sr} = g_{rs}$.

Hence, the number of molecules of species s with velocity in $d\boldsymbol{v}$ and impact parameter in $d\omega$, colliding with a fixed target molecule of species r located in $d\boldsymbol{x}$ with velocity in $d\boldsymbol{w}$, is given by

$$f_s(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{v} \, g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) d\omega dt \, .$$

To obtain the total number of collisions, we multiply by the number of target molecules present, which is

$$f_r(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{w} d\boldsymbol{x} \, ,$$

reaching

$$g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) f_s(\boldsymbol{x}, \boldsymbol{v}, t) f_r(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{x} d\boldsymbol{w} d\omega dt \, .$$

The total number of collisions occurring in $d\boldsymbol{x}$ and dt that remove a molecule from the velocity range $d\boldsymbol{v}$ is therefore given by integrating over all target molecules and all admissible solid angles, namely

$$Q^-_{sr} = \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) f_s(\boldsymbol{x}, \boldsymbol{v}, t) f_r(\boldsymbol{x}, \boldsymbol{v}, t) d\boldsymbol{w} d\omega \, .$$

To construct the gain term Q^+_{sr}, we introduce the notion of a **dual collision**, in which the post-collisional velocities from the direct interaction are interpreted as incoming collisional velocities. Specifically, a gain of particles in $d\boldsymbol{v}$ in the direct collision corresponds to a loss of particles in $d\boldsymbol{v}$ in the dual collision. This observation allows us to recast the gain term as a loss term associated with the dual process.
Using the dual collision method, and observing that

$$\left| \frac{\partial(\boldsymbol{Y}, \boldsymbol{y})}{\partial(\boldsymbol{v}, \boldsymbol{w})} \right| = 1 \quad \Longrightarrow \ d\boldsymbol{v} d\boldsymbol{w} d\omega = d\boldsymbol{v}' d\boldsymbol{w}' d\omega',$$

we have

$$Q^+_{sr} = \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) f_s(\boldsymbol{v}'_{sr}, \boldsymbol{x}, t) f_r(\boldsymbol{w}'_{sr}, \boldsymbol{x}, t) d\boldsymbol{w} d\omega.$$

Eventually, from (1.6),

$$Q_{sr}(f_s, f_r) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) \left[f_s(\boldsymbol{v}'_{sr}) f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) \right] d\boldsymbol{w} d\omega. \tag{1.7}$$

In the case of collisions between molecules of the same species, we find the Boltzmann collision operator for single gas

$$Q_{ss} = \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_{ss}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) \left[f_s(\boldsymbol{v}'_s) f_s(\boldsymbol{w}'_s) - f_s(\boldsymbol{v}) f_s(\boldsymbol{w}) \right] d\boldsymbol{w} d\omega.$$

1.3 Properties of the Boltzmann equations

In each elastic collision, molecules undergo a variation of their molecular velocity and thus a transfer of momentum and kinetic energy between the species involved in the collision.
Since we have assumed the mixture to be inert and therefore the mass of each species is preserved, the transfer of such quantities from species s to species r is the opposite of the corresponding transfer from species r to species s.
Consequently, defining the following scalar product as

$$\langle \varphi(\boldsymbol{v}), \psi(\boldsymbol{v}) \rangle = \int_{\mathbb{R}^3} \varphi(\boldsymbol{v})\psi(\boldsymbol{v}) d\boldsymbol{v}\,,$$

and upon summing over all molecular velocities, we expect to recover

$$\begin{aligned} m_s \langle Q_{sr}(f_s, f_r), \boldsymbol{v} \rangle + m_r \langle Q_{rs}(f_r, f_s), \boldsymbol{v} \rangle &= \mathbf{0}, \\ m_s \langle Q_{sr}(f_s, f_r), v^2 \rangle + m_r \langle Q_{rs}(f_r, f_s), v^2 \rangle &= 0. \end{aligned} \tag{1.8}$$

We prove it analytically through the general weak formulations of binary Boltzmann operators, with test functions $\varphi_s(\boldsymbol{v}) = m_s \boldsymbol{v}, m_s v^2$:

$$\begin{aligned} &\langle Q_{sr}, \varphi_s(\boldsymbol{v}) \rangle + \langle Q_{rs}, \varphi_r(\boldsymbol{v}) \rangle \qquad (1.9) \\ &= \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_s(\boldsymbol{v}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_s(\boldsymbol{v}'_{sr})f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v})f_r(\boldsymbol{w})\big] d\boldsymbol{v} d\boldsymbol{w} d\omega \\ &+ \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_r(\boldsymbol{v}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_r(\boldsymbol{v}'_{rs})f_s(\boldsymbol{w}'_{rs}) - f_r(\boldsymbol{v})f_s(\boldsymbol{w})\big] d\boldsymbol{v} d\boldsymbol{w} d\omega\ . \end{aligned}$$

Now, we reformulate these integrals using the following change of variable

$$\begin{aligned} \boldsymbol{v} &\to \boldsymbol{w} \\ \boldsymbol{w} &\to \boldsymbol{v} \\ \omega &\to -\omega\ , \end{aligned} \tag{1.10}$$

from which

$$\begin{aligned} \boldsymbol{v}'_{sr} &\to \alpha_{sr}\boldsymbol{w} + \alpha_{rs}(\boldsymbol{v} - \boldsymbol{y}\cdot\omega) = \boldsymbol{w}'_{rs} \\ \boldsymbol{w}'_{sr} &\to \alpha_{rs}\boldsymbol{v} + \alpha_{sr}(\boldsymbol{w} + \boldsymbol{y}\cdot\omega) = \boldsymbol{v}'_{rs}\ . \end{aligned}$$

Then

$$\begin{aligned} &\langle Q_{sr}, \varphi_s(\boldsymbol{v}) \rangle + \langle Q_{rs}, \varphi_r(\boldsymbol{v}) \rangle \qquad (1.11) \\ &= \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_s(\boldsymbol{w}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_s(\boldsymbol{w}'_{rs})f_r(\boldsymbol{v}'_{rs}) - f_s(\boldsymbol{w})f_r(\boldsymbol{v})\big] d\boldsymbol{v} d\boldsymbol{w} d\omega \\ &+ \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_r(\boldsymbol{w}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_r(\boldsymbol{w}'_{sr})f_s(\boldsymbol{v}'_{sr}) - f_r(\boldsymbol{w})f_s(\boldsymbol{v})\big] d\boldsymbol{v} d\boldsymbol{w} d\omega\ . \end{aligned}$$

In (1.9), by switching now pre- and post-collisional velocities, that is

$$\begin{aligned} \boldsymbol{v} &\to \boldsymbol{v}'_{sr} \\ \boldsymbol{w} &\to \boldsymbol{w}'_{sr} \\ \omega &\to \omega' \ , \end{aligned} \tag{1.12}$$

in the first integral, and

$$\begin{aligned} \boldsymbol{v} &\to \boldsymbol{v}'_{rs} \\ \boldsymbol{w} &\to \boldsymbol{w}'_{rs} \\ \omega &\to \omega' \ , \end{aligned} \tag{1.13}$$

in the second integral, we get the following reformulation

$$\begin{aligned} &\langle Q_{sr}, \varphi_s(\boldsymbol{v})\rangle + \langle Q_{rs}, \varphi_r(\boldsymbol{v})\rangle \qquad (1.14) \\ &= -\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_s(\boldsymbol{v}'_{sr}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_s(\boldsymbol{v}'_{sr})f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{w})f_r(\boldsymbol{v})\big] d\boldsymbol{v}d\boldsymbol{w}d\omega \\ &- \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_r(\boldsymbol{v}'_{rs}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_r(\boldsymbol{v}'_{rs})f_s(\boldsymbol{w}'_{rs}) - f_r(\boldsymbol{v})f_s(\boldsymbol{w})\big] d\boldsymbol{v}d\boldsymbol{w}d\omega \ , \end{aligned}$$

thanks also to $d\boldsymbol{v}'d\boldsymbol{w}'d\omega = d\boldsymbol{v}d\boldsymbol{w}d\omega$.

Combining the previous changes of variables, we also get

$$\begin{aligned} &\langle Q_{sr}, \varphi_s(\boldsymbol{v})\rangle + \langle Q_{rs}, \varphi_r(\boldsymbol{v})\rangle \\ &= -\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_s(\boldsymbol{w}'_{rs}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_s(\boldsymbol{w}'_{rs})f_r(\boldsymbol{v}'_{rs}) - f_s(\boldsymbol{w})f_r(\boldsymbol{v})\big] d\boldsymbol{v}d\boldsymbol{w}d\omega \\ &- \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} \varphi_r(\boldsymbol{w}'_{sr}) g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big[f_r(\boldsymbol{w}'_{sr})f_s(\boldsymbol{v}'_{sr}) - f_r(\boldsymbol{w})f_s(\boldsymbol{v})\big] d\boldsymbol{v}d\boldsymbol{w}d\omega \ . \end{aligned} \tag{1.15}$$

Since (1.9), (1.11), (1.14) and (1.15) are equivalent formulations of $\langle Q_{sr}, \varphi_s(\boldsymbol{v})\rangle + \langle Q_{rs}, \varphi_r(\boldsymbol{v})\rangle$, we can recast it as

$$\begin{aligned} &\langle Q_{sr}, \varphi_s(\boldsymbol{v})\rangle + \langle Q_{rs}, \varphi_r(\boldsymbol{v})\rangle \\ &= -\frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} [\varphi_s(\boldsymbol{v}'_{sr}) + \varphi_r(\boldsymbol{w}'_{sr}) - \varphi_s(\boldsymbol{v}) - \varphi_r(\boldsymbol{w})] \\ &\times [f_s(\boldsymbol{v}'_{sr}) + f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v}) - f_r(\boldsymbol{w})]\, d\boldsymbol{v}d\boldsymbol{w}d\omega \qquad (1.16) \\ &- \frac{1}{4}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} [\varphi_r(\boldsymbol{v}'_{rs}) + \varphi_s(\boldsymbol{w}'_{rs}) - \varphi_r(\boldsymbol{v}) - \varphi_s(\boldsymbol{w})] \\ &\times [f_r(\boldsymbol{v}'_{rs}) + f_s(\boldsymbol{w}'_{rs}) - f_r(\boldsymbol{v}) - f_s(\boldsymbol{w})]\, d\boldsymbol{v}d\boldsymbol{w}d\omega \ . \end{aligned}$$

Setting $\varphi_s = m_s\boldsymbol{v}, m_s v^2$ and recalling (1.4), we have proved (1.8).

Obviously, if $s = r$, we have

$$m_s \langle Q_{ss}(f_s), \boldsymbol{v} \rangle = \mathbf{0}\,, \quad m_s \langle Q_{ss}(f_s), v^2 \rangle = 0\,.$$

In the case of a constant test function, i.e. $\varphi_s(\boldsymbol{v}) = 1$, switching pre- and post-collisional velocities as in (1.12) and (1.13) leads to

$$\begin{aligned} \langle Q_{sr}, 1 \rangle = \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} & g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) [f_s(\boldsymbol{v}'_{sr}) f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) \\ & - f_s(\boldsymbol{v}'_{sr}) f_r(\boldsymbol{w}'_{sr}) + f_s(\boldsymbol{v}) f_r(\boldsymbol{w})] = 0\,, \end{aligned} \tag{1.17}$$

confirming preservation of species number densities.

1.4 Collision invariants and equilibrium distributions

Given a regular test function $\varphi_s(\boldsymbol{v})$, using changes of variables analogous to those presented in the previous section and summing on all species, the **weak form of the Boltzmann equation** may be cast as

$$\begin{aligned} & \sum_{s=1}^{N} \langle \frac{\partial f_s}{\partial t},\ \varphi_s(\boldsymbol{v}) \rangle + \langle \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s,\ \varphi_s(\boldsymbol{v}) \rangle \\ & = -\frac{1}{4} \sum_{r,s=1}^{N} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) \left[\varphi_s(\boldsymbol{v}'_{sr}) + \varphi_r(\boldsymbol{w}'_{sr}) - \varphi_s(\boldsymbol{v}) - \varphi_r(\boldsymbol{w}) \right] \\ & \times \left[f_s(\boldsymbol{v}'_{sr}) f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v}) - f_r(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w} d\omega. \end{aligned} \tag{1.18}$$

It can also be easily checked, by exchanging pre- and post–collision velocities, that an additional equivalent formulation of the weak form of each bi-species Boltzmann operator is

$$\begin{aligned} \langle Q_{sr}(f_s, f_r), \varphi_s(\boldsymbol{v}) \rangle = -\frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} & g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \boldsymbol{\omega}) \left[\varphi_s(\boldsymbol{v}'_{sr}) - \varphi_s(\boldsymbol{v}) \right] \\ & \times \left[f_s(\boldsymbol{v}'_{sr}) f_r(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w} d\omega\,. \end{aligned} \tag{1.19}$$

We define a **collisional invariant** as a molecular property that is conserved in the collisional process. More rigorously, according to equation (1.16), the following condition must be satisfied

$$\varphi_s(\boldsymbol{v}'_{sr}) + \varphi_r(\boldsymbol{w}'_{sr}) = \varphi_s(\boldsymbol{v}) + \varphi_r(\boldsymbol{w}) \quad \forall \boldsymbol{v}, \boldsymbol{w}, \omega, \quad r, s = 1, \dots, N. \tag{1.20}$$

As in a single gas, collisional invariants are suitable combinations of the principal molecular properties.
It is possible to prove (see, for instance, [42] for details) that the collisional invariants take the form

$$\varphi_s(\boldsymbol{v}) = a + \boldsymbol{b} \cdot m_s \boldsymbol{v} + \frac{c}{2} m_s v^2\ , \tag{1.21}$$

and can be written as linear combination of the following $N+4$ linearly independent vectors

$$\overline{\psi}^{(1)}(\boldsymbol{v}) = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad , \quad \dots , \quad \overline{\psi}^{(N)}(\boldsymbol{v}) = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix} \quad , \quad \overline{\psi}^{(N+1)}(\boldsymbol{v}) = \begin{pmatrix} m_1 v_x \\ m_2 v_x \\ \vdots \\ m_N v_x \end{pmatrix} \quad ,$$

$$\overline{\psi}^{(N+2)}(\boldsymbol{v}) = \begin{pmatrix} m_1 v_y \\ m_2 v_y \\ \vdots \\ m_N v_y \end{pmatrix} \quad , \quad \overline{\psi}^{(N+3)}(\boldsymbol{v}) = \begin{pmatrix} m_1 v_z \\ m_2 v_z \\ \vdots \\ m_N v_z \end{pmatrix} \quad , \quad \overline{\psi}^{(N+4)}(\boldsymbol{v}) = \frac{1}{2} \begin{pmatrix} m_1 v^2 \\ m_2 v^2 \\ \vdots \\ m_N v^2 \end{pmatrix} .$$

which constitute a basis for the associated linear subspace.

In the full-Boltzmann description, we have proved the mass conservation of every species

$$\langle Q_s, 1 \rangle = 0, \quad s = 1, \dots, N, \tag{1.22}$$

and of global momentum and kinetic energy

$$\sum_{s=1}^{N} \langle Q_s, m_s \boldsymbol{v} \rangle = \boldsymbol{0}, \quad \sum_{s=1}^{N} \langle Q_s, m_s v^2 \rangle = 0 \, . \tag{1.23}$$

Starting from the weak form, taking moments of the Boltzmann equation with respect to $N+4$ collision invariants of the basis, the corresponding $N+4$ macroscopic conservation equations for the hydrodynamic variables $n_s, \boldsymbol{u}$ and T can be derived

$$\begin{cases} \dfrac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}_s) = 0 \\ \dfrac{\partial}{\partial t}(\rho \boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (nT + \underline{\boldsymbol{\Pi}}) = \boldsymbol{0} \\ \dfrac{\partial}{\partial t} \left(\dfrac{1}{2} \rho u^2 + \dfrac{3}{2} nT \right) + \nabla_{\boldsymbol{x}} \cdot \left[\left(\dfrac{1}{2} \rho u^2 + \dfrac{5}{2} nT \right) \boldsymbol{u} \right] + \nabla_{\boldsymbol{x}} \cdot (\underline{\boldsymbol{\Pi}} \cdot \boldsymbol{u} + \boldsymbol{q}) = 0 \, , \end{cases}$$

where, in addition to the hydrodynamic variables, the $3N-3$ independent components of the diffusion velocities $\boldsymbol{u}_s$, the five independent components of the viscous stress tensor $\underline{\boldsymbol{\Pi}}$ and the three components of the heat flux vector $\boldsymbol{q}$ appear, for which constitutive equations will be required in order to close the system.

We define **collisional equilibria** those distribution functions $\boldsymbol{f}$ which nullify the collisional operator Q_s, i.e.

$$Q_s(\boldsymbol{f}(\boldsymbol{v})) = \boldsymbol{0} \ , \quad \forall s, \boldsymbol{v} \, ;$$

it can be proven that the **principle of detailed balance** holds true also for mixtures, namely

$$
\begin{aligned}
& Q_s(\boldsymbol{f}(\boldsymbol{v})) = \mathbf{0} \ , \quad \forall s, \boldsymbol{v} \\
\iff \ & f_s(\boldsymbol{v}'_{sr}) f_r(\boldsymbol{w}'_{sr}) = f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) \quad \forall s, r, \boldsymbol{v}, \boldsymbol{w}, \omega \\
\iff \ & \log \boldsymbol{f}(\boldsymbol{v}) \ \text{is a collisional invariant} \ ,
\end{aligned}
$$

where

$$
\log \boldsymbol{f}(\boldsymbol{v}) = \begin{pmatrix} \log f_1 \\ \log f_2 \\ \vdots \\ \log f_N \end{pmatrix} \ .
$$

Using the form of the collision invariant (1.21) and the detailed balance principle, if $\log \boldsymbol{f}(\boldsymbol{v})$ is a collisional invariant, then there exist $a, \boldsymbol{b}$ and c such that

$$
f_s(\boldsymbol{v}) = \exp\left(a + \boldsymbol{b} \cdot m_s \boldsymbol{v} + c \frac{1}{2} m_s v^2\right) \ , \quad \forall s = 1, \ldots, N, \tag{1.24}
$$

where c is required to be negative to ensure that $f_s \in L^1$.

It can be shown, after a suitable reformulation, that the **collisional equilibria** $\mathcal{M}_s^{eq}$ take the Maxwellian distribution form

$$
\mathcal{M}_s^{eq} := \mathcal{M}\left(\boldsymbol{v}; n_s, \boldsymbol{u}, \frac{T}{m_s}\right) = n_s \left(\frac{m_s}{2\pi T}\right) \exp\left(-\frac{m_s}{2T} (\boldsymbol{v} - \boldsymbol{u})^2\right) .
$$

We observe that the equilibrium Maxwellian distributions allow the species densities to be independent, while prescribe the same velocity and temperature for all distributions, i.e. $\boldsymbol{u}_1 = \ldots = \boldsymbol{u}_N$, $T_1 = \ldots = T_N$.
It follows that the collisional equilibria remain local Maxwellians and constitute an $N+4$-parameter family, depending on the macroscopic fields $n_s, \boldsymbol{u}$ and T, which can be expressed as suitable moments of $\mathcal{M}_s^{eq}$ or appropriate combination of them.

By some standard computations, we get the zeroth, first, and second order moment of $\mathcal{M}_s^{eq}$

$$
\begin{cases}
\langle \mathcal{M}_s^{eq}, 1 \rangle = n_s \\
\langle \mathcal{M}_s^{eq}, \boldsymbol{v} \rangle = n_s \boldsymbol{u} \\
\langle \mathcal{M}_s^{eq}, v^2 \rangle = n_s \left(u^2 + \dfrac{3T}{m_s}\right) .
\end{cases}
$$

Furthermore, the $N+4$ parameters characterizing the collisional equilibria are in one to one correspondence with the $N+4$ scalar functions identifying the collisional invariants, this correspondence being explicitly given in (1.24).

1.5 The BGK collisional operator

Kinetic Boltzmann-type models are particularly difficult to handle both analytically and numerically, due to the presence of nonlinear integral operators. These difficulties are amplified when moving from a single gas to a mixture, since the collision operator for each component is a sum of binary integral operators. For this reason, simplified models are desirable, allowing the preservation of the fundamental properties without entering into the details of microscopic collisions. The most famous one, originally built up for a single gas [3], is the BGK model, where the Boltzmann collision integral is replaced by a relaxation-type operator, forcing the distribution towards a local Maxwellian equilibrium. The first mathematically rigorous BGK model for mixtures of monoatomic gases, proposed in 2002 in [1], considers a single relaxation operator for the entire collision process, thus losing the structure of the Boltzmann operator characterized by a sum of binary terms. Starting from [1], more refined models have been proposed (see for instance [15]), that also take into account the polyatomic structure of components or the possibility of chemical interactions between molecules [4, 11, 16, 28, 35].
A different way of modeling, based on the pioneering work by McCormack [39], considers a collision term provided by a sum of binary operators, thus mimicking the structure of the classical Boltzmann collision operator for mixtures [31, 33]. The recent paper [13] by Bobylev and co-authors fits into this research line, and proposes a model valid for general intermolecular potentials. The collision operator is given by

$$\hat{Q}_s = \sum_{r=1}^{N} \hat{Q}_{sr},$$

with

$$\hat{Q}_{sr} = \nu_{sr}\big(\mathcal{M}_{sr} - f_s\big), \tag{1.25}$$

where ν_{sr} is a parameter independent of $\boldsymbol{v}$ to be fixed, representing the collision frequency, having units of t^{-1}, and $\mathcal{M}_{sr}$, dependent on the **fictitious parameters**

$$n_{sr}\,, \quad \boldsymbol{u}_{sr}\,, \quad T_{sr}\,,$$

is a suitable local Maxwellian,

$$\mathcal{M}_{sr} = \mathcal{M}\left(\boldsymbol{v}; n_{sr}, \boldsymbol{u}_{sr}, \frac{T_{sr}}{m_s}\right), \quad s, r = 1, ..., N. \tag{1.26}$$

Remark. *Contrary to the case of a single gas, the local Maxwellian $\mathcal{M}_{sr}$ in* (1.26) *depends on auxiliary fields $n_{sr}, \boldsymbol{u}_{sr}$ and T_{sr} different from the actual moments of the distribution function f_s.*

The equation governing the evolution of the generic species s will therefore be

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = \sum_{r=1}^{N} \nu_{sr}\big(\mathcal{M}_{sr} - f_s\big).$$

It is necessary to determine fictitious parameters involved in the Maxwellian attractors. We observe that, following the natural choice of setting $n_{ss} = n_s$, $\boldsymbol{u}_{ss} = \boldsymbol{u}_s$, and $T_{ss} = T_s$ (i.e., the parameters related to collisions of species s with itself coincide with the moments of the distribution function f_s), there still remain $5(N^2-N)$ fictitious parameters to be fixed, while only $N+4$ conservation laws are available (the N continuity equations, one for each species, plus the global conservation of momentum and kinetic energy).

To determine the fictitious parameters, in [13] it is imposed that the mass of the molecules is conserved in each collision, as it occurs for the Boltzmann operator, i.e.,

$$\langle \hat{Q}_{sr}, 1 \rangle = \langle Q_{sr}, 1 \rangle = 0, \tag{1.27}$$

and that the transfer of momentum and kinetic energy through each binary inter-species BGK operator coincides with the respective transfer of molecular properties in the corresponding binary Boltzmann operator, i.e.,

$$\langle Q_{sr} - \hat{Q}_{sr}, \boldsymbol{v} \rangle = \mathbf{0}\,,\ \langle Q_{sr} - \hat{Q}_{sr}, v^2 \rangle = 0\,. \tag{1.28}$$

These assumptions are sufficient to determine the fictitious parameters in terms of the main macroscopic species fields.
For the obtained model, it is possible to prove the positivity of the fictitious temperatures T_{sr} and the consistency of the model. The proof techniques are similar to those we will use in the next chapter to analyze the mixed model proposed in this thesis.

Before proceeding to express the fictitious parameters in terms of the macroscopic species ones, we observe that equations (1.27) and (1.28) provide themselves the conservation of mass, total momentum and kinetic energy. Indeed, the exchanged amount of any of these molecular properties is the same when the collision is described by either the Boltzmann or the BGK operator.

Going through the same calculations computed in previous sections for the global and species Maxwellian, we are able to explicitly determine zero-th, first- and second-order momentum of the fictitious Maxwellian $\mathcal{M}_{sr}$

$$\begin{cases} \langle \mathcal{M}_{sr}, 1 \rangle = n_{sr} \\ \langle \mathcal{M}_{sr}, \boldsymbol{v} \rangle = n_{sr} \boldsymbol{u}_{sr} \\ \langle \mathcal{M}_{sr}, v^2 \rangle = n_{sr} \left(u_{sr}^2 + \dfrac{3T_{sr}}{m_s} \right) . \end{cases}$$

Let us now compute the explicit expression of the fictitious parameters.
Recalling the mass conservation (1.27), we get

$$
\begin{aligned}
\langle \hat{Q}_{sr}, 1\rangle &= \nu_{sr}\int_{\mathbb{R}^3}\big(\mathcal{M}_{sr}-f_s\big)d\boldsymbol{v}\\
&= \nu_{sr}\left(\int_{\mathbb{R}^3}\mathcal{M}_{sr}d\boldsymbol{v}-\int_{\mathbb{R}^3}f_s d\boldsymbol{v}\right)\\
&= \nu_{sr}\big(n_{sr}-n_s\big)=0,
\end{aligned}
$$

and so

$$
n_{sr}=n_s\,,\qquad \forall s,r=1,...,N. \tag{1.29}
$$

Therefore, the fictitious densities coincide with the species densities.

Computing the exchange of momentum relative to the BGK collisional operator, we find

$$
\begin{aligned}
\langle \hat{Q}_{sr}, \boldsymbol{v}\rangle &= \nu_{sr}\int_{\mathbb{R}^3}\big(\mathcal{M}_{sr}-f_s\big)\boldsymbol{v}d\boldsymbol{v}\\
&= \nu_{sr}\left(\int_{\mathbb{R}^3}\mathcal{M}_{sr}\boldsymbol{v}d\boldsymbol{v}-\int_{\mathbb{R}^3}f_s\boldsymbol{v}d\boldsymbol{v}\right)=\nu_{sr}n_s\big(\boldsymbol{u}_{sr}-\boldsymbol{u}_s\big)\,.
\end{aligned} \tag{1.30}
$$

As regards kinetic energy, we have

$$
\begin{aligned}
\langle \hat{Q}_{sr}, v^2\rangle &= \nu_{sr}\langle \mathcal{M}_{sr}-f_s, v^2\rangle\\
&= \nu_{sr}\big[\langle \mathcal{M}_{sr}, v^2\rangle-\langle f_s, v^2\rangle\big]\\
&= \nu_{sr}n_s\left[3\frac{T_{sr}-T_s}{m_s}+u_{sr}^2-u_s^2\right]\,.
\end{aligned} \tag{1.31}
$$

First and second order moments of the Boltzmann integral Q_{sr} are computed making use the weak form

$$
\langle Q_{sr}, \varphi_s(\boldsymbol{v})\rangle=\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} g_{sr}\left(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega\right)\big(\varphi_s(\boldsymbol{v}'_{sr})-\varphi_s(\boldsymbol{v})\big)f_s(\boldsymbol{v})f_r(\boldsymbol{w})d\boldsymbol{v}d\boldsymbol{w}d\omega\,,
$$

obtained by exchanging the pre- and post-collisional velocities.
Inserting $\varphi_s(\boldsymbol{v})=\boldsymbol{v}$, and referring to Appendix A for detailed computation, we

obtain

$$
\begin{aligned}
\langle Q_{sr}, \boldsymbol{v}\rangle &= \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big(\boldsymbol{v}'_{sr} - \boldsymbol{v}\big) f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) d\boldsymbol{v} d\boldsymbol{w} d\omega \\
&= -\frac{m_r}{m_s+m_r}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big(\boldsymbol{y} - |\boldsymbol{y}|\omega\big) f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) d\boldsymbol{v} d\boldsymbol{w} d\omega \\
&= -\frac{2\pi m_r}{m_s+m_r}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v}) f_r(\boldsymbol{w})\boldsymbol{y}\int_{-1}^{1}(1-\mu) g_{sr}(|\boldsymbol{y}|,\mu) d\mu d\boldsymbol{v} d\boldsymbol{w} \\
&= -\frac{m_r}{m_s+m_r}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v}) f_r(\boldsymbol{w})(\boldsymbol{v}-\boldsymbol{w}) g^{(1)}_{sr}(|\boldsymbol{v}-\boldsymbol{w}|) d\boldsymbol{v} d\boldsymbol{w},
\end{aligned}
\tag{1.32}
$$

in which we have defined

$$
g^{(1)}_{sr}(|\boldsymbol{y}|) = 2\pi\int_{-1}^{1}(1-\mu) g_{sr}(|\boldsymbol{y}|,\mu) d\mu.
$$

Inserting now $\varphi(\boldsymbol{v}) = v^2$ in the weak form and once again referring to Appendix A for further details, for the second order moment of Q_{sr}, we obtain

$$
\begin{aligned}
\langle Q_{sr}, v^2\rangle &= \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big(v'^2_{sr} - v^2\big) f_s(\boldsymbol{v}) f_r(\boldsymbol{w}) d\boldsymbol{v} d\boldsymbol{w} d\omega \\
&= -\frac{2m_r}{(m_s+m_r)^2}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v}) f_r(\boldsymbol{w})\big(m_s\boldsymbol{v} + m_r\boldsymbol{w}\big)\cdot\int_{\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\big(\boldsymbol{y} - |\boldsymbol{y}|\omega\big) d\omega d\boldsymbol{v} d\boldsymbol{w} \\
&= -\frac{2m_r}{(m_s+m_r)^2}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v}) f_r(\boldsymbol{w})\big(m_s\boldsymbol{v} + m_r\boldsymbol{w}\big)\cdot\big(\boldsymbol{v}-\boldsymbol{w}\big) g^{(1)}_{sr}(|\boldsymbol{v}-\boldsymbol{w}|) d\boldsymbol{v} d\boldsymbol{w}.
\end{aligned}
\tag{1.33}
$$

The terms just computed are obtained for an arbitrary interaction potential; from this point onward, **we fix the potential to that of Maxwellian molecules** [18]. In this case, the collision kernel $g_{sr}(|\boldsymbol{y}|,\mu)$ is independent of $|\boldsymbol{y}|$, and therefore $g^{(1)}_{sr}$ becomes a definite integral in $d\mu$ of a function depending only on μ. Thus, it is a constant and we set

$$
g^{(1)}_{sr} = \Lambda_{sr} = \text{constant}. \tag{1.34}
$$

Remark. *It is possible to represent in this framework, also more general interaction potentials, as proposed in [13], by approximating $g^{(1)}_{sr}(|\boldsymbol{y}|)$ by its value in* *some typical point* $\bar{\boldsymbol{y}}$*, like, for instance, in an average of the relative speed*

$$\bar{\boldsymbol{y}} = \left(\frac{1}{n_s n_r}\int_{\mathbb{R}^3\times\mathbb{R}^3}(\boldsymbol{v}-\boldsymbol{w})^2 f_s(\boldsymbol{v})f_r(\boldsymbol{w})d\boldsymbol{v}d\boldsymbol{w}\right)^{\frac{1}{2}}$$
$$= \left[3\left(\frac{T_s}{m_s}+\frac{T_r}{m_r}\right)+(\boldsymbol{u}_s-\boldsymbol{u}_r)^2\right]^{\frac{1}{2}}.$$

Hence, (1.32) can be reformulated into

$$\begin{aligned}
\langle Q_{sr},\boldsymbol{v}\rangle &= -\frac{m_r}{m_s+m_r}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v})f_r(\boldsymbol{w})\boldsymbol{y}g_{sr}^{(1)}d\boldsymbol{v}d\boldsymbol{w}\\
&= -\frac{m_r}{m_s+m_r}\Lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v})f_r(\boldsymbol{w})(\boldsymbol{v}-\boldsymbol{w})d\boldsymbol{v}d\boldsymbol{w}\\
&= -\frac{m_r}{m_s+m_r}\Lambda_{sr}\left(\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v})f_r(\boldsymbol{w})\boldsymbol{v}d\boldsymbol{v}d\boldsymbol{w}-\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v})f_r(\boldsymbol{w})\boldsymbol{w}d\boldsymbol{v}d\boldsymbol{w}\right)\\
&= -\frac{m_r}{m_s+m_r}\Lambda_{sr}n_s n_r\big(\boldsymbol{u}_s-\boldsymbol{u}_r\big)\,,
\end{aligned} \tag{1.35}$$

while (1.33) provides

$$\begin{aligned}
\langle Q_{sr},v^2\rangle &= -\frac{2m_r}{(m_s+m_r)^2}\Lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v})f_r(\boldsymbol{w})\big(m_s\boldsymbol{v}+m_r\boldsymbol{w}\big)\cdot\big(\boldsymbol{v}-\boldsymbol{w}\big)d\boldsymbol{v}d\boldsymbol{w}\\
&= -\frac{2m_r}{(m_s+m_r)^2}\Lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3} f_s(\boldsymbol{v})f_r(\boldsymbol{w})\Big[m_s v^2-m_r w^2+\big(m_r-m_s\big)\boldsymbol{v}\cdot\boldsymbol{w}\Big]d\boldsymbol{v}d\boldsymbol{w}\\
&= -\frac{2m_r}{(m_s+m_r)^2}\Lambda_{sr}n_s n_r\Big[3\big(T_s-T_r\big)+m_s u_s^2-m_r u_r^2+\big(m_r-m_s\big)\boldsymbol{u}_s\cdot\boldsymbol{u}_r\Big]\\
&= -\frac{2m_r}{(m_s+m_r)^2}\Lambda_{sr}n_s n_r\Big[3\big(T_s-T_r\big)+\big(m_s\boldsymbol{u}_s+m_r\boldsymbol{u}_r\big)\cdot\big(\boldsymbol{u}_s-\boldsymbol{u}_r\big)\Big].
\end{aligned} \tag{1.36}$$

We are eventually capable of writing the explicit form of (1.28)

$$\begin{aligned}
\langle\hat{Q}_{sr},m_s\boldsymbol{v}\rangle &= -\frac{m_s m_r}{m_s+m_r}\Lambda_{sr}n_s n_r(\boldsymbol{u}_s-\boldsymbol{u}_r),\\
\langle\hat{Q}_{rs},m_s v^2\rangle &= -\frac{2m_s m_r}{(m_s+m_r)^2}\Lambda_{sr}n_s n_r\big[3(T_s-T_r)+(m_s\boldsymbol{u}_s-m_r\boldsymbol{u}_r)\cdot(\boldsymbol{u}_s-\boldsymbol{u}_r)\big],
\end{aligned} \tag{1.37}$$

and thus, taking into account (1.30) and (1.31), we can write the fictitious parameters $\boldsymbol{u}_{sr}$ and T_{sr} in terms of the macroscopic species fields.

From the equality of the momentum exchange, we get

$$
\begin{aligned}
&-\frac{m_r}{m_s+m_r}\Lambda_{sr} n_s n_r \big(\boldsymbol{u}_s - \boldsymbol{u}_r\big) = \nu_{sr} n_s \big(\boldsymbol{u}_{sr} - \boldsymbol{u}_s\big) \\
&\iff \boldsymbol{u}_{sr} = -\frac{m_r n_r \lambda_{sr}}{(m_s+m_r)\,\nu_{sr}} \big(\boldsymbol{u}_s - \boldsymbol{u}_r\big) + \boldsymbol{u}_s;
\end{aligned}
$$

setting

$$
a_{sr} = \frac{m_r n_r \Lambda_{sr}}{\nu_{sr}\big(m_s+m_r\big)}\,, \tag{1.38}
$$

we can write

$$
\boldsymbol{u}_{sr} = (1-a_{sr})\,\boldsymbol{u}_s + a_{sr}\boldsymbol{u}_r. \tag{1.39}
$$

On the other hand, from the equality of the kinetic energy exchange, we get

$$
\begin{aligned}
&-\frac{2m_r}{(m_s+m_r)^2}\Lambda_{sr} n_s n_r \Big[3\big(T_s - T_r\big) + \big(m_s\boldsymbol{u}_s + m_r\boldsymbol{u}_r\big)\cdot\big(\boldsymbol{u}_s - \boldsymbol{u}_r\big)\Big] \\
&= \nu_{sr} n_s \Big[3\frac{T_{sr}-T_s}{m_s} + u_{sr}^2 - u_s^2\Big] \\
&\iff -\frac{2m_s m_r}{(m_s+m_r)^2}\frac{\Lambda_{sr} n_r}{\nu_{12}}\Big[3T_s - 3T_r + m_s u_s^2 - m_r u_r^2 - \big(m_s - m_r\big)\boldsymbol{u}_s\cdot\boldsymbol{u}_r\Big] \\
&= 3T_{sr} - 3T_s + m_s\big\{\,[(1-a_{sr})\boldsymbol{u}_s + a_{sr}\boldsymbol{u}_r]^2 - u_s^2\big\};
\end{aligned}
$$

setting

$$
b_{sr} = \frac{2m_r n_r \Lambda_{sr}}{\nu_{sr}\big(m_s+m_r\big)}\frac{m_s}{m_s+m_r} = \frac{2a_{sr}m_s}{m_s+m_r}, \tag{1.40}
$$

we can compute

$$
\begin{aligned}
&-b_{sr}\Big[3T_s - 3T_r + m_s u_s^2 - m_r u_r^2 - \big(m_s - m_r\big)\boldsymbol{u}_s\cdot\boldsymbol{u}_r\Big] \\
&= 3T_{sr} - 3T_s + m_s\big[(1+a_{sr}^2 - 2a_{sr})u_s^2 + a_{sr}^2 u_r^2 + (2a_{sr} - 2a_{sr}^2)\boldsymbol{u}_s\cdot\boldsymbol{u}_r - u_s^2\big],
\end{aligned}
$$

which, through further computations, becomes

$$
\begin{aligned}
&3T_{sr} = 3\big[\big(1-b_{rs}\big)T_s + b_{sr}T_r\big] + m_s\big(2a_{sr} - b_{sr} - a_{sr}^2\big)u_s^2 \\
&\ + \big(m_r b_{sr} - m_s a_{sr}^2\big)u_r^2 + \big(b_{sr}(m_s - m_r) - 2m_s(a_{sr} - a_{sr}^2)\big)\boldsymbol{u}_s\cdot\boldsymbol{u}_r.
\end{aligned} \tag{1.41}
$$

At this point, recalling (1.40), we find

$$
\begin{aligned}
&m_s\big(2a_{sr} - b_{sr} - a_{sr}^2\big) = m_s\bigg(2a_{sr} - \frac{2a_{sr}m_s}{m_s+m_r} - a_{sr}^2\bigg) \\
&= m_s a_{sr}\bigg(\frac{2m_r}{m_s+m_r} - a_{sr}\bigg),
\end{aligned} \tag{1.42}
$$

$$m_r b_{sr} - m_s a_{sr}^2 = m_s a_{sr} \left(\frac{2m_r}{m_s + m_r} - a_{sr} \right), \tag{1.43}$$

and

$$b_{sr}(m_s - m_r) + m_s a_{sr}(2a_{sr} - 2) = -2m_s a_{sr} \left(\frac{2m_r}{m_s + m_r} - a_{sr} \right). \tag{1.44}$$

Finally, using the computations above and setting

$$\gamma_{sr} = \frac{m_s a_{sr}}{3} \left(\frac{2m_r}{m_s + m_r} - a_{sr} \right), \tag{1.45}$$

we find an explicit expression for the fictitious temperature T_{sr}

$$T_{sr} = \big(1 - b_{sr}\big)T_s + b_{sr}T_r + \gamma_{sr} u_s^2 + \gamma_{sr} u_r^2 - 2\gamma_{sr} \boldsymbol{u}_s \cdot \boldsymbol{u}_r$$

$$= \big(1 - b_{sr}\big)T_s + b_{sr}T_r + \gamma_{sr} \left(\boldsymbol{u}_s - \boldsymbol{u}_r\right)^2 .$$

Summarizing, we obtain the expressions of the fictitious moments in terms of the macroscopic fields

$$\begin{cases} \boldsymbol{u}_{sr} = \big(1 - a_{sr}\big)\boldsymbol{u}_s + a_{sr}\boldsymbol{u}_r \\ T_{sr} = \big(1 - b_{sr}\big)T_s + b_{sr}T_r + \gamma_{sr} \left(\boldsymbol{u}_s - \boldsymbol{u}_r\right)^2 , \end{cases} \tag{1.46}$$

along with

$$\begin{cases} a_{sr} = \dfrac{m_r n_r \Lambda_{sr}}{\nu_{sr}\big(m_s + m_r\big)} \\ b_{sr} = \dfrac{2a_{sr} m_s}{m_s + m_r} \\ \gamma_{sr} = \dfrac{m_s a_{sr}}{3} \left(\dfrac{2m_r}{m_s + m_r} - a_{sr} \right). \end{cases} \tag{1.47}$$

Proposition. *The fictitious temperatures T_{sr} provided in* (1.46) *are well defined, i.e. $T_{sr} > 0$, if collision frequencies fulfill the constraint*

$$\nu_{sr} \geq \frac{1}{2} \Lambda_{sr} n_r \tag{1.48}$$

for each $s, r = 1, \ldots, N$, $r \neq s$.

Proof. By definition, it follows that

$$a_{sr} > 0 , \qquad b_{sr} > 0 ; \tag{1.49}$$

moreover, under (1.48), we have

$$b_{sr} = 2\,\frac{\Lambda_{sr}}{\nu_{sr}}\,n_r\,\frac{m_s\,m_r}{(m_s+m_r)^2} \le 4\,\frac{m_s\,m_r}{(m_s+m_r)^2} = 4\,\frac{m_s}{m_s+m_r}\left(1-\frac{m_s}{m_s+m_r}\right) \\ \le 4\cdot\frac{1}{4} = 1\,, \tag{1.50}$$

and

$$\gamma_{sr} = \frac{1}{3}m_s a_{sr}\left(\frac{2\,m_r}{m_s+m_r} - \frac{\Lambda_{sr}\,m_r\,n_r}{\nu_{sr}\,(m_s+m_r)}\right) \ge 0\,. \tag{1.51}$$

Hence, the positiveness of the fictitious temperatures trivially follows. □

Remark. *Regarding the choice of the collision frequencies ν_{sr}, one possibility is provided by estimating the number of collisions between species s and r as done in [43], which leads to relating them to the first moment of the impact parameter functions $g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)$, obtaining*

$$\nu_{sr} = n_r \int_{\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)d\omega\,.$$

However, in this work, to maintain the greatest generality and possibly reproduce the correct Prandtl number in the Navier-Stokes expansion, we deliberately leave them free and not fix them.

Any BGK model must satisfy the main consistency properties verified by the Boltzmann operator; in particular, for the model proposed in [13] the following must holds:

- conservation of mass, momentum, and kinetic energy:

$$\langle \hat{Q}_{sr}, 1\rangle = 0 \quad s,r = 1,...,N; \quad \sum_{s=1}^N m_s\langle \hat{Q}_s, \boldsymbol{v}\rangle = \boldsymbol{0}; \quad \sum_{s=1}^N m_s\langle \hat{Q}_s, v^2\rangle = 0; \tag{1.52}$$

- uniqueness of collisional equilibria:

$$\hat{Q}_s = 0 \quad s = 1,...,N \implies f_s = \mathcal{M}_s^{eq}\big(\boldsymbol{v}; n_s, \boldsymbol{u}, \frac{T}{m_s}\big) \quad s = 1,...,N \quad , \tag{1.53}$$

- the $H-$theorem:

$$\sum_{s=1}^N \langle \hat{Q}_s, \log f_s\rangle \le 0 \quad . \tag{1.54}$$

The proofs of these properties can be found in [13] and will be partially revisited in the next chapter.

Chapter 2

The mixed Boltzmann-BGK model

In this chapter, we propose a mixed Boltzmann–BGK model that combines the positive aspects of the two previous descriptions, which can be regarded as complementary; the corresponding results have been published in [5]. The Boltzmann operator allows for a high level of accuracy in the interaction dynamics and for the derivation of precise transport coefficients. However, being a 5-dimensional integral hard to handle either analytically or computationally, numerical solutions are often very demanding. On the other hand, the BGK operator comes with analytical convenience, allowing explicit calculations, and computational efficiency, since its simplified relaxation structure makes it possible to obtain numerical solutions with far less effort compared to the Boltzmann operator. However, these advantages come at the cost of a slightly approximated representation of collisional dynamics.
A remarkable property of the hybrid model we will construct is that it allows for the study of different asymptotic regimes, where the dominant role in the evolution is played either by the whole collision process or by any of the binary interactions.

The general mixed Boltzmann–BGK model for an inert mixture of N gaseous species reads as

$$\begin{aligned} \frac{\partial f_s}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s &= Q_s \\ &= \sum_{r=1}^{N}\Big[\chi_{sr}\, Q_{sr}(f_s,f_r) + (1-\chi_{sr})\,\hat{Q}_{sr}(f_s)\Big]\,, \quad s=1,\dots,N\,, \end{aligned} \tag{2.1}$$

where $Q_{sr}(f_s, f_r)$ is the bi–species Boltzmann operator defined in (1.7), and $\hat{Q}_{sr}(f_s) = \nu_{sr}(\mathcal{M}_{sr} - f_s)$ is the BGK operator (1.25) constructed in Chapter 1, with the auxiliary Maxwellian $\mathcal{M}_{sr}$ depending on the fictitious moments (1.46) involving coefficients (1.47); moreover, coefficients $\chi_{sr} \in \{0, 1\}$ are such

that $\chi_{sr} = \chi_{rs}$, $\forall\ s, r = 1, \dots, N$. This means that if $\chi_{sr} = 1$ the interactions between particles s and r are modeled by a Boltzmann operator, while if $\chi_{sr} = 0$ a BGK term is used.
Notice that the option $\chi_{sr} = 1$, $\forall (s, r)$ provides the pure Boltzmann model for inert mixtures, while the option $\chi_{sr} = 0$, $\forall (s, r)$ allows to recover the full BGK model proposed in [1].
The general collision operator in (2.1) takes into account that, for any pair (s, r), with $s, r = 1, \dots, N$, we can choose to describe the interactions between particles of species s and r by means of a classical Boltzmann operator (keeping all the details of the intermolecular interaction potential), or by means of a simpler BGK operator that, as described in the previous sections, introduces some proper approximations. A possible reasonable choice could be to model the dominant collisions (for instance the ones involving particles with much larger mass) with Boltzmann terms, and the others, providing momentum and energy exchanging on a slower time scale, with BGK terms. Many other choices can be put in this frame, including also not symmetric scenarios like, for instance, $\chi_{11} = 1$ and $\chi_{sr} = 0$ for any pair $(s, r) \neq (1, 1)$, suitable to describe a mixture in which the component labelled by 1 is much heavier than the others. If two gas components s and r are similar, namely with particle masses of the same order of magnitude and with analogous interaction potentials, one should choose $\chi_{sj} = \chi_{rj}$, $\forall\ j = 1, \dots, N$; consequently, the particular limiting case where all species become equal should be described only by the full Boltzmann model (with all coefficients equal to 1) or by the full BGK approximation (with all coefficients equal to 0).

2.1 Consistency of the model

We show now that the mixed description introduced above satisfies the **consistency properties**; more precisely, we prove

A) conservation of species masses, global momentum and energy, i.e.

$$\begin{aligned} \langle Q_{ss}, 1 \rangle = \langle \hat{Q}_{ss}, 1 \rangle = 0\,, &\quad s = 1, \dots, N \\ \langle Q_{sr}, 1 \rangle = \langle \hat{Q}_{sr}, 1 \rangle = 0\,, &\quad s, r = 1, \dots, N\,, \quad r \neq s\,, \end{aligned} \tag{2.2}$$

and

$$\sum_{s=1}^{N} \sum_{r=1}^{N} \langle \chi_{sr}\, Q_{sr}(f_s, f_r) + (1 - \chi_{sr})\, \hat{Q}_{sr}(f_s), \varphi_s(\boldsymbol{v}) \rangle = 0\,, \tag{2.3}$$

for $\varphi_s(\boldsymbol{v}) = m_s\, \boldsymbol{v}$ and $\varphi_s(\boldsymbol{v}) = m_s v^2$.

B) the validity of Boltzmann H-theorem, in particular of the entropy dissipation estimate, i.e.

$$\sum_{s=1}^{N} \langle Q_s, \log f_s \rangle \leq 0\,; \tag{2.4}$$

C) preservation of Boltzmann equilibrium distribution functions, i.e.

$$Q_s = 0\,, \quad s = 1, \ldots, N \iff f_s = \mathcal{M}_s^{eq} = n_s \left(\frac{m_s}{2\pi T}\right)^{3/2} \exp\left[-\frac{m_s}{2T}\left(\boldsymbol{v} - \boldsymbol{u}\right)^2\right]\,, \tag{2.5}$$

where $\boldsymbol{u}$ and T are the global mean velocity and temperature, respectively.

In the following, Proposition 1 will be devoted to the proof of item A), Proposition 2 to the proof of item B), and Proposition 3 to the proof of item C).

Proposition 1. *The conservation laws (2.2) and (2.3) hold for the mixed model (2.1).*

Proof. The conservation of species number densities trivially follows from the constraint (1.27).

As concerns the conservation of momentum and kinetic energy, we start by proving that

$$\begin{aligned} \langle \hat{Q}_{sr}, m_s\boldsymbol{v}\rangle &= -\langle \hat{Q}_{rs}, m_r\boldsymbol{v}\rangle, \\ \langle \hat{Q}_{sr}, m_s v^2\rangle &= -\langle \hat{Q}_{rs}, m_r v^2\rangle. \end{aligned} \tag{2.6}$$

Having imposed that the exchange of momentum and kinetic energy between species s and r described by the Boltzmann operator equals the one due to the BGK operator, we have

$$\langle \hat{Q}_{sr}, m_s\boldsymbol{v}\rangle = -\frac{m_s m_r}{m_s + m_r}\Lambda_{sr} n_s n_r \left(\boldsymbol{u}_s - \boldsymbol{u}_r\right),$$

and since $\lambda_{sr} = \lambda_{rs}$,

$$\langle \hat{Q}_{rs}, m_r\boldsymbol{v}\rangle = -\frac{m_s m_r}{m_s + m_r}\Lambda_{rs} n_s n_r \left(\boldsymbol{u}_r - \boldsymbol{u}_s\right) = -\langle \hat{Q}_{sr}, m_s\boldsymbol{v}\rangle. \tag{2.7}$$

Analogously

$$\langle \hat{Q}_{sr}, m_s|\boldsymbol{v}|^2\rangle = -\frac{2m_s m_r}{\left(m_s + m_r\right)^2}\Lambda_{sr} n_s n_r \left[3\left(T_s - T_r\right) + \left(m_s\boldsymbol{u}_s + m_r\boldsymbol{u}_r\right)\cdot\left(\boldsymbol{u}_s - \boldsymbol{u}_r\right)\right],$$

and

$$\begin{aligned} \langle \hat{Q}_{rs}, m_r v^2\rangle &= \frac{2m_s m_r}{\left(m_s + m_r\right)^2}\Lambda_{rs} n_s n_r \left[3\left(T_s - T_r\right) + \left(m_s\boldsymbol{u}_s + m_r\boldsymbol{u}_r\right)\cdot\left(\boldsymbol{u}_s - \boldsymbol{u}_r\right)\right] \\ &= -\langle \hat{Q}_{sr}, m_s v^2\rangle. \end{aligned} \tag{2.8}$$

Now, equation (2.3) may be rewritten as

$$\begin{aligned} &\sum_{s=1}^{N}\langle \chi_{ss}\, Q_{ss}(f_s, f_s) + (1 - \chi_{ss})\, \hat{Q}_{ss}(f_s), \varphi_s(\boldsymbol{v})\rangle \\ &+ \sum_{s=1}^{N}\sum_{\substack{r=1 \\ r\neq s}}^{N}\langle \chi_{sr}\, Q_{sr}(f_s, f_r) + (1 - \chi_{sr})\, \hat{Q}_{sr}(f_s), \varphi_s(\boldsymbol{v})\rangle = 0\,. \end{aligned} \tag{2.9}$$

The first sum vanishes, since $\varphi_s(\boldsymbol{v}) = m_s\, \boldsymbol{v}$ and $\varphi_s(\boldsymbol{v}) = m_s v^2$ are collision invariants for the single–species Boltzmann operators, and BGK contributions (1.37) also vanish when $r = s$.
As concerns the second sum, involving interactions between different species, by exchanging indices r and s and recalling that $\chi_{rs} = \chi_{sr}$ we get

$$
\begin{aligned}
&\sum_{s=1}^{N}\sum_{\substack{r=1\\ r\neq s}}^{N}\langle \chi_{sr}\, Q_{sr}(f_s,f_r) + (1-\chi_{sr})\,\hat{Q}_{sr}(f_s), \varphi_s(\boldsymbol{v})\rangle \\
&= \frac{1}{2}\sum_{s=1}^{N}\sum_{\substack{r=1\\ r\neq s}}^{N}\Big[\chi_{sr}\Big(\langle Q_{sr}(f_s,f_r),\varphi_s(\boldsymbol{v})\rangle + \langle Q_{rs}(f_r,f_s),\varphi_r(\boldsymbol{v})\rangle\Big) \\
&+ (1-\chi_{sr})\Big(\langle \hat{Q}_{sr}(f_s),\varphi_s(\boldsymbol{v})\rangle + \langle \hat{Q}_{rs}(f_r),\varphi_r(\boldsymbol{v})\rangle\Big)\Big].
\end{aligned}
$$

Owing to (1.8), we see that Boltzmann contributions vanish due to conservations of momentum and energy in each collision; even BGK contributions vanish as already proved in (2.7)-(2.8), therefore also the second sum in (2.9) is equal to zero, concluding thus the proof of conservation laws. □

We prove now the validity of two lemmas that will be used in the demonstration of the H-theorem and the uniqueness of equilibrium solutions.

Lemma 1. *Let $\{\kappa_{ij}\,, i,j = 1,\ldots,N\,, i\neq j\}$ be a set of $N(N-1)$ positive numbers such that $\kappa_{ij} = \kappa_{ji}$ for each admissible pair. Then, the linear system*

$$\sum_{\substack{j=1\\ j\neq i}}^{N}\kappa_{ij}(\xi_j - \xi_i) = 0\,,\quad i = 1,\ldots,N \tag{2.10}$$

admits only the trivial solution $\xi_1 = \ldots = \xi_N = const.$

Proof. We multiply each equation by ξ_i and we sum over i; we obtain

$$\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\kappa_{ij}(\xi_i^2 - \xi_i\xi_j) = \frac{1}{2}\sum_{i=1}^{N}\sum_{\substack{j=1\\ j\neq i}}^{N}\kappa_{ij}(\xi_i - \xi_j)^2 = 0\,. \tag{2.11}$$

Since all coefficients κ_{ij} are positive, the only admissible solution is $\xi_i - \xi_j = 0$ for each pair of indices. □

Lemma 2. *For any $s = 1,\ldots,N$, we have*

$$\sum_{s=1}^{N}\sum_{\substack{r=1,\\ r\neq s}}^{N}\langle \hat{Q}_{sr}, \log f_s\rangle \leq 0 \ , \tag{2.12}$$

and

$$\sum_{s=1}^{N}\sum_{\substack{r=1,\\ r\neq s}}^{N}\langle \hat{Q}_{sr}, \log f_s\rangle = 0 \iff f_s = \mathcal{M}_s^{eq} \ . \tag{2.13}$$

Proof.

$$\begin{aligned}\sum_{s=1}^{N}\sum_{\substack{r=1\\r\neq s}}^{N}\langle\hat{Q}_{sr},\log f_s\rangle &= \sum_{s=1}^{N}\sum_{\substack{r=1\\r\neq s}}^{N}\nu_{sr}\langle\mathcal{M}_{sr}-f_s,\log f_s\rangle\\ &\leq \sum_{s=1}^{N}\sum_{\substack{r=1\\r\neq s}}^{N}\nu_{sr}\left[\langle\mathcal{M}_{sr},\log\mathcal{M}_{sr}-1\rangle-\langle f_s,\log f_s-1\rangle\right] \qquad (2.14)\\ &= \sum_{s=1}^{N}\sum_{\substack{r=1\\r\neq s}}^{N}\nu_{sr}\left[\langle\mathcal{M}_{sr},\log\mathcal{M}_{sr}\rangle-\langle f_s,\log f_s\rangle\right],\end{aligned}$$

where in the last equality we have taken into account that $\langle\mathcal{M}_{sr},1\rangle=\langle f_s,1\rangle=n_s$ and the inequality follows from

$$(y-x)\log x\leq y(\log y-1)-x(\log x-1)\,,\qquad \text{for any } x,y>0\,. \tag{2.15}$$

In fact,

$$\begin{aligned}&(y-x)\log x\leq y(\log y-1)-x(\log x-1)\\ &\iff y\log x\leq y\log y-y+x\\ &\iff \log\frac{x}{y}\leq\frac{x}{y}-1\,,\end{aligned}$$

that holds for any x, $y>0$.
Now, we can use the classical inequality

$$\langle f_s,\log f_s\rangle\;\geq\;\langle\mathcal{M}_s,\log\mathcal{M}_s\rangle\,, \tag{2.16}$$

where $\mathcal{M}_s:=\mathcal{M}\left(\boldsymbol{v};n_s,\boldsymbol{u}_s,\dfrac{T_s}{m_s}\right)$ is a Maxwellian function having the same moments as f_s; it follows that

$$\sum_{s=1}^{N}\sum_{\substack{r=1\\r\neq s}}^{N}\nu_{sr}\left[\langle\mathcal{M}_{sr},\log\mathcal{M}_{sr}\rangle-\langle\mathcal{M}_s,\log\mathcal{M}_s\rangle\right]\,. \tag{2.17}$$

We compute explicitly

$$\begin{aligned}\langle\mathcal{M}_{sr},\log\mathcal{M}_{sr}\rangle &= \langle\mathcal{M}_{sr},\log n_s+\frac{3}{2}\log\left(\frac{m_s}{2\pi T_{sr}}\right)-\frac{m_s}{2T_{sr}}|\boldsymbol{v}-\boldsymbol{u}_{sr}|^2\rangle\\ &=\left[\log n_s+\frac{3}{2}\log\left(\frac{m_s}{2\pi T_{sr}}\right)\right]\langle\mathcal{M}_{sr},1\rangle-\frac{m_s}{2T_{sr}}\langle\mathcal{M}_{sr},|\boldsymbol{v}-\boldsymbol{u}_{sr}|^2\rangle\\ &=n_s\left[\log n_s+\frac{3}{2}\log\left(\frac{m_s}{2\pi T_{sr}}\right)\right]-\frac{m_s}{2T_{sr}}n_s\left(\frac{m_s}{2\pi T_{sr}}\right)^{3/2}\frac{3}{2}\pi^{3/2}\left(\frac{m_s}{2T_{sr}}\right)^{-5/2}\\ &=n_s\left[\log n_s+\frac{3}{2}\log\left(\frac{m_s}{2\pi T_{sr}}\right)-\frac{3}{2}\right],\end{aligned} \tag{2.18}$$

hence

$$\sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \langle \hat{Q}_{sr}, \log f_s \rangle \leq -\frac{3}{2} \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} n_s \log \frac{T_{sr}}{T_s} \,. \tag{2.19}$$

From the expressions of auxiliary temperatures given in (1.46), we have

$$\begin{aligned} &T_{sr} \geq (1 - b_{sr}) T_s + b_{sr} T_r \\ \Longrightarrow &\log T_{sr} \geq \log[(1 - b_{sr}) T_s + b_{sr} T_r] \geq (1 - b_{sr}) \log T_s + b_{sr} \log T_r \,, \end{aligned} \tag{2.20}$$

where last inequality follows from concavity arguments, recalling that $b_{sr} < 1$; by such result, we can rewrite

$$\log \frac{T_{sr}}{T_s} = \log T_{sr} - \log T_s \geq (1 - b_{sr}) \log T_s + b_{sr} \log T_r - \log T_s = b_{sr} \log \frac{T_r}{T_s} \,, \tag{2.21}$$

and

$$\begin{aligned} \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \langle \hat{Q}_{sr}, \log f_s \rangle &\leq -\frac{3}{2} \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r \neq s}}^{N} \nu_{sr} n_s b_{sr} \log \frac{T_r}{T_s} \\ &= -\frac{3}{2} \sum_{s=1}^{N} \sum_{\substack{r=1 \\ r > s}}^{N} \nu_{sr} n_s b_{sr} \left(\log \frac{T_r}{T_s} + \log \frac{T_s}{T_r} \right) = 0 \,, \end{aligned} \tag{2.22}$$

where using (1.47) we have noted that $\nu_{rs} n_r b_{rs} = \nu_{sr} n_s b_{sr}$. □

We are now ready to prove the analogous of the Boltzmann H-theorem for our mixed Boltzmann–BGK model.

Proposition 2. *In the space homogeneous case, the functional*

$$\mathcal{H}[\boldsymbol{f}] = \sum_{s=1}^{N} \langle f_s, \log f_s \rangle = \sum_{s=1}^{N} \int_{\mathbb{R}^3} f_s(\boldsymbol{v}) \, \log \big(f_s(\boldsymbol{v}) \big) \, d\mathbf{v} \tag{2.23}$$

is a Lyapunov functional, namely $\dfrac{d\mathcal{H}}{dt} \leq 0$ *along each solution of the mixed Boltzmann–BGK system (2.1), and* $\mathcal{H}(\boldsymbol{f}) > \mathcal{H}(\boldsymbol{\mathcal{M}^{eq}})$ *for any* $\boldsymbol{f} \neq \boldsymbol{\mathcal{M}^{eq}}$*, with* $\boldsymbol{\mathcal{M}^{eq}} := (\mathcal{M}_1^{eq}, \ldots, \mathcal{M}_N^{eq})^T$*, where* $\mathcal{M}_s^{eq}$ *are the Maxwellian equilibrium distributions defined in* (1.53).

Proof. In order to verify the validity of the theorem we have to prove that along any solution of the mixed model (2.1) in space homogeneous conditions we have

$\frac{d\mathcal{H}}{dt} \le 0$. Similarly to (2.1), it can be checked that

$$\begin{aligned}\frac{d\mathcal{H}}{dt} &= \sum_{s=1}^{N}\sum_{r=1}^{N}\langle \chi_{sr}\, Q_{sr}(f_s,f_r) + (1-\chi_{sr})\,\hat{Q}_{sr}(f_s), \log f_s\rangle \\ &= \sum_{s=1}^{N}\langle \chi_{ss}\, Q_{ss}(f_s,f_s) + (1-\chi_{ss})\,\hat{Q}_{ss}(f_s), \log f_s\rangle \\ &+ \sum_{s=1}^{N}\sum_{\substack{r=1\\ r\neq s}}^{N}\langle \chi_{sr}\, Q_{sr}(f_s,f_r) + (1-\chi_{sr})\,\hat{Q}_{sr}(f_s), \log f_s\rangle.\end{aligned}$$

Since $Q_{ss}(f_s,f_s)$ is the one–species Boltzmann operator [18] and $\hat{Q}_{ss}(f_s)$ is the standard BGK operator for a single gas [3], it is well known that $\langle Q_{ss}(f_s,f_s),\log f_s\rangle \le 0$ and $\langle \hat{Q}_{ss}(f_s),\log f_s\rangle \le 0$. As concerns contributions involving operators with $r \neq s$, for the BGK ones we have already proved in lemma 2

$$\langle Q_{sr}(f_s), \log f_s\rangle + \langle Q_{rs}(f_r), \log f_r\rangle \le 0\,,$$

while for the Boltzmann terms, recalling the weak form (1.19), we have

$$\begin{aligned}&\langle Q_{sr}(f_s,f_r), \log f_s\rangle + \langle Q_{rs}(f_r,f_s), \log f_r\rangle \\ &\qquad = -\frac{1}{2}\iiint_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} g_{sr}(\boldsymbol{y}, \hat{\boldsymbol{y}}\cdot\boldsymbol{\omega}) \log\left(\frac{f_s(\boldsymbol{v}'_{sr})f_r(\boldsymbol{w}'_{sr})}{f_s(\boldsymbol{v})f_r(\boldsymbol{w})}\right) \\ &\qquad \times \left[\frac{f_s(\boldsymbol{v}'_{sr})f_r(\boldsymbol{w}'_{sr})}{f_s(\boldsymbol{v})f_r(\boldsymbol{w})} - 1\right] f_s(\boldsymbol{v})f_r(\boldsymbol{w}) d\boldsymbol{v} d\boldsymbol{w} d\omega \le 0\,,\end{aligned}$$

where the inequality holds since $(y-1)\log y \ge 0$, $\forall y > 0$. In conclusion, the inequality $\frac{d\mathcal{H}}{dt} \le 0$ is fulfilled and, more specifically, $\frac{d\mathcal{H}}{dt}$ may be seen as a sum of non–positive contributions as follows:

$$\begin{aligned}\frac{d\mathcal{H}}{dt} &= \sum_{s=1}^{N}\chi_{ss}\, \underbrace{\langle Q_{ss}(f_s,f_s), \log f_s\rangle}_{\le 0} + \sum_{s=1}^{N}(1-\chi_{ss})\, \underbrace{\langle \hat{Q}_{ss}(f_s), \log f_s\rangle}_{\le 0} \\ &+ \sum_{s=1}^{N}\sum_{\substack{r=1\\ r>s}}^{N}\chi_{sr}\Big(\underbrace{\langle Q_{sr}(f_s,f_r), \log f_s\rangle + \langle Q_{rs}(f_r,f_s), \log f_r\rangle}_{\le 0}\Big) \\ &+ \sum_{s=1}^{N}\sum_{\substack{r=1\\ r>s}}^{N}(1-\chi_{sr})\Big(\underbrace{\langle \hat{Q}_{sr}(f_s), \log f_s\rangle + \langle \hat{Q}_{rs}(f_r), \log f_r >}_{\le 0}\Big).\end{aligned} \tag{2.24}$$

We note that each addend of the right-hand side above vanishes only if $\boldsymbol{f}$ is a stationary state, i.e. $\boldsymbol{f} = \boldsymbol{\mathcal{M}^{eq}}$. Hence the the proof is concluded.

□

Proposition 3. *The equilibrium solutions of the Boltzmann–BGK model (2.1) are provided by Maxwellian functions depending on global mean velocity and temperature, i.e.*

$$Q_s = 0\,, \quad s = 1, \ldots, N \iff f_s = \mathcal{M}_s^{eq} = n_s \left(\frac{m_s}{2\pi T}\right)^{3/2} \exp\left[-\frac{m_s}{2T}\,(\boldsymbol{v}-\boldsymbol{u})^2\right]. \tag{2.25}$$

Proof. Firstly we observe that one of the two implications is trivial: if the Maxwellian distribution functions share the same mean velocity and temperature then each term in Q_s vanishes. For the reverse implication, we remark that in (2.24) we have shown that $\dfrac{d\mathcal{H}}{dt}$ is a sum of non–negative terms, therefore if $\boldsymbol{f} = (f_1, \ldots, f_N)$ is a stationary state, then $\dfrac{d\mathcal{H}}{dt}$ must vanish.
By considering at first the interactions between particles of the same species we get that, for any $s = 1, ..., N$, if $\chi_{ss} = 1$ then $\langle Q_{ss}(f_s, f_s), \log f_s\rangle = 0$, while if $\chi_{ss} = 0$ then $\langle \hat{Q}_{ss}(f_s), \log f_s\rangle = 0$; in both cases this obviously yields (recalling classical results for one–species Boltzmann and BGK H-theorem)

$$f_s = \mathcal{M}_s\left(\boldsymbol{v};\, n_s,\, \boldsymbol{u}_s,\, \frac{T_s}{m_s}\right) = n_s\left(\frac{m_s}{2\pi T_s}\right)^{3/2} \exp\left[-\frac{m_s}{2T_s}\,|\boldsymbol{v}-\boldsymbol{u}_s|^2\right], \tag{2.26}$$

namely it is a Maxwellian distribution with species macroscopic fields n_s, $\mathbf{u}_s$ and T_s.
Taking into account this result, let us consider the interactions between different constituents. For any (s, r) with $r \neq s$ such that $\chi_{sr} = 1$, from the computations above and from the well known detailed balance principle for bi–species Boltzmann operators [19], we have that the pertinent contribution to the entropy dissipation estimate (2.24) vanishes only if

$$\log\big(f_s(\boldsymbol{v}'_{sr})\big) + \log\big(f_r(\boldsymbol{w}'_{sr})\big) = \log\big(f_s(\boldsymbol{v})\big) + \log\big(f_r(\boldsymbol{w})\big)\,, \quad \forall \boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^3, \omega \in \mathbb{S}^2\,.$$

By substituting into this equality the expressions of the local Maxwellian $\mathcal{M}_s$ and $\mathcal{M}_r$ given in (2.26) we get

$$\frac{m_s}{T_s}|\boldsymbol{v}'_{sr} - \boldsymbol{u}_s|^2 + \frac{m_r}{T_r}|\boldsymbol{w}'_{sr} - \boldsymbol{u}_r|^2 = \frac{m_s}{T_s}|\boldsymbol{v} - \boldsymbol{u}_s|^2 + \frac{m_r}{T_r}|\boldsymbol{w} - \boldsymbol{u}_r|^2,$$

hence

$$\frac{m_s}{T_s}\left(|\boldsymbol{v}'_{sr}|^2 - |\boldsymbol{v}|^2\right) + \frac{m_r}{T_r}\left(|\boldsymbol{w}'_{sr}|^2 - |\boldsymbol{w}|^2\right) - 2\frac{m_s}{T_s}\,(\boldsymbol{v}'_{sr} - \boldsymbol{v})\cdot\boldsymbol{u}_s - 2\frac{m_r}{T_r}\,(\boldsymbol{w}'_{sr} - \boldsymbol{w})\cdot\boldsymbol{u}_r = 0\,;$$

choosing $\boldsymbol{w} = -\boldsymbol{v}$ and $\boldsymbol{\omega} = -\boldsymbol{v}/|\boldsymbol{v}|$ we get $\boldsymbol{v}'_{sr} = \left(1 - 4\,\dfrac{m_r}{m_s + m_r}\right)\boldsymbol{v}$ and $\boldsymbol{w}'_{sr} = \left(4\,\dfrac{m_s}{m_r + m_s} - 1\right)\boldsymbol{v}$, and consequently

$$8\,\frac{m_s\, m_r}{m_s + m_r}\left(2\,\frac{m_r}{m_s + m_r} - 1\right)\left(\frac{1}{T_s} - \frac{1}{T_r}\right)|\boldsymbol{v}|^2 + 8\,\frac{m_s\, m_r}{m_s + m_r}\,\boldsymbol{v}\cdot\left(\frac{\boldsymbol{u}_s}{T_s} - \frac{\boldsymbol{u}_r}{T_r}\right) = 0\,.$$

Since such equality must hold $\forall \boldsymbol{v} \in \mathbb{R}^3$, we obtain $\boldsymbol{u}_r = \boldsymbol{u}_s$ and $T_r = T_s$ for all pairs (s,r) with $\chi_{sr} = 1$. Under these constraints, distributions (2.26) are such that $Q_{sr}(\mathcal{M}_s, \mathcal{M}_r) = Q_{rs}(\mathcal{M}_r, \mathcal{M}_s) = 0$, for any (s,r) with $\chi_{rs} = 1$. Therefore, by multiplying the s-th collision operator in (2.1) by $m_s\, \boldsymbol{v}$, only BGK contributions remain:

$$\sum_{r=1}^{N} \langle \chi_{sr}\, \hat{Q}_{sr}(\mathcal{M}_s, \mathcal{M}_r) + (1-\chi_{sr})\, \hat{Q}_{sr}(\mathcal{M}_s), m_s\, \boldsymbol{v} \rangle$$
$$= \sum_{\substack{r=1 \\ r\neq s}}^{N} (1-\chi_{sr}) \langle Q_{sr}(\mathcal{M}_s), m_s\, \boldsymbol{v} \rangle = \sum_{\substack{r=1 \\ r\neq s}}^{N} (1-\chi_{sr}) \mathcal{C}_{sr}(\boldsymbol{u}_r - \boldsymbol{u}_s)\,,$$

with coefficients $\mathcal{C}_{sr} = \Lambda_{sr} \dfrac{m_s m_r}{m_s + m_r} n_s n_r > 0$ (see (1.37)).
At the equilibrium we have thus

$$\sum_{r \in \Xi_s} \mathcal{C}_{sr}(\mathbf{u}_r - \mathbf{u}_s) = \mathbf{0}\,, \qquad s = 1, \ldots, N,$$

where Ξ_s denotes the set of indices $r = 1, \ldots, N$ such that $\chi_{sr} = 0$. According to Lemma 1, these equalities hold if and only if $\mathbf{u}_r = \mathbf{u}_s$ for any (s,r) such that $\chi_{rs} = 0$. Using this result in the weak form of the s-th collision operator in (2.1) with weight $m_s\, v^2$ we obtain

$$\sum_{r=1}^{N} \langle \chi_{sr}\, Q_{sr}(\mathcal{M}_s, \mathcal{M}_r) + (1-\chi_{sr})\, \hat{Q}_{sr}(\mathcal{M}_s), m_s\, v^2 \rangle$$
$$= \sum_{\substack{r=1 \\ r\neq s}}^{N} (1-\chi_{sr}) \langle \hat{Q}_{sr}(\mathcal{M}_s), m_s\, v^2 \rangle = \sum_{\substack{r=1 \\ r\neq s}}^{N} (1-\chi_{sr}) \mathcal{D}_{sr}(T_r - T_s)\,,$$

with coefficients $\mathcal{D}_{sr} = 2\mathcal{C}_{sr}/(m_s + m_r) > 0$, see again (1.37), and the same arguments as above imply $T_r = T_s$ for any (s,r) such that $\chi_{sr} = 0$. This concludes the proof of equalization of mean velocities and temperatures of all species in any equilibrium configuration.

□

2.2 Dimensionless equations

We now turn to the dimensionless form of the kinetic equations in order to introduce the Knudsen number and other dimensionless numbers able to identify the role of various collision processes. This formulation will enable the analysis of different regimes and, in particular, the identification of the hydrodynamic limits of these equations. To begin, we order the masses of the components; without loss of generality, we may assume that

$$0 < m_1 \leq m_2 \leq \ldots \leq m_{N-1} < m_N \quad ,$$

and we set

$$\tilde{m}_s = \frac{m_s}{m_N}, \quad \forall s = 1, ..., N,$$

hence $\tilde{m}_N = 1$.

Let us consider a reference temperature T_0 and introduce a velocity defined as

$$\tau = \left(\frac{T_0}{m_N}\right)^{\frac{1}{2}} \quad .$$

We also denote by n_0 a suitable reference molecular density, and write

$$\tilde{n}_s = \frac{n_s}{n_0} \ , \qquad \tilde{T}_s = \frac{T_s}{T_0} \ , \qquad \tilde{\boldsymbol{v}} = \frac{\boldsymbol{v}}{\tau} \ , \qquad \tilde{\boldsymbol{u}}_s = \frac{\boldsymbol{u}_s}{\tau} \ .$$

and we then normalize the distribution functions as follows

$$\tilde{f}_s = \tau^3 \frac{f_s}{n_0} \ .$$

Finally, recalling that the collision frequencies have the unit measure of the inverse of time, we rescale the spatial and temporal variables as follows

$$\tilde{t} = \nu t \ , \quad \tilde{\boldsymbol{x}} = \frac{\nu \boldsymbol{x}}{\tau} \ ,$$

where ν is a reference value for the collision frequencies.
In order to study different hydrodynamic regimes, characterized by different dominant collisional phenomena, we rescale the collision frequencies and the differential cross sections by introducing the constants β_{sr} and ε

$$\tilde{\nu}_{sr} = \frac{\varepsilon \nu_{sr}}{\beta_{sr}\nu} \, , \quad \tilde{g}_{sr} = \frac{\varepsilon n_0}{\beta_{sr}\nu} g_{sr} \, , \qquad \forall\, s, r = 1, \dots, N. \tag{2.27}$$

specifically, $\boldsymbol{\varepsilon}$ is the **Knudsen number**, the small parameter representative of the ratio between microscopic and macroscopic scale, while β_{sr} will allow us to analyze different hydrodynamic regimes.

We recall the equation of the system describing the evolution of the s-th species

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = \sum_{r=1}^{N} \left[\chi_{sr} Q_{sr} + (1 - \chi_{sr}) \hat{Q}_{sr} \right] \tag{2.28}$$

and make it dimensionless.

Exploiting the dimensionless variables above, first addend of the left-hand side becomes

$$\frac{\partial f_s}{\partial t} = \nu \frac{\partial f_s}{\partial \tilde{t}} = \frac{\nu n_0}{\tau^3} \frac{\partial \tilde{f}_s}{\partial \tilde{t}}, \tag{2.29}$$

and the second

$$\begin{aligned}
&\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s = \tau\tilde{\boldsymbol{v}}\cdot\nabla_{\boldsymbol{x}}\left(\frac{n_0}{\tau^3}\tilde{f}\right)\\
&= \frac{\nu}{\tau}\tau\frac{n_0}{\tau^3}\tilde{\boldsymbol{v}}\cdot\nabla_{\tilde{\boldsymbol{x}}}\tilde{f}_s \qquad (2.30)\\
&\Longleftrightarrow\ \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s = \frac{\nu n_0}{\tau^3}\ \tilde{\boldsymbol{v}}\cdot\nabla_{\tilde{\boldsymbol{x}}}\tilde{f}_s\,.
\end{aligned}$$

Boltzmann collisional operator thus turns into

$$\begin{aligned}
Q_{sr} &= \int_{\mathbb{R}^3\times\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|,\hat{\boldsymbol{y}}\cdot\omega)\Big[f_s(\boldsymbol{v}'_{sr})f_s(\boldsymbol{w}'_{sr}) - f_s(\boldsymbol{v})f_s(\boldsymbol{w})\Big]d\boldsymbol{w}d\omega\\
&= \frac{\beta_{sr}\nu}{\varepsilon n_0}\frac{n_0}{\tau^3}\frac{n_0}{\tau^3}\int_{\mathbb{R}^3\times\mathbb{S}^2}\tilde{g}_{sr}(|\boldsymbol{y}|,\hat{\boldsymbol{y}}\cdot\omega)\Big[\tilde{f}_s(\boldsymbol{v}'_{sr})\tilde{f}_s(\boldsymbol{w}'_{sr}) - \tilde{f}_s(\boldsymbol{v})\tilde{f}_s(\boldsymbol{w})\Big]d\boldsymbol{w}d\omega\\
&= \frac{\beta_{sr}}{\varepsilon}\frac{\nu n_0}{\tau^3}\int_{\mathbb{R}^3\times\mathbb{S}^2}\tilde{g}_{sr}(|\boldsymbol{y}|,\hat{\boldsymbol{y}}\cdot\omega)\Big[\tilde{f}_s(\boldsymbol{v}'_{sr})\tilde{f}_s(\boldsymbol{w}'_{sr}) - \tilde{f}_s(\boldsymbol{v})\tilde{f}_r(\boldsymbol{w})\Big]d\tilde{\boldsymbol{w}}d\omega,
\end{aligned}$$

hence

$$Q_{sr} = \frac{\beta_{sr}}{\varepsilon}\frac{\nu n_0}{\tau^3}\tilde{Q}_{sr}. \qquad (2.31)$$

Focusing now on the BGK collisional operator $\hat{Q}_{sr}$, we need to adimensionalize the the fictitious parameter $\boldsymbol{u}_{sr}$ and T_{sr}.
Recalling the expression of their coefficients

$$\begin{cases}
a_{sr} = \dfrac{m_r n_r \Lambda_{sr}}{\nu_{sr}\big(m_s+m_r\big)}\\
b_{sr} = \dfrac{2a_{sr}m_s}{m_s+m_r}\\
\gamma_{sr} = \dfrac{m_s a_{sr}}{3}\left(\dfrac{2m_r}{m_s+m_r} - a_{sr}\right)
\end{cases},$$

we notice that a_{sr} and b_{sr} are already pure numbers, i.e. we can write $a_{sr} = \tilde{a}_{sr}$, $b_{sr} = \tilde{b}_{sr}$, while γ_{sr} has the dimension of a mass: we then introduce

$$\tilde{\gamma}_{sr} = \frac{\gamma_{sr}}{m_N}\ .$$

We set now

$$\tilde{\boldsymbol{u}}_{sr} = \frac{\boldsymbol{u}_{sr}}{\tau}\ ,\quad \tilde{T}_{sr} = \frac{T_s}{T_0}\ ,$$

from which

$$\begin{aligned}
&\boldsymbol{u}_{sr} = (1-a_{sr})\,\boldsymbol{u}_s + a_{sr}\boldsymbol{u}_r\\
&\Longrightarrow\ \tilde{\boldsymbol{u}}_{sr} = (1-\tilde{a}_{sr})\,\tilde{\boldsymbol{u}}_s + \tilde{a}_{sr}\tilde{\boldsymbol{u}}_r\ ,
\end{aligned}$$

and

$$T_s = (1 - b_{sr})\, T_s + b_{sr} T_r + \gamma_{sr}\, (\boldsymbol{u}_s - \boldsymbol{u}_r)^2$$

$$\Longrightarrow\ \tilde{T}_{sr} = \left(1 - \tilde{b}_{sr}\right) \tilde{T}_s + \tilde{b}_{sr} \tilde{T}_r + \tilde{\gamma}_{sr}\, (\tilde{\boldsymbol{u}}_s - \tilde{\boldsymbol{u}}_r)^2 \ ,$$

where we have used $m_N \tau^2 = T_0$.

We now concentrate on the fictitious Maxwellian $\mathcal{M}_{sr}$: dividing both numerator and denominator by m_N and exploiting the relations computed above, we obtain

$$\mathcal{M}_{sr} = n_0 \tilde{n}_s \left(\frac{\tilde{m}_s}{2\pi \tilde{T}_{sr} \frac{T_0}{m_N}} \right)^{\frac{3}{2}} \exp \left(- \frac{\tilde{m}_s}{2\tilde{T}_{rs} \frac{T_0}{m_N}} \tau^2 |\tilde{\boldsymbol{v}} - \tilde{\boldsymbol{u}}_{sr}|^2 \right)$$

$$= \frac{n_0}{\tau^3}\ \tilde{n}_s \left(\frac{\tilde{m}_s}{2\pi \tilde{T}_{sr}} \right)^{\frac{3}{2}} \exp \left(\frac{\tilde{m}_s}{2\tilde{T}_{sr}} |\tilde{\boldsymbol{v}} - \tilde{\boldsymbol{u}}_{sr}|^2 \right) ,$$

then

$$\mathcal{M}_{sr} = \frac{n_0}{\tau^3} \tilde{\mathcal{M}}_{sr} \ .$$

Hence, the BGK operator accounting for the collision between species s and r can be reformulated as

$$\begin{aligned} \hat{Q}_{sr} &= \frac{\beta_{sr}\nu}{\varepsilon} \tilde{\nu}_{sr} \big(\frac{n_0}{\tau^3} \tilde{\mathcal{M}}_{sr} - \frac{n_0}{\tau^3} \tilde{f}_s \big) \\ &= \frac{\beta_{sr}}{\varepsilon}\ \frac{\nu n_0}{\tau^3}\ \tilde{\nu}_{sr} \big(\tilde{\mathcal{M}}_{sr} - \tilde{f}_s \big) = \frac{\beta_{sr}}{\varepsilon}\ \frac{\nu n_0}{\tau^3}\ \hat{\tilde{Q}}_{sr} \ . \end{aligned} \tag{2.32}$$

We are now ready to write the dimensionless form of the Boltzmann equations which drives the evolution of the system. Using (2.29), (2.30), (2.31) and (2.32), simplifying $\dfrac{\nu n_0}{\tau^3}$ and omitting the symbol $\sim$ we finally obtain

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = \sum_{r=1}^{N} \frac{\beta_{sr}}{\varepsilon} \left[\chi_{sr} Q_{sr} + (1 - \chi_{sr}) \hat{Q}_{sr} \right] , \tag{2.33}$$

which will allow us to study different hydrodynamic regimes.
In particular, throughout this thesis, thanks to (2.33), we will be able to study the classical collision-dominated regime, the regime dominated by intra–species collisions, and the fluid–kinetic regime, corresponding to a binary mixture in which one species is significantly heavier than the other.

Remark. *The possibility of choosing which interactions are described by the classical Boltzmann operator and which by the BGK terms includes in particular the case where the Boltzmann operators model intra-species interactions, while the BGK operators account for inter-species interactions.*
This choice could be motivated by the fact that in some physical problems, like

ε-mixtures of heavy and light masses or in astro-physics problems, particles of the same species exchange energy faster than particles with disparate masses, and consequently Boltzmann's description of intra-species collisions is the most adequate. Moreover, in the regime dominated by the intra-species collisions only, this approach allows for the correct reproduction of species Prandtl number in the hydrodynamic limit [8], a property that is not satisfied by the full-BGK description [9].

Chapter 3

Classical collision dominated regime

3.1 Chapman-Enskog expansion

In this chapter we analyze the classical fluid–dynamic regime, where molecules are subject to a huge number of collisions with particles of all species. In order to enforce the dominance of the entire collisional phenomenon, both intra- and inter-species, in the dimensionless kinetic equation (2.33), we set

$$\beta_{sr} = 1\,, \quad \forall\, s, r = 1, \ldots, N;$$

The evolution equation for the s-th species will then be

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = \frac{1}{\varepsilon} \left[\sum_{r=1}^{N} \chi_{sr} Q_{sr} + (1 - \chi_{sr}) \hat{Q}_{sr} \right], \tag{3.1}$$

where we recall that ε represents the Knudsen number, ratio between the molecular mean free path and a macroscopic length, that is small in a collision dominated regime.

To analyze this regime, we employ the Chapman–Enskog expansion, an asymptotic procedure aimed at obtaining the closure of the macroscopic conservation equations. In this expansion, the hydrodynamic variables, which are moments of the distribution function corresponding to the collisional invariants, are not expanded in powers of ε; rather, they are treated as standalone entities, representative of the corresponding physical quantities. In the case where all collisions are dominant, the collisional invariants for the entire collision operator are those of the mixture, namely the density n_s of each species, the velocity $\boldsymbol{u}$ and the temperature T. The expansions of n_s, $\boldsymbol{u}$ and T are considered as a single $O(1)$ term corresponding to the leading-order f_0 of the asymptotic series

$$f_s(\boldsymbol{x}, \boldsymbol{v}, t, \varepsilon) := \sum_{n=0}^{+\infty} \varepsilon^n f_s^{(n)}\left(\boldsymbol{x}, \boldsymbol{v}, t\right), \tag{3.2}$$

of which in this thesis we will investigate the first two terms, neglecting $O(\varepsilon^2)$ corrections: we consider the first order expansion

$$f_s = f_s^{(0)} + \varepsilon f_s^{(1)}.$$

By substituting this expansion in (3.1), we get

$$\begin{aligned}
&\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s^{(0)} + \varepsilon\left(\frac{\partial f_s^{(1)}}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s^{(1)}\right)\\
&= \frac{1}{\varepsilon}\Bigg\{ \sum_{r=1}^{N}\chi_{sr}\Big[Q_{sr}(f_s^{(0)}, f_r^{(0)}) + \varepsilon\big(Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)})\big)\Big] \qquad (3.3)\\
&+ \sum_{r=1}^{N}(1-\chi_{sr})\big(\nu_{sr}^{(0)} + \varepsilon\nu_{sr}^{(1)}\big)\Big(\mathcal{M}_{sr}^{(0)} + \varepsilon\mathcal{M}_{sr}^{(1)} - f_s^{(0)} - \varepsilon f_s^{(1)}\Big)\Bigg\}.
\end{aligned}$$

As for the distribution functions, the macroscopic variables of the species $\boldsymbol{u}_s$ and T_s, as well as the global pressure tensor $\underline{\boldsymbol{P}}$ and the global heat flux vector $\boldsymbol{q}$, are also expanded with respect to ε

$$\begin{aligned}
\boldsymbol{u}_s &= \boldsymbol{u}_s^{(0)} + \varepsilon\boldsymbol{u}_s^{(1)}\,;\\
T_s &= T_s^{(0)} + \varepsilon T_s^{(1)}\,;\\
\underline{\boldsymbol{P}} &= \underline{\boldsymbol{P}}^{(0)} + \varepsilon\underline{\boldsymbol{P}}^{(1)}\,;\\
\boldsymbol{q} &= \boldsymbol{q}^{(0)} + \varepsilon\boldsymbol{q}^{(1)}\,.
\end{aligned} \qquad (3.4)$$

Similar expansions are also introduced for the auxiliary parameters ν_{sr}, $\boldsymbol{u}_{sr}$, and T_{sr}, as well as for the constants appearing in these parameters a_{sr}, b_{sr}, γ_{sr} and Λ_{sr}, from which

$$\begin{aligned}
\boldsymbol{u}_{sr} = \boldsymbol{u}_{sr}^{(0)} + \varepsilon\boldsymbol{u}_{sr}^{(1)} &= \left(1 - a_{sr}^{(0)} - \varepsilon a_{sr}^{(1)}\right)\left(\boldsymbol{u}_s^{(0)} + \varepsilon\boldsymbol{u}_s^{(1)}\right)\\
&+ \left(a_{sr}^{(0)} + \varepsilon a_{sr}^{(1)}\right)\left(\boldsymbol{u}_r^{(0)} + \varepsilon\boldsymbol{u}_r^{(1)}\right)\,,
\end{aligned}$$

then

$$\begin{cases}
\boldsymbol{u}_{sr}^{(0)} = \left(1 - a_{sr}^{(0)}\right)\boldsymbol{u}_s^{(0)} + a_{sr}^{(0)}\boldsymbol{u}_r^{(0)}\\
\boldsymbol{u}_{sr}^{(1)} = \left(1 - a_{sr}^{(0)}\right)\boldsymbol{u}_s^{(1)} + a_{sr}^{(0)}\boldsymbol{u}_r^{(1)} + a_{sr}^{(1)}\left(\boldsymbol{u}_r^{(0)} - \boldsymbol{u}_s^{(0)}\right)\,,
\end{cases} \qquad (3.5)$$

and analogously

$$\begin{cases}
T_{sr}^{(0)} = \left(1 - b_{sr}^{(0)}\right)T_s^{(0)} + b_{sr}^{(0)}T_r^{(0)} + \gamma_{sr}^{(0)}\left(\boldsymbol{u}_s^{(0)} - \boldsymbol{u}_r^{(0)}\right)^2\\
T_{sr}^{(1)} = \left(1 - b_{sr}^{(0)}\right)T_s^{(1)} + b_{sr}^{(0)}T_r^{(1)} + 2\gamma_{sr}^{(0)}\left(\boldsymbol{u}_s^{(1)} - \boldsymbol{u}_r^{(1)}\right)\cdot\left(\boldsymbol{u}_s^{(0)} - \boldsymbol{u}_r^{(0)}\right)\\
+b_{sr}^{(1)}\left(T_r^{(0)} - T_s^{(0)}\right) + \gamma_{sr}^{(1)}\left(\boldsymbol{u}_s^{(0)} - \boldsymbol{u}_r^{(0)}\right)^2\,,
\end{cases}$$

(3.6)

where

$$
\begin{cases}
a_{sr}^{(0)} &= \dfrac{\Lambda_{sr} n_r^{(0)} m_r}{\nu_{sr}^{(0)}\,(m_s+m_r)} \\
a_{sr}^{(1)} &= \dfrac{\Lambda_{sr} m_r}{\nu_{sr}^{(0)}\,(m_s+m_r)}\left(n_r^{(1)} - \dfrac{n_r^{(0)}\nu_{sr}^{(1)}}{\nu_{sr}^{(0)}}\right) \\
b_{sr}^{(0)} &= \dfrac{2a_{sr}^{(0)} m_s}{m_s+m_r} \\
b_{sr}^{(1)} &= \dfrac{2a_{sr}^{(1)} m_s}{m_s+m_r} \\
\gamma_{sr}^{(0)} &= \dfrac{m_s a_{sr}^{(0)}}{3}\left(\dfrac{2m_r}{m_s+m_r} - a_{sr}^{(0)}\right) \\
\gamma_{sr}^{(1)} &= \dfrac{2}{3} a_{sr}^{(1)}\left(m_{sr} - m_s a_{sr}^{(0)}\right) .
\end{cases}
\tag{3.7}
$$

At leading order of (3.3), we find the following

$$
\sum_{r=1}^{N}\left[\chi_{sr}\mathcal{Q}_{sr}(f_s^{(0)}, f_r^{(0)}) + (1-\chi_{sr})\nu_{sr}^{(0)}\left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)}\right)\right] = 0\,,
$$

that by the uniqueness of the equilibrium distribution, proved in Proposition 3, implies

$$
f_s^{(0)} = \mathcal{M}_s^{eq} = n_s\left(\frac{m_s}{2\pi T}\right)\exp\left[-\frac{m_s}{2T}|\boldsymbol{v}-\boldsymbol{u}|^2\right], \tag{3.8}
$$

which through some standard computations provides the zeroth, first, and second order moment of $f_s^{(0)}$

$$
\int_{\mathbb{R}^3} f_s^{(0)}(\boldsymbol{v})d\boldsymbol{v} = n_s\,, \quad \int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(0)}(\boldsymbol{v})d\boldsymbol{v} = n_s\boldsymbol{u}\,, \quad \int_{\mathbb{R}^3} v^2 f_s^{(0)}(\boldsymbol{v})d\boldsymbol{v} = n_s\left(u^2 + \frac{3T}{m_s}\right) . \tag{3.9}
$$

As previously anticipated, in the Chapman-Enskog procedure, the hydrodynamic variables –moments of the distribution function corresponding to the collisional invariants –must remain unexpanded. In our case, therefore, the species densities n_s, along with global velocity $\boldsymbol{u}$ and temperature T, remain unexpanded, i.e.

$$
n_s = n_s^{(0)}\,, \qquad \boldsymbol{u} = \boldsymbol{u}_s^{(0)}\,, \qquad T = T_s^{(0)}\,.
$$

The species densities non-expansion directly implies

$$
\int_{\mathbb{R}^3}\left(f_s^{(0)}(\boldsymbol{v}) + \varepsilon f_s^{(1)}(\boldsymbol{v})\right)d\boldsymbol{v} = n_s \implies \int_{\mathbb{R}^3} f_s^{(1)}(\boldsymbol{v})d\boldsymbol{v} = n_s^{(1)} = 0\,. \tag{3.10}
$$

As regards the first order momentum, we have

$$
\int_{\mathbb{R}^3}\boldsymbol{v}(f_s^{(0)} + \varepsilon f_s^{(1)})d\boldsymbol{v} = n_s(\boldsymbol{u} + \varepsilon\boldsymbol{u}_s^{(1)}) \implies \int_{\mathbb{R}^3}\boldsymbol{v} f_s^{(1)} d\boldsymbol{v} = n_s\boldsymbol{u}_s^{(1)}\,. \tag{3.11}
$$

Neglecting $O(\varepsilon^2)$ corrections, for the temperatures we find

$$
\begin{aligned}
&\int_{\mathbb{R}^3} v^2 (f_s^{(0)} + \varepsilon f_s^{(1)}) d\boldsymbol{v} = n_s \left(u^2 + 2\varepsilon \boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + 3 \frac{T + \varepsilon T_s^{(1)}}{m_s} \right) \\
&\implies \int_{\mathbb{R}^3} v^2 f_s^{(1)} d\boldsymbol{v} = n_s \left(2\boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + 3 \frac{T_s^{(1)}}{m_s} \right) .
\end{aligned}
\tag{3.12}
$$

Recalling the definition of global velocity and temperature, we find the constraints

$$
\boldsymbol{u} = \frac{1}{\rho} \sum_{s=1}^{N} \rho_s \boldsymbol{u}_s = \frac{1}{\rho} \sum_{s=1}^{N} \rho_s (\boldsymbol{u} + \varepsilon \boldsymbol{u}_s^{(1)}) \implies \sum_{s=1}^{N} \rho_s \boldsymbol{u}_s^{(1)} = \boldsymbol{0} \, , \tag{3.13}
$$

and

$$
T = \frac{1}{n} \sum_{s=1}^{N} n_s (T + \varepsilon T_s^{(1)}) + O(\varepsilon^2) \implies \sum_{s=1}^{N} n_s T_s^{(1)} = 0 \, . \tag{3.14}
$$

Formulas (3.13) and (3.14), in conjunction with $n_s^{(1)} = 0 \, , \quad \forall s = 1, \ldots, N$, provide the **compatibility constraints**.

We are now ready to compute the $N+4$ macroscopic conservation equations. The first N scalar collision invariants provide

$$
\begin{aligned}
&\int_{\mathbb{R}^3} \frac{\partial (f_s^{(0)} + \varepsilon f_s^{(1)})}{\partial t} d\boldsymbol{v} + \int_{\mathbb{R}^3} \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} (f_s^{(0)} + \varepsilon f_s^{(1)}) d\boldsymbol{v} \\
&= \frac{\partial}{\partial t} \left[\int_{\mathbb{R}^3} f_s^{(0)} d\boldsymbol{v} + \varepsilon \int_{\mathbb{R}^3} f_s^{(1)} d\boldsymbol{v} \right] + \nabla_{\boldsymbol{x}} \cdot \left[\int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(0)} d\boldsymbol{v} + \varepsilon \int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(1)} d\boldsymbol{v} \right] \\
&= \frac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}) + \varepsilon \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}_s^{(1)}) = 0 \ , \quad \text{for } s = 1, \ldots, N.
\end{aligned}
$$

Exploiting the compatibility constraints, the test function $m_s \boldsymbol{v}$ yield the following

$$
\begin{aligned}
&\sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} \boldsymbol{v} \frac{\partial (f_s^{(0)} + \varepsilon f_s^{(1)})}{\partial t} d\boldsymbol{v} \\
&= \frac{\partial}{\partial t} \sum_{s=1}^{N} m_s n_s \boldsymbol{u} + \varepsilon \frac{\partial}{\partial t} \sum_{s=1}^{N} m_s n_s \boldsymbol{u}_s^{(1)} = \frac{\partial}{\partial t} (\rho \boldsymbol{u}) \, ;
\end{aligned}
$$

furthermore, with regard to the spatial derivatives, adopting the Einstein convention on repeated indices we obtain

$$\begin{aligned}
&\sum_{s=1}^{N}\int_{\mathbb{R}^3} m_s v_i v_j \frac{\partial(f_s^{(0)}+\varepsilon f_s^{(1)})}{\partial x_j} d\boldsymbol{v} \\
&= \frac{\partial}{\partial x_j}\sum_{s=1}^{N}\int_{\mathbb{R}^3} m_s\big(u_i+c_i\big)\big(u_j+c_j\big)\big(f_s^{(0)}+\varepsilon f_s^{(1)}\big)d\boldsymbol{v} \\
&= \frac{\partial}{\partial x_j}\sum_{s=1}^{N} m_s u_i u_j \int_{\mathbb{R}^3}\big(f_s^{(0)}+\varepsilon f_s^{(1)}\big)d\boldsymbol{v} + \frac{\partial}{\partial x_j}\sum_{s=1}^{N} m_s\int_{\mathbb{R}^3} c_i c_j\big(f_s^{(0)}+\varepsilon f_s^{(1)}\big)d\boldsymbol{v} \\
&= \frac{\partial}{\partial x_j}\sum_{s=1}^{N} u_i u_j m_s n_s + \frac{\partial}{\partial x_j}\sum_{s=1}^{N} m_s\left[\int_{\mathbb{R}^3} c_i c_j f_s^{(0)} d\boldsymbol{v} + \varepsilon\int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v}\right] \\
&= \frac{\partial}{\partial x_j}\big(\rho u_i u_j\big) + \frac{\partial}{\partial x_j}\big(nT\big) + \varepsilon\frac{\partial P_{ij}^{(1)}}{\partial x_j}\,,
\end{aligned}$$

where we used that $\underline{\boldsymbol{P}} = nT\underline{\boldsymbol{I}} + \underline{\boldsymbol{\Pi}}$ and that at collisional equilibrium the viscous stress tensor $\underline{\boldsymbol{\Pi}}$ vanishes. Writing in vector form what we have just derived becomes

$$\nabla_{\boldsymbol{x}}\cdot\big(\rho\boldsymbol{u}\otimes\boldsymbol{u}\big) + \nabla_{\boldsymbol{x}}\big(nT\big) + \varepsilon\nabla_{\boldsymbol{x}}\cdot\underline{\boldsymbol{P}}^{(1)}\,.$$

Ultimately, we consider as a test function $\frac{1}{2}m_s v^2$.

We first focus on the term related to $f_s^{(0)}$, subsequently to the one related to $f_s^{(1)}$.

$$\begin{aligned}
&\sum_{s=1}^{N}\int_{\mathbb{R}^3}\frac{1}{2}m_s v^2\frac{\partial f_s^{(0)}}{\partial t}d\boldsymbol{v} + \sum_{s=1}^{N}\int_{\mathbb{R}^3}\frac{1}{2}m_s v^2\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s^{(0)} d\boldsymbol{v} \\
&= \frac{\partial}{\partial t}\sum_{s=1}^{N}\int_{\mathbb{R}^3}\frac{1}{2}m_s\big(u^2+2\boldsymbol{u}\cdot\boldsymbol{c}+c^2\big)f_s^{(0)}d\boldsymbol{v} + \frac{\partial}{\partial x_j}\sum_{s=1}^{N}\int_{\mathbb{R}^3}\frac{1}{2}m_s v^2\big(u_j+c_j\big)f_s^{(0)}d\boldsymbol{v} \\
&= \frac{\partial}{\partial t}\left[\frac{1}{2}u^2\sum_{s=1}^{N} m_s n_s + \frac{3}{2}nT\right] + \frac{\partial}{\partial x_j}\left[u_j\left(\frac{1}{2}\rho u^2+\frac{3}{2}nT\right)\right] \\
&+ \frac{\partial}{\partial x_j}\sum_{s=1}^{N}\int_{\mathbb{R}^3} c_j\frac{1}{2}m_s\big(u^2+2\boldsymbol{u}\cdot\boldsymbol{c}+c^2\big)f_s^{(0)}d\boldsymbol{v} \\
&= \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2+\frac{3}{2}nT\right) + \frac{\partial}{\partial x_j}\left[u_j\left(\frac{1}{2}\rho u^2+\frac{3}{2}nT\right)\right] \\
&+ \frac{\partial}{\partial x_j}\sum_{s=1}^{N} m_s\int_{\mathbb{R}^3} c_j\boldsymbol{u}\cdot\boldsymbol{c} f_s^{(0)}d\boldsymbol{v} + \frac{\partial}{\partial x_j}\sum_{s=1}^{N}\frac{1}{2}m_s\int_{\mathbb{R}^3} c_j c^2 f_s^{(0)}d\boldsymbol{v}\,.
\end{aligned}$$

The third addend is related to the pressure tensor $\underline{\boldsymbol{P}}$, which at the collisional equilibrium reduces to the purely hydrostatic part $nT\underline{\boldsymbol{I}}$; the fourth addend is related to the heat flux vector $\boldsymbol{q}$, which vanishes at the collisional equilibrium. Therefore we find

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2 + \frac{3}{2}nT\right) + \frac{\partial}{\partial x_j}\left[\left(\frac{1}{2}\rho u^2 + \frac{5}{2}nT\right)u_j\right],$$

that, in vector form, provides

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2 + \frac{3}{2}nT\right) + \nabla_{\boldsymbol{x}}\cdot\left[\left(\frac{1}{2}\rho u^2 + \frac{5}{2}nT\right)\boldsymbol{u}\right].$$

As regards the term related to $f_s^{(1)}$, we go through an analogous computation

$$\begin{aligned}
&\sum_{s=1}^{N}\frac{1}{2}m_s\int_{\mathbb{R}^3} v^2\frac{\partial f_s^{(1)}}{\partial t}d\boldsymbol{v} + \frac{\partial}{\partial x_j}\Bigg[\sum_{s=1}^{N}\frac{1}{2}m_s u^2\int_{\mathbb{R}^3} f_s^{(1)}d\boldsymbol{v} + \frac{3}{2}\underbrace{\sum_{s=1}^{N} n_s T_s^{(1)}}_{=0}\Bigg]\\
&+\frac{\partial}{\partial x_j}\sum_{s=1}^{N}\int_{\mathbb{R}^3} c_j\frac{1}{2}m_s\big(u^2 + 2\boldsymbol{c}\cdot\boldsymbol{u} + c^2\big)f_s^{(1)}d\boldsymbol{v}\\
&=\frac{\partial}{\partial t}\sum_{s=1}^{N}\frac{1}{2}m_s u^2\underbrace{\int_{\mathbb{R}^3} f_s^{(1)}d\boldsymbol{v}}_{=n_s^{(1)}=0} + \frac{\partial}{\partial t}\sum_{s=1}^{N}\frac{1}{2}m_s\int_{\mathbb{R}^3} c^2 f_s^{(1)}d\boldsymbol{v}\\
&+\frac{\partial}{\partial x_j}u_i\sum\frac{1}{2}m_s\int_{\mathbb{R}^3} c_i c_j f_s^{(1)}d\boldsymbol{v} + \frac{\partial}{\partial x_j}\sum_{s=1}^{N}\int_{\mathbb{R}^3} c_j\frac{1}{2}m_s c^2 f_s^{(1)}d\boldsymbol{v}\\
&=\frac{1}{2}\frac{\partial}{\partial t}\underbrace{\sum_{s=1}^{N} n_s T_s^{(1)}}_{=0} + \frac{\partial}{\partial x_j}\big[P_{ij}^{(1)}u_i + q_j^{(1)}\big] = \nabla_{\boldsymbol{x}}\cdot(\underline{\boldsymbol{P}}^{(1)}\cdot\boldsymbol{u} + \boldsymbol{q}^{(1)}),
\end{aligned}$$

where we used the compatibility constraint.
Recalling the Knudsen number ε multiplying the term related to $f_s^{(1)}$, we can produce the last macroscopic conservation equation

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho u^2 + \frac{3}{2}nT\right] + \nabla_{\boldsymbol{x}}\cdot\left[\left(\frac{1}{2}\rho u^2 + \frac{5}{2}nT\right)\boldsymbol{u}\right] + \varepsilon\nabla_{\boldsymbol{x}}\cdot\big(\underline{\boldsymbol{P}}^{(1)}\cdot\boldsymbol{u} + \boldsymbol{q}^{(1)}\big) = 0.$$

The system of macroscopic conservation equations, with first-order corrections, gives rise to the structure of the **Navier–Stokes hydrodynamic equations**

$$\begin{cases}
\dfrac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}}\cdot(n_s\boldsymbol{u}) + \varepsilon\nabla_{\boldsymbol{x}}\cdot(n_s\boldsymbol{u}_s^{(1)}) = 0\\[2ex]
\dfrac{\partial}{\partial t}\big(\rho\boldsymbol{u}\big) + \nabla_{\boldsymbol{x}}\cdot\big(\rho\boldsymbol{u}\otimes\boldsymbol{u}\big) + \nabla_{\boldsymbol{x}}\big(nT\big) + \varepsilon\nabla_{\boldsymbol{x}}\cdot\underline{\boldsymbol{P}}^{(1)} = \boldsymbol{0}\\[2ex]
\dfrac{\partial}{\partial t}\left[\dfrac{1}{2}\rho u^2 + \dfrac{3}{2}nT\right] + \nabla_{\boldsymbol{x}}\cdot\left[\left(\dfrac{1}{2}\rho u^2 + \dfrac{5}{2}nT\right)\boldsymbol{u}\right] + \varepsilon\nabla_{\boldsymbol{x}}\cdot\big(\underline{\boldsymbol{P}}^{(1)}\cdot\boldsymbol{u} + \boldsymbol{q}^{(1)}\big) = 0\,,
\end{cases} \tag{3.15}$$

which involves $4N + 9$ unknowns.
These are

- the N species densities n_s;
- the 3 components of the macroscopic velocity of the mixture $\boldsymbol{u}$;
- the temperature of the mixture T;
- the $3N - 3$ independent components of the diffusion velocities $\boldsymbol{u}_s^{(1)}$, first order corrections of the species velocities, representative for the deviation with respect to the mean velocity $\boldsymbol{u}$;
- the 5 independent components of the first order corrections of the symmetric and traceless viscous stress tensor $\underline{\boldsymbol{\Pi}}$;
- the 3 components of the first order corrections of the heat flux vector $\boldsymbol{q}$.

We designate the first $N + 4$ unknowns $n_s, \boldsymbol{u}$ and T as **main unknowns** (since they correspond to the collision invariants of the whole dominant collision operator), and the remaining $3N + 5$ **secondary unknowns**.

The Chapman–Enskog asymptotic expansion aims to derive constitutive equations for the secondary unknowns, allowing the fields beyond the primary ones to be explicitly expressed and the macroscopic conservation equations to be closed, leading to the Navier–Stokes equations—a closed system of partial differential equations approximating the dynamics near equilibrium. This approach inevitably introduces approximations to the exact conservation laws, as the constitutive relations are obtained from truncated expansions of the distribution functions and, consequently, from the mixed Boltzmann-BGK equations at subsequent orders of approximation.

3.2 Euler equations

The simplest closure of the system described above is obtained by truncating at zeroth order, approximating the distribution functions by their equilibrium forms. This is equivalent to setting

$$\begin{cases} \boldsymbol{u}_s = \boldsymbol{u} \\ \underline{\boldsymbol{\Pi}} = \underline{\boldsymbol{0}} \\ \boldsymbol{q} = \boldsymbol{0}\,. \end{cases} \tag{3.16}$$

Although these constitutive relations are very simple, they provide a reasonable approximation in situations close to equilibrium. By closing the macroscopic equations using the Maxwellian equilibrium, one obtains the Euler hydrodynamic equations:

$$\begin{cases} \dfrac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}) = 0 \\ \dfrac{\partial}{\partial t}(\rho \boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla_{\boldsymbol{x}}(nT) = \boldsymbol{0} \\ \dfrac{\partial}{\partial t}\left[\dfrac{1}{2}\rho u^2 + \dfrac{3}{2} nT\right] + \nabla_{\boldsymbol{x}} \cdot \left[\left(\dfrac{1}{2}\rho u^2 + \dfrac{5}{2} nT\right) \boldsymbol{u}\right] = 0\,. \end{cases} \tag{3.17}$$

Equivalently, the same result can be obtained by setting $\varepsilon = 0$ in the Navier–Stokes system (3.15), thereby recovering a closed set of partial differential equations describing the dynamics near equilibrium.

3.3 Navier-Stokes equations

In order to close the Navier–Stokes system (3.15), one needs to specify the constitutive relations for the first-order corrections, namely the secondary fields. Terms $O(1)$ in expanded equation (3.3) yield

$$\begin{aligned} &\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} \\ &= \sum_{r=1}^{N} \Big\{ \chi_{sr} \big[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)}) \big] + (1-\chi_{sr}) \nu_{sr}^{(0)} \big(\mathcal{M}_{sr}^{(1)} - f_s^{(1)} \big) \Big\} \\ &\iff \sum_{r=1}^{N} (1-\chi_{sr}) \nu_{sr}^{(0)} f_s^{(1)} = -\frac{\partial f_s^{(0)}}{\partial t} - \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} \\ &+ \sum_{r=1}^{N} \Big\{ \chi_{sr} \Big[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)}) \Big] + (1-\chi_{sr}) \nu_{sr}^{(0)} \mathcal{M}_{sr}^{(1)} \Big\}\,. \end{aligned} \tag{3.18}$$

Now, the first-order term of the attractor $\mathcal{M}_{sr}^{(1)}$ corresponds to the coefficient of the linear term in the Taylor expansion of the attractor with respect to the expansion parameter ε, that is

$$\mathcal{M}_{sr}^{(1)} = \frac{\partial}{\partial \varepsilon} \mathcal{M}\left(\boldsymbol{v}; n_s, \boldsymbol{u} + \varepsilon \boldsymbol{u}_{sr}^{(1)}, \frac{T + \varepsilon T_{sr}^{(1)}}{m_s} \right)\Bigg|_{\varepsilon=0}, \tag{3.19}$$

where

$$\begin{aligned} &\mathcal{M}\left(\boldsymbol{v}; n_s, \boldsymbol{u} + \varepsilon \boldsymbol{u}_{sr}^{(1)}, \frac{T + \varepsilon T_{sr}^{(1)}}{m_s} \right) \\ &= n_s \left(\frac{m_s}{2\pi} \right)^{\frac{3}{2}} \big(T + \varepsilon T_{sr}^{(1)} \big)^{-\frac{3}{2}} \exp\left[-\frac{m_s}{2} \big(T + \varepsilon T_{sr}^{(1)} \big)^{-1} \big(\boldsymbol{v} - \boldsymbol{u} - \varepsilon \boldsymbol{u}_{sr}^{(1)} \big)^2 \right]. \end{aligned}$$

Then

$$
\begin{aligned}
\mathcal{M}_{sr}^{(1)} &= -\frac{3}{2} n_s \Big(\frac{m_s}{2\pi T}\Big)^{\frac{3}{2}} \frac{1}{T} T_{sr}^{(1)} \exp\Big[-\frac{m_s}{2T} \big(\boldsymbol{v}-\boldsymbol{u}\big)^2 \Big] \\
&+ \Big(\frac{m_s}{2\pi T}\Big)^{\frac{3}{2}} \exp\Big[-\frac{m_s}{2T} \big(\boldsymbol{v}-\boldsymbol{u}\big)^2 \Big] \Big(\frac{m_s}{2T^2} T_{sr}^{(1)} c^2 + \frac{m_s}{2T} 2\boldsymbol{c}\cdot\boldsymbol{u}_{sr}^{(1)} \Big) \\
\iff \mathcal{M}_{sr}^{(1)} &= f_s^{(0)} \Big[\frac{m_s}{T} \boldsymbol{c}\cdot\boldsymbol{u}_{sr}^{(1)} + \Big(\frac{m_s}{2T} c^2 - \frac{3}{2} \Big) \frac{T_{sr}^{(1)}}{T} \Big] \,.
\end{aligned} \tag{3.20}
$$

Taking advantage of $f_s^{(0)} = \mathcal{M}_s^{eq}$ and of the computations made in [5], we get

$$
\begin{aligned}
&\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_s^{(0)} \\
&= f_s^{(0)} \Big[\frac{1}{n_s} \Big(\frac{\partial n_s}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} n_s \Big) + \frac{m_s \boldsymbol{c}}{T} \cdot \Big(\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} \boldsymbol{u} \Big) \\
&+ \frac{1}{T} \Big(\frac{m_s}{2T} c^2 - \frac{3}{2} \Big) \Big(\frac{\partial T}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} T \Big) \Big] \,.
\end{aligned} \tag{3.21}
$$

To rewrite the terms appearing inside the parentheses in (3.21), we can make use of the macroscopic Euler equations (3.17), since any further approximation introduced would be of second order in the small parameter and is therefore neglected.

First Euler equation provides

$$
\begin{aligned}
&\frac{\partial n_s}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} n_s - \boldsymbol{c}\cdot\nabla_{\boldsymbol{x}} n_s + n_s \nabla_{\boldsymbol{x}}\cdot\boldsymbol{u} = 0 \\
\iff &\frac{\partial n_s}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} n_s = \boldsymbol{c}\cdot\nabla_{\boldsymbol{x}} n_s - n_s \nabla_{\boldsymbol{x}}\cdot\boldsymbol{u} \,.
\end{aligned} \tag{3.22}
$$

The second one results in

$$
\begin{aligned}
&\frac{\partial}{\partial t} \left(\rho u_i\right) + \frac{\partial}{\partial x_j} \left(\rho u_i u_j\right) + \frac{\partial \left(nT\right)}{\partial x_i} \\
&= \rho \frac{\partial u_i}{\partial t} + u_i \frac{\partial \rho}{\partial t} + u_i u_j \frac{\partial \rho}{\partial x_j} + \rho u_i \frac{\partial u_j}{\partial x_j} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial (nT)}{\partial x_i} \\
&= \rho \frac{\partial u_i}{\partial t} + \rho v_j \frac{\partial u_i}{\partial x_j} - \rho c_j \frac{\partial u_i}{\partial x_j} + \frac{\partial (nT)}{\partial x_i} = 0 \\
\iff &\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} \boldsymbol{u} = \boldsymbol{c}\cdot\nabla_{\boldsymbol{x}} \boldsymbol{u} - \frac{1}{\rho} \nabla_{\boldsymbol{x}} \left(nT\right) = 0 \,,
\end{aligned} \tag{3.23}
$$

where we have exploited (3.22).

Finally, the third one yields

$$\frac{\partial}{\partial t}\left[\frac{1}{2}\rho u^2+\frac{3}{2}nT\right]+\nabla_{\boldsymbol{x}}\cdot\left[\left(\frac{1}{2}\rho u^2+\frac{5}{2}nT\right)\boldsymbol{u}\right]=\frac{u^2}{2}\frac{\partial\rho}{\partial t}+\rho\boldsymbol{u}\cdot\frac{\partial\boldsymbol{u}}{\partial t}+\frac{3}{2}n\frac{\partial T}{\partial t}$$

$$+\frac{3}{2}T\frac{\partial n}{dt}+\frac{1}{2}\rho u^2\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\frac{5}{2}nT\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\frac{\boldsymbol{u}}{2}\cdot\nabla_{\boldsymbol{x}}\left(\rho u^2\right)+\frac{5}{2}\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}\left(nT\right)$$

$$=\frac{u^2}{2}\frac{\partial\rho}{\partial t}+\rho\boldsymbol{u}\cdot\frac{\partial\boldsymbol{u}}{\partial t}+\frac{3}{2}n\frac{\partial T}{\partial t}+\frac{3}{2}T\frac{\partial n}{\partial t}+\frac{1}{2}\rho u^2\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\frac{5}{2}nT\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\frac{u^2}{2}\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}\rho$$

$$+\rho u^2\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\frac{5}{2}n\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}T+\frac{5}{2}T\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}n=0\,,$$

that, thanks to (3.22) and (3.23), becomes

$$\begin{aligned}
&\frac{3}{2}n\frac{\partial T}{\partial t}-n\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}T-T\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}n+T\nabla_{\boldsymbol{x}}\cdot(n\boldsymbol{u})+n\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}T+\frac{3}{2}n\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}T=0\\
&\iff T\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\frac{3}{2}\boldsymbol{u}\cdot\nabla_{\boldsymbol{x}}T+\frac{3}{2}\frac{\partial T}{\partial t}=0\\
&\iff \frac{\partial T}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}T=\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}T-\frac{2}{3}T\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\,.
\end{aligned}$$

Hence, we have found

$$\begin{cases}
\dfrac{\partial n_s}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}n_s=\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}n_s-n_s\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\\[2ex]
\dfrac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{u}=\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{u}-\dfrac{1}{\rho}\nabla_{\boldsymbol{x}}\left(nT\right)\\[2ex]
\dfrac{\partial T}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}T=\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}T-\dfrac{2}{3}T\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\,,
\end{cases}\tag{3.24}$$

that reformulates (3.21) into

$$\frac{\partial f_s^{(0)}}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}f_s^{(0)}=f_s^{(0)}\left[\frac{1}{n_s}\big(-n_s\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}+\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}n_s\big)\right.\tag{3.25}$$

$$\left.+\frac{m_s}{T}\boldsymbol{c}\cdot\left(\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}\boldsymbol{u}-\frac{1}{\rho}\nabla_{\boldsymbol{x}}\left(nT\right)\right)+\frac{1}{T}\left(\frac{m_s}{2T}c^2-\frac{3}{2}\right)\left(\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}T-\frac{2}{3}T\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\right)\right].$$

Collecting the terms involving the gradients of the species densities, of the velocity of the mixture and of the temperature, we obtain

$$\frac{1}{n_s}\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}n_s-\frac{m_s}{\rho}\boldsymbol{c}\cdot\nabla_{\boldsymbol{x}}n=m_s\boldsymbol{c}\cdot\left(\frac{\nabla_{\boldsymbol{x}}n_s}{m_sn_s}-\frac{\nabla_{\boldsymbol{x}}n}{\rho}\right),$$

$$
\begin{aligned}
&- \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} + \frac{m_s}{T} \boldsymbol{c} \otimes \boldsymbol{c} : \nabla_{\boldsymbol{x}} \boldsymbol{u} - \frac{2}{3} T \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} \left(\frac{m_s}{2T} c^2 - \frac{3}{2} \right) \frac{1}{T} \\
&= -\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} + \frac{m_s}{T} \boldsymbol{c} \otimes \boldsymbol{c} : \nabla_{\boldsymbol{x}} \boldsymbol{u} - \frac{1}{3} \frac{m_s}{T} c^2 \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} + \frac{1}{T} T \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} \\
&= \frac{m_s}{T} \left(\boldsymbol{c} \otimes \boldsymbol{c} - \frac{1}{3} c^2 \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u} \,,
\end{aligned}
$$

and

$$
- \frac{m_s}{T} \frac{n}{\rho} \boldsymbol{c} \cdot \nabla_{\boldsymbol{x}} T + \frac{1}{T} \left(\frac{m_s}{2T} c^2 - \frac{3}{2} \right) \boldsymbol{c} \cdot \nabla_{\boldsymbol{x}} T = \boldsymbol{c} \cdot \frac{\nabla_{\boldsymbol{x}} T}{T} \left(\frac{m_s}{2T} c^2 - \frac{m_s n}{\rho} - \frac{3}{2} \right) .
$$

Thus, (3.21) eventually becomes

$$
\begin{aligned}
&\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} = f_s^{(0)} \Bigg[m_s \boldsymbol{c} \cdot \left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho} \right) \\
&+ \frac{m_s}{T} \left(\boldsymbol{c} \otimes \boldsymbol{c} - \frac{c^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u} + \left(\frac{m_s}{2T} c^2 - \frac{3}{2} - \frac{m_s n}{\rho} \right) \boldsymbol{c} \cdot \frac{\nabla_{\boldsymbol{x}} T}{T} \Bigg] .
\end{aligned}
$$

So, (3.18) yields

$$
\begin{aligned}
\sum_{r=1}^{N} (1 - \chi_{sr}) \nu_{sr}^{(0)} f_s^{(1)} &= -f_s^{(0)} \Bigg[m_s \boldsymbol{c} \cdot \left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho} \right) + \frac{m_s}{T} \left(\boldsymbol{c} \otimes \boldsymbol{c} - \frac{c^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u} \\
&+ \left(\frac{m_s}{2T} c^2 - \frac{3}{2} - \frac{m_s n}{\rho} \right) \boldsymbol{c} \cdot \frac{\nabla_{\boldsymbol{x}} T}{T} \Bigg] \qquad (3.26) \\
&+ \sum_{r=1}^{N} \left\{ \chi_{sr} \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)}) \right] + (1 - \chi_{sr}) \nu_{sr}^{(0)} \mathcal{M}_{sr}^{(1)} \right\} .
\end{aligned}
$$

Using (3.20), we obtain the ultimate implicit expression of $f_s^{(1)}$

$$
\begin{aligned}
\sum_{r=1}^{N} (1 - \chi_{sr}) \nu_{sr}^{(0)} f_s^{(1)} &= -f_s^{(0)} \Bigg[m_s \boldsymbol{c} \cdot \left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho} \right) + \frac{m_s}{T} \left(\boldsymbol{c} \otimes \boldsymbol{c} - \frac{c^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u} \\
&+ \left(\frac{m_s}{2T} c^2 - \frac{3}{2} - \frac{m_s n}{\rho} \right) \boldsymbol{c} \cdot \frac{\nabla_{\boldsymbol{x}} T}{T} \Bigg] + \sum_{r=1}^{N} \chi_{sr} \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)}) \right] \qquad (3.27) \\
&+ f_s^{(0)} \left[\frac{m_s}{T} \boldsymbol{c} \cdot \sum_{r=1}^{N} (1 - \chi_{sr}) \nu_{sr}^{(0)} \boldsymbol{u}_{sr}^{(1)} + \left(\frac{m_s}{2T} c^2 - \frac{3}{2} \right) \frac{1}{T} \sum_{r=1}^{N} (1 - \chi_{sr}) \nu_{sr}^{(0)} T_{sr}^{(1)} \right] .
\end{aligned}
$$

In order to find the closure of the Navier-Stokes equations (3.15), we need to provide the secondary unknowns $\boldsymbol{u}_s^{(1)}$, $\underline{\boldsymbol{P}}^{(1)}$ and $\boldsymbol{q}^{(1)}$ and make sure that we either obtain an explicit expression for them or at least prove that such expression always exist and may be numerically computed when we know the parameters (initial values and collision frequencies) of the mixture under investigation.

Remark. *Throughout the following computations we will repeatedly use the identities*

$$\int_{\mathbb{R}^3} c_\ell^2 \, f_s^{(0)}(\boldsymbol{v}) \, d\boldsymbol{v} = \int_{\mathbb{R}^3} c_\ell v_\ell \, f_s^{(0)}(\boldsymbol{v}) \, d\boldsymbol{v} = \frac{n_s T}{m_s}, \qquad \forall \; \ell \in \{i, j, k\}, \tag{3.28}$$

which can be obtained from standard Gaussian-moment calculations.
Moreover, any integral of the form

$$\int_{\mathbb{R}^3} c_i^{\beta_i} c_j^{\beta_j} c_k^{\beta_k} \, f_s^{(0)}(\boldsymbol{v}) \, d\boldsymbol{v} = 0 \,, \tag{3.29}$$

if at least one among $\beta_i, \beta_j, \beta_k$ is a positive odd integer. In fact, the integral in (3.29) *vanishes by symmetry, due to the oddness and isotropy of the integrand. For the same reasons, it also holds*

$$\int_{\mathbb{R}^3} c_\ell v_m f_s^{(0)}(\boldsymbol{v}) d\boldsymbol{v} = 0 \,, \quad \forall \ell \neq m, \;\; \ell, m \in \{i, j, k\} \,. \tag{3.30}$$

We begin with the first-order approximation of the species velocities $\boldsymbol{u}_s^{(1)}$, exploiting

$$u_i^{s^{(1)}} = \frac{1}{n_s} \int_{\mathbb{R}^3} v_i f_s^{(1)} d\boldsymbol{v} \,.$$

Making use of the linearity of the integral, we derive the contribution of single addends on the right hand side of (3.27). So, the first, using (3.28) and (3.30), provides

$$\begin{aligned}
&\frac{m_s}{n_s} \sum_{\ell = i.j,k} \left(\frac{\partial n_s}{\partial x_\ell} \frac{1}{\rho_s} - \frac{\partial n}{\partial x_\ell} \frac{1}{\rho} \right) \int_{\mathbb{R}^3} c_l v_i f_s^{(0)} d\boldsymbol{v} \\
&= \frac{m_s}{n_s} \left(\frac{\partial n_s}{\partial x_i} \frac{1}{\rho_s} - \frac{\partial n}{\partial x_i} \frac{1}{\rho} \right) \int_{\mathbb{R}^3} c_i v_i f_s^{(0)} d\boldsymbol{v} \\
&= \left(\frac{\partial n_s}{\partial x_i} \frac{1}{\rho_s} - \frac{\partial n}{\partial x_i} \frac{1}{\rho} \right) T \,.
\end{aligned} \tag{3.31}$$

The second addend provides

$$\begin{aligned}
&\frac{m_s}{n_s T} \sum_{\ell,m=i,j,k} \frac{\partial u_\ell}{\partial x_m} \int_{\mathbb{R}^3} \left(c_\ell c_m - \frac{c^2}{3}\delta_{\ell m} \right) v_i f_s^{(0)} d\boldsymbol{v} \\
&= \frac{m_s}{n_s T} u_i \sum_{\ell,m=i,j,k} \frac{\partial u_\ell}{\partial x_m} \int_{\mathbb{R}^3} \left(c_\ell c_m - \frac{c^2}{3}\delta_{lm} \right) f_s^{(0)} d\boldsymbol{v} \qquad (3.32) \\
&= \frac{m_s}{n_s T} u_i \sum_{\ell=i,j,k} \frac{\partial u_\ell}{\partial x_\ell} \int_{\mathbb{R}^3} \left(c_\ell^2 - \frac{c^2}{3} \right) f_s^{(0)} d\boldsymbol{v} = 0 \,.
\end{aligned}$$

Now, the third addend yields

$$\begin{aligned}
&-\frac{1}{n_s T} \sum_{\ell=i.j,k} \frac{\partial T}{\partial x_\ell} \int_{\mathbb{R}^3} c_\ell \left[\frac{m_s}{2T}\left(c_i^2 + c_j^2 + c_k^2\right) - \frac{3}{2} - \frac{m_s n}{\rho} \right] v_i f_s^{(0)} d\boldsymbol{v} \\
&= -\frac{1}{n_s T} \frac{\partial T}{\partial x_i} \int_{\mathbb{R}^3} \left[\frac{m_s}{2T}\left(c_i^4 + c_i^2 c_j^2 + c_i^2 c_k^2\right) - \left(\frac{3}{2} + \frac{m_s n}{\rho} \right) c_i^2 \right] f_s^{(0)} d\boldsymbol{v} \,,
\end{aligned}$$

where we used (3.29).
Than, recalling the Gaussian integrals reported in Appendix B, in formulas (B.2) and (B.3), we obtain

$$= -\frac{1}{T}\left(\frac{5T}{2m_s} - \frac{3T}{2m_s} - \frac{nT}{\rho} \right) \frac{\partial T}{\partial x_i} = -\left(\frac{1}{m_s} - \frac{n}{\rho} \right) \frac{\partial T}{\partial x_i} \,. \qquad (3.33)$$

The fourth addend is related to the Boltzmann collisional operator Q_{sr} and Q_{rs}, we have to make its contribution explicit by computing

$$\int_{\mathbb{R}^3} v_i [Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)})] d\boldsymbol{v} \,. \qquad (3.34)$$

Remark. *Since this contribution cannot be made explicit for a generic interaction potential, consistently with the standard Maxwellian molecules assumption* $g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) = g_{sr}(\mu)$, *so that*

$$g_{sr}^{(1)} = 2\pi \int_{-1}^{1} (1-\mu) g_{sr}(\mu) d\mu = \Lambda_{sr} \,, \qquad (3.35)$$

we adopt the following choice

$$g_{sr}(|\boldsymbol{y}|, \mu) = \lambda_{sr} = const \,, \qquad (3.36)$$

that leads to

$$\Lambda_{sr} = 4\pi \lambda_{sr} \,.$$

When $s = r$, *we will denote*

$$\Lambda_{ss} := \Lambda_s \,, \quad \lambda_{ss} := \lambda_s \,.$$

Remark. *Under assumption* (3.36), *constants coefficients* a_{sr}, b_{sr} *and* γ_{sr} *depend on the Knudsen number* ε *only through collision frequencies* ν_{sr} *and their expression can be simplified into*

$$\begin{cases} a_{sr}^{(0)} &= 4\pi \dfrac{\alpha_{rs}\lambda_{sr}n_r}{\nu_{sr}^{(0)}} \\ b_{sr}^{(0)} &= 2\alpha_{sr}a_{sr}^{(0)} \\ \gamma_{sr}^{(0)} &= \dfrac{1}{3}m_s a_{sr}^{(0)}\left(2\alpha_{rs} - a_{sr}^{(0)}\right) \\ a_{sr}^{(1)} &= -\dfrac{\nu_{sr}^{(0)}}{\nu_{sr}^{(1)}}a_{sr}^{(0)} \\ b_{sr}^{(1)} &= -\dfrac{\nu_{sr}^{(0)}}{\nu_{sr}^{(1)}}b_{sr}^{(0)} \\ \gamma_{sr}^{(1)} &= -\dfrac{\nu_{sr}^{(0)}}{\nu_{sr}^{(1)}}\left(\gamma_{sr}^{(0)} - \dfrac{1}{3}m_s(a_{sr}^{(0)})^2\right) . \end{cases} \tag{3.37}$$

Now, (3.34) leads to

$$\begin{aligned} &\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i \underbrace{g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)}_{=\lambda_{sr}} \Big[f_s^{(0)}(\boldsymbol{v}'_{sr})f_r^{(1)}(\boldsymbol{w}'_{sr}) + f_s^{(1)}(\boldsymbol{v}'_{sr})f_r^{(0)}(\boldsymbol{w}'_{sr}) \\ &- f_s^{(0)}(\boldsymbol{v}) \underbrace{f_r^{(1)}(\boldsymbol{w})}_{=n_r^{(1)}=0} - \underbrace{f_s^{(1)}(\boldsymbol{v})}_{n_s u_i^{s^{(1)}}} \underbrace{f_r^{(0)}(\boldsymbol{w})}_{n_r} \Big] d\boldsymbol{v}d\boldsymbol{w}d\omega \qquad (3.38) \\ &= \lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i \left[f_s^{(0)}(\boldsymbol{v}'_{sr})f_r^{(1)}(\boldsymbol{w}'_{sr}) + f_s^{(1)}(\boldsymbol{v}'_{sr})f_r^{(0)}(\boldsymbol{w}'_{sr})\right] d\boldsymbol{v}d\boldsymbol{w}d\omega - 4\pi\lambda_{sr}n_s n_r u_i^{s^{(1)}} \end{aligned}$$

Recalling $\boldsymbol{v}'_{sr} = \alpha_{sr}\boldsymbol{v} + \alpha_{rs}\boldsymbol{w} + \alpha_{rs}g\omega'$ and by exchanging pre- and post-collisional velocities, we obtain

$$\begin{aligned} &\lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} (\alpha_{sr}v_i + \alpha_{rs}w_i + \alpha_{rs}g\omega'_i)\left[f_s^{(0)}(\boldsymbol{v})f_r^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v})f_r^{(0)}(\boldsymbol{w})\right] d\boldsymbol{v}d\boldsymbol{w}d\omega \\ &- 4\pi\lambda_{sr}n_s n_r u_i^{s^{(1)}} \qquad (3.39) \\ &= 4\pi\lambda_{sr}\left[\alpha_{sr}n_r\int_{\mathbb{R}^3} v_i f_s^{(1)} d\boldsymbol{v} + \alpha_{rs}n_s\int_{\mathbb{R}^3} w_i f_r^{(1)} d\boldsymbol{w} - n_s n_r u_i^{s^{(1)}}\right] \\ &= 4\pi\lambda_{sr}n_s n_r\left[(\alpha_{sr}-1)u_i^{s^{(1)}} + \alpha_{rs}u_i^{r^{(1)}}\right] = 4\pi\lambda_{sr}n_s n_r\alpha_{rs}\left(u_i^{r^{(1)}} - u_i^{s^{(1)}}\right) . \qquad (3.40) \end{aligned}$$

Hence, the fourth addend provides

$$4\pi\sum_{r=1}^{N}\chi_{sr}\lambda_{sr}\alpha_{rs}n_r(u_i^{r^{(1)}} - u_i^{s^{(1)}}) , \tag{3.41}$$

which we can see it vanishes when $s = r$, consistently with the fact that $\boldsymbol{v}$ belongs to the kernel of the linearized Boltzmann operator in the intra-species case.
We now focus of the fifth addend of the right-hand side of (3.27), which, thanks to (3.28), yields

$$\frac{m_s}{n_s T}\sum_{r=1}^{N}\nu_{sr}^{(0)}\int_{\mathbb{R}^3}\left(u_i^{sr^{(1)}}c_i + u_j^{sr^{(1)}}c_j + u_k^{sr^{(1)}}c_k\right)v_i f_s^{(1)} d\boldsymbol{v} = \sum_{\substack{r=1,\\ r\neq s}}^{N}\nu_{sr}^{(0)}u_i^{sr^{(1)}}\,. \tag{3.42}$$

Ultimately, from the sixth addend, we obtain

$$\begin{aligned}
&\frac{1}{n_s T}\sum_{\substack{r=1,\\ r\neq s}}^{N}\nu_{sr}^{(0)}T_{sr}^{(1)}\int_{\mathbb{R}^3}\left(\frac{m_s}{2T}c^2-\frac{3}{2}\right)v_i f_s^{(0)} d\boldsymbol{v}\\
&=\frac{1}{n_s T}\sum_{\substack{r=1,\\ r\neq s}}^{N}\nu_{sr}^{(0)}T_{sr}^{(1)}\left(\frac{m_s}{2T}\underbrace{\int_{\mathbb{R}^3}c_i c^2 f_s^{(0)} d\boldsymbol{v}}_{=0}+\frac{m_s}{2T}u_i\int_{\mathbb{R}^3}c^2 f_s^{(0)} d\boldsymbol{v}-\frac{3}{2}n_s u_i\right)\\
&=\frac{1}{n_s T}\sum_{r=1}^{N}\nu_{sr}^{(0)}T_{sr}^{(1)}\left(\frac{3}{2T}n_s u_i T-\frac{3}{2}n_s u_i\right)=0\,.
\end{aligned}$$

Collecting (3.31), (3.33), (3.40) and (3.42), and recasting it in vector notation, we get

$$\begin{aligned}
&\sum_{r=1}^{N}(1-\chi_{sr})\nu_{sr}^{(0)}\boldsymbol{u}_s^{(1)} = -\left[T\left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s}-\frac{\nabla_{\boldsymbol{x}} n}{\rho}\right)+\left(\frac{1}{m_s}-\frac{n}{\rho}\right)\nabla_{\boldsymbol{x}} T\right]\\
&+\sum_{r=1}^{N}\left[\nu_{sr}^{(0)}(1-\chi_{sr})\boldsymbol{u}_{sr}^{(1)}+4\pi\chi_{sr}\lambda_{sr}\alpha_{rs}n_r(\boldsymbol{u}_r^{(1)}-\boldsymbol{u}_s^{(1)})\right]\,,
\end{aligned}$$

and, from $\boldsymbol{u}_{sr}^{(1)} = \boldsymbol{u}_s^{(1)} + a_{sr}^{(0)}(\boldsymbol{u}_r^{(1)} - \boldsymbol{u}_s^{(1)})$ and rearranging the terms involving the gradients of the densities and the temperatures, we obtain

$$\begin{aligned}
&\sum_{r=1}^{N}\left[(1-\chi_{sr})\nu_{sr}^{(0)}a_{sr}^{(0)}+4\pi\chi_{sr}\lambda_{sr}\alpha_{rs}n_r\right](\boldsymbol{u}_s^{(1)}-\boldsymbol{u}_r^{(1)})\\
&=-\frac{\nabla_{\boldsymbol{x}}(n_s T)}{\rho_s}+\frac{\nabla_{\boldsymbol{x}}(nT)}{\rho}\,.
\end{aligned} \tag{3.43}$$

Now, recalling the expression of $a_{sr}^{(0)}$ from (3.37), multiplying both sides for $m_s n_s$ and noticing that s-th term of the sum vanishes, we obtain

$$4\pi\sum_{\substack{r=1,\\ r\neq s}}^{N}\lambda_{sr}\mu_{sr}n_s n_r(\boldsymbol{u}_s^{(1)}-\boldsymbol{u}_r^{(1)}) = -\nabla_{\boldsymbol{x}}(n_s T)+\frac{\rho_s}{\rho}\nabla_{\boldsymbol{x}}(nT)\,, \tag{3.44}$$

which is a linear system for the unknowns $\boldsymbol{u}_s^{(1)}$.

Remark. *We notice that the linear system that provides the first order approximation of the diffusion velocities does not depend on the coefficients χ_{sr}. Therefore, any choice of the Boltzmann or BGK operators will reproduce the same results.*

By summing on s the N equations of system (3.43), thanks to $n = \sum_{s=1}^N n_s$ and $\rho = \sum_{s=1}^N \rho_s$, we have both sides vanishing, which implies that the solution is not unique. By restricting to the first $N-1$ rows and columns of the coefficient matrix, we obtain the following coefficient sub-matrix,

$$A_{ss} = 4\pi \sum_{\substack{r=1,\\ r\neq s}}^{N} \lambda_{sr}\mu_{sr} n_s n_r \,, \tag{3.45}$$

$$A_{sr} = -4\pi \lambda_{sr}\mu_{sr} n_s n_r \,, \quad s \neq r \,, \quad s, r = 1, \dots, N-1 \,.$$

Since any strictly diagonal dominant $M \times M$ matrix A, namely that fulfills

$$|A_{ss}| > \sum_{\substack{r=1,\\ r\neq s}}^{M} |A_{sr}| \,, \quad \forall s = 1, \dots, M, \tag{3.46}$$

is non-singular, and we notice that conditions (3.46) is satisfied by the $(N-1) \times (N-1)$ sub-matrix considered in (3.45), since

$$\sum_{\substack{r=1,\\ r\neq s}}^{N} \lambda_{sr}\mu_{sr} n_s n_r > \sum_{\substack{r=1\\ r\neq s}}^{N-1} \lambda_{sr}\mu_{sr} n_s n_r \,,$$

then the $N-1$ equations are independent and there exists ∞^1 solutions at most. The additional condition that ensures the uniqueness of the solution is provided by the compatibility constraint

$$\sum_{s=1}^{N} \rho_s \boldsymbol{u}_s^{(1)} = \mathbf{0} \,,$$

which follows from the requirement that the global velocity is unexpanded.
It can be shown as in [9], that (3.43) along with the compatibility constraint, leads to

$$\boldsymbol{u}_s^{(1)} = \nabla_{\mathbf{x}} n_s \sum_{r=1}^{N} \mathcal{F}_{sr} + \alpha_s \nabla_{\mathbf{x}} T \;\; , \quad \text{for } \; s = 1, \dots, N,$$

where $\mathcal{F}_{sr}$ denote the entries of the Fick matrix and α_s the Soret coefficients.

Remark. *Unlike the BGK mixture model [9], in the case of the mixed model, due to the difficulty of making explicit the inverse of the linearized operator, it is not possible to obtain a closed-form expression for the first-order correction of the distribution function* (3.27)*. Due to this and to the large number of variables and terms in the systems we will derive, obtaining a closed-form expression of* $\underline{\boldsymbol{P}}^{(1)}$ *and* $\boldsymbol{q}^{(1)}$ *is impractical.*
What we will derive are two linear systems in which the unknowns will be, respectively,

$$m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}\,, \quad m_s \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}\,,$$

and, in order to prove the invertibility of the coefficient matrixes, we will demonstrate their diagonal dominance.
On the other hand, in real mixtures the number of species N is typically not very large, and the variables involved reduce to strictly positive real numbers. In such cases, the coefficient matrix can be inverted straightforwardly using standard mathematical software.

Remark. *Due to the length of the computations related to the first-order approximation of the pressure tensor and the heat flux vector, in order to preserve the flow of the reading, we have decided to place most of them in Appendix C and to focus in the main body on the theoretical aspects of the procedure.*

We now turn our attention to the global pressure tensor $\underline{\boldsymbol{P}}^{(1)}$, defined as

$$\underline{\boldsymbol{P}}^{(1)} = \sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} \boldsymbol{c} \otimes \boldsymbol{c} f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}\,,$$

and, by the explicit expression of $f_s^{(1)}$ given in (3.27),we multiply the single addends by the test function $\varphi_s = m_s \boldsymbol{c} \otimes \boldsymbol{c}$.
The computations corresponding to the first, second, third, fifth, and sixth terms are analogous to those carried out for $\boldsymbol{u}_s^{(1)}$, and their contribution is also made explicit in [9]. Therefore, we focus on the fourth addend, the one involving the intra- and inter-species Boltzmann collisional operator

$$\begin{aligned} & m_s \int_{\mathbb{R}^3} c_i c_j \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)}) \right] d\boldsymbol{v} \\ &= m_s \lambda_{sr} \int_{\mathbb{R}^3} \left(v_i v_j - u_i v_j - u_j v_i + \underbrace{u_i u_j}_{=0} \right) \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)}) \right] d\boldsymbol{v} \end{aligned}$$

where in the round brackets the last addend vanishes due to mass preservation and the second and third addends, taking advantage of (3.40), yield

$$-4\pi \lambda_{sr} n_s n_r \mu_{sr} \left[u_j (u_i^{r^{(1)}} - u_i^{s^{(1)}}) + u_i (u_j^{r^{(1)}} - u_i^{s^{(1)}}) \right] . \tag{3.47}$$

Then, it is left to compute

$$
\begin{aligned}
& m_s\lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i v_j \Bigg[f_s^{(0)}(\boldsymbol{v}'_{sr}) f_r^{(1)}(\boldsymbol{w}'_{sr}) + f_s^{(1)}(\boldsymbol{v}'_{sr}) f_r^{(0)}(\boldsymbol{w}'_{sr}) \\
& - f_s^{(0)}(\boldsymbol{v}) \underbrace{f_r^{(1)}(\boldsymbol{w})}_{=n_r^{(1)}=0} - f_s^{(1)}(\boldsymbol{v}) \underbrace{f_r^{(0)}(\boldsymbol{w})}_{n_r} \Bigg] d\boldsymbol{v}d\boldsymbol{w}d\omega \\
& = m_s\lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_{sr}^{i'} v_{sr}^{j'} \left[f_s^{(0)}(\boldsymbol{v}) f_r^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_r^{(0)}(\boldsymbol{w}) \right] d\boldsymbol{v}d\boldsymbol{w}d\omega \\
& - 4\pi m_s \lambda_{sr} n_r \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v}\,,
\end{aligned} \tag{3.48}
$$

where we have exploited (3.38) and exchanged pre- and post-collision velocities. Now, referring to the Appendix A for the product of post-collision velocities $\int_{\mathbb{S}^2} v_{sr}^{i'} v_{sr}^{j'} d\omega$, (A.9), and the computations for the first integral of (3.48), explicitly carried out in (C.1), (3.48) becomes

$$
\begin{aligned}
& 4\pi\lambda_{sr}\mu_{sr}\Bigg[n_r(-1-\alpha_{sr})\int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + n_s\alpha_{rs}\int_{\mathbb{R}^3} v_i v_j f_r^{(1)} d\boldsymbol{v} \\
& + \alpha_{sr} n_s n_r \left(u_i u_j^{r^{(1)}} + u_j u_i^{s^{(1)}} + u_i u_j^{s^{(1)}} + u_j u_i^{r^{(1)}} \right) + \delta_{ij}\alpha_{rs} n_s n_r \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r} \right) \Bigg],
\end{aligned} \tag{3.49}
$$

where we made use of the derivations (C.1), reported in Appendix C.
We quickly compute

$$
\int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} = \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + n_s \left(u_i u_j^{s^{(1)}} + u_j u_i^{s^{(1)}} \right), \tag{3.50}
$$

and obviously the same for $\int_{\mathbb{R}^3} v_i v_j f_r^{(1)} d\boldsymbol{v}$. Inserting both these in (3.49), it provides

$$
\begin{aligned}
& 4\pi\lambda_{sr}\mu_{sr}\Bigg\{ n_r(-1-\alpha_{sr})\int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + n_s\alpha_{rs}\int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v} \\
& + n_s n_r \left[u_i \left(u_j^{r^{(1)}} - u_j^{s^{(1)}} \right) + u_j \left(u_i^{r^{(1)}} - u_i^{s^{(1)}} \right) \right] + \delta_{ij}\alpha_{rs} n_s n_r \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r} \right) \Bigg\},
\end{aligned}
$$

which, along with (3.47), finally provides

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} c_i c_j \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{sr}(f_s^{(1)}, f_r^{(0)}) \right] d\boldsymbol{v} \\
& = 4\pi \lambda_{sr} \mu_{sr} \left\{ n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + n_s \alpha_{rs} \int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v} \right. \\
& \left. + \delta_{ij} \alpha_{rs} n_s n_r \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r} \right) \right\}. \qquad (3.51)
\end{aligned}
$$

Hence, as previously stated, by analogous computations to the ones carried out for the velocities $\boldsymbol{u}_s^{(1)}$, we obtain

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \sum_{r=1}^N (1-\chi_{sr}) \nu_{sr}^{(0)} = \delta_{ij} n_s T_s^{(1)} \sum_{r=1}^N (1-\chi_{sr}) \nu_{sr}^{(0)} \\
& - n_s T \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} \delta_{ij} \right] + 4\pi \sum_{r=1}^N \chi_{sr} \lambda_{sr} \mu_{sr} \left\{ n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} \right. \\
& \left. + n_s \alpha_{rs} \int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v} + \delta_{ij} \alpha_{rs} n_s n_r \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r} \right) \right\}, \qquad (3.52)
\end{aligned}
$$

which, reformulated, becomes

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \left\{ \sum_{\substack{r=1, \\ r \neq s}}^N \left[(1-\chi_{sr}) \nu_{sr}^{(0)} + 4\pi \chi_{sr} \lambda_{sr} \alpha_{rs} n_r (1+\alpha_{sr}) \right] \right. \qquad (3.53) \\
& \left. + (1-\chi_{ss}) \nu_{ss}^{(0)} + 2\pi \chi_{ss} \lambda_s n_s \right\} - 4\pi \sum_{\substack{r=1, \\ r \neq s}}^N \chi_{sr} \lambda_{sr} \mu_{sr} n_s \alpha_{rs} \int_{\mathbb{R}^3} c_i c_j f_r^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \\
& = \delta_{ij} n_s T_s^{(1)} \sum_{r=1}^N (1-\chi_{sr}) \nu_{sr}^{(0)} - n_s T \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} \delta_{ij} \right] \\
& + 4\pi \delta_{ij} n_s \sum_{r=1}^N \chi_{sr} \lambda_{sr} \mu_{sr} n_r \alpha_{rs} \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r} \right). \qquad (3.54)
\end{aligned}
$$

This leads to an $N \times N$ linear system for the unknowns

$$
m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \,,
$$

whose right-hand side coincides with that of the equation above.
Our next goal is to prove the invertibility of the coefficient matrix by establishing its diagonal dominance. In order to do so, we rescale the unknowns as

$$
\frac{m_s}{n_s} \int_{\mathbb{R}^3} c_i c_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \,, \quad \text{for } s = 1, \dots, N.
$$

Let A denote the coefficient matrix. Its entries read

$$
\begin{aligned}
(A)_{ss} = n_s \Bigg\{ \sum_{\substack{r=1,\\ r\neq s}}^{N} & \left[(1-\chi_{sr})\nu_{sr}^{(0)} + 4\pi\chi_{sr}\lambda_{sr}n_r\alpha_{rs}(1+\alpha_{sr}) \right] \\
& + (1-\chi_{ss})\nu_{ss}^{(0)} + 2\pi\chi_{ss}\lambda_s n_s \Bigg\}, \\
(A)_{sr} = -4\pi\chi_{sr}\lambda_{sr}&\alpha_{sr}\alpha_{rs}n_s n_r\,, \quad \forall s \neq r.
\end{aligned}
$$

We note that

$$
\begin{aligned}
4\pi\chi_{sr}\lambda_{sr}\alpha_{rs}(1+\alpha_{sr})n_s n_r &> 4\pi\chi_{sr}\lambda_{sr}\alpha_{sr}\alpha_{rs}n_s n_r \\
\iff 1+\alpha_{sr} &> \alpha_{sr},
\end{aligned}
$$

which proves that A is strictly diagonally dominant, namely $|A_{ss}| > \sum_{r\neq s}|A_{sr}|$, hence invertible. Consequently, the linear system above always admits a unique solution.

Remark. *For the first-order approximation of the heat flux vector $\boldsymbol{q}^{(1)}$, we adopt the same approach leveraged for the pressure tensor. Hence, for the first, second, third, fifth and sixth addends on the right-hand side of* (3.27)*, we will exploit the computations already made for the first-order approximation of the velocities and made explicit in [9], and we focus on the addend involving the Boltzmann collisional operators $Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)})$.*
Eventually, we will obtain a linear system of unknowns similar to the one derived for $m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v}$ and we will prove its diagonal dominance.

So, from

$$
\boldsymbol{q}^{(1)} = \frac{1}{2}\sum_{s=1}^{N} m_s \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)}(\boldsymbol{v})d\boldsymbol{v}\,,
$$

to provide the fourth addend explicit expression we must compute

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} c_i c^2 \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)}) \right] d\boldsymbol{v} \\
& = m_s \int_{\mathbb{R}^3} v_i v^2 \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)}) \right] d\boldsymbol{v} && (3.55) \\
& + m_s \int_{\mathbb{R}^3} \left[-u_i v^2 + u^2 v_i - 2(u_i v_i^2 + u_j v_i v_j + u_k v_i v_k) + 2u_i \boldsymbol{u}\cdot\boldsymbol{v} \right] && (3.56) \\
& \times \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)}) \right] d\boldsymbol{v}
\end{aligned}
$$

As concerns the contribution given from (3.55) and (3.56), the long computations are similar to the ones carried out for the pressure tensor and they are made explicit in Appendix C, respectively in (C.3) and (C.5). Combining those, we notice that most of the terms vanish and we ultimately obtain

$$\frac{1}{2}m_s \int_{\mathbb{R}^3} c_i c^2 \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)})\right] d\boldsymbol{v} = 2\pi\lambda_{sr}\mu_{sr}$$

$$\times \Bigg\{ -\left(1 + 2\alpha_{sr}^2 - \frac{2}{3}\alpha_{sr}\alpha_{rs}\right) n_r \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} + \frac{8}{3}\alpha_{rs}^2 n_s \int_{\mathbb{R}^3} c_i c^2 f_r^{(1)} d\boldsymbol{v}$$

$$+ 5n_s n_r \left[\left(1 - \frac{8}{3}\alpha_{sr}\alpha_{rs}\right) u_i^{r^{(1)}} \frac{T}{m_s} + 2\alpha_{rs}\left(1 - \frac{4}{3}\alpha_{rs}\right) u_i^{s^{(1)}} \frac{T}{m_r}\right] \Bigg\}. \tag{3.57}$$

Referring once again to [9] for the computation of the leftover addends and coming back to the vector notation, we get

$$\frac{1}{2}m_s \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \sum_{r=1}^{N} (1 - \chi_{sr})\nu_{sr}^{(0)} = 2\pi \sum_{r=1}^{N} \chi_{sr}\lambda_{sr}\mu_{sr}$$

$$\times \Bigg\{ -\left(1 + 2\alpha_{sr}^2 - \frac{2}{3}\alpha_{sr}\alpha_{rs}\right) n_r \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)} d\boldsymbol{v} + \frac{8}{3}\alpha_{rs}^2 n_s \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_r^{(1)} d\boldsymbol{v}$$

$$+ 5n_s n_r \left[\left(1 - \frac{8}{3}\alpha_{sr}\alpha_{rs}\right) \boldsymbol{u}_r^{(1)} \frac{T}{m_s} + 2\alpha_{rs}\left(1 - \frac{4}{3}\alpha_{rs}\right) \boldsymbol{u}_s^{(1)} \frac{T}{m_r}\right] \Bigg\} \tag{3.58}$$

$$+ \frac{5}{2} n_s T \Bigg\{ \sum_{r=1}^{N} (1 - \chi_{sr})\nu_{sr}^{(0)} \boldsymbol{u}_{sr}^{(1)} - T\left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho}\right) - 2\left(\frac{2}{m_s} - \frac{n}{\rho}\right)\nabla_{\boldsymbol{x}} T \Bigg\}.$$

Exploiting the same procedure we used for the pressure tensor, we have reached a linear system for the unknowns

$$\frac{m_s}{n_s} \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)} d\boldsymbol{v}\,,$$

having the following coefficient matrix A

$$(A)_{ss} = n_s \Bigg\{ \sum_{\substack{r=1,\\ r\neq s}}^{N} \left[(1 - \chi_{sr})\nu_{sr}^{(0)} + 4\pi\chi_{sr}\lambda_{sr} n_r \left(1 + 2\alpha_{sr}^2 - \frac{2}{3}\alpha_{sr}\alpha_{rs}\right)\right] \tag{3.59}$$

$$+ (1 - \chi_{ss})\nu_{ss}^{(0)} + \frac{4}{3}\pi\chi_{ss}\lambda_s n_s \Bigg\}, \quad s = 1, \ldots, N; \tag{3.60}$$

$$(A)_{sr} = -4\pi n_s \chi_{sr}\lambda_{sr} \frac{8}{3}\alpha_{sr}\alpha_{rs}^2 n_r\,, \quad \forall\, s \neq r\,;$$

and known terms

$$5n_s T \Bigg\{ 4\pi \sum_{r=1}^{N} \chi_{sr}\lambda_{sr} n_r \left[\left(1 - \frac{8}{3}\alpha_{sr}\alpha_{rs}\right)\alpha_{rs}\boldsymbol{u}_r^{(1)} + 2\alpha_{sr}\alpha_{rs}\left(1 - \frac{4}{3}\alpha_{rs}\right)\boldsymbol{u}_s^{(1)}\right]$$

$$+ \frac{1}{2}\left[\sum_{r=1}^{N} (1 - \chi_{sr})\nu_{sr}^{(0)} \boldsymbol{u}_{sr}^{(1)} - T\left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho}\right) - 2\left(\frac{2}{m_s} - \frac{n}{\rho}\right)\nabla_{\boldsymbol{x}} T\right] \Bigg\}.$$

We easily check that

$$\left(1+2\alpha_{sr}^2-\frac{2}{3}\alpha_{sr}\alpha_{rs}\right)\alpha_{rs} > \frac{8}{3}\alpha_{sr}\alpha_{rs}^2$$
$$\iff 1+2\alpha_{sr}^2 > \frac{10}{3}\alpha_{sr}\alpha_{rs}\,,$$

which holds true since $\alpha_{rs}\alpha_{sr} \leq \frac{1}{4}$.
Altogether, this establishes the invertibility of the coefficient matrix, and therefore the existence and uniqueness of the solution vector. Consequently, it becomes possible to determine the explicit expression of $\boldsymbol{q}^{(1)}$, thereby ultimately closing the Navier–Stokes fluid dynamic equations (3.15).

Remark. *It is worth noting that the present closure at the Navier–Stokes level remains valid for arbitrary intermolecular potentials. The only simplification arising in the case of Maxwell molecules considered here is that the expressions of the diffusion velocities and the heat flux involve constant parameters like* λ_{sr} *or* Λ_{sr}*; in contrast, for other interaction potentials these parameters could depend on the macroscopic fields* $\boldsymbol{u}_s$ *and* T_s*.*

Chapter 4

Navier-Stokes equations in the case of Boltzmann intra-species operators

In this section we introduce in detail the model in which, by setting $\chi_{sr} = \delta_{sr}$, intra–species collisions are governed by a one–species Boltzmann operator, whereas inter–species collisions are described by the binary BGK operators (1.25). The well-posedness of this hybrid model—namely, the fulfillment of conservation laws, the validity of the Boltzmann H-theorem, and the preservation of the correct Maxwellian equilibria—has already been established in Chapter 2.
The adoption of this choice of kinetic operators—taking advantage of the analytical convenience of the Boltzmann-type operators for intra–species collisions and the BGK-type operator for inter–species collisions—enables us to study not only the classical collision-dominated regime, as in the previous chapter, but also the scenario in which intra–species collisions constitute the prevailing mechanism and for both regimes we are able to abtain a close form of $\underline{\boldsymbol{P}}^{(1)}$ and $\boldsymbol{q}^{(1)}$, providing an explicit closure of the Navier-Stokes equations.
The choice of the Boltzmann model for intra–species interactions and a proper BGK model for inter–species ones is also motivated by the fact that in some physical problems particles of the same species exchange energy faster than particles with disparate masses. This occurs for instance in ε-mixtures of heavy and light gases [26] or in astro-physics problems [49], but also some phenomena in plasma physics are studied neglecting inter–species interactions (as the so–called Z–pinch dynamics, meaning anomalous resistivity and plasma sheath formation [40]). Therefore, we consider the following integro–differential equations:

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = Q_s = Q_{ss} + \sum_{r=1}^{N} \nu_{sr}(\mathcal{M}_{sr} - f_s)\,. \tag{4.1}$$

As regards the dimensionless form of the equation (4.1), we take advantage of the computations carried out in Chapter 2 and simply set $\chi_{sr} = \delta_{sr}$ in (2.33), obtaining

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = \frac{\beta_{ss}}{\varepsilon} Q_{ss} + \frac{\beta_{sr}}{\varepsilon} \sum_{\substack{r=1, \\ r \neq s}}^{N} \hat{Q}_{sr} \,, \tag{4.2}$$

which under the assumption of $\chi_{sr} = \delta_{sr}$ will allow us to study either the classical collision dominated regime and the intra-species collision dominated one.

4.1 Classical collision dominated regime

Implementing $\beta_{sr} = 1$ for all $s, r = 1, \dots, N$, in (4.2), we get the collision dominated regime already investigated in previous chapter for the general mixed model:

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s = \frac{1}{\varepsilon} \left(Q_{ss} + \sum_{\substack{r=1, \\ r \neq s}}^{N} \hat{Q}_{sr} \right) . \tag{4.3}$$

We notice that expanding $f_s = f_s^{(0)} + \varepsilon f_s^{(1)}$, at the leading order of (4.3) we have

$$\mathcal{Q}_{ss}(f_s^{(0)}) + \sum_{\substack{r=1, \\ r \neq s}}^{N} \nu_{sr}^{(0)} \left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right) = 0 \,,$$

that by the uniqueness of equilibrium distributions, still implies

$$f_s^{(0)} = \mathcal{M}_s^{eq} \,.$$

The results on the hydrodynamic variables, on the main moments of expanded distributions given (3.10), (3.11) and (3.12) and the related compatibility constraints (3.13), (3.14) still hold.
Before computing the implicit expression of $f_s^{(1)}$, we rewrite the first-order approximation of the distribution function $f_s^{(1)}$ as $f_s^{(1)} = f_s^{(0)} h_s^{(1)}$, where $h_s^{(1)}$ stands for the realtive perturbation, and introduce the linearized intra-species Boltzmann operator $\mathcal{L}(h_s^{(1)})$ defined in [42], given by

$$\mathcal{L}(h_s^{(1)}) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} g_{ss}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) \left[h_s^{(1)}(\boldsymbol{v}'_s) + h_s^{(1)}(\boldsymbol{w}'_s) - h_s^{(1)}(\boldsymbol{v}) - h_s^{(1)}(\boldsymbol{w}) \right] d\boldsymbol{v} d\omega \,,$$

for which it holds

$$\ker \left(f_s^{(0)} \mathcal{L}(h_s^{(1)}) \right) = \mathrm{span}\{1, \boldsymbol{v}, v^2\} \,, \tag{4.4}$$

meaning that it shares the same kernel of the intra-species Boltzmann operator. The linearized Boltzmann intra-species operator allows us to write

$$Q_{ss}(f_s^{(0)}, f_s^{(1)}) + Q_{ss}(f_s^{(1)}, f_s^{(0)}) = f_s^{(0)} \mathcal{L}(h_s^{(1)})\,.$$

Rearranging the terms $O(1)$ in the expanded equation yields

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

where

- $\mathcal{M}_{sr}^{(1)} = \dfrac{\partial}{\partial \boldsymbol{\varepsilon}} \mathcal{M}_{sr} \left(\mathbf{v}; \mathbf{u} + \boldsymbol{\varepsilon}\, u_{sr}^{(1)}, \dfrac{T + \boldsymbol{\varepsilon} T_{sr}^{(1)}}{m_s} \right) \Bigg|_{\boldsymbol{\varepsilon}=0}$
- $\dfrac{\partial f_s^{(0)}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_s^{(0)}$ may be computed owing to Euler equations
- $f_s^{(0)} \mathcal{L}(h_s^{(1)})$ involves the linearized Boltzmann operator defined above, for which we set
$$\mathcal{L}_s := f_s^{(0)} \mathcal{L}(h_s^{(1)})\,.$$

Analogous computations lead to the Navier-Stokes system of equations (3.15) and to the following implicit expression of $f_s^{(1)}$

$$\begin{aligned} f_s^{(1)} = \frac{f_s^{(0)}}{\sum_{r=1}^{N} \nu_{sr}^{(0)}} \Bigg[&- m_s \boldsymbol{c} \cdot \left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} + \frac{\nabla_{\boldsymbol{x}} n}{\rho} \right) + \frac{m_s}{T} \left(\boldsymbol{c} \otimes \boldsymbol{c} - \frac{c^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u} \\ &+ \left(\frac{m_s}{2T} c^2 - \frac{3}{2} - \frac{m_s n}{\rho} \right) \boldsymbol{c} \cdot \frac{\nabla_{\boldsymbol{x}} T}{T} + \mathcal{L}(h_s^{(1)}) + \\ &+ \frac{m_s}{T} \boldsymbol{c} \cdot \sum_{r=1}^{N} (1 - \chi_{sr}) \nu_{sr}^{(0)} \boldsymbol{u}_{sr}^{(1)} + \left(\frac{m_s}{2T} c^2 - \frac{3}{2} \right) \frac{1}{T} \sum_{r=1}^{N} (1 - \chi_{sr}) \nu_{sr}^{(0)} T_{sr}^{(1)} \Bigg]. \end{aligned} \tag{4.5}$$

4.2 Existence of solutions to the linearized problem

In the following section we will derive the Navier–Stokes equations for the classical collision-dominated regime. We believe that it is appropriate to investigate first the analytical properties of the kinetic operators underlying these derivations. In this section we focus on the Boltzmann operator associated with intra-species collisions in its linearized form. We show that this operator is always invertible with finite norm, a property that ensures the consistency of the hydrodynamic equations and provides a solid basis for treating the slow collisional exchanges between different species.

We begin by introducing the linear operator

$$\tilde{\mathcal{L}}_s = Id - \frac{1}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}} \mathcal{L}_s \,,$$

where $\mathcal{L}_s$ is the standard Boltzmann linearized operator

$$\begin{aligned}\mathcal{L}_s &= f_s^{(0)} \mathcal{L}(h_s^{(1)}) \\ &= \int_{\mathbb{R}^3\times\mathbb{S}^2} g_{ss}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega) f_s^{(0)} \left[h_s^{(1)}(\boldsymbol{v}'_s) + h_s^{(1)}(\boldsymbol{w}'_s) - h_s^{(1)}(\boldsymbol{v}) - h_s^{(1)}(\boldsymbol{w}) \right] d\boldsymbol{w} d\omega \,,\end{aligned}$$

with

$$f_s^{(0)}(\boldsymbol{v}) = \mathcal{M}_s^{eq} \,.$$

We consider now the real Hilbert space

$$\aleph_s := L^2(\mathbb{R}^3; \mathcal{M}_s^{eq} d\boldsymbol{v}) \,,$$

with inner product

$$\langle f, g\rangle_{\mathcal{M}_s^{eq}} = \int_{\mathbb{R}^3} f g \, \mathcal{M}_s^{eq} \, d\boldsymbol{v} \,, \quad f, g \in \aleph_s \,.$$

By standard arguments, one can show that $\mathcal{L}_s$ is a non-positive coercive symmetric operator with the set of collision invariants as kernel in $\aleph_s$, i.e.

$$\langle f, \mathcal{L}_s g\rangle_{\mathcal{M}_s^{eq}} = \langle \mathcal{L}_s f, g\rangle_{\mathcal{M}_s^{eq}} \,; \quad \langle g, \mathcal{L}_s g\rangle_{\mathcal{M}_s^{eq}} \leq 0; \quad \mathcal{L}_s = \mathrm{span}\big\{1, \boldsymbol{v}, v^2\big\} \,.$$

Hence, clearly, $\tilde{\mathcal{L}}_s$ is a coercive symmetric operator with a trivial kernel in $\aleph_s$, such that

$$\langle f, \tilde{\mathcal{L}}_s g\rangle_{\mathcal{M}_s^{eq}} = \langle \tilde{\mathcal{L}}_s f, g\rangle_{\mathcal{M}_s^{eq}} \,; \quad \langle g, \tilde{\mathcal{L}}_s g\rangle_{\mathcal{M}_s^{eq}} \geq \langle g, g\rangle_{\mathcal{M}_s^{eq}} \,; \quad \ker \tilde{\mathcal{L}}_s = \{0\} \,.$$

The linearized operator $\mathcal{L}_s$ can be decomposed as

$$\mathcal{L}_s = K_s - \eta_s \,,$$

where η_s is the positive multiplication operator

$$\eta_s g := \theta_s g$$

for the collision frequency

$$\theta_s = \int_{\mathbb{R}^3\times\mathbb{S}^2} g_{ss}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega) f_s^{(0)}(\boldsymbol{w}) d\boldsymbol{w} d\omega \,,$$

while

$$K_s g = \int_{\mathbb{R}^3\times\mathbb{S}^2} g_{ss}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega) f_s^{(0)}(\boldsymbol{w}) \big[g(\boldsymbol{v}'_s) + g(\boldsymbol{w}'_s) - g(\boldsymbol{w}) \big] d\boldsymbol{w} d\omega \,.$$

The linear operator K_s is a compact operator on $\aleph_s$ under, for instance, Grad's assumption on the collision kernel, i.e.

$$g_{ss}(|\boldsymbol{y}|, \hat{\boldsymbol{y}} \cdot \omega) \leq b_s \left(|\boldsymbol{y}| + \frac{1}{|\boldsymbol{y}|^{1-\varepsilon}} \right) ,$$

for some positive constants $b_s > 0$ and $0 < \varepsilon < 1$, acknowledging that Grad's assumption is fulfilled for hard-sphere potentials, as well as, cut-off inverse power-law potentials, including Maxwell molecules.
Assume that the above operator K_s is compact on $\aleph_s$. Then $\mathcal{L}_s$ is a self-adjoint operator with the domain

$$D(\mathcal{L}_s) = \{ f \in \aleph_s \, ; \quad \theta_s f \in \aleph_s \} \, .$$

Furthermore, η_s is, at least under Grad's assumption, a closed, densely defined, and self-adjoint operator and is also Fredholm if and only if η_s is coercive. Hence, $\mathcal{L}_s$ is a Fredholm operator if and only if η_s is coercive; indeed Fredholmness is conserved under addition of compact operators. The multiplication operator η_s is coercive for e.g. hard-sphere potentials, as well as, cut-off hard potentials and Maxwell molecules. On the other hand,

$$\tilde{\mathcal{L}_s} = Id + \eta_s - K_s \, ,$$

hence $\tilde{\mathcal{L}_s}$ is a Fredholm operator, since, clearly, $Id+\eta_s$ is coercive. Then the linear operator $\tilde{\mathcal{L}_s}$ is Fredholm, with a trivial kernel, therefore $\tilde{\mathcal{L}_s}$ is also invertible, with an inverse operator $\tilde{\mathcal{L}_s}^{-1}$, such that

$$\left|\left| \tilde{\mathcal{L}_s}^{-1} \right|\right| \leq 1 \, .$$

4.3 First order macroscopic fields

Once the existence of the solution $f_s^{(1)}$ has been proved, we can proceed to the explicit computation of its moments. We compute them without making use of the explicit expression of the first order distribution functions, since the presence of $f_s^{(1)}$ inside the linearized intra-species operator prevents its calculation.
With regard to $\boldsymbol{u}_s^{(1)}$, we need to multiply equation (4.5) by $\varphi_s(\boldsymbol{v}) = \boldsymbol{v}$; we simply notice that

$$\int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} = \boldsymbol{0} \, ,$$

and using the computations carried out for the general mixed model we reach the following

$$\boldsymbol{u}_s^{(1)} = \frac{1}{\sum_{\substack{r=1,\\ r\neq s}}^{N} \nu_{sr}^{(0)}} \left[\sum_{\substack{r=1,\\ r\neq s}}^{N} \nu_{sr}^{(0)} \boldsymbol{u}_{sr}^{(1)} - T \left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho} \right) - \left(\frac{1}{m_s} - \frac{n}{\rho} \right) \nabla_{\boldsymbol{x}} T \right] . \tag{4.6}$$

Recalling the expression of $\boldsymbol{u}_{sr}^{(1)} = \boldsymbol{u}_s^{(1)} + a_{sr}^{(0)}(\boldsymbol{u}_r^{(1)} - \boldsymbol{u}_s^{(1)})$ and multiplying both sides for $m_s n_s$, we obtain, as expected, the same linear system of (3.44) for the diffusion velocities, independently from the choice of the collisional operators between Boltzmann and BGK

$$4\pi \sum_{\substack{r=1,\\ r\neq s}}^{N} \lambda_{sr} n_s n_r \mu_{sr} \left(\boldsymbol{u}_s^{(1)} - \boldsymbol{u}_r^{(1)}\right) = -\nabla_{\boldsymbol{x}} \left(n_s T\right) + \frac{\rho_s}{\rho} \nabla_{\boldsymbol{x}} \left(nT\right) \, .$$

Hence, it leads again to

$$\boldsymbol{u}_s^{(1)} = \sum_{\substack{r=1,\\ r\neq s}}^{N} \mathcal{F}_{sr} \nabla_{\boldsymbol{x}} n_s + \alpha_s \nabla_{\boldsymbol{x}} T \, ,$$

with the same Fick matrix entries $\mathcal{F}_{sr}$ and Soret coefficients α_s.

Remark. *As regards the first-order approximation of the pressure tensor* $\underline{\boldsymbol{P}}^{(1)}$ *and of the heat flux vector* $\boldsymbol{q}^{(1)}$*, we notice from* (4.5) *that in the explicit expression of* $f_s^{(1)}$*, the only Boltzmann collisional operator involved is the linearized operator for single gas* $\mathcal{L}(h_s^{(1)})$*.*
Hence, the computations of

$$m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} \, , \quad m_s \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} \, , \tag{4.7}$$

do not depend on other species moments of $m_r \int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v}$ *or* $m_r \int_{\mathbb{R}^3} c_i c^2 f_r^{(1)} d\boldsymbol{v}$ *respectively, and is therefore possible to factor out both terms in* (4.7) *and to obtain a closed expression for either* $\underline{\boldsymbol{P}}^{(1)}$ *and* $\boldsymbol{q}^{(1)}$*.*
Furthermore, we focus on deriving

$$m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \, , \quad m_s \int_{\mathbb{R}^3} c_i c^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \, , \tag{4.8}$$

since the computations of moments of other addends appearing in (4.5) are identical to the ones already carried out for the general model.

As in Chapter 3, some technical details on the computations of moments of the linearized Boltzmann operator are given in Appendix C. Specifically, using (A.11) and the symmetry with respect to the variables $\boldsymbol{v}$ and $\boldsymbol{w}$ of the linearized intra-species operator, for $m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v}$ we have

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \\
& = \pi m_s \lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3} \left\{ 2v_i v_j + 2 v_i w_j + \frac{\delta_{ij}}{3}\left(v^2 + w^2 - 2\boldsymbol{v}\cdot\boldsymbol{w}\right) \right\} \\
& \times \left[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(0)}(\boldsymbol{w}) f_s^{(1)}(\boldsymbol{v}) \right] d\boldsymbol{v} d\boldsymbol{w} - 4\pi m_s \lambda_s n_s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \\
& = 2\pi m_s \lambda_s n_s \Bigg[\int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + n_s (u_i u_j^{s^{(1)}} + u_j u_i^{s^{(1)}}) + \frac{2}{3}\delta_{ij} n_s \left(2\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} + 3\frac{T_s^{(1)}}{m_s} \right) \\
& - \frac{4}{3}\delta_{ij} n_s \boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} \Bigg]
\end{aligned}
\tag{4.9}
$$

$$
\begin{aligned}
& = 2\pi m_s \lambda_s n_s \Bigg[- \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} - u_i \int_{\mathbb{R}^3} (v_j - u_j) f_s^{(1)} d\boldsymbol{v} - u_j \int_{\mathbb{R}^3} (v_i - u_i) f_s^{(1)} d\boldsymbol{v} \\
& + n_s (u_i u_j^s + u_j u_i^s) + \delta_{ij} n_s \frac{T_s^{(1)}}{m_s} \Bigg] = 2\pi m_s \lambda_s n_s \left(- \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + \delta_{ij} n_s \frac{T_s^{(1)}}{m_s} \right).
\end{aligned}
\tag{4.10}
$$

Therefore, from (3.52) and (4.10), we obtain

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} = \delta_{ij} n_s T_s^{(1)} + \frac{n_s T}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\delta_{ij} \right) \\
& + \frac{2\pi m_s \lambda_s n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}} \left(- \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + \delta_{ij} n_s \frac{T_s^{(1)}}{m_s} \right) \\
& \iff m_s \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} = \delta_{ij} n_s T_s^{(1)} \left(1 + \frac{2\pi\lambda_s n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}} \right) \frac{1}{1 + \frac{2\pi\lambda_s n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}} \\
& - \frac{n_s T}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}} \; \frac{1}{1 + \frac{2\pi\lambda_s n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\delta_{ij} \right),
\end{aligned}
$$

and, taking into account the constraint $\sum_{s=1}^N n_s T_s^{(1)} = 0$, we get that the global pressure tensor is provided by

$$
P_{ij}^{(1)} = - \sum_{s=1}^N \frac{n_s T}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)} + 2\pi\lambda_s n_s} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\delta_{ij} \right). \tag{4.11}
$$

Hence, the tensor $\underline{\boldsymbol{P}}^{(1)}$ takes the following form

$$\underline{\boldsymbol{P}}^{(1)} = -\mu\underline{\boldsymbol{\tau}}\,,$$

where μ is a proper viscosity coefficient and $\underline{\boldsymbol{\tau}}$ is the strain rate tensor, provided by

$$\mu = T\sum_{s=1}^{N}\frac{n_s}{\sum_{\substack{r=1,\\ r\neq s}}^{N}\nu_{sr}^{(0)} + 2\pi\lambda_s n_s}\,, \qquad \tau_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}\delta_{ij}\,.$$

Remark. *From* (4.11)*, it can be easily verified that Tr*($\underline{\boldsymbol{P}}^{(1)}$) $= 0$*, consistently with the fact that the viscous stress tensor represents the traceless deviatoric part of the pressure tensor.*

Referring, once again, to Appendix C for the long computations, analogous to those already carried out, (C.6) provides the following for $m_s\int_{\mathbb{R}^3} c_i c^2 f_s^{(0)}\mathcal{L}(h_s^{(1)})d\boldsymbol{v}$,

$$\begin{aligned}
&\frac{1}{2}m_s\int_{\mathbb{R}^3} c_i c^2 f_s^{(0)}\mathcal{L}(h_s^{(1)})d\boldsymbol{v} = \frac{1}{2}m_s\int_{\mathbb{R}^3} v_i v^2 f_s^{(0)}\mathcal{L}(h_s^{(1)})d\boldsymbol{v}\\
&- 2\pi u_i m_s\lambda_s n_s\Big\{-\int_{\mathbb{R}^3} v_i^2 f_s^{(1)}d\boldsymbol{v} + 2n_s u_i u_i^{s^{(1)}} + n_s\frac{T_s^{(1)}}{m_s}\Big\}\\
&- 2\pi u_j m_s\lambda_s n_s\Big\{-\int_{\mathbb{R}^3} v_i v_j f_s^{(1)}d\boldsymbol{v} + n_s\left(u_i u_j^{s^{(1)}} + u_j u_i^{s^{(1)}}\right)\Big\}\\
&- 2\pi u_k m_s\lambda_s n_s\Big\{-\int_{\mathbb{R}^3} v_i v_k f_s^{(1)}d\boldsymbol{v} + n_s\left(u_i u_k^{s^{(1)}} + u_k u_i^{s^{(1)}}\right)\Big\},
\end{aligned} \tag{4.12}$$

and, with regards to $m_s\int_{\mathbb{R}^3} v_i v^2 f_s^{(0)}\mathcal{L}(h_s^{(1)})d\boldsymbol{v}$, from (C.7), we get

$$\begin{aligned}
&\frac{1}{2}m_s\int_{\mathbb{R}^3} v_i v^2 f_s^{(0)}\mathcal{L}(h_s^{(1)})d\boldsymbol{v} = \frac{2}{3}\pi m_s\lambda_s n_s\Big\{-\int_{\mathbb{R}^3} c_i c^2 f_s^{(1)}d\boldsymbol{v} - 3u_i\int_{\mathbb{R}^3} v_i^2 f_s^{(1)}d\boldsymbol{v}\\
&- 3u_j\int_{\mathbb{R}^3} v_i v_j f_s^{(1)}d\boldsymbol{v} - 3u_k\int_{\mathbb{R}^3} v_i v_k f_s^{(1)}d\boldsymbol{v} + n_s u^2 u_i^{s^{(1)}} - n_s u_i\frac{3T_s^{(1)}}{m_s}\\
&+ 2n_s u_i^{s^{(1)}}\left(u^2 + \frac{3T}{m_s}\right) + 2n_s u_i\left(2\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s}\right) - n_s\left(u_i\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} + u_i^{s^{(1)}}\frac{T}{m_s}\right)\Big\}.
\end{aligned} \tag{4.13}$$

Now, plugging (4.13) into (4.12) and referring to (C.7) for details, we get the following

$$\frac{1}{2}m_s\int_{\mathbb{R}^3} c_i c^2 f_s^{(0)}\mathcal{L}(h_s^{(1)})d\boldsymbol{v} = \frac{2}{3}\pi m_s\lambda_s n_s\left(-\int_{\mathbb{R}^3} c_i c^2 f_s^{(1)}d\boldsymbol{v} + 5n_s u_i^{s^{(1)}}\frac{T}{m_s}\right). \tag{4.14}$$

Hence, exploiting (3.58) for the computation of the remaining addends, we thus find

$$
\begin{aligned}
&\frac{1}{2}m_s \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)}(\boldsymbol{v})d\boldsymbol{v} = \frac{5}{2}\frac{n_s T}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\Bigg\{ -\frac{\nabla_{\boldsymbol{x}} T}{m_s} \\
&\underbrace{+\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}\boldsymbol{u}_{sr}^{(1)} - T\left(\frac{\nabla_{\boldsymbol{x}} n_s}{\rho_s} - \frac{\nabla_{\boldsymbol{x}} n}{\rho}\right) - \nabla_{\boldsymbol{x}} T\left(\frac{1}{m_s} - \frac{n}{\rho}\right)\Bigg\}}_{=\boldsymbol{u}_s^{(1)}} \\
&+\frac{2}{3}\frac{\pi m_s \lambda_s n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\left(-\int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)} d\boldsymbol{v} + 5 n_s \boldsymbol{u}_s^{(1)}\frac{T}{m_s}\right) \\
&= -\frac{5}{2}\frac{n_s T}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\frac{\nabla_{\boldsymbol{x}} T}{m_s} + 5 n_s \boldsymbol{u}_s^{(1)} T\left(1 + \frac{4}{3}\frac{\pi n_s \lambda_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\right) \\
&-\frac{2}{3}\frac{\pi m_s \lambda_s n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)} d\boldsymbol{v} \\
&\iff \frac{1}{2}m_s \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)} d\boldsymbol{v} = -\left(1 + \frac{4}{3}\frac{\pi n_s \lambda_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\right)^{-1} \\
&\times\left(\frac{5}{2}\frac{n_s T}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}}\frac{\nabla_{\boldsymbol{x}} T}{m_s}\right) + \frac{5}{2} n_s \boldsymbol{u}_s^{(1)} T\,.
\end{aligned}
$$

We can finally formulate the explicit expression of $\boldsymbol{q}^{(1)}$

$$
\begin{aligned}
\boldsymbol{q}^{(1)} &= \sum_{s=1}^N m_s \int_{\mathbb{R}^3} \boldsymbol{c}c^2 f_s^{(1)}(\boldsymbol{v})d\boldsymbol{v} = -\frac{5}{2}T\sum_{s=1}^N \frac{n_s}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)} + \frac{4}{3}\pi n_s \lambda_s}\frac{\nabla_{\boldsymbol{x}} T}{m_s} + \frac{5}{2}T\sum_{s=1}^N n_s \boldsymbol{u}_s^{(1)} \\
&= -\xi \nabla_{\boldsymbol{x}} T + \frac{5}{2}T\sum_{s=1}^N n_s \boldsymbol{u}_s^{(1)}\,,
\end{aligned}
$$

with thermal conductivity coefficient

$$
\xi = \frac{5}{2}T\sum_{s=1}^N \frac{n_s m_s^{-1}}{\sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)} + \frac{4}{3}\pi n_s \lambda_s}\,.
$$

Remark. *Viscosity and conduction coefficients depend on collision frequencies only through the combinations* $\bar{\nu}_s = \sum_{\substack{r=1,\\ r\neq s}}^N \nu_{sr}^{(0)}$, $s = 1, \ldots, N$, *which play the role of overall collision frequencies for single species. It is possible to tune the* *collision frequencies $\bar{\nu}_s$, which we remind to be free parameters, in order to reproduce the correct physical ratio $\frac{c_P \mu}{\lambda}$, the Prandtl number, where c_P is the specific heat at constant pressure, of the gas mixture under investigation. This allows in principle to overcome the main drawback of the BGK approximation, namely that for a single gas it is not able to reproduce the correct Prandtl number.*

Chapter 5

Various hydrodynamic limits for a binary mixture

In this chapter, we consider a binary mixture, which naturally arises in many physical contexts, such as ε-mixtures of heavy and light gases [26], or in plasmas constituted by ions and electrons [40], focusing on two relevant regimes.
The first concerns intra-species dominated collisions, where self-interactions govern the relaxation dynamics and inter-species collisions act as small perturbations, that will lead to multi-velocity and multi-temperature Navier-Stokes equations, with source terms accounting for the slow collisional dynamics and, consequently, for the transfer of momentum and kinetic energy between the two components.
The second one addresses a mixture of heavy and light particles, in which only the heaviest intra-species collisions play a dominant role while the binary lightest intra-species encounters account for the slowest process.
By sticking to the case $\chi_{sr} = \delta_{sr}$,where Boltzmann operators are used for intra-species collisions only, the dimensionless system for a binary mixture reads as

$$\begin{cases} \dfrac{\partial f_1}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_1 = \dfrac{\beta_{11}}{\varepsilon} Q_{11} + \dfrac{\beta_{12}}{\varepsilon} \nu_{12} (\mathcal{M}_{12} - f_1) \\ \dfrac{\partial f_2}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_2 = \dfrac{\beta_{21}}{\varepsilon} \nu_{12} (\mathcal{M}_{21} - f_2) + \dfrac{\beta_{22}}{\varepsilon} Q_{22} \,, \end{cases} \tag{5.1}$$

in which the different choices of the β-coefficients will allow for the study of the regimes cited above.

5.1 Binary mixture with intra-species dominant collisions

The regime with dominant intra-species collisions corresponds to the choice

$$\beta_{11} = \beta_{22} = 1 \,, \qquad \beta_{12} = \beta_{21} = \varepsilon \,,$$

in (5.1), leading to

$$\begin{cases} \dfrac{\partial f_1}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_1 = \dfrac{1}{\varepsilon} Q_{11} + \nu_{12}(\mathcal{M}_{12} - f_1) \\ \dfrac{\partial f_2}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_2 = \nu_{12}(\mathcal{M}_{21} - f_2) + \dfrac{1}{\varepsilon}\ Q_{22} \,. \end{cases}$$

This scaling defines the so-called $\varepsilon-$mixture regime, which arises when the mixture is composed of particles with strongly different masses with both intra-species interactions playing a dominant role and energy transfer between species occurring on a much slower timescale than within each species [26]. A prominent example is provided by plasma physics, where light electrons coexist with much heavier constituents such as atoms, molecules, and ions [44].

By expanding the macroscopic and the fictitious parameters as we did in the classical collision dominated regime, we get

$$\begin{aligned} &\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} + \varepsilon \left(\frac{\partial f_s^{(1)}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(1)} \right) \\ &= \frac{1}{\varepsilon} \left[Q_{ss}(f_s^{(0)}) + \varepsilon \left(Q_{ss}(f_s^{(0)}, f_s^{(1)}) + Q_{ss}(f_s^{(1)}, f_s^{(0)}) \right) + \varepsilon^2 Q_{ss}(f_s^{(1)}) \right] \\ &+ (\nu_{sr}^{(0)} + \varepsilon \nu_{sr}^{(1)}) \left(\mathcal{M}_{sr}^{(0)} + \varepsilon \mathcal{M}_{sr}^{(1)} - f_s^{(0)} - \varepsilon f_s^{(1)} \right) , \quad s, r = 1, 2 \,, \quad s \neq r \,; \end{aligned} \tag{5.2}$$

which, at the leading order, yields

$$Q_{ss}(f_s^{(0)}) = 0 \,,$$

which implies that leading order distributions are equilibria of the single species Boltzmann operators, hence Maxwellians depending on species fields:

$$f_s^{(0)} = \mathcal{M} \left(\boldsymbol{v}; n_s, \boldsymbol{u}_s, \frac{T_s}{m_s} \right) , \quad s = 1, 2. \tag{5.3}$$

The hydrodynamic variables that remain unexpanded in the Chapman-Enskog procedure correspond to the collision invariants of leading order operators, namely of the single species Boltzmann ones; therefore, they are the species density n_s, mean velocity $\boldsymbol{u}_s$ and temperature T_s, which means

$$\begin{cases} n_s^{(0)} = n_s \\ \boldsymbol{u}_s^{(0)} = \boldsymbol{u} \\ T_s^{(0)} = T_s \end{cases} \implies \begin{cases} n_s^{(1)} = 0 \\ \boldsymbol{u}_s^{(1)} = \boldsymbol{0} \\ T_s^{(1)} = 0 \end{cases} \tag{5.4}$$

From this, it also follows that $\langle f_s^{(1)}, \varphi_s(\boldsymbol{v}) \rangle = 0$, for any of $\varphi_s(\boldsymbol{v}) = 1, m_s \boldsymbol{v}, m_s v^2$.

With regard to the fictitious parameters, exploiting (5.4), we find

$$\begin{cases} \boldsymbol{u}_{sr}^{(0)} = (1 - a_{sr}^{(0)}) \boldsymbol{u}_s + a_{sr}^{(0)} \boldsymbol{u}_r \\ \boldsymbol{u}_{sr}^{(1)} = a_{sr}^{(1)} (\boldsymbol{u}_r - \boldsymbol{u}_s) \\ T_{sr}^{(0)} = (1 - b_{sr}^{(0)}) T_s + b_{sr}^{(0)} T_r + \gamma_{sr}^{(0)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \\ T_{sr}^{(1)} = b_{sr}^{(1)} (T_r - T_s) + \gamma_{sr}^{(1)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \,. \end{cases} \tag{5.5}$$

From (5.5), we get

$$\mathcal{M}_{sr}^{(0)} = n_s \left(\frac{m_s}{2\pi T_{sr}^{(0)}} \right)^{\frac{3}{2}} \exp\left[-\frac{m_s}{2T_{sr}^{(0)}} \left(\boldsymbol{v} - \boldsymbol{u}_{sr}^{(0)} \right)^2 \right] ,$$

thus, the computation of the zeroth, first and second order moment of $\mathcal{M}_{sr}^{(0)}$ yields

$$\begin{cases} \langle \mathcal{M}_{sr}^{(0)}, 1 \rangle = n_s \\ \langle \mathcal{M}_{sr}^{(0)}, \boldsymbol{v} \rangle = n_s \boldsymbol{u}_{sr}^{(0)} \\ \langle \mathcal{M}_{sr}^{(0)}, v^2 \rangle = n_s \left({u_{sr}^{(0)}}^2 + \dfrac{3T_{sr}^{(0)}}{m_s} \right) . \end{cases} \tag{5.6}$$

Regarding $\mathcal{M}_{sr}^{(1)}$, by considering the derivative of the Maxwellian attractor with respect to the small parameter, with computations analogous to those leading to (3.20), but with $\boldsymbol{u}$ replaced by $\boldsymbol{u}_{sr}^{(0)}$ and T replaced by $T_{sr}^{(0)}$, we obtain

$$\mathcal{M}_{sr}^{(1)} = \mathcal{M}_{sr}^{(0)} \left[\frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \cdot \boldsymbol{c}_{sr}^{(0)} + \frac{1}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \left(\frac{m_s}{T_{sr}^{(0)}} (\boldsymbol{c}_{sr}^{(0)})^2 - 3 \right) \right] , \tag{5.7}$$

where $\boldsymbol{c}_{sr}^{(0)} = \boldsymbol{v} - \boldsymbol{u}_{sr}^{(0)}$.
As for its moments, we have

$$\begin{aligned} \langle \mathcal{M}_{sr}^{(1)}, 1 \rangle &= \frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \underbrace{\int_{\mathbb{R}^3} \boldsymbol{c}_{sr}^{(0)} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}}_{=0} + \frac{1}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \left(\frac{m_s}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} (\boldsymbol{c}_{sr}^{(0)})^2 \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - 3 \int_{\mathbb{R}^3} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} \right) \\ &= \frac{1}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \left(\frac{m_s}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} (v^2 + (\boldsymbol{u}_{sr}^{(0)})^2 - 2\boldsymbol{v} \cdot \boldsymbol{u}_{sr}^{(0)}) \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - 3n_s \right) \\ &= \frac{1}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \left(\frac{m_s}{T_{sr}^{(0)}} (\boldsymbol{u}_{sr}^{(0)})^2 + 3n_s + \frac{m_s}{T_{sr}^{(0)}} (\boldsymbol{u}_{sr}^{(0)})^2 - 2 \frac{m_s}{T_{sr}^{(0)}} (\boldsymbol{u}_{sr}^{(0)})^2 - 3n_s \right) = 0 , \end{aligned}$$

$$\langle \mathcal{M}_{sr}^{(1)}, \boldsymbol{v} \rangle = \frac{m_s}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} \boldsymbol{v}(\boldsymbol{u}_{sr}^{(1)} \cdot \boldsymbol{c}_{sr}^{(0)}) \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} + \frac{1}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \frac{m_s}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} \Big((\boldsymbol{c}_{sr}^{(0)})^2 - 3 \Big) \boldsymbol{v} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}$$
$$= \frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \cdot \int \boldsymbol{v} \otimes \boldsymbol{v} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - \frac{m_s}{T_{sr}^{(0)}} (\boldsymbol{u}_{sr}^{(1)} \cdot \boldsymbol{u}_{sr}^{(0)}) \int_{\mathbb{R}^3} \boldsymbol{v} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}$$
$$+ \frac{T_{sr}^{(1)}}{(T_{sr}^{(0)})^2} \boldsymbol{q}_{sr}^{(0)} + \frac{1}{2} \frac{T_{sr}^{(1)}}{(T_{sr}^{(0)})^2} \boldsymbol{u}_{sr}^{(0)} \int_{\mathbb{R}^3} (\boldsymbol{c}_{sr}^{(0)})^2 \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - \frac{3}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} \boldsymbol{v} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}$$
$$= \frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \cdot \Big(n_s \boldsymbol{u}_{sr}^{(0)} \otimes \boldsymbol{u}_{sr}^{(0)} + \underline{\boldsymbol{P}}_{sr}^{(0)} \Big) - \frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \cdot (n_s \boldsymbol{u}_{sr}^{(0)} \otimes \boldsymbol{u}_{sr}^{(0)})$$
$$+ \frac{1}{2} \frac{m_s T_{sr}^{(1)}}{(T_{sr}^{(0)})^2} \boldsymbol{u}_{sr}^{(0)} \int_{\mathbb{R}^3} (v^2 + (\boldsymbol{u}_{sr}^{(0)})^2 - 2\boldsymbol{v} \cdot \boldsymbol{u}_{sr}^{(0)}) \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - \frac{3}{2} \frac{n_s T_{sr}^{(1)}}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(0)}$$
$$= \frac{n_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} T_{sr}^{(0)} + \frac{m_s T_{sr}^{(1)}}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(0)} \Big(n_s (\boldsymbol{u}_{sr}^{(0)})^2 + n_s (\boldsymbol{u}_{sr}^{(0)})^2 - 2 n_s (\boldsymbol{u}_{sr}^{(0)})^2 \Big) = n_s \boldsymbol{u}_{sr}^{(1)} \,,$$

where

$$\underline{\boldsymbol{P}}_{sr}^{(0)} = m_s \int_{\mathbb{R}^3} (\boldsymbol{c}_{sr}^{(0)} \otimes \boldsymbol{c}_{sr}^{(0)}) \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} = n_s T_{sr}^{(0)} \underline{\boldsymbol{I}} \,,$$

since the strain rate tensor and the heat flux vector

$$\boldsymbol{q}_{sr}^{(0)} = \frac{1}{2} m_s \int_{\mathbb{R}^3} \boldsymbol{c}_{sr}^{(0)} (\boldsymbol{c}_{sr}^{(0)})^2 \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}$$

vanish at local equilibrium $\mathcal{M}_{sr}^{(0)}$.

Eventually,

$$\langle \mathcal{M}_{sr}^{(1)}, v^2 \rangle = \frac{m_s}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} v^2 (\boldsymbol{u}_{sr}^{(1)} \cdot \boldsymbol{c}_{sr}^{(0)}) \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}$$
$$+ \frac{1}{2} \frac{T_{sr}^{(1)}}{T_{sr}^{(0)}} \left(\frac{m_s}{T_{sr}^{(0)}} \int_{\mathbb{R}^3} (\boldsymbol{c}_{sr}^{(0)})^2 v^2 \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - 3 \int_{\mathbb{R}^3} v^2 \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} \right),$$

where the first term of the right hand side leads to

$$\frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \cdot \int_{\mathbb{R}^3} \Big[(\boldsymbol{c}_{sr}^{(0)})^2 + (\boldsymbol{u}_{sr}^{(0)})^2 + 2\boldsymbol{c}_{sr}^{(0)} \cdot \boldsymbol{u}_{sr}^{(0)} \Big] \boldsymbol{c}_{sr}^{(0)} \mathcal{M}_{sr}^{(0)} d\boldsymbol{v}$$
$$= 2 \frac{m_s}{T_{sr}^{(0)}} \boldsymbol{u}_{sr}^{(1)} \cdot \left(\boldsymbol{u}_{sr}^{(0)} \cdot \int_{\mathbb{R}^3} (\boldsymbol{c}_{sr}^{(0)} \otimes \boldsymbol{c}_{sr}^{(0)}) \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} \right) = 2 n_s \boldsymbol{u}_{sr}^{(0)} \cdot \boldsymbol{u}_{sr}^{(1)} \,,$$

while the second one to

$$\frac{1}{2} \frac{m_s T_{sr}^{(1)}}{(T_{sr}^{(0)})^2} \int_{\mathbb{R}^3} (\boldsymbol{c}_{sr}^{(0)})^2 \Big[(\boldsymbol{c}_{sr}^{(0)})^2 + (\boldsymbol{u}_{sr}^{(0)})^2 + 2\boldsymbol{c}_{sr}^{(0)} \cdot \boldsymbol{u}_{sr}^{(0)} \Big] \mathcal{M}_{sr}^{(0)} d\boldsymbol{v} - \frac{3}{2} \frac{n_s T_{sr}^{(1)}}{T_{sr}^{(0)}} \left((\boldsymbol{u}_{sr}^{(0)})^2 + \frac{3 T_{sr}^{(0)}}{m_s} \right)$$
$$= \frac{T_{sr}^{(1)}}{(T_{sr}^{(0)})^2} \left[\frac{15}{2} \frac{n_s}{m_s} (T_{sr}^{(0)})^2 + \frac{3}{2} (\boldsymbol{u}_{sr}^{(0)})^2 n_s T_{sr}^{(0)} \right] - \frac{3}{2} \frac{n_s T_{sr}^{(1)}}{T_{sr}^{(0)}} \left((\boldsymbol{u}_{sr}^{(0)})^2 + \frac{3 T_{sr}^{(0)}}{m_s} \right)$$
$$= \frac{15}{2} n_s \frac{T_{sr}^{(1)}}{m_s} - \frac{9}{2} n_s \frac{T_{sr}^{(1)}}{m_s} = 3 n_s \frac{T_{sr}^{(1)}}{m_s} \,,$$

where we took advantage of the Gaussian integral (B.2).
Therefore, we obtain

$$\langle \mathcal{M}_{sr}^{(1)}, v^2 \rangle = 2n_s \boldsymbol{u}_{sr}^{(0)} \cdot \boldsymbol{u}_{sr}^{(1)} + 3n_s \frac{T_{sr}^{(1)}}{m_s} \,,$$

and summarizing

$$\begin{cases} \langle \mathcal{M}_{sr}^{(1)}, 1 \rangle = 0 \\ \langle \mathcal{M}_{sr}^{(1)}, \boldsymbol{v} \rangle = n_s \boldsymbol{u}_{sr}^{(1)} \\ \langle \mathcal{M}_{sr}^{(1)}, v^2 \rangle = 2n_s \boldsymbol{u}_{sr}^{(0)} \cdot \boldsymbol{u}_{sr}^{(1)} + 3n_s \dfrac{T_{sr}^{(1)}}{m_s} \,. \end{cases} \tag{5.8}$$

Macroscopic equations can be achieved by computing the weak form of equation (5.2) with respect to the test functions $\varphi_s(\boldsymbol{v}) = 1, m_s\boldsymbol{v}, \frac{1}{2}m_s v^2$, which is

$$\begin{aligned} &\frac{\partial}{\partial t}\int_{\mathbb{R}^3} \varphi_s(\boldsymbol{v}) f_s^{(0)} d\boldsymbol{v} + \nabla_{\boldsymbol{x}} \cdot \int_{\mathbb{R}^3} \varphi_s(\boldsymbol{v}) \boldsymbol{v} f_s^{(0)} d\boldsymbol{v} + \varepsilon \nabla_{\boldsymbol{x}} \cdot \int_{\mathbb{R}^3} \varphi_s(\boldsymbol{v}) \boldsymbol{v} f_s^{(1)} d\boldsymbol{v} \\ &= \int_{\mathbb{R}^3} \underbrace{\Big(Q_{ss}(f_s^{(0)}, f_s^{(1)}) + Q_{ss}(f_s^{(1)}, f_s^{(0)}) \Big)}_{= f_s^{(0)} \mathcal{L}(h_s^{(1)})} d\boldsymbol{v} + \varepsilon \int_{\mathbb{R}^3} \varphi_s(\boldsymbol{v}) Q_{ss}(f_s^{(1)}) d\boldsymbol{v} \qquad (5.9) \\ &+ \int_{\mathbb{R}^3} \varphi_s(\boldsymbol{v}) \left\{ \nu_{sr}^{(0)} (\mathcal{M}_{sr}^{(0)} - f_s^{(0)}) + \varepsilon \left[\nu_{sr}^{(1)} \left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right) + \nu_{sr}^{(0)} \left(\mathcal{M}_{sr}^{(1)} - f_s^{(1)} \right) \right] \right\} d\boldsymbol{v} \,, \end{aligned}$$

for $s, r = 1, 2 \,,\ r \neq s$.
Recalling (5.4), as regards the left-hand side, we get for $\varphi_s(\boldsymbol{v}) = 1$

$$\frac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}_s) \,, \tag{5.10}$$

for $\varphi_s(\boldsymbol{v}) = m_s \boldsymbol{v}$

$$\begin{aligned} &\frac{\partial}{\partial t}(\rho_s u_i^s) + m_s \frac{\partial}{\partial x_j} \int_{\mathbb{R}^3} v_i v_j (f_s^{(0)} + \varepsilon f_s^{(1)}) d\boldsymbol{v} \\ &= \frac{\partial}{\partial t}(\rho_s u_i^s) + m_s \frac{\partial}{\partial x_j} \int_{\mathbb{R}^3} \left[u_i^s u_j^s + c_i^s c_j^s + u_i^s c_j^s + u_j^s c_i^s \right] (f_s^{(0)} + \varepsilon f_s^{(1)}) d\boldsymbol{v} \\ &= \frac{\partial}{\partial t}(\rho_s u_i^s) + \frac{\partial}{\partial x_j} \left[\rho_s u_i^s u_j^s + m_s \int_{\mathbb{R}^3} c_i^s c_j^s f_s^{(0)} d\boldsymbol{v} + \varepsilon m_s \int_{\mathbb{R}^3} c_i^s c_j^s f_s^{(1)} d\boldsymbol{v} \right] \\ &= \frac{\partial}{\partial t}(\rho_s \boldsymbol{u}_s) + \nabla_{\boldsymbol{x}} \cdot [\rho_s (\boldsymbol{u}_s \otimes \boldsymbol{u}_s) + n_s T_s \underline{\boldsymbol{I}}] + \varepsilon \nabla_{\boldsymbol{x}} \cdot \underline{\boldsymbol{P}}_s^{(1)} \,, \qquad (5.11) \end{aligned}$$

and for $\varphi_s(\boldsymbol{v}) = \frac{1}{2}m_s v^2$

$$
\begin{aligned}
&\frac{1}{2}m_s\frac{\partial}{\partial t}\int_{\mathbb{R}^3} v^2 f_s^{(0)}d\boldsymbol{v} + \frac{1}{2}m_s\nabla_{\boldsymbol{x}}\cdot\int_{\mathbb{R}^3} v^2(\boldsymbol{u}_s+\boldsymbol{c}_s)(f_s^{(0)}+\varepsilon f_s^{(1)})d\boldsymbol{v}\\
&= \frac{\partial}{\partial t}\left(\frac{1}{2}\rho_s u_s^2 + \frac{3}{2}n_s T_s\right) + \frac{1}{2}m_s\nabla_{\boldsymbol{x}}\cdot\boldsymbol{u}_s\int_{\mathbb{R}^3} v^2(f_s^{(0)}+\varepsilon f_s^{(1)})d\boldsymbol{v}\\
&+ \frac{1}{2}m_s\nabla_{\boldsymbol{x}}\cdot\int_{\mathbb{R}^3}(u_s^2+c_s^2+2\boldsymbol{u}_s\cdot\boldsymbol{c}_s)\boldsymbol{c}_s(f_s^{(0)}+\varepsilon f_s^{(1)})d\boldsymbol{v}\\
&= \frac{\partial}{\partial t}\left(\frac{1}{2}\rho_s u_s^2 + \frac{3}{2}n_s T_s\right) + \nabla_{\boldsymbol{x}}\cdot\left[\boldsymbol{u}_s\left(\frac{1}{2}\rho_s u_s^2+\frac{3}{2}n_s T_s\right)\right]\\
&+ m_s\nabla_{\boldsymbol{x}}\cdot\left(\boldsymbol{u}_s\int_{\mathbb{R}^3}(\boldsymbol{c}_s\otimes\boldsymbol{c}_s)(f_s^{(0)}+\varepsilon f_s^{(1)})d\boldsymbol{v}\right) + \frac{\varepsilon}{2}m_s\nabla_{\boldsymbol{x}}\cdot\int_{\mathbb{R}^3}\boldsymbol{c}_s c_s^2 f_s^{(1)}d\boldsymbol{v}\\
&= \frac{\partial}{\partial t}\left(\frac{1}{2}\rho_s u_s^2 + \frac{3}{2}n_s T_s\right) + \nabla_{\boldsymbol{x}}\cdot\left[\left(\frac{5}{2}\rho_s u_s^2+\frac{3}{2}n_s T_s\right)\boldsymbol{u}_s\right] + \varepsilon\nabla_{\boldsymbol{x}}\cdot\left(\underline{\boldsymbol{P}}_s^{(1)}\cdot\boldsymbol{u}_s^{(1)}+\boldsymbol{q}_s^{(1)}\right)\,.
\end{aligned}
\tag{5.12}
$$

Concerning the right-hand side of (5.9), from the theory for the single gas Boltzmann collisional operator, we know that $\varphi_s(\boldsymbol{v}) = 1, m_s\boldsymbol{v}, \frac{1}{2}m_s v^2$ are collision invariants for both the whole operator Q_{ss} and the linearized Boltzmann intra-species one $\mathcal{L}(h_s^{(1)})$. Hence,

$$
\int_{\mathbb{R}^3}\varphi_s(\boldsymbol{v})Q_{ss}(f_s^{(1)})d\boldsymbol{v} = \int_{\mathbb{R}^3}\varphi_s(\boldsymbol{v})\mathcal{L}(h_s^{(1)})d\boldsymbol{v} = 0\,,
$$

for any of our test functions $\varphi_s(\boldsymbol{v})$. As for

$$
\int_{\mathbb{R}^3}\varphi_s(\boldsymbol{v})\left[\nu_{sr}^{(1)}(\mathcal{M}_{sr}^{(0)}-f_s^{(0)})+\nu_{sr}^{(0)}(\mathcal{M}_{sr}^{(1)}-f_s^{(1)})\right]d\boldsymbol{v}\,,
$$

the moments of $\mathcal{M}_{sr}^{(1)}$ given in (5.8) allow to show that it vanishes.
Indeed, making use of (5.4), (5.5), (3.37), and (5.8), we obtain

$$
\begin{aligned}
&\nu_{sr}^{(1)}\int_{\mathbb{R}^3}(\mathcal{M}_{sr}^{(0)}-f_s^{(0)})d\boldsymbol{v} + \nu_{sr}^{(0)}\int_{\mathbb{R}^3}(\mathcal{M}_{sr}^{(1)}-f_s^{(1)})d\boldsymbol{v} = 0\,,\\
&m_s\nu_{sr}^{(1)}\int_{\mathbb{R}^3}\boldsymbol{v}(\mathcal{M}_{sr}^{(0)}-f_s^{(0)})d\boldsymbol{v} + m_s\nu_{sr}^{(0)}\int_{\mathbb{R}^3}\boldsymbol{v}(\mathcal{M}_{sr}^{(1)}-f_s^{(1)})d\boldsymbol{v}\\
&\quad= \rho_s\nu_{sr}^{(1)}(\boldsymbol{u}_{sr}^{(0)}-\boldsymbol{u}_s) + \rho_s\nu_{sr}^{(0)}\boldsymbol{u}_{sr}^{(1)} = \rho_s(\nu_{sr}^{(1)}a_{sr}^{(0)}-\nu_{sr}^{(0)}a_{sr}^{(1)})(\boldsymbol{u}_r-\boldsymbol{u}_s) = \boldsymbol{0}\,,
\end{aligned}
$$

and

$$
\begin{aligned}
&\frac{1}{2} m_s \nu_{sr}^{(1)} \int_{\mathbb{R}^3} v^2 (\mathcal{M}_{sr}^{(0)} - f_s^{(0)}) d\boldsymbol{v} + \frac{1}{2} \nu_{sr}^{(0)} \int_{\mathbb{R}^3} v^2 (\mathcal{M}_{sr}^{(1)} - f_s^{(1)}) d\boldsymbol{v} \\
&= \frac{1}{2} \nu_{sr}^{(1)} \left[\rho_s (\boldsymbol{u}_{sr}^{(0)})^2 + 3 n_s T_{sr}^{(0)} - \rho_s u_s^2 - 3 n_s T_s \right] + \nu_{sr}^{(0)} \left(\rho_s \boldsymbol{u}_{sr}^{(0)} \cdot \boldsymbol{u}_{sr}^{(1)} + \frac{3}{2} n_s T_{sr}^{(1)} \right) \\
&= -\frac{1}{2} \nu_{sr}^{(0)} \rho_s a_{sr}^{(1)} \left[a_{sr}^{(0)} (\boldsymbol{u}_s - \boldsymbol{u}_r) + 2 \boldsymbol{u}_s \right] \cdot (\boldsymbol{u}_s - \boldsymbol{u}_r) \\
&- \frac{3}{2} n_s \nu_{sr}^{(0)} \left[b_{sr}^{(1)} (T_s - T_r) + \left(\gamma_{sr}^{(1)} - \frac{1}{3} m_s \frac{\nu_{sr}^{(1)}}{\nu_{sr}^{(0)}} (a_{sr}^{(0)}) \right) (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \right] \\
&+ \nu_{sr}^{(0)} \rho_s a_{sr}^{(1)} \left[\boldsymbol{u}_s \cdot (\boldsymbol{u}_s - \boldsymbol{u}_r) + a_{sr}^{(0)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \right] + \frac{3}{2} \nu_{sr}^{(0)} n_s \left[b_{sr}^{(1)} (T_r - T_s) + \gamma_{sr}^{(1)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \right] \\
&= -\frac{1}{2} \nu_{sr}^{(0)} \left[\rho_s a_{sr}^{(1)} \left(a_{sr}^{(0)} (\boldsymbol{u}_s - \boldsymbol{u}_r) + 2 \boldsymbol{u}_s \right) \cdot (\boldsymbol{u}_s - \boldsymbol{u}_r) + \rho_s a_{sr}^{(0)} a_{sr}^{(1)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \right] \\
&+ \nu_{sr}^{(0)} \rho_s a_{sr}^{(1)} \left[\boldsymbol{u}_s \cdot (\boldsymbol{u}_r - \boldsymbol{u}_s) + a_{sr}^{(0)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \right] = 0 \,.
\end{aligned}
$$

Ultimately, with respect to

$$
\nu_{sr}^{(0)} \int_{\mathbb{R}^3} \varphi_s(\boldsymbol{v}) (\mathcal{M}_{sr}^{(0)} - f_s^{(0)}) d\boldsymbol{v} \,,
$$

it also trivially vanishes for $\varphi_s(\boldsymbol{v}) = 1$.
With test functions $\varphi_s(\boldsymbol{v}) = m_s \boldsymbol{v}$, $\frac{1}{2} m_s v^2$, however, it yields some source terms.
In particular

$$
\begin{aligned}
\mathbf{R}_{sr} &= m_s \nu_{sr}^{(0)} \int_{\mathbb{R}^3} \boldsymbol{v} (\mathcal{M}_{sr}^{(0)} - f_s^{(0)}) d\boldsymbol{v} = \nu_{sr}^{(0)} \rho_s \left(\boldsymbol{u}_{sr}^{(0)} - \boldsymbol{u}_s \right) \\
&= \nu_{sr}^{(0)} \rho_s a_{sr}^{(0)} (\boldsymbol{u}_r - \boldsymbol{u}_s) = \mu_{sr} \Lambda_{sr} n_s n_r (\boldsymbol{u}_r - \boldsymbol{u}_s) \,.
\end{aligned}
\tag{5.13}
$$

Turning to the energy exchanges, we obtain

$$
\begin{aligned}
\mathrm{S}_{sr} &= \frac{1}{2} m_s \nu_{sr}^{(0)} \int_{\mathbb{R}^3} v^2 \left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right) d\boldsymbol{v} = \frac{1}{2} \nu_{sr}^{(0)} n_s \left[3 \left(T_{sr}^{(0)} - T_s \right) + m_s \left((\boldsymbol{u}_{sr}^{(0)})^2 - u_s^2 \right) \right] \\
&= \frac{1}{2} \nu_{sr}^{(0)} n_s \left[3 \left(b_{sr}^{(0)} (T_r - T_s) + \gamma_{sr}^{(0)} (\boldsymbol{u}_s - \boldsymbol{u}_r)^2 \right) + m_s \left((1 - a_{sr}^{(0)}) \boldsymbol{u}_s + a_{sr}^{(0)} \boldsymbol{u}_r \right)^2 - m_s u_s^2 \right] \\
&= \alpha_{rs} \Lambda_{sr} n_s n_r \left[3 \alpha_{sr} (T_r - T_s) + \frac{1}{2} m_s (2 \alpha_{rs} - a_{sr}^{(0)}) (u_s^2 + u_r^2 - \boldsymbol{u}_s \cdot \boldsymbol{u}_r) \right] \\
&+ \alpha_{rs} \Lambda_{sr} n_s n_r m_s \left[\frac{1}{2} a_{sr}^{(0)} (u_s^2 + u_r^2) - u_s^2 + (1 - a_{sr}^{(0)}) \boldsymbol{u}_s \cdot \boldsymbol{u}_r \right] \\
&= 3 \alpha_{sr} \alpha_{rs} \Lambda_{sr} n_s n_r (T_r - T_s) + \alpha_{rs} \Lambda_{sr} n_s n_r \alpha_{sr} m_r (u_s^2 + u_r^2) \\
&- \alpha_{rs} \Lambda_{sr} n_s n_r m_s \alpha_{sr} \left(\frac{m_s}{m_r} - 1 \right) \boldsymbol{u}_s \cdot \boldsymbol{u}_r - \alpha_{rs} \alpha_{sr} \Lambda_{sr} n_s n_r (m_s + m_r) u_s^2 \\
&= \alpha_{sr} \alpha_{rs} \Lambda_{sr} n_s n_r [3 (T_r - T_s) - (m_s \boldsymbol{u}_s + m_r \boldsymbol{u}_r) \cdot (\boldsymbol{u}_s - \boldsymbol{u}_r)] \,.
\end{aligned}
\tag{5.14}
$$

Collecting (5.10), (5.11), (5.12), (5.13) and (5.14), we are finally ready to provide the Navier-Stokes equations

$$\begin{cases} \dfrac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}_s) = 0 \\[2ex] \dfrac{\partial}{\partial t}\big(\rho_s \boldsymbol{u}_s\big) + \nabla_{\boldsymbol{x}} \cdot \big(\rho_s \boldsymbol{u}_s \otimes \boldsymbol{u}_s + n_s T_s \underline{\boldsymbol{I}}\big) + \varepsilon \nabla_{\boldsymbol{x}} \cdot \underline{\boldsymbol{P}}_s^{(1)} = \mathbf{R}_{sr} \\[2ex] \dfrac{\partial}{\partial t}\left[\dfrac{1}{2}\rho_s u_s^2 + \dfrac{3}{2} n_s T_s\right] + \nabla_{\boldsymbol{x}} \cdot \left[\left(\dfrac{1}{2}\rho_s u_s^2 + \dfrac{5}{2} n_s T_s\right)\boldsymbol{u}_s\right] + \varepsilon \nabla_{\boldsymbol{x}} \cdot \big(\underline{\boldsymbol{P}}_s^{(1)} \cdot \boldsymbol{u}_s + \boldsymbol{q}_s^{(1)}\big) = \mathrm{S}_{sr}\,, \end{cases} \tag{5.15}$$

where

$$\begin{aligned} \mathbf{R}_{sr} &= \Lambda_{sr} \alpha_{rs} m_s n_s n_r (\boldsymbol{u}_r - \boldsymbol{u}_s) \\ \mathrm{S}_{sr} &= \Lambda_{sr} \alpha_{sr} \alpha_{rs} n_s n_r \big[3(T_r - T_s) + (m_s \boldsymbol{u}_s + m_r \boldsymbol{u}_r) \cdot (\boldsymbol{u}_r - \boldsymbol{u}_s)\big]\,. \end{aligned}$$

for any $s, r = 1, 2,\ r \neq s$.
The system above involves the following unknowns

- the species densities n_1, n_2;
- the 6 components of the species velocities $\boldsymbol{u}_1$, $\boldsymbol{u}_2$;
- the species temperatures T_1, T_2;
- the 10 independent components of the first order corrections of the viscous stress tensors $\underline{\boldsymbol{\Pi}}_1^{(1)}$, $\underline{\boldsymbol{\Pi}}_2^{(1)}$;
- the 6 components of the first order corrections of the heat flux vector $\boldsymbol{q}_1^{(1)}$, $\boldsymbol{q}_2^{(1)}$.

We observe that the resulting multi-velocity and multi-temperature equations are not conservation equations but take the form of balance equations, with source terms $\mathbf{R}_{sr}$ and S_{sr}accounting for the slow collisional dynamics and, consequently, for the transfer of momentum and energy between the different components. In contrast to the global equations in the classical collision dominated regime (3.15), which describe inter-species interactions only through diffusion and transport coefficients, the present system explicitly includes additional source terms that model the slow collisional exchange of momentum and energy.

Multi-velocities and multi-temperatures Euler-like equations

As done in Chapter 3, the simplest closure of the system above is obtained by truncating at zeroth order, approximating the distribution functions by their equilibrium form. In this regime, this is equivalent to setting

$$\begin{cases} \underline{\mathbf{\Pi}}_s^{(1)} = \underline{\mathbf{0}} \\ \boldsymbol{q}_s^{(1)} = \mathbf{0}\,, \end{cases}$$

obtaining

$$\begin{cases} \dfrac{\partial n_s}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_s \boldsymbol{u}_s) = 0 \\[2ex] \dfrac{\partial}{\partial t}\big(\rho_s \boldsymbol{u}_s\big) + \nabla_{\boldsymbol{x}} \cdot \big(\rho_s \boldsymbol{u}_s \otimes \boldsymbol{u}_s + n_s T_s \underline{\boldsymbol{I}}\big) = \mathbf{R}_{sr} \\[2ex] \dfrac{\partial}{\partial t}\left[\dfrac{1}{2}\rho_s u_s^2 + \dfrac{3}{2} n_s T_s\right] + \nabla_{\boldsymbol{x}} \cdot \left[\left(\dfrac{1}{2}\rho_s u_s^2 + \dfrac{5}{2} n_s T_s\right)\boldsymbol{u}_s\right] = \mathrm{S}_{sr}\,, \quad s,r = 1,2\,, \quad r \neq s\,. \end{cases} \tag{5.16}$$

As in the classical collision dominated-regime, despite its simplicity, such closure still provides an efficient approximation in situations close to equilibrium.

Multi-velocities and multi-temperatures Navier-Stokes equations

In order to close the macroscopic equations system (5.15), we need to provide constitutive relations for the first-order approximations of the following

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

For this purpose, we start by equating $O(1)$ terms in the expansion of (5.2)

$$\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} = \underbrace{Q_{ss}(f_s^{(0)}, f_s^{(1)}) + Q_{ss}(f_s^{(1)}, f_s^{(0)})}_{= f_s^{(0)} \mathcal{L}(h_s^{(1)})} + \nu_{sr}^{(0)}(\mathcal{M}_{sr}^{(0)} - f_s^{(0)}) \tag{5.17}$$

Now, it can be easily computed that

$$\frac{\partial f_s^{(0)}}{\partial t} = \left[\frac{1}{n_s}\frac{\partial n_s}{\partial t} + \frac{1}{2T_s}\left(\frac{m_s c_s^2}{T_s} - 3\right)\frac{\partial T_s}{\partial t} + \frac{m_s}{T_s}\boldsymbol{c}_s \cdot \frac{\partial \boldsymbol{u}_s}{\partial t}\right] f_s^{(0)}\,, \tag{5.18}$$

and

$$\begin{aligned} &\nabla_{\boldsymbol{x}} f_s^{(0)} = \left[\frac{1}{n_s}\nabla_{\boldsymbol{x}} n_s + \frac{1}{2T_s}\left(\frac{m_s c_s^2}{T_s} - 3\right)\nabla_{\boldsymbol{x}} T_s + \frac{m_s}{T_s}\nabla_{\boldsymbol{x}} \boldsymbol{u}_s \cdot \boldsymbol{c}_s\right] f_s^{(0)} \\ &\implies \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} = \left[\frac{1}{n_s}\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} n_s + \frac{1}{2T_s}\left(\frac{m_s c_s^2}{T_s} - 3\right)\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} T_s + \frac{m_s}{T_s}(\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} \boldsymbol{u}_s) \cdot \boldsymbol{c}_s\right] f_s^{(0)}\,. \end{aligned} \tag{5.19}$$

Making use of the computations that led to (3.24), Euler-like equations (5.16) can be rearranged into

$$\begin{cases} \dfrac{\partial n_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} n_s = \boldsymbol{c}_s \cdot \nabla_{\boldsymbol{x}} n_s - n_s \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u}_s \\ \dfrac{\partial \boldsymbol{u}_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} \boldsymbol{u}_s = \boldsymbol{c}_s \cdot \nabla_{\boldsymbol{x}} \boldsymbol{u}_s - \dfrac{1}{\rho_s} \nabla_{\boldsymbol{x}} (n_s T_s) + \dfrac{1}{\rho_s} \mathbf{R}_{sr} \\ \dfrac{\partial T_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} T_s = \boldsymbol{c}_s \cdot \nabla_{\boldsymbol{x}} T_s - \dfrac{2}{3} T_s \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u}_s + \dfrac{2}{3} \dfrac{1}{n_s} \left(\mathrm{S}_{sr} - \boldsymbol{u}_s \cdot \mathbf{R}_{sr} \right) . \end{cases} \tag{5.20}$$

Now, (5.18), (5.19) and (5.20) altogether provide

$$\frac{\partial f_s^{(0)}}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_s^{(0)} = \left[\frac{1}{n_s T_s} \boldsymbol{c}_s \cdot \mathbf{R}_{sr} + \frac{m_s}{T_s} \left(\boldsymbol{c}_s \otimes \boldsymbol{c}_s - \frac{c_s^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u}_s \right.$$
$$\left. + \frac{2}{3} \frac{1}{n_s T_s} \left(\frac{m_s}{2T_s} c_s^2 - \frac{3}{2} \right) \left(\mathrm{S}_{sr} - \boldsymbol{u}_s \cdot \mathbf{R}_{sr} \right) + \left(\frac{m_s}{2T_s} c_s^2 - \frac{5}{2} \right) \boldsymbol{c}_s \cdot \frac{\nabla_{\boldsymbol{x}} T_s}{T_s} \right] f_s^{(0)} .$$

Hence, (5.17) can be reformulated into

$$\mathcal{L}(h_s^{(1)}) = \left[\frac{1}{n_s T_s} \boldsymbol{c}_s \cdot \mathbf{R}_{sr} + \frac{m_s}{T_s} \left(\boldsymbol{c}_s \otimes \boldsymbol{c}_s - \frac{c_s^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u}_s \right.$$
$$\left. + \frac{2}{3} \frac{1}{n_s T_s} \left(\frac{m_s}{2T_s} \boldsymbol{c}_s^2 - \frac{3}{2} \right) \left(\mathrm{S}_{sr} - \boldsymbol{u}_s \cdot \mathbf{R}_{sr} \right) + \left(\frac{m_s}{2T_s} c_s^2 - \frac{5}{2} \right) \boldsymbol{c}_s \cdot \frac{\nabla_{\boldsymbol{x}} T_s}{T_s} \right] f_s^{(0)} \tag{5.21}$$
$$- \nu_{sr}^{(0)} \left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right) .$$

Remark. *Since in the first-order expansion* (5.17), $f_s^{(1)}$ *appears only within the integrals defining* $\mathcal{L}(h_s^{(1)})$, *it is not possible to derive an explicit expression for it, as done in* (3.27) *for the classical collision dominated regime. Nonetheless, by computing the weak form of* (5.21) *with respect to the test functions* $\varphi_s = m_s \boldsymbol{c}_s \otimes \boldsymbol{c}_s$, $\frac{1}{2} m_s \boldsymbol{c}_s c_s^2$, *we can still obtain explicit expressions for* $\underline{\boldsymbol{P}}_s^{(1)}$ *and* $\boldsymbol{q}_s^{(1)}$.

Remark. *As for the right-hand side of the weak form of* (5.21) *with respect to the test functions* $\varphi_s = m_s \boldsymbol{c}_s \otimes \boldsymbol{c}_s$, $\frac{1}{2} m_s \boldsymbol{c}_s c_s^2$, *the computations are analogous to those performed for the classical collision-dominated regime, and the corresponding results can be directly recovered from [8], [9].*

We now compute $m_s \int_{\mathbb{R}^3} c_i^s c_j^s \mathcal{L}(h_s^{(1)}) d\boldsymbol{v}$. Writing

$$c_i^s c_j^s = v_i v_j - u_i^s v_j - u_j^s v_i + u_i^s u_j^s ,$$

and recalling that $\ker(\mathcal{L}(h_s^{(1)})) = \mathrm{span}\{1, \boldsymbol{v}, v^2\}$, the contribution from the second, third and fourth term vanish when paired to $\mathcal{L}(h_s^{(1)})$. Hence it suffices to consider

$$m_s \int_{\mathbb{R}^3} v_i v_j \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \,.$$

For it, recalling that under the assumption (3.36) $g_s(\mu) = \lambda_s = \text{const.}$, from which $\Lambda_s = 4\pi\lambda_s$, we obtain

$$\begin{aligned}
& m_s\lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i v_j \Big[f_s^{(0)}(\boldsymbol{v}'_s) f_s^{(1)}(\boldsymbol{w}'_s) + f_s^{(1)}(\boldsymbol{v}'_s) f_s^{(0)}(\boldsymbol{w}'_s) \\
& - f_s^{(0)}(\boldsymbol{v}) \underbrace{f_s^{(1)}(\boldsymbol{w})}_{=n_r^{(1)}=0} - f_s^{(1)}(\boldsymbol{v}) \underbrace{f_s^{(0)}(\boldsymbol{w})}_{=n_r} \Big] d\boldsymbol{v} d\boldsymbol{w} d\omega \\
& = m_s\lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i v_j \Big[f_s^{(0)}(\boldsymbol{v}'_s) f_s^{(1)}(\boldsymbol{w}'_s) + f_s^{(1)}(\boldsymbol{v}'_s) f_s^{(0)}(\boldsymbol{w}'_s) \Big] d\boldsymbol{v} d\boldsymbol{w} d\omega \\
& - 4\pi m_s \lambda_s n_s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}
\end{aligned}$$

By exchanging pre- and post-collision velocities in the first integral and recalling the integral on post-collision velocities (A.11), we get

$$\begin{aligned}
& = \pi m_s \lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3} \Big[v_i v_j + w_i w_j + \frac{\delta_{ij}}{3}(v^2 + w^2 - 2\boldsymbol{v}\cdot\boldsymbol{w}) + v_i w_j + v_j w_i \Big] \\
& \times \Big[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_s^{(0)}(\boldsymbol{w}) \Big] d\boldsymbol{v} d\boldsymbol{w} - 4\pi m_s \lambda_s n_s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \\
& = \pi \lambda_s m_s \Bigg(n_s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} + n_s \int_{\mathbb{R}^3} w_i w_j f_s^{(1)}(\boldsymbol{w}) d\boldsymbol{w} + \frac{\delta_{ij}}{3} n_s \underbrace{\int_{\mathbb{R}^3} v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0} \\
& + \frac{\delta_{ij}}{3} n_s \underbrace{\int_{\mathbb{R}^3} w^2 f_s^{(1)}(\boldsymbol{w}) d\boldsymbol{v}}_{=0} - \frac{2}{3}\delta_{ij} \int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(0)}(\boldsymbol{v}) d\boldsymbol{v} \cdot \underbrace{\int_{\mathbb{R}^3} \boldsymbol{w} f_s^{(1)}(\boldsymbol{w}) d\boldsymbol{w}}_{=0} \\
& - \frac{2}{3}\delta_{ij} \underbrace{\int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0} \cdot \int_{\mathbb{R}^3} \boldsymbol{w} f_s^{(0)}(\boldsymbol{w}) d\boldsymbol{w} \\
& + \int_{\mathbb{R}^3} v_i f_s^{(0)}(\boldsymbol{v}) d\boldsymbol{v} \underbrace{\int_{\mathbb{R}^3} w_j f_s^{(1)}(\boldsymbol{w}) d\boldsymbol{w}}_{=0} + \underbrace{\int_{\mathbb{R}^3} v_i f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0} \int_{\mathbb{R}^3} w_j f_s^{(0)}(\boldsymbol{w}) d\boldsymbol{w} \\
& + \int_{\mathbb{R}^3} v_j f_s^{(0)}(\boldsymbol{v}) d\boldsymbol{v} \underbrace{\int_{\mathbb{R}^3} w_i f_s^{(1)}(\boldsymbol{w}) d\boldsymbol{w}}_{=0} + \underbrace{\int_{\mathbb{R}^3} v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0} \int_{\mathbb{R}^3} w_i f_s^{(0)}(\boldsymbol{w}) d\boldsymbol{w} - 4n_s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} \Bigg) \\
& = -2\pi\lambda_s \rho_s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \,,
\end{aligned}$$

where we made use of (5.4).
Furthermore,

$$\int_{\mathbb{R}^3} v_i v_j f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \tag{5.22}$$
$$= \int_{\mathbb{R}^3} c_i^s c_j^s f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} + u_j^s \underbrace{\int_{\mathbb{R}^3} (v_i - u_i^s) f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0} + u_i^s \underbrace{\int_{\mathbb{R}^3} (v_j - u_j^s) f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0} + u_i^s u_j^s \underbrace{\int_{\mathbb{R}^3} f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}}_{=0},$$

and we have reached

$$m_s \int_{\mathbb{R}^3} c_i^s c_j^s \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} = -2\pi\lambda_s \rho_s \int_{\mathbb{R}^3} c_i^s c_j^s f_s^{(1)}(\boldsymbol{v}) = -2\pi\lambda_s n_s P_{ij}^{s^{(1)}}, \tag{5.23}$$

hence, from (5.21), we find

$$P_{ij}^{s^{(1)}} = -\frac{m_s}{2\pi\lambda_s n_s} \Bigg\{ \frac{1}{n_s T_s} \int_{\mathbb{R}^3} (c_i^s c_j^s \boldsymbol{c}_s \cdot \mathbf{R}_{sr}) f_s^{(0)} d\boldsymbol{v} + \frac{m_s}{T_s} \int_{\mathbb{R}^3} \left[c_i^s c_j^s \left(\boldsymbol{c}_s \otimes \boldsymbol{c}_s - \frac{c_s^2}{3} \underline{\boldsymbol{I}} \right) : \nabla_{\boldsymbol{x}} \boldsymbol{u}_s \right] f_s^{(0)}$$
$$+ \frac{2}{3} \frac{1}{n_s T_s} \int_{\mathbb{R}^3} \left[c_i^s c_j^s \left(\frac{m_s}{2T_s} c_s^2 - \frac{3}{2} \right) (\mathrm{S}_{sr} - \boldsymbol{u}_s \cdot \mathbf{R}_{sr}) \right] f_s^{(0)} d\boldsymbol{v}$$
$$+ \int_{\mathbb{R}^3} \left[c_i^s c_j^s \left(\frac{m_s}{2T_s} c_s^2 - \frac{5}{2} \right) \boldsymbol{c}_s \cdot \frac{\nabla_{\boldsymbol{x}} T_s}{T_s} \right] f_s^{(0)} d\boldsymbol{v} \Bigg\} - \nu_{sr}^{(0)} \int_{\mathbb{R}^3} c_i^s c_j^s \left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)} \right) d\boldsymbol{v}.$$

As concerns the right-hand side, computations are analogous to the ones performed in the classical collision-dominated regime and referring to [9, 8] for a more detailed view of those, it yields

$$\underline{\boldsymbol{P}}_s^{(1)} = -\frac{T_s}{2\pi\lambda_s} \left(\frac{\partial u_i^s}{\partial x_j} + \frac{\partial u_j^s}{\partial x_i} - \frac{2}{3} \nabla_{\boldsymbol{x}} \cdot \boldsymbol{u}_s \delta_{ij} \right)$$
$$+ \frac{1}{2\pi\lambda_s n_s} \nu_{sr}^{(0)} \rho_s (a_{sr}^{(0)})^2 \left[(\boldsymbol{u}_r - \boldsymbol{u}_s) \otimes (\boldsymbol{u}_r - \boldsymbol{u}_s) - \frac{1}{3} |\boldsymbol{u}_r - \boldsymbol{u}_s|^2 \underline{\boldsymbol{I}} \right], \quad s, r = 1, 2, \quad r \neq s.$$

in which we can notice the strain tensor multiplied by the viscosity coefficient

$$\mu_s = \frac{T_s}{2\pi\lambda_s}$$

and also additional contributions involving the differences among species mean velocities, specific of the present multi-velocity and multi-temperature hydrodynamic regime.

As regards the first-order approximation of the heat flux vector $\boldsymbol{q}_s^{(1)}$, starting from

$$c_i c_s^2 = v_i v^2 + v_i u_s^2 - 2(u_i^s v_i^2 + u_j^s v_i v_j + u_k^s v_i v_k) - u_i^s v^2 - u_i^s u_s^2 + 2u_i^s \boldsymbol{u}_s \cdot \boldsymbol{v}, \tag{5.24}$$

and recalling that $\ker(\mathcal{L}(h_s^{(1)})) = \operatorname{span}\{1, \boldsymbol{v}, v^2\}$, we get

$$\frac{1}{2}m_s \int_{\mathbb{R}^3} c_i^s c_s^2 \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} = \frac{1}{2}m_s \int_{\mathbb{R}^3} v_i v^2 \mathcal{L}(h_s^{(1)}) d\boldsymbol{v}$$
$$- m_s u_i^s \int_{\mathbb{R}^3} v_i^2 \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} - m_s u_j^s \int_{\mathbb{R}^3} v_i v_j \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} - m_s u_k^s \int_{\mathbb{R}^3} v_i v_k \mathcal{L}(h_s^{(1)}) d\boldsymbol{v}$$
$$= \frac{1}{2}m_s \int_{\mathbb{R}^3} v_i v^2 \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} + 2\pi\lambda_s n_s \left(u_i^s P_{ii}^{s^{(1)}} + u_j^s P_{ij}^{s^{(1)}} + u_k^s P_{ik}^{s^{(1)}} \right), \qquad (5.25)$$

where we used (5.22), (5.23).
Now, recalling (5.4) and (A.10), we derive

$$\frac{1}{2}m_s \int_{\mathbb{R}^3} v_i v^2 \mathcal{L}(h_s^{(1)}) d\boldsymbol{v}$$
$$= \frac{1}{2}m_s\lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i v^2 \Big[f_s^{(0)}(\boldsymbol{v}'_s) f_s^{(1)}(\boldsymbol{w}'_s) + f_s^{(1)}(\boldsymbol{v}'_s) f_s^{(0)}(\boldsymbol{w}'_s) - f_s^{(0)}(\boldsymbol{v}) \underbrace{f_s^{(1)}(\boldsymbol{w})}_{=n_s^{(1)}=0} - f_s^{(1)}(\boldsymbol{v}) \underbrace{f_s^{(0)}(\boldsymbol{w})}_{=n_s} \Big] d\boldsymbol{v} d\boldsymbol{w} d\omega$$
$$= \frac{1}{2}m_s\lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v'_i v'^2 \Big[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_s^{(0)}(\boldsymbol{w}) \Big] d\boldsymbol{v} d\boldsymbol{w} d\omega - 2\pi m_s n_s \lambda_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}$$
$$= \frac{\pi}{2}m_s\lambda_s \int_{\mathbb{R}^3\times\mathbb{R}^3} \Big[v_i v^2 + w_i w^2 + \underbrace{v^2 w_i + v_i w^2}_{=0} + \frac{1}{3}(v^2 + w^2 - 2v_i w_i - 2v_j w_j - 2v_k w_k)(v_i + w_i) \Big]$$
$$\times \Big[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_s^{(0)}(\boldsymbol{w}) \Big] d\boldsymbol{v} d\boldsymbol{w} - 2\pi\lambda_s\rho_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}$$

$$= \frac{\pi}{2}m_s\lambda_s \Bigg\{ 2n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}$$
$$+ \frac{1}{3} \int_{\mathbb{R}^3\times\mathbb{R}^3} \big(v_i v^2 + w_i w^2 + \underbrace{v^2 w_i + v_i w^2}_{=0} - 2v_i^2 w_i - 2v_i w_i^2 - 2v_i v_j w_j - 2v_j w_i w_j - 2v_i v_k w_k - 2v_k w_i w_k \big)$$
$$\times \Big[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_s^{(0)}(\boldsymbol{w}) \Big] d\boldsymbol{v} d\boldsymbol{w} \Bigg\} - 2\pi\lambda_s n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}$$
$$= \frac{\pi}{2}m_s\lambda_s \Bigg(\frac{8}{3}n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} - \frac{4}{3}n_s u_i^s \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} - \frac{4}{3}n_s u_j^s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v}$$
$$- \frac{4}{3}n_s u_k^s \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} \Bigg) - 2\pi\lambda_s n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v}$$
$$= -\frac{2}{3}\pi\lambda_s\rho_s \Bigg(\int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} + u_i^s \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} + u_j^s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + u_k^s \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} \Bigg).$$

As concerns $\int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v}$, from (5.4), (5.24), we have

$$\int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} = \int_{\mathbb{R}^3} c_i^s c_s^2 f_s^{(1)} d\boldsymbol{v} + 2\Bigg(u_i^s \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} + u_j^s \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + u_k^s \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} \Bigg).$$

Hence, using (5.22), (5.23) we obtain

$$
\begin{aligned}
&\frac{1}{2}m_s\int_{\mathbb{R}^3} v_i v^2\mathcal{L}(h_s^{(1)})d\boldsymbol{v} = -\frac{2}{3}\pi\lambda_s\rho_s\int_{\mathbb{R}^3} c_i^s c_s^2 f_s^{(1)}d\boldsymbol{v}\\
&-2\pi\lambda_s\rho_s\left(u_i^s\int_{\mathbb{R}^3} v_i^2 f_s^{(1)}d\boldsymbol{v} + u_j^s\int_{\mathbb{R}^3} v_i v_j f_s^{(1)}d\boldsymbol{v} + u_k^s\int_{\mathbb{R}^3} v_i v_k f_s^{(1)}d\boldsymbol{v}\right)\\
&= -\frac{2}{3}\pi\lambda_s\rho_s\int_{\mathbb{R}^3} c_i^s c_s^2 f_s^{(1)}d\boldsymbol{v} - 2\pi\lambda_s n_s\left(u_i^s P_{ii}^{s^{(1)}} + u_j^s P_{ij}^{s^{(1)}} + u_k^s P_{ik}^{s^{(1)}}\right).
\end{aligned}
$$

Ultimately, from (5.25), we obtain

$$
m_s\int_{\mathbb{R}^3} c_i^s c_s^2\mathcal{L}(h_s^{(1)})d\boldsymbol{v} = -\frac{4}{3}\pi\lambda_s n_s q_i^{s^{(1)}}.
$$

As for the pressure tensor, we resort to [9, 8] for the computation of the following from (5.21)

$$
\begin{aligned}
q_i^{s^{(1)}} &= -\frac{3m_s}{4\pi\lambda_s n_s}\Bigg\{\frac{1}{n_sT_s}\int_{\mathbb{R}^3}(c_i^s c_s^2\boldsymbol{c}_s\cdot\mathbf{R}_{sr})f_s^{(0)}d\boldsymbol{v} + \frac{m_s}{T_s}\int_{\mathbb{R}^3}\left[c_i^s c_s^2\left(\boldsymbol{c}_s\otimes\boldsymbol{c}_s - \frac{c_s^2}{3}\underline{\boldsymbol{I}}\right) : \nabla_{\boldsymbol{x}}\boldsymbol{u}_s\right]f_s^{(0)}\\
&+\frac{2}{3}\frac{1}{n_sT_s}\int_{\mathbb{R}^3}\left[c_i^s c_s^2\left(\frac{m_s}{2T_s}\boldsymbol{c}_s^2 - \frac{3}{2}\right)(\mathrm{S}_{sr} - \boldsymbol{u}_s\cdot\mathbf{R}_{sr})\right]f_s^{(0)}d\boldsymbol{v} + \int_{\mathbb{R}^3}\left[c_i^s c_s^2\left(\frac{m_s}{2T_s}c_s^2 - \frac{5}{2}\right)\boldsymbol{c}_s\cdot\frac{\nabla_{\boldsymbol{x}}T_s}{T_s}\right]f_s^{(0)}d\boldsymbol{v}\\
&-\nu_{sr}^{(0)}\int_{\mathbb{R}^3} c_i^s c_s^2\left(\mathcal{M}_{sr}^{(0)} - f_s^{(0)}\right)d\boldsymbol{v},
\end{aligned}
$$

we obtain

$$
\begin{aligned}
\boldsymbol{q}_s^{(1)} &= -\frac{15T_s}{8\pi m_s\lambda_s}\nabla_{\boldsymbol{x}}T_s + \frac{15}{4\pi\lambda_s}\alpha_{sr}\nu_{sr}^{(0)}(a_{sr}^{(0)})^2(T_r - T_s)(\boldsymbol{u}_r - \boldsymbol{u}_s)\\
&+\frac{4}{\pi\lambda_s}\nu_{sr}^{(0)}(a_{sr}^{(0)})^2(5\alpha_{rs} - a_{sr}^{(0)})(\boldsymbol{u}_r - \boldsymbol{u}_s)^3, \quad s, r = 1, 2, \quad r\neq s,
\end{aligned}
$$

where the first term on the right-hand-side is proportional to the opposite of the gradient of species temperature by means of the conductivity coefficient

$$
\xi_s = \frac{15T_s}{8\pi m_s\lambda_s}.
$$

As in the case of the pressure tensor, the additional contributions involving differences between species velocities and species temperatures are due to the considered asymptotic limit in which only intra-species collisions play the dominant role.

Remark. *The same computations can be repeated with the standard Maxwellian assumption*

$$
g_s = g_s(\mu),
$$

where μ is the deflection angle $\mu = \hat{\mu}\cdot\omega$, obtaining the same results, provided that one substitutes

$$
\frac{8\pi}{3}\lambda_s \quad \textit{with} \quad \lambda_s^{(2)} = 2\pi\int_0^\pi g_{ss}(\mu)(1-\cos^2(\mu))\sin(\mu)d\mu.
$$

5.2 Fluid-kinetic equations for mixtures

Sticking to the assumption $\chi_{sr} = \delta_{sr}$, as in (5.1), we consider a binary gas mixture in which one species has a mass much heavier than the other, i.e., $m_1 >> m_2$.

By setting

$$\beta_{11} = \varepsilon\,, \quad \beta_{12} = \beta_{12} = 1\,, \quad \beta_{22} = \frac{1}{\varepsilon}\,,$$

in the dimensionless system (5.1), we obtain the following scaling

$$\begin{cases} \dfrac{\partial f_1}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_1 = \dfrac{1}{\varepsilon} Q_{11} + \nu_{12} \left(\mathcal{M}_{12} - f_1 \right) \\ \dfrac{\partial f_2}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_2 = \nu_{21} \left(\mathcal{M}_{21} - f_2 \right) + \varepsilon Q_{22}\,. \end{cases} \tag{5.26}$$

This framework defines a rescaled kinetic system that in the asymptotic limit will lead to the so-called fluid–kinetic regime, which arises when the components of a mixture experience collisions on different timescales. In such situations, it can be seen how the different timescales influence the trend to equilibrium: one species rapidly attains local equilibrium and can be described by macroscopic balance equations, while the other remains out of equilibrium and requires a kinetic description, [22, 33].

In the regime considered here, the asymmetry between the two species originates from their strongly disparate masses. The heavier component relaxes toward equilibrium much faster than the lighter one, as its larger mass implies smaller velocity variations in individual collisions and thus a faster equilibration process on the kinetic timescale. Accordingly, its distribution function is expanded as

$$f_1 = f_1^{(0)} + \varepsilon f_1^{(1)}\,,$$

and we can apply the standard Chapman-Enskog expansion.

In contrast, the light component undergoes more significant changes in velocity during collisions and relaxes on a slower timescale. Its distribution function is therefore written as

$$f_2 = \mathcal{M}_2 + g_2,$$

without introducing the small parameter ε, since g_2 may represent a deviation of order one from local equilibrium.

This scaling emphasizes the physical structure of the fluid–kinetic mixture: the heavy species rapidly equilibrates and behaves as a fluid, while the light species evolves on a kinetic timescale, exchanging momentum and energy with the species 1, active as a background.

Going through the standard Chapman-Enskog expansion for species 1, making use of what computed in the previous section, at the leading order we find

$$Q_{11}(f_1^{(0)}) = 0\,. \tag{5.27}$$

and this implies

$$f_1^{(0)} = \mathcal{M}_1 = n_1 \left(\frac{m_1}{2\pi T_1}\right)^{\frac{3}{2}} \exp\left\{-\frac{(\boldsymbol{v}-\boldsymbol{u}_1)^2}{2T_1}\right\}\,,$$

and that the hydrodynamic variables will be the macroscopic fields of species 1, so that

$$\begin{cases} n_1^{(0)} = n_1 \quad n_1^{(1)} = 0 \\ \boldsymbol{u}_1^{(0)} = \boldsymbol{u}_1 \quad \boldsymbol{u}_1^{(1)} = \mathbf{0} \\ T_1^{(0)} = T_1\,, \quad T_1^{(1)} = 0\,. \end{cases}$$

By following the same procedure performed in the previous section, we directly find the Navier-Stokes balance equations for the macroscopic fields $n_1, \boldsymbol{u}_1, T_1$

$$\begin{cases} \dfrac{\partial n_1}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (n_1 \boldsymbol{u}_1) = 0 \\[2ex] \dfrac{\partial}{\partial t}\big(\rho_1 \boldsymbol{u}_1\big) + \nabla_{\boldsymbol{x}} \cdot \big(\rho_1 \boldsymbol{u}_1 \otimes \boldsymbol{u}_1 + n_1 T_1 \underline{\boldsymbol{I}}\big) + \varepsilon \nabla_{\boldsymbol{x}} \cdot \underline{\boldsymbol{P}}_1^{(1)} = \mathbf{R}_{12} \\[2ex] \dfrac{\partial}{\partial t}\left[\dfrac{1}{2}\rho_1 u_1^2 + \dfrac{3}{2} n_1 T_1\right] \nabla_{\boldsymbol{x}} \cdot \left[\left(\dfrac{1}{2}\rho_1 u_1^2 + \dfrac{5}{2} n_1 T_1\right)\boldsymbol{u}_1\right] + \varepsilon \nabla_{\boldsymbol{x}} \cdot \big(\underline{\boldsymbol{P}}_1^{(1)} \cdot \boldsymbol{u}_1 + \boldsymbol{q}_1^{(1)}\big) = \mathrm{S}_{12}\,, \end{cases} \tag{5.28}$$

where

$$\mathbf{R}_{12} = \Lambda_{12} \alpha_{21} m_1 n_1 n_2 (\boldsymbol{u}_2 - \boldsymbol{u}_1)$$
$$\mathrm{S}_{12} = \Lambda_{12} \alpha_{12} \alpha_{21} n_1 n_2 \big[3(T_2 - T_1) + (m_1 \boldsymbol{u}_1 + m_2 \boldsymbol{u}_2) \cdot (\boldsymbol{u}_2 - \boldsymbol{u}_1)\big]\,,$$

and the closure of the system above is provided by

$$\begin{aligned} \underline{\boldsymbol{P}}_1^{(1)} &= -\frac{T_1}{2\pi\lambda_1}\left(\frac{\partial u_i^1}{\partial x_j} + \frac{\partial u_j^1}{\partial x_i} - \frac{2}{3}\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u}_1 \delta_{ij}\right) \\ &+ \frac{1}{2\pi\lambda_1 n_1} \nu_{12}^{(0)} \rho_1 \big(a_{12}^{(0)}\big)^2 \left[(\boldsymbol{u}_2 - \boldsymbol{u}_1) \otimes (\boldsymbol{u}_2 - \boldsymbol{u}_1) - \frac{1}{3}|\boldsymbol{u}_2 - \boldsymbol{u}_1|^2 \underline{\boldsymbol{I}}\right]\,, \\ \mathbf{q}_1^{(1)} &= -\frac{15 T_1}{8\pi m_1 \lambda_1} \nabla_{\boldsymbol{x}} T_1 + \frac{15}{4\pi\lambda_1} \alpha_{12} \nu_{12}^{(0)} (a_{12}^{(0)})^2 (T_2 - T_1)(\boldsymbol{u}_2 - \boldsymbol{u}_1) \\ &+ \frac{4}{\pi\lambda_1} \nu_{12}^{(0)} \big(a_{12}^{(0)}\big)^2 (5\alpha_{21} - a_{12}^{(0)})(\boldsymbol{u}_2 - \boldsymbol{u}_1)^3\,. \end{aligned}$$

As concerns species 2, we aim to extend the micro–macro decomposition introduced in [2, 21]. This approach, originally developed for numerical schemes applied to Boltzmann-type equations for mixtures, allows one to accurately capture the compressible Navier–Stokes dynamics at small–Knudsen-number. The central idea is to express the distribution function as the sum of its local equilibrium, which satisfies a fluid-type equation, and a kinetic remainder accounting for deviations from equilibrium. Accordingly, we decompose f_2 as follows

$$f_2 = \mathcal{M}_2 + g_2 \,,$$

and since f_2 and $\mathcal{M}_2$ share the same zeroth, first and second order moments, we have $\langle g_2, \varphi_2\rangle = 0$, for $\varphi_2 = 1, \boldsymbol{v}, v^2$.

Using the decomposition above, the equation for species 2 can be reformulated as

$$\begin{aligned}\frac{\partial \mathcal{M}_2}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}\mathcal{M}_2 + \frac{\partial g_2}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} g_2 & \qquad (5.29)\\ = \nu_{21}\left(\mathcal{M}_{21} - \mathcal{M}_2 - g_2\right) + \varepsilon\big[\underbrace{Q_{22}(\mathcal{M}_2)}_{=0} + \mathcal{L}_2(\mathcal{M}_2, g_2) + Q_{22}(g_2)\big]\,, &\end{aligned}$$

where $\mathcal{L}_2(\mathcal{M}_2, g_2)$ is the linearized Boltzmann operator of species 2, i.e.

$$\mathcal{L}_2(\mathcal{M}_2, g_2) = Q_{22}(\mathcal{M}_2, g_2) + Q_{22}(g_2, \mathcal{M}_2)\,,$$

which, by standard arguments, can be shown to possess the same collision invariants $1, \boldsymbol{v}, v^2$ as the linearized Boltzmann intra–species operator $\mathcal{L}(h_s^{(1)})$ introduced in the previous chapters.

Let us consider the Hilbert space $L^2_{\mathcal{M}_2}$,

$$L^2_{\mathcal{M}_2} := \left\{\phi : \phi\mathcal{M}_2^{-\frac{1}{2}} \in L^2 d\boldsymbol{v}\right\}\,,$$

with the weighted inner product

$$(\phi, \psi) := \int_{\mathbb{R}^3} \phi\psi\mathcal{M}_2^{-1} d\boldsymbol{v}\,.$$

Given its subspace

$$\mathcal{N}_2 = \operatorname{span}\left\{\mathcal{M}_2, \boldsymbol{v}\mathcal{M}_2, v^2\mathcal{M}_2\right\}\,,$$

we call $\Pi_{\mathcal{M}_2}$ the orthogonal projection in $L^2_{\mathcal{M}_2}$ on the subspace $\mathcal{N}_2$.
Given the orthonormal basis $\mathcal{B}_2$ of $\mathcal{N}_2$, we have

$$\mathcal{B}_2 = \operatorname{span}\left\{ n_2^{-\frac{1}{2}}\mathcal{M}_2,\quad \frac{1}{\sqrt{3}}\frac{\boldsymbol{v}-\boldsymbol{u}_2}{\left(\frac{T_2}{m_2}\right)^{\frac{1}{2}}} n_2^{-\frac{1}{2}}\mathcal{M}_2,\quad \sqrt{\frac{1}{6}}\left(\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right) n_2^{-\frac{1}{2}}\mathcal{M}_2 \right\} := \{b_2^1, b_2^2, b_2^3\}\,,$$

and

$$\begin{aligned}\Pi_{\mathcal{M}_2}(\phi) &= \sum_{n=1}^{3} (\phi, b_2^n) b_2^n \qquad (5.30)\\ &= \frac{\mathcal{M}_2}{n_2}\left\{\langle\phi, 1\rangle + \frac{m_2}{3T_2}(\boldsymbol{v}-\boldsymbol{u}_2)\cdot\langle(\boldsymbol{v}-\boldsymbol{u}_2), \phi\rangle + \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\langle\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right], \phi\rangle\right\}\end{aligned}$$

Lemma 3. *From standard properties of the orthogonal projection on an Hilbert space, it holds that*

$$
\begin{aligned}
&(I-\Pi_{\mathcal{M}_2})(\mathcal{M}_2) = (I-\Pi_{\mathcal{M}_2})\left(\frac{\partial \mathcal{M}_2}{\partial t}\right) = 0\,,\\
&\Pi_{\mathcal{M}_2}(g_2) = \Pi_{\mathcal{M}_2}\left(\frac{\partial g_2}{\partial t}\right) = 0\,,\\
&\Pi_{\mathcal{M}_2}(\mathcal{L}_2(\mathcal{M}_2, g_2)) = \Pi_{\mathcal{M}_2}(Q_{22}(g_2)) = 0\,,
\end{aligned}
$$

and

$$
\begin{aligned}
\Pi_{\mathcal{M}_2}(\mathcal{M}_{21}) = \mathcal{M}_2 \Bigg\{ & 1 + \frac{m_2 a_{21}(\boldsymbol{u}_1 - \boldsymbol{u}_2)\cdot(\boldsymbol{v}-\boldsymbol{u}_2)}{3T_2} + \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right] \\
\times & \left[\frac{3T_{21}}{T_2} + \frac{m_2}{T_2}\left(\boldsymbol{u}_{21}^2 + a_{21}\boldsymbol{u}_2\cdot(\boldsymbol{u}_2 - \boldsymbol{u}_1)\right) - 3\right]\Bigg\}.
\end{aligned}
$$

Proof.

- Since $\Pi_{\mathcal{M}_2}(\mathcal{M}_2) = \mathcal{M}_2$, it holds $(I-\Pi_{\mathcal{M}_2})(\mathcal{M}_2) = 0$.
- From (5.18), $\dfrac{\partial \mathcal{M}_2}{\partial t}$ is a linear combination of $\mathcal{M}_2, \boldsymbol{v}\mathcal{M}_2, v^2\mathcal{M}_2$. Hence $\frac{\partial \mathcal{M}_2}{\partial t} \in \mathcal{N}_2$ and therefore $\Pi_{\mathcal{M}_2}\left(\frac{\partial \mathcal{M}_2}{\partial t}\right) = \frac{\partial \mathcal{M}_2}{\partial t}$.
- From $\langle \varphi_2(\boldsymbol{v}), g_2\rangle = 0$, for $\varphi_2(\boldsymbol{v}) = 1, \boldsymbol{v}, v^2$, it follows that the weighted integral

$$
(\varphi_2(\boldsymbol{v})\mathcal{M}_2, g_2) = \int_{\mathbb{R}^3} \varphi_2(\boldsymbol{v}) g_2 d\boldsymbol{v} = 0 \implies g_2 \perp \mathcal{N}_2 \implies \Pi_{\mathcal{M}_2}(g_2) = 0\,.
$$

- Analogously

$$
\left(\varphi_2(\boldsymbol{v})\mathcal{M}_2, \frac{\partial g_2}{\partial t}\right) = \frac{\partial}{\partial t}(\varphi_2(\boldsymbol{v})\mathcal{M}_2, g_2) = 0 \implies \Pi_{\mathcal{M}_2}\left(\frac{\partial g_2}{\partial t}\right) = 0\,.
$$

- From (5.30) and the fact that 1, $\boldsymbol{v}$, v^2 are collision invariants for both $\mathcal{L}(\mathcal{M}_2, g_2)\,,\ Q_{22}(g_2)$ it follows that they are orthogonal to $\mathcal{N}_2$ and then

$$
\Pi_{\mathcal{M}_2}(\mathcal{L}(\mathcal{M}_2, g_2)) = \Pi_{\mathcal{M}_2}(Q_{22}(g_2)) = 0\,.
$$

- From $\Pi_{\mathcal{M}_2}(\phi) = \sum_{n=1}^{3}(\phi, b_2^n)b_2^n$, we get

$$
\begin{aligned}
&\Pi_{\mathcal{M}_2}(\mathcal{M}_{21}) = \sum_{n=1}^{3}(\mathcal{M}_{21}, b_2^n)b_2^n = \sum_{n=1}^{3} b_2^n \int_{\mathbb{R}^3} \mathcal{M}_{21} b_2^n \mathcal{M}_2^{-1} d\boldsymbol{v}\\
&= \frac{\mathcal{M}_2}{n_2}\int_{\mathbb{R}^3} \mathcal{M}_{21} d\boldsymbol{v} + \frac{1}{3}\frac{m_2(\boldsymbol{v}-\boldsymbol{u}_2)}{T_2}\frac{\mathcal{M}_2}{n_2}\cdot \int_{\mathbb{R}^3}(\boldsymbol{v}-\boldsymbol{u}_2)\mathcal{M}_{21} d\boldsymbol{v}\\
&+ \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\frac{\mathcal{M}_2}{n_2}\int_{\mathbb{R}^3}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\mathcal{M}_{21} d\boldsymbol{v}\\
&= \mathcal{M}_2 + \frac{1}{3}\frac{m_2 a_{21}(\boldsymbol{u}_1-\boldsymbol{u}_2)\cdot(\boldsymbol{v}-\boldsymbol{u}_2)}{T_2}\mathcal{M}_2 + \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\frac{\mathcal{M}_2}{n_2}\\
&\times\left[\frac{m_2}{T_2}\int_{\mathbb{R}^3}(v^2+u_2^2-2\boldsymbol{u}_2\cdot\boldsymbol{v})\mathcal{M}_{21} d\boldsymbol{v} - 3n_2\right]
\end{aligned}
$$

$$
\begin{aligned}
&= \mathcal{M}_2\Bigg\{1 + \frac{m_2 a_{21}(\boldsymbol{u}_1-\boldsymbol{u}_2)\cdot(\boldsymbol{v}-\boldsymbol{u}_2)}{3T_2} + \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\\
&\times\left[\frac{m_2}{T_2}\left(\boldsymbol{u}_{21}^2 + \frac{3T_{21}}{m_2} + \boldsymbol{u}_2\cdot(\boldsymbol{u}_2-\boldsymbol{u}_{21})\right) - 3\right]\Bigg\}\\
&= \mathcal{M}_2\Bigg\{1 + \frac{m_2 a_{21}(\boldsymbol{u}_1-\boldsymbol{u}_2)\cdot(\boldsymbol{v}-\boldsymbol{u}_2)}{3T_2} + \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\\
&\times\left[\frac{3T_{21}}{T_2} + \frac{m_2}{T_2}\left(\boldsymbol{u}_{21}^2 + a_{21}\boldsymbol{u}_2\cdot(\boldsymbol{u}_2-\boldsymbol{u}_1)\right) - 3\right]\Bigg\}.
\end{aligned}
$$

□

We now apply the orthogonal projection $I - \Pi_{\mathcal{M}_2}$ to the kinetic equation (5.29) and, using lemma 3, we obtain

$$
\begin{aligned}
&\frac{\partial g_2}{\partial t} + (I-\Pi_{\mathcal{M}_2})(\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}\mathcal{M}_2) + (I-\Pi_{\mathcal{M}_2})(\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} g_2)\\
&= \nu_{21}(I-\Pi_{\mathcal{M}_2})\left(\mathcal{M}_{21}-\mathcal{M}_2-g_2\right) + \varepsilon\left[\mathcal{L}(\mathcal{M}_2,g_2) + Q_{22}(g_2)\right]\\
&= \nu_{21}\Bigg\{\mathcal{M}_{21} - \mathcal{M}_2\Bigg\{1 + \frac{m_2 a_{21}(\boldsymbol{u}_1-\boldsymbol{u}_2)\cdot(\boldsymbol{v}-\boldsymbol{u}_2)}{3T_2} + \frac{1}{6}\left[\frac{(\boldsymbol{v}-\boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3\right]\\
&\times\left[\frac{3T_{21}}{T_2} + \frac{m_2}{T_2}\left(\boldsymbol{u}_{21}^2 + a_{21}\boldsymbol{u}_2\cdot(\boldsymbol{u}_2-\boldsymbol{u}_1)\right) - 3\right]\Bigg\} - g_2\Bigg\} + \varepsilon\left[\mathcal{L}(\mathcal{M}_2,g_2) + Q_{22}(g_2)\right].
\end{aligned}
$$

On the other hand, computing the weak form of (5.29) with the collision invariants $\varphi_2(\boldsymbol{v}) = 1, \boldsymbol{v}, v^2$, along with $\langle\varphi_2(\boldsymbol{v}), g_2\rangle = 0$, we get

$$
\begin{aligned}
&\frac{\partial}{\partial t}\langle\varphi_2(\boldsymbol{v}),\mathcal{M}_2\rangle + \nabla_{\boldsymbol{x}}\cdot\langle\varphi_2(\boldsymbol{v}),\boldsymbol{v}\mathcal{M}_{21}\rangle + \nabla_{\boldsymbol{x}}\cdot\langle\varphi_2(\boldsymbol{v}),\boldsymbol{v} g_2\rangle\\
&= \nu_{21}\langle\varphi_2(\boldsymbol{v}),\mathcal{M}_{21}-\mathcal{M}_2\rangle\,.
\end{aligned}
$$

Altogether, this yields a coupled microscopic–macroscopic system for the lighter species

$$\begin{cases} \dfrac{\partial g_2}{\partial t} + (I - \Pi_{\mathcal{M}_2})(\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} \mathcal{M}_2) + (I - \Pi_{\mathcal{M}_2})(\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} g_2) \\ \qquad = \nu_{21} \Bigg\{ \mathcal{M}_{21} - \mathcal{M}_2 \Bigg\{ 1 + \dfrac{m_2 a_{21} (\boldsymbol{u}_1 - \boldsymbol{u}_2) \cdot (\boldsymbol{v} - \boldsymbol{u}_2)}{3 T_2} + \dfrac{1}{6} \left[\dfrac{(\boldsymbol{v} - \boldsymbol{u}_2)^2}{\frac{T_2}{m_2}} - 3 \right] \\ \qquad \times \left[\dfrac{3 T_{21}}{T_2} + \dfrac{m_2}{T_2} \big(\boldsymbol{u}_{21}^2 + a_{21} \boldsymbol{u}_2 \cdot (\boldsymbol{u}_2 - \boldsymbol{u}_1) \big) - 3 \right] \Bigg\} - g_2 \Bigg\} + \varepsilon \left[\mathcal{L}(\mathcal{M}_2, g_2) + Q_{22}(g_2) \right] \\ \dfrac{\partial}{\partial t} \langle \varphi_2(\boldsymbol{v}), \mathcal{M}_2 \rangle + \nabla_{\boldsymbol{x}} \cdot \langle \varphi_2(\boldsymbol{v}), \boldsymbol{v} \mathcal{M}_{21} \rangle + \nabla_{\boldsymbol{x}} \cdot \langle \varphi_2(\boldsymbol{v}), \boldsymbol{v} g_2 \rangle = \nu_{21} \langle \varphi_2(\boldsymbol{v}), \mathcal{M}_{21} - \mathcal{M}_2 \rangle \, . \end{cases}$$

Analogously to what was done for the full-BGK model in [2, 44], it can be proved that the Boltzmann-BGK equation for f_2 in (5.26), is equivalent to the above system of equations for g_2 and $\mathcal{M}_2$.

Chapter 6

Convergence results

In this chapter we investigate the challenging problems of finding convergence results for our mixed Boltzmann-BGK model. Specifically, we look for the rate of convergence of distribution functions towards the Maxwellian ones.
This problem has been studied extensively for single species Boltzmann equation. In particular, in 1979 Cercignani proposed the following conjecture for a single gas [17]:

$$D(f) \geq c\, H(f|\mathcal{M}),$$

where $D(f)$ is the entropy production functional, defined as

$$D(f) = -\int_{\mathbb{R}^3} Q(f) \log f \, d\boldsymbol{v},$$

$H(f|\mathcal{M})$ is the relative entropy with respect to the local Maxwellian $\mathcal{M}$

$$H(f|\mathcal{M}) = \int_{\mathbb{R}^3} f \log \frac{f}{\mathcal{M}} d\boldsymbol{v}\,, \tag{6.1}$$

and c is a positive constant. Subsequent investigations have shown that this conjecture is generally false for all distributions f, due to the presence of very slow relaxation tails [14]. However, a weaker form of the conjecture,

$$D(f) \geq c\, H(f \mid \mathcal{M})^{1+\varepsilon},$$

has been proven to hold under the assumption of hard potentials with angular cut-off [24], while exponential convergence has been established for distributions sufficiently close to equilibrium [37].
Regarding the BGK operator, the stronger version of the conjecture is known to hold for a single in the space homogeneous case and it follows directly from the ordinary differential equation

$$\partial_t f = \nu(\mathcal{M} - f)\,,$$

and from the fact that $\mathcal{M}$ does not depend on t.
In the case of a mixture, the problem is more difficult to deal with and it has

not been fully investigated yet in the present literature. For this reason, in this chapter, we are going to derive the exponential convergence rate towards the Maxwellian species distributions for a hybrid Boltzmann–BGK model for a binary mixture, with Boltzmann intra-species operators.
Restricting ourselves, as is often done in this context, to the spatially homogeneous case, we obtain the following system

$$\begin{cases} \partial_t f_1 = Q_{11} + \nu_{12}(\mathcal{M}_{12} - f_1) \\ \\ \partial_t f_2 = \nu_{21}(\mathcal{M}_{21} - f_2) + Q_{22} \,. \end{cases} \tag{6.2}$$

We begin by proving the exponential decay rate for the difference of the velocities and temperatures.

Theorem 1. *In the space-homogeneous case* (6.2)*, we have the following decay rate of the velocities*

$$\boldsymbol{u}_2 - \boldsymbol{u}_1 = e^{-c_{\boldsymbol{u}} t}(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0) \ , \tag{6.3}$$

with $c_{\boldsymbol{u}} = \nu_{12}a_{12} + \nu_{21}a_{21}$*, and* $\boldsymbol{u}_1^0$*,* $\boldsymbol{u}_2^0$ *denote the initial values of the diffusion velocities.*

Proof. By the fact that $\boldsymbol{v}$ is a collision invariant for the Boltzmann intra-species operator,

$$\begin{aligned} &\partial_t \int_{\mathbb{R}^3} \boldsymbol{v} f_1 d\boldsymbol{v} = \nu_{12} \int_{\mathbb{R}^3} \boldsymbol{v}(\mathcal{M}_{12} - f_1) d\boldsymbol{v} \\ &\iff \partial_t \boldsymbol{u}_1 = \nu_{12}(\boldsymbol{u}_{12} - \boldsymbol{u}_1) = \nu_{12}a_{12}(\boldsymbol{u}_2 - \boldsymbol{u}_1) \ . \end{aligned}$$

Analogously,

$$\partial_t \boldsymbol{u}_2 = \nu_{21}a_{21}(\boldsymbol{u}_1 - \boldsymbol{u}_2)$$

Hence

$$\begin{aligned} &\partial_t(\boldsymbol{u}_2 - \boldsymbol{u}_1) = -(\nu_{12}a_{12} + \nu_{21}a_{21})(\boldsymbol{u}_2 - \boldsymbol{u}_1) \\ &\implies \boldsymbol{u}_2 - \boldsymbol{u}_1 = e^{-c_{\boldsymbol{u}} t}(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0) \ . \end{aligned}$$

□

By an analogous reasoning, albeit with a slightly more involved computation, we obtain the following

Theorem 2. *In the space-homogeneous case* (6.2)*, we have the following decay rate of the temperatures*

$$T_2 - T_1 = e^{-c_T t}\left[T_2^0 - T_1^0 - \frac{c_1}{c_2}\left(e^{-c_2 t} - 1\right)\right] \ , \tag{6.4}$$

with

$$\begin{cases} c_T = \nu_{12}b_{12} + \nu_{21}b_{21} \\ c_1 = \dfrac{1}{3}\dfrac{\mu_{12}(\nu_{21}a_{21} - \nu_{12}a_{12})(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0)^2(m_1+m_2)^2}{\Lambda_{12}(m_1^2 n_1 + m_2^2 n_2)} \\ c_2 = \dfrac{2\Lambda_{12}\left(m_1^2 n_1 + m_2^2 n_2\right)}{(m_1+m_2)^2} . \end{cases}$$

Proof. Again, since v^2 is a collision invariant of the single species Boltzmann operator, we have

$$m_1\partial_t \int_{\mathbb{R}^3} v^2 f_1 d\boldsymbol{v} = m_1\nu_{12}\int_{\mathbb{R}^3} v^2(\mathcal{M}_{12} - f_1)d\boldsymbol{v}$$

$$\iff m_1\partial_t\left[u_1^2 + \frac{3T_1}{m_1}\right] = m_1\nu_{12}\left[u_{12}^2 - u_1^2 + \frac{3}{m_1}(T_{12}-T_1)\right]$$

$$\iff 2m_1\boldsymbol{u}_1\cdot\partial_t\boldsymbol{u}_1 + 3\partial_t T_1$$

$$= m_1\nu_{12}a_{12}\left[a_{12}(\boldsymbol{u}_2-\boldsymbol{u}_1)^2 + 2\boldsymbol{u}_1\cdot(\boldsymbol{u}_2-\boldsymbol{u}_1)\right] + 3\nu_{12}\left[b_{12}(T_2-T_1) + \gamma_{12}(\boldsymbol{u}_2-\boldsymbol{u}_1)^2\right]$$

$$= 2m_1\nu_{12}a_{12}\boldsymbol{u}_1\cdot(\boldsymbol{u}_2-\boldsymbol{u}_1) + 3\nu_{12}b_{12}(T_2-T_1) + 2m_1\nu_{12}a_{12}\alpha_{21}(\boldsymbol{u}_2-\boldsymbol{u}_1)^2,$$

since $\gamma_{12} = m_1\nu_{12}a_{12}(\alpha_{12} - a_{12})$.
Then

$$3\partial_t T_1 = 3\nu_{12}b_{12}(T_2-T_1) + 2m_1\nu_{12}a_{12}\alpha_{21}(\boldsymbol{u}_2-\boldsymbol{u}_1)^2 \ .$$

In the same way, we reach

$$3\partial_t T_2 = 3\nu_{21}b_{21}(T_1-T_2) + 2m_2\nu_{21}a_{21}\alpha_{12}(\boldsymbol{u}_2-\boldsymbol{u}_1)^2 \ .$$

Hence, taking advantage of (6.3), we find

$$\partial_t(T_2-T_1) = -\underbrace{(\nu_{12}b_{12} + \nu_{21}b_{21})}_{:=c_T}(T_2-T_1) + \frac{2}{3}\mu_{12}(\nu_{21}a_{21} - \nu_{12}a_{12})(\boldsymbol{u}_2-\boldsymbol{u}_1)^2$$

$$= -c_T(T_2-T_1) + \underbrace{\frac{2}{3}\mu_{12}(\nu_{21}a_{21} - \nu_{12}a_{12})(\boldsymbol{u}_2^0-\boldsymbol{u}_1^0)^2}_{:=c_1} e^{-2c_{\boldsymbol{u}}t}$$

$$\iff \partial_t(T_2-T_1) = -c_T(T_2-T_1) + c_1 e^{-2c_{\boldsymbol{u}}t} \ .$$

Duhamel formula gives

$$T_2 - T_1 = e^{-c_T t}\left[T_2^0 - T_1^0 + c_1\int_0^t e^{(c_T - 2c_{\boldsymbol{u}})s}ds \ ,\right]$$

where

$$c_T - 2c_{\boldsymbol{u}} = -2\Lambda_{12}\frac{\left(m_1^2 n_1 + m_2^2 n_2\right)}{(m_1+m_2)^2} := -c_2 < 0 \ .$$

Redefining c_1 as

$$c_1 := \frac{c_1}{c_2} = \frac{1}{3}\frac{\mu_{12}(\nu_{21}a_{21} - \nu_{12}a_{12})(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0)^2(m_1 + m_2)^2}{\Lambda_{12}(m_1^2 n_1 + m_2^2 n_2)} \ ,$$

we have

$$T_2 - T_1 = e^{-c_T t}\left[T_2^0 - T_1^0 - c_1\left(e^{-c_2 t} - 1\right)\right] \ .$$

□

From Theorem 1 and 2, it follows

Theorem 3. *For the space homogeneous system* (6.2)*, for any species $s = 1, 2$, the difference between $\boldsymbol{u}_s$ (or T_s) and the corresponding mixture field $\boldsymbol{u}$ (or T) exponentially decreases in time according to:*

$$\begin{aligned}
\boldsymbol{u} - \boldsymbol{u}_s &= \frac{\rho_r}{\rho}(\boldsymbol{u}_r^0 - \boldsymbol{u}_s^0)e^{-c_{\boldsymbol{u}} t} \\
T - T_s &= \frac{n_r}{n}e^{-c_T t}\left[T_r^0 - T_s^0 - \frac{c_1}{c_2}(e^{-c_2 t} - 1)\right] + \frac{\rho_s\rho_r}{3\rho}(\boldsymbol{u}_r^0 - \boldsymbol{u}_s^0)^2 e^{-2c_{\boldsymbol{u}} t} \, ,
\end{aligned}$$

with $s, r = 1, 2 ,, \ r \neq s$*, the constant c_1, c_2, $c_{\boldsymbol{u}}$ and c_T defined in Theorem 1 and 2 and $\boldsymbol{u}_1^{(0)}$, $\boldsymbol{u}_2^{(0)}$, $T_1^{(0)}$ and $T_2^{(0)}$ are the initial values for species velocities and temperatures.*

Proof. From the definition of $\boldsymbol{u}$,

$$\boldsymbol{u} = \frac{\rho_1 \boldsymbol{u}_1 + \rho_2 \boldsymbol{u}_2}{\rho_1 + \rho_2} \, ,$$

we obtain

$$\boldsymbol{u} - \boldsymbol{u}_1 = \frac{\rho_2}{\rho}(\boldsymbol{u}_2 - \boldsymbol{u}_1) = \frac{\rho_2}{\rho}(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0)e^{-c_{\boldsymbol{u}} t} \, .$$

On the other hand, the definition of T,

$$T = \frac{n_1 T_1 + n_2 T_2}{n_1 + n_2} + \frac{1}{3}\left[\rho_1(\boldsymbol{u} - \boldsymbol{u}_1)^2 + \rho_2(\boldsymbol{u} - \boldsymbol{u}_2)^2\right] \, ,$$

implies

$$\begin{aligned}
T - T_1 &= \frac{n_2(T_2 - T_1)}{n_1 + n_2} + \frac{1}{3}\left[\frac{\rho_1\rho_2^2}{(\rho_1 + \rho_2)^2} + \frac{\rho_1^2\rho_2}{(\rho_1 + \rho_2)^2}\right](\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0)^2 e^{-2c_{\boldsymbol{u}} t} \\
&= \frac{n_2}{n}e^{-c_T t}\left[T_2^0 - T_1^0 - \frac{c_1}{c_2}(e^{-c_2 t} - 1)\right] + \frac{\rho_1\rho_2}{3\rho}(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0)^2 e^{-2c_{\boldsymbol{u}} t} \, .
\end{aligned}$$

Obviously, $\boldsymbol{u} - \boldsymbol{u}_2$ and $T - T_2$ are derived analogously. □

We show now some elementary properties of the distribution function f_s and of the Maxwellian distributions $\mathcal{M}_s$ which will be used in the subsequent theorem.

Lemma 4. *For a space homogeneous inert gas mixture, if we denote with $\mathcal{M}_s$ the Maxwellian function characterized by the same fields n_s, $\boldsymbol{u}_s$, T_s of the species distribution f_s, it holds*

$$\int_{\mathbb{R}^3} f_s \frac{\partial_t \mathcal{M}_s}{\mathcal{M}_s} d\boldsymbol{v} = 0 \ .$$

Proof. Since we are in the space homogeneous case,

$$\partial_t \mathcal{M}_s = \left\{ \frac{\partial_t n_s}{n_s} + \frac{m_s}{T_s} \partial_t \boldsymbol{u}_s \cdot (\boldsymbol{v} - \boldsymbol{u}_s) + \left[\frac{m_s}{2T_s^2} (\boldsymbol{v} - \boldsymbol{u}_s)^2 - \frac{3}{2T_s} \right] \partial_t T_s \right\} \mathcal{M}_s \,, \tag{6.5}$$

then, taking into account that in an inert space-homogeneous mixture $\partial_t n_s = 0$,

$$\frac{\partial_t \mathcal{M}_s}{\mathcal{M}_s} = \frac{m_s}{T_s} \partial_t \boldsymbol{u}_s \cdot (\boldsymbol{v} - \boldsymbol{u}_s) + \left[\frac{m_s}{2T_s^2} (\boldsymbol{v} - \boldsymbol{u}_s)^2 - \frac{3}{2T_s} \right] \partial_t T_s \,.$$

Hence,

$$\int_{\mathbb{R}^3} f_s \frac{\partial_t \mathcal{M}_s}{\mathcal{M}_s} d\boldsymbol{v} = \frac{m_s}{T_s} \partial_t \boldsymbol{u}_s \cdot \underbrace{\int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u}_s) f_s d\boldsymbol{v}}_{= n_s \boldsymbol{u}_s - n_s \boldsymbol{u}_s = 0} + \left[\frac{m_s}{2T_s^2} \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u}_s)^2 f_s d\boldsymbol{v} - \frac{3n_s}{2T_s} \right] \partial_t T_s$$

$$= \left[\frac{3n_s}{2T_s} - \frac{3n_s}{2T_s} \right] \partial_t T_s = 0 \ .$$

□

Lemma 5. *As in lemma 4, for a space homogeneous inert gas mixture, it holds*

$$\int_{\mathbb{R}^3} \partial_t \mathcal{M}_s d\boldsymbol{v} = 0 \ .$$

Proof. By (6.5), we have

$$\int_{\mathbb{R}^3} \partial_t \mathcal{M}_s d\boldsymbol{v} = \frac{m_s \partial_t \boldsymbol{u}_s}{T_s} \cdot \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u}_s) \mathcal{M}_s d\boldsymbol{v} + \partial_t T_s \left[\frac{m_s}{2T_s^2} \int_{\mathbb{R}^3} (\boldsymbol{v} - \boldsymbol{u}_s)^2 \mathcal{M}_s d\boldsymbol{v} - \frac{3}{2} \frac{n_s}{T_s} \right]$$

$$= \partial_t T_s \left(\frac{1}{2T_s^2} 3 n_s T_s - \frac{3}{2} \frac{n_s}{T_s} \right) = 0 \,.$$

□

We now prove the upcoming lemma.

Lemma 6. *Let H denote the classical Boltzmann H-functional*

$$H(f) := \int_{\mathbb{R}^3} f(\boldsymbol{v}) \log(f) d\boldsymbol{v} \,.$$

Given masses m_s, densities n_s, velocities u_s, temperatures T_s $(s = 1, 2)$, the following relation holds, connecting the H-functional computed in the Maxwellian attractors $\mathcal{M}_{12}$, $\mathcal{M}_{21}$ defined in (1.26) *with the one computed in the local Maxwellians $\mathcal{M}_1$, M_2:*

$$\nu_{12} H(\mathcal{M}_{12}) + \nu_{21} H(\mathcal{M}_{21}) \leq \nu_{12} H(\mathcal{M}_1) + \nu_{21} H(\mathcal{M}_2)$$

Proof. One easily checks that

$$\log \mathcal{M}_s = \log n_s + \frac{3}{2} \log \left(\frac{m_s}{2\pi T_s} \right) - \frac{m_s}{2T_s} (\boldsymbol{v} - \boldsymbol{u}_s)^2 \tag{6.6}$$

$$\log \mathcal{M}_{sr} = \log n_s + \frac{3}{2} \log \left(\frac{m_s}{2\pi T_{sr}} \right) - \frac{m_s}{2T_{sr}} (\boldsymbol{v} - \boldsymbol{u}_{sr})^2 \ ,$$

that leads to

$$H(\mathcal{M}_s) = n_s \left\{ \log n_s + \frac{3}{2} \log \left(\frac{m_s}{2\pi T_s} \right) - \frac{3}{2} \right\}$$

$$H(\mathcal{M}_{sr}) = n_s \left\{ \log n_s + \frac{3}{2} \log \left(\frac{m_s}{2\pi T_{sr}} \right) - \frac{3}{2} \right\} \ ,$$

and the inequality we aim to prove becomes equivalent to

$$\nu_{12} n_1 \left\{ \log \left[n_1 \left(\frac{m_1}{2\pi} \right)^{\frac{3}{2}} \right] - \frac{3}{2} \log T_{12} \right\} + \nu_{21} n_2 \left\{ \log \left[n_2 \left(\frac{m_2}{2\pi} \right)^{\frac{3}{2}} \right] - \frac{3}{2} \log T_{21} \right\}$$

$$\leq \nu_{12} n_1 \left\{ \log \left[n_1 \left(\frac{m_1}{2\pi} \right)^{\frac{3}{2}} \right] - \frac{3}{2} \log T_1 \right\} + \nu_{21} n_2 \left\{ \log \left[n_2 \left(\frac{m_2}{2\pi} \right)^{\frac{3}{2}} \right] - \frac{3}{2} \log T_2 \right\} ,$$

namely

$$\iff \nu_{12} n_1 \log T_{12} + \nu_{21} n_2 \log T_{21} \geq \nu_{12} n_1 \log T_1 + \nu_{21} n_2 \log T_2 \, .$$

The only condition we have imposed on ν_{sr} is $\nu_{sr} \geq \frac{1}{2} \lambda_{sr} n_r$, guarantees the positivity of the coefficients γ_{sr} appearing in T_{sr}, hence by the monotonicity of the logarithm, the left-hand side of the last inequality becomes

$$\nu_{12} n_1 \log \left[(1 - b_{12}) T_1 + b_{12} T_2 + \gamma_{12} (\boldsymbol{u}_1 - \boldsymbol{u}_2)^2 \right]$$

$$+ \nu_{21} n_2 \log \left[(1 - b_{21}) T_2 + b_{21} T_1 + \gamma_{21} (\boldsymbol{u}_1 - \boldsymbol{u}_2)^2 \right]$$

$$\geq \nu_{12} n_1 \log \left[(1 - b_{12}) T_1 + b_{12} T_2 \right] + \nu_{21} n_2 \log \left[(1 - b_{21}) T_2 + b_{21} T_1 \right] \ .$$

Knowing that $0 < b_{sr} < 1$ and exploiting the concavity of the logarithm, the inequality to be proven develops into

$$\nu_{12} n_1 \left[(1 - b_{12}) \log T_1 + b_{12} \log T_2 \right] + \nu_{21} n_2 \left[(1 - b_{21}) \log T_2 + b_{21} \log T_1 \right]$$

$$\geq \nu_{12} n_1 \log T_1 + \nu_{21} n_2 \log T_2$$

$$\iff \nu_{12} n_1 b_{12} \log \frac{T_2}{T_1} + \nu_{21} n_2 b_{21} \log \frac{T_1}{T_2} \geq 0 \ .$$

By the definition of b_{ij}, we have

$$\nu_{12} n_1 b_{12} = 2 n_1 n_2 \frac{m_1 m_2}{(m_1+m_2)^2} \Lambda_{12} = \nu_{21} n_2 b_{21} \ ,$$

and the thesis is proven. $\square$

We are now ready to prove the convergence rate of each species distribution f_s towards the corresponding local Maxwell species distribution $\mathcal{M}_s$.

Theorem 4. *In the space homogeneous case, with the relative entropy $H(f|g)$ defined as in* (6.1)*, we have the following convergence rate of the distribution functions f_1 and f_2 towards the local Maxwellians $\mathcal{M}_1$ and $\mathcal{M}_2$*

$$||f_s - \mathcal{M}_s||_{L^1(d\boldsymbol{v})} \leq 4 e^{-\frac{1}{2}\nu t} \left[H(f_1^0|\mathcal{M}_1^0) + H(f_2^0|\mathcal{M}_2^0) \right] + \frac{k}{\nu - 2c} e^{-\nu t} \left(e^{(\nu-2c)t} - 1 \right) , \quad s = 1, 2,$$

where $\mathcal{M}_1^0$ and $\mathcal{M}_2^0$ are the local Maxwellians depending on the initial values for species velocities and temperatures, and

$$\begin{cases} \nu = \min\{\nu_{12}, \nu_{21}\} \\ k = \dfrac{m_1 m_2 n_1 n_2 \Lambda_{12}}{(m_1+m_2)^2 k_T} \max\left\{ \dfrac{3}{k_T} \left[T_2^0 - T_1^0 + c_1 \right], (m_1+m_2)(\boldsymbol{u}_2^0 - \boldsymbol{u}_1^0)^2 \right\} \\ c = \min\{c_{\boldsymbol{u}}, c_T\}, \end{cases}$$

with $k_T = \min\{T_1^0, T_2^0\}$.

Proof. We consider the entropy production of each species $D_s(f_s, f_r) := -\langle \log f_s, Q_s \rangle$,

$$D_1(f_1, f_2) = -\int_{\mathbb{R}^3} \log f_1 Q_{11} d\boldsymbol{v} - \nu_{12} \int_{\mathbb{R}^3} (\mathcal{M}_{12} - f_1) \log f_1 d\boldsymbol{v} \, .$$

Since the function $h(x) := x \log x - x$ satisfies $h'(x) = \log x$ and is convex, we can deduce

$$\begin{aligned} D_1(f_1, f_2) &= -\int_{\mathbb{R}^3} \log f_1 Q_{11} d\boldsymbol{v} - \nu_{12} \int_{\mathbb{R}^3} h'(f_1)(\mathcal{M}_{12} - f_1) d\boldsymbol{v} \\ &\geq -\int_{\mathbb{R}^3} \log f_1 Q_{11} d\boldsymbol{v} + \nu_{12} \int_{\mathbb{R}^3} [h(f_1) - h(\mathcal{M}_{12})] d\boldsymbol{v} \\ &= -\int_{\mathbb{R}^3} \log f_1 Q_{11} d\boldsymbol{v} + \nu_{12} [H(f_1) - H(\mathcal{M}_{12})] \, . \end{aligned}$$

In the same way we get a similar expression for $D_2(f_2, f_1)$.

By recalling the expression of $\log \mathcal{M}_s$ provided in (6.6), and bearing in mind that f_s and $\mathcal{M}_s$ have the same moments, we have

$$\int_{\mathbb{R}^3} (\mathcal{M}_s - f_s) \log \mathcal{M}_s d\boldsymbol{v} = 0\,,$$

then

$$H(f_s|\mathcal{M}_s) = \int_{\mathbb{R}^3} f_s(\log f_s - \log \mathcal{M}_s) d\boldsymbol{v} = \int_{\mathbb{R}^3} [f_s(\log f_s - \log \mathcal{M}_s) - (\mathcal{M}_s - f_s)\log \mathcal{M}_s] d\boldsymbol{v}$$

$$= \int_{\mathbb{R}^3} f_s \log f_s d\boldsymbol{v} - \int_{\mathbb{R}^3} \mathcal{M}_s \log \mathcal{M}_s d\boldsymbol{v} = H(f_s) - H(\mathcal{M}_s)\,.$$

Moreover, from lemma 6 and from the well known inequality $\int_{\mathbb{R}^3} \log f_s Q_{ss}(f_s) d\boldsymbol{v} \leq 0$, we get

$$\begin{aligned}
D_1(f_1, f_2) + D_2(f_2, f_1) &\geq -\int_{\mathbb{R}^3} \log f_1 Q_{11} d\boldsymbol{v} + \nu_{12}(H(f_1) - H(\mathcal{M}_1)) \\
&\quad - \int_{\mathbb{R}^3} \log f_2 Q_{22} d\boldsymbol{v} + \nu_{21}(H(f_2) - H(\mathcal{M}_2)) \\
&\geq \nu_{12} H(f_1|\mathcal{M}_1) + \nu_{21} H(f_2|\mathcal{M}_2) \\
&\iff -[D_1(f_1, f_2) + D_2(f_2, f_1)] \leq -[\nu_{12} H(f_1|\mathcal{M}_1) + \nu_{21} H(f_2|\mathcal{M}_2)]\,. \quad (6.7)
\end{aligned}$$

Using lemma 4, we now compute

$$\begin{aligned}
&\frac{\partial}{\partial t}\left[H(f_1|\mathcal{M}_1) + H(f_2|\mathcal{M}_2)\right] \\
&= \int_{\mathbb{R}^3} \partial_t \left[f_1 \log \frac{f_1}{\mathcal{M}_1}\right] d\boldsymbol{v} + \int_{\mathbb{R}^3} \partial_t \left[f_2 \log \frac{f_2}{\mathcal{M}_2}\right] d\boldsymbol{v} \\
&= \int_{\mathbb{R}^3} \left\{ \partial_t f_1 (\log f_1 - \log \mathcal{M}_1) + \underbrace{f_1 \left[\frac{1}{f_1}\partial_t f_1 - \frac{\partial_t \mathcal{M}_1}{\mathcal{M}_1}\right]}_{=0} \right\} d\boldsymbol{v} \\
&+ \int_{\mathbb{R}^3} \left\{ \partial_t f_2 (\log f_2 - \log \mathcal{M}_2) + \underbrace{f_2 \left[\frac{1}{f_2}\partial_t f_2 - \frac{\partial_t \mathcal{M}_2}{\mathcal{M}_2}\right]}_{=0} \right\} d\boldsymbol{v} \\
&= \int_{\mathbb{R}^3} [\partial_t f_1 (\log f_1 - \log \mathcal{M}_1)]\, d\boldsymbol{v} + \int_{\mathbb{R}^3} [\partial_t f_2 (\log f_2 - \log \mathcal{M}_2)]\, d\boldsymbol{v}\ .
\end{aligned}$$

By recalling the expression of $\partial_t f_s$ from the space homogeneous system (6.2), we get

$$\frac{\partial}{\partial t}[H(f_1|\mathcal{M}_1)] + \frac{\partial}{\partial t}[H(f_2|\mathcal{M}_2)] \tag{6.8}$$
$$= \int_{\mathbb{R}^3} [Q_{11} + \nu_{12}(\mathcal{M}_{12} - f_1)] \log \frac{f_1}{\mathcal{M}_1} d\boldsymbol{v} + \int_{\mathbb{R}^3} [\nu_{21}(\mathcal{M}_{21} - f_2) + Q_{22}] \log \frac{f_2}{\mathcal{M}_2} d\boldsymbol{v}$$

$$= \underbrace{\int_{\mathbb{R}^3} [Q_{11} + \nu_{12}(\mathcal{M}_{12} - f_1)] \log f_1 d\boldsymbol{v}}_{-D_1(f_1,f_2)} + \underbrace{\int_{\mathbb{R}^3} [\nu_{21}(\mathcal{M}_{21} - f_2) + Q_{22}] \log f_2}_{-D_2(f_2,f_1)}$$
$$- \left[\nu_{12} \int_{\mathbb{R}^3} (\mathcal{M}_{12} - f_1) \log \mathcal{M}_1 d\boldsymbol{v} + \nu_{21} \int_{\mathbb{R}^3} (\mathcal{M}_{21} - f_2) \log \mathcal{M}_2 d\boldsymbol{v}\right] \ ,$$

where in the last equality we used that $\log \mathcal{M}_s$ provided in(6.6) is a linear combination of collision invariants for the Boltzmann intra-species operator.
We now focus on

$$- \nu_{12} \int_{\mathbb{R}^3} (\mathcal{M}_{12} - f_1) \log \mathcal{M}_1 d\boldsymbol{v} = -\nu_{12} \int_{\mathbb{R}^3} (\mathcal{M}_{12} - f_1) \left\{ \log \left[n_1 \left(\frac{m_1}{2\pi T_1} \right)^{\frac{3}{2}} \right] - \frac{m_1}{2T_1} (\boldsymbol{v} - \boldsymbol{u}_1)^2 \right\} d\boldsymbol{v}$$
$$= \nu_{12} \frac{m_1}{2T_1} \int_{\mathbb{R}^3} (\mathcal{M}_{12} - f_1)(\boldsymbol{v}^2 + \boldsymbol{u}_1^2 - 2\boldsymbol{u}_1 \cdot \boldsymbol{v}) d\boldsymbol{v}$$
$$= \nu_{12} n_1 \frac{m_1}{2T_1} (\boldsymbol{u}_{12}^2 - \boldsymbol{u}_1^2) + \frac{3n_1}{2T_1} \nu_{12}(T_{12} - T_1) - \nu_{12} n_1 \frac{m_1}{2T_1} a_{12}(\boldsymbol{u}_2 - \boldsymbol{u}_1) \cdot \boldsymbol{u}_1$$
$$= \frac{n_1}{2T_1} \{ m_1 a_{12} \left[a_{12}(\boldsymbol{u}_2 - \boldsymbol{u}_1)^2 - 2\boldsymbol{u}_1 \cdot (\boldsymbol{u}_1 - \boldsymbol{u}_2) \right]$$
$$+ 3\nu_{12} b_{12}(T_2 - T_1) + 3\nu_{12}\gamma_{12}(\boldsymbol{u}_2 - \boldsymbol{u}_1)^2 - 2\nu_{12} m_1 a_{12} \boldsymbol{u}_1 \cdot (\boldsymbol{u}_2 - \boldsymbol{u}_1) \}$$
$$= \frac{\nu_{12} n_1}{2T_1} \left[3b_{12}(T_2 - T_1) + m_1 a_{12} 2\alpha_{21}(\boldsymbol{u}_2 - \boldsymbol{u}_1)^2 \right] = \frac{\nu_{12} a_{12} \alpha_{12} n_1}{T_1} \left[3b_{12}(T_2 - T_1) + m_2(\boldsymbol{u}_2 - \boldsymbol{u}_1)^2 \right]$$
$$= \frac{a}{T_1} \left[3b_{12}(T_2 - T_1) + m_2(\boldsymbol{u}_2 - \boldsymbol{u}_1)^2 \right] \quad ,$$

having set

$$\nu_{12} a_{12} \alpha_{12} n_1 = \nu_{21} a_{21} \alpha_{21} n_2 = \frac{m_1 m_2 n_1 n_2 \lambda_{12}}{(m_1 + m_2)^2} := a \ .$$

Obviously, analogous computations lead to

$$-\nu_{21} \int_{\mathbb{R}^3} (\mathcal{M}_{21} - f_2) \log \mathcal{M}_2 d\boldsymbol{v} = \frac{a}{T_2} \left[3b_{21}(T_1 - T_2) + m_2(\boldsymbol{u}_2 - \boldsymbol{u}_1)^2 \right] \ .$$

Hence the sum of the two yields

$$3a\left[\frac{1}{T_1}(T_2-T_1)+\frac{1}{T_2}(T_1-T_2)\right]+a(\boldsymbol{u}_2-\boldsymbol{u}_1)^2\left[\frac{m_2}{T_1}+\frac{m_1}{T_2}\right]$$
$$=3a\frac{(T_2-T_1)^2}{T_1T_2}+a(\boldsymbol{u}_2-\boldsymbol{u}_1)^2\left[\frac{m_2}{T_1}+\frac{m_1}{T_2}\right] \ .$$

So, recalling the decay rate of the velocities and temperatures proved in Theorem 1 and Theorem 2, we get

$$-\nu_{12}\int_{\mathbb{R}^3}(\mathcal{M}_{12}-f_1)\log\mathcal{M}_1 d\boldsymbol{v}-\nu_{21}\int_{\mathbb{R}^3}(\mathcal{M}_{21}-f_2)\log\mathcal{M}_2 d\boldsymbol{v}$$
$$=3ae^{-2c_T t}\left[T_2^0-T_1^0-c_1\left(e^{-c_2 t}-1\right)\right]\frac{1}{T_1T_2}+a(\boldsymbol{u}_2^0-\boldsymbol{u}_1^0)^2e^{-2c_{\boldsymbol{u}}t}\left[\frac{m_2}{T_1}+\frac{m_1}{T_2}\right] \ .$$

Using the exponential decay of the temperatures difference along with $k_T := \min\{T_1^0, T_2^0\}$, and the fact that $0 \leq 1-e^{-kt} \leq 1$ for any $k>0$, the latter expression can be controlled from above with

$$3a\left[T_2^0-T_1^0+c_1\right]\frac{1}{k_T^2}e^{-2c_T t}+\frac{a}{k_T}(\boldsymbol{u}_2^0-\boldsymbol{u}_1^0)^2(m_1+m_2)e^{-2c_{\boldsymbol{u}}t}\leq ke^{-2ct} \ ,$$

with

$$\begin{cases} k = a\max\left\{\frac{3}{k_T^2}\left[T_2^0-T_1^0+c_1\right], \frac{m_1+m_2}{k_T}(\boldsymbol{u}_2^0-\boldsymbol{u}_1^0)^2\right\} \\ c=\min\{c_{\boldsymbol{u}}, c_T\} \ . \end{cases}$$

Hence

$$\partial_t\big[H(f_1|\mathcal{M}_1)+H(f_2|\mathcal{M}_2)\big]\leq -\left[D_1(f_1,f_2)+D_2(f_2,f_1)\right]+ke^{-2ct}$$
$$\leq -\min\{\nu_{12},\nu_{21}\}\left[H(f_1|\mathcal{M}_1)+H(f_2|\mathcal{M}_2)\right]+ke^{-2ct} \ .$$

We set $\nu := \min\{\nu_{12}, \nu_{21}\}$ and apply Duhamel formula

$$H(f_1|\mathcal{M}_1)+H(f_2|\mathcal{M}_2)\leq e^{-\nu t}\left[H(f_1^0|\mathcal{M}_1^0)+H(f_2^0|\mathcal{M}_2^0)\right]+ke^{-\nu t}\int_0^t e^{(\nu-2c)s}ds$$
$$=e^{-\nu t}\left[H(f_1^0|\mathcal{M}_1^0)+H(f_2^0|\mathcal{M}_2^0)\right]+\frac{k}{\nu-2c}\left(e^{-2ct}-e^{-\nu t}\right) \ .$$

With the Ciszar-Kullback inequality (see appendix D) we get

$$||f_s-\mathcal{M}_s||_{L^1(d\boldsymbol{v})}\leq\sum_{s=1,2}||f_s-\mathcal{M}_s||_{L^1(d\boldsymbol{v})}$$
$$\leq 4e^{-\frac{1}{2}\nu t}\left[H(f_1^0|\mathcal{M}_1^0)+H(f_2^0|\mathcal{M}_2^0)\right]+\frac{k}{\nu-2c}e^{-\nu t}\left(e^{(\nu-2c)t}-1\right) \ .$$

The positivity of the right-hand side is assured by the fact that both $\frac{\nu k}{\nu - 2c}$ and $e^{(\nu-2c)t} - 1$ are positive if $\nu > 2c$, and both are negative if $\nu < 2c$.

$\square$

Remark. *The proof still holds for the full BGK description, with the only difference that we find*

$$-[D_1(f_1, f_2) + D_2(f_2, f_1)] \leq -\left[(\nu_{11} + \nu_{12})H(f_1|\mathcal{M}_1) + (\nu_{21} + \nu_{22})H(f_2|\mathcal{M}_2)\right] ,$$

and then $\nu = \min\{\nu_{11}+\nu_{12}, \nu_{21}+\nu_{22}\}$*, where* ν_{11}*,* ν_{22} *are the collision frequencies of the intra-species BGK operator* $\hat{Q}_{11}$*,* $\hat{Q}_{22}$*.*

Remark. *Since we have demonstrated, in Theorem 3, that velocities and temperatures converge exponentially towards the mixture velocity and temperature respectively, Theorem 4 could be considered representative of the exponential convergence of the distribution functions towards the Maxwellian equilibrium distribution.*

Conclusions

We have proposed and investigated a mixed Boltzmann–BGK kinetic model for an inert gas mixtures of N constituents which allows some kind of interactions to be modeled by Boltzmann operators and others by the binary BGK relaxation terms built up in [13]. As well known, the Boltzmann description is able to take into suitable account the intermolecular potential and the microscopic impact parameters of each collision. On the other hand, a BGK approximation neglects some microscopic details of single interactions, preserving only some basic features as conservation laws and entropy dissipation, but it turns out to be more manageable from the numerical point of view and also in the analytical derivation of hydrodynamic closures [9].
Some possible combined uses of nonlinear terms coming from Boltzmann descriptions and of linear contributions from BGK operators have already been proposed in literature in view of numerical approximations [36, 45], but for the first time in this thesis we have proved that a general mixed Boltzmann-BGK description is consistent even from the theoretical point of view. Specifically, we have shown that our general model correctly reproduces conservation laws and Maxwellian equilibria of the Boltzmann kinetic equations, and even the entropy dissipation property is fulfilled. The proof of the H-theorem is based on the fact that entropy dissipation holds separately for the single–species Boltzmann or BGK operators, and for the two symmetric operators relevant to each pair of interacting species (s, r), with $r \neq s$, both of Boltzmann or of BGK type.
In several problems for mixtures of rarefied gases, differences between the results corresponding to various interaction potentials may be more appreciated in presence of nonlinear terms [48]. On the other hand, it is known that the evolution is driven by heaviest molecules, leading to unexpected behaviors in high order moments, as heat flux [30]. In this respect, our hybrid model is devised to describe the evolution of gas mixtures whose constituents show different features, and allows to treat the most meaningful binary interactions, as the ones involving heavy particles or higher collision frequencies, by accurate Boltzmann operators, and to approximate by simpler BGK terms the interactions playing a minor role in the global evolution of the mixture.
The framework of this model allows for the study of different hydrodynamic regimes. In this respect, we have performed at first the Chapman–Enskog asymptotic procedure at Euler and Navier-Stokes accuracy for the classical collision dominated regime. In particular, the linear system of the diffusion velocities

does not depend on the coefficients χ_{sr} ruling the choice of the collision operators, showing that their expressions are independent of which interactions have been chosen to be modeled by the Boltzmann or BGK operators. As concerns the first order correction of the pressure tensor and of the heat flux vector, the simultaneous presence of the linearized Boltzmann operators and of the first order correction of BGK relaxation terms makes their explicit computations impracticable. Nonetheless, we demonstrated the non-singularity of the system matrix associated to them and thus leading to an effective closure of the Navier-Stokes equations.

Within the same collisional regime, we have investigated the particular case with intra–species collisions modeled by Boltzmann operators and inter–species interactions by BGK terms. In this case, it is possible to prove the existence and uniqueness of the first order distribution functions, whose expression, however, cannot be made explicit. Anyway, taking advantage that the only linearized Boltzmann operators involved in the computations are the single-species ones, we established an explicit expressions for any of the additional macroscopic unknowns of the Navier-Stokes system.

In the last part of the thesis we focus on binary mixtures, investigating two different collisional regimes. In the first one both intra-species collisions play a dominant role. This scaling defines the so-called $\varepsilon-$mixtures, namely mixtures composed by particles with strongly different masses, with energy transfer between different species occurring on a much slower timescale than within each species [26]. In this case, the Chapman-Enskog procedure leads to a multi-velocities and multi-temperatures Navier-Stokes system, where source terms on the right-hand side are representative of the slow collisional dynamics and, consequently, of the transfer of momentum and kinetic energy between the two components.

The second regime addresses a mixture of heavy and light particles, in which only the heaviest intra-species collisions play a dominant role, while the lightest intra-species encounters account for the slowest process. The asymmetry between the two species stems from the large difference in their masses. Because the heavier particles experience smaller velocity changes during collisions, they approach equilibrium much more quickly than the lighter ones. As a result, their distribution relaxes on a significantly shorter timescale, while the lightest species remains far from equilibrium and retains a kinetic description [22, 33]. This results in a coupled microscopic–macroscopic system, where the evolution of the heaviest species is governed by Navier-Stokes equations, while the lightest species retains a mesoscopic description.

In the last chapter, we have derived the exponential convergence rate towards the Maxwellian species distributions for a hybrid Boltzmann–BGK model for a binary mixture, with Boltzmann intra-species operators. Restricting ourselves to the spatially homogeneous case, as often done in this context, we have first demonstrated the exponential decay rate of the velocities and the temperatures and then the exponential convergence rate of the distribution functions towards the local Maxwellians, depending on collision frequencies and relaxation parameters.

The present results suggest some further research lines. First, the intra-species dominated regime, investigated in this thesis only in the case when the intra-species collisions are described by Boltzmann operators and inter-species interactions by BGK terms, could be studied for the more general model with arbitrary chosen collision operators.
Second, we would like to extend to an arbitrary number of species N the fluid-kinetic description performed in Chapter 5 for a binary mixture. Furthermore, it would be interesting to investigate the exponential convergence of the distribution functions towards species Maxwellian or towards global distributions in the case of a generic $N-$components mixtures. Some preliminary attempts show that additional difficulties arise in the decay rate estimates for velocities and temperatures and the exponential convergence may be lost.

Appendix A

Computations on pre- and post-collisional velocities

Recalling the expressions of post-collision velocities in an inert gas mixtures

$$\begin{cases} \boldsymbol{v}'_{sr} = \alpha_{sr}\boldsymbol{v} + \alpha_{rs}\left(\boldsymbol{w} + |\boldsymbol{y}|\omega\right) \\ \boldsymbol{w}'_{sr} = \alpha_{rs}\boldsymbol{w} + \alpha_{sr}\left(\boldsymbol{v} - |\boldsymbol{y}|\omega\right) \end{cases}, \tag{A.1}$$

we obtain

$$\boldsymbol{v}'_{sr} = \frac{m_s\boldsymbol{v} + m_r\boldsymbol{w}}{m_s + m_r} + \frac{m_r}{m_s + m_r}|\boldsymbol{y}|\omega\,, \tag{A.2}$$

thus

$$\begin{aligned} \boldsymbol{v}'_{sr} - \boldsymbol{v} &= \frac{m_s\boldsymbol{v} + m_r\boldsymbol{w}}{m_r + m_s} + \frac{m_r}{m_s + m_r}|\boldsymbol{v} - \boldsymbol{w}|\omega - \boldsymbol{v} \\ &\frac{m_s\boldsymbol{v} + m_r\boldsymbol{w}}{m_r + m_s} + \frac{m_r}{m_s + m_r}|\boldsymbol{v} - \boldsymbol{w}|\omega - \frac{m_s\boldsymbol{v} + m_r\boldsymbol{v}}{m_s + m_r} \\ &= \frac{m_s\boldsymbol{v} + m_r\boldsymbol{w} + m_r|\underline{y}|\omega - m_s\boldsymbol{v} - m_r\boldsymbol{v}}{m_s + m_r} \\ &= \frac{m_r}{m_s + m_r}\big(\boldsymbol{w} - \boldsymbol{v} + |\boldsymbol{y}|\omega\big) \\ &= -\frac{m_r}{m_s + m_r}\big(\boldsymbol{y} - |\boldsymbol{y}|\omega\big)\,. \end{aligned} \tag{A.3}$$

Analogously,

$$v_{sr}'^2 - v^2 = \frac{(m_s\boldsymbol{v} + m_r\boldsymbol{w})^2}{(m_s + m_r)^2} + \frac{m_r^2}{(m_s + m_r)^2} y^2\omega^2$$

$$+ \frac{2m_r}{(m_s + m_r)^2}\big(m_s\boldsymbol{v} + m_r\boldsymbol{w}\big) \cdot |\boldsymbol{y}|\omega - v^2$$

$$= \frac{m_s^2 v^2 + m_r^2 w^2 + 2m_s m_r \boldsymbol{v}\cdot\boldsymbol{w} + m_r^2(v^2 + w^2 - 2\boldsymbol{v}\cdot\boldsymbol{w})}{(m_s + m_r)^2}$$

$$+ \frac{2m_r(m_s\boldsymbol{v} + m_r\boldsymbol{w}) \cdot |\boldsymbol{y}|\omega - (m_s^2 + m_r^2 + 2m_s m_r)v^2}{(m_s + m_r)^2}$$

$$= -\frac{2m_r}{(m_s + m_r)^2}\Big[m_s v^2 - m_r w^2 - (m_s\boldsymbol{v} + m_r\boldsymbol{w}) \cdot |\boldsymbol{y}|\omega + (m_r - m_s)\boldsymbol{v}\cdot\boldsymbol{w}\Big].$$

The term within the square brackets provides

$$\begin{aligned} & m_s v^2 - m_r w^2 - (m_s\boldsymbol{v} + m_r\boldsymbol{w}) \cdot |\boldsymbol{y}|\omega + (m_r - m_s)\boldsymbol{v}\cdot\boldsymbol{w} \\ & = (m_s\boldsymbol{v} + m_r\boldsymbol{w}) \cdot \big(\boldsymbol{y} - |\boldsymbol{y}|\omega\big)\,, \end{aligned} \tag{A.4}$$

hence

$$v_{sr}'^2 - v^2 = -\frac{2m_r}{(m_s + m_r)^2}\big(m_s\boldsymbol{v} + m_r\boldsymbol{w}\big) \cdot \big(\boldsymbol{y} - |\boldsymbol{y}|\omega\big)\,. \tag{A.5}$$

We now rewrite in polar coordinates

$$\int_{\mathbb{S}^2} g_{sr}(|\boldsymbol{y}|, \hat{\boldsymbol{y}}\cdot\omega)\omega d\omega = \hat{\boldsymbol{y}} 2\pi \int_{-1}^{1} \mu g_{sr}(|\boldsymbol{y}|, \mu) d\mu\ , \tag{A.6}$$

and we define

$$g_{sr}^{(1)}(|\boldsymbol{y}|) = 2\pi \int_{-1}^{1} (1-\mu) g_{sr}(|\boldsymbol{y}|, \mu) d\mu \quad . \tag{A.7}$$

Product of post-collision velocities

Recalling (A.1) for $\boldsymbol{v}'_{sr}$ and $\boldsymbol{w}'_{sr}$, and using the following integrals on the unit sphere

$$\begin{aligned} & \int_{\mathbb{S}^2} d\omega = 4\pi\,, \qquad \int_{\mathbb{S}^2} \omega_\ell d\omega = 0\,, \qquad \int_{\mathbb{S}^2} \omega_\ell^2 d\omega = \frac{4\pi}{3}\,, \quad \ell = i,j,k \\ & \int_{\mathbb{S}^2} \omega_\ell \omega_m d\omega = 0\,, \qquad \ell \neq m\,, \quad \ell, m = i,j,k\,; \end{aligned} \tag{A.8}$$

we obtain

$$\int_{\mathbb{S}^2} v_i^{sr'} v_j^{sr'} d\omega = \int_{\mathbb{S}^2} (\alpha_{sr} v_i + \alpha_{rs} w_i + \alpha_{rs} g\omega_i)(\alpha_{sr} v_j + \alpha_{rs} w_j + \alpha_{rs} g\omega_j)\, d\omega$$
$$= 4\pi \Big[\alpha_{sr}^2 v_i v_j + \alpha_{rs}^2 w_i w_j + \frac{\delta_{ij}}{3} \alpha_{rs}^2 |\boldsymbol{y}|^2 + \alpha_{sr}\alpha_{rs}(v_i w_j + v_j w_i) \Big]. \tag{A.9}$$

Now,

$$v_{sr}'^2 = (\alpha_{sr}^2 + \alpha_{rs}^2) v^2 + 2\alpha_{rs}^2 w^2 + (v_i w_i + v_j w_j + v_k w_k)(\alpha_{sr}\alpha_{rs} - \alpha_{rs}^2)$$
$$+ 2\alpha_{rs} g \left[\omega_i(\alpha_{sr} v_i + \alpha_{rs} w_i) + \omega_j(\alpha_{sr} v_j + \alpha_{rs} w_j) + \omega_k(\alpha_{sr} v_k + \alpha_{rs} w_k) \right],$$

hence

$$\int_{\mathbb{S}^2} v_i^{sr'} v_{sr}'^2 d\omega = \int_{\mathbb{S}^2} \Bigg[\left(\alpha_{sr}^3 + \alpha_{sr}\alpha_{rs}^2\right) v_i v^2 + 2\alpha_{rs}^3 w_i w^2 + 2\alpha_{sr}\alpha_{rs}^2 v_i w^2$$
$$+ \left(\alpha_{sr}^2 \alpha_{rs} + \alpha_{rs}^2\right) v^2 w_i + 2\left(\alpha_{sr}^2\alpha_{rs} - \alpha_{sr}\alpha_{rs}^2\right)\left(v_i^2 w_i v_i v_j w_j + v_i v_k w_k\right)$$
$$+ 2(\alpha_{sr}\alpha_{rs}^2 - \alpha_{rs}^3)(v_i w_i^2 + v_j w_i w_j + v_k w_i w_k) + 2\alpha_{rs}^2 \omega_i^2 (\alpha_{sr} v_i + \alpha_{rs} w_i)$$
$$\times \left[v^2 + w^2 - 2(v_i w_i + v_j w_j + v_k w_k) \right] \Bigg] d\omega$$
$$= 4\pi \Bigg[\left(\alpha_{sr}^3 + \frac{5}{3}\alpha_{sr}\alpha_{rs}^2 \right) v_i v^2 + \frac{8}{3}\alpha_{rs}^3 w_i w^2 + \frac{8}{3}\alpha_{sr}\alpha_{rs}^2 v_i w^2 + \left(\alpha_{sr}^2 \alpha_{rs} + \frac{5}{3}\alpha_{rs}^3 \right) v^2 w_i$$
$$+ 2\left(\alpha_{sr}^2\alpha_{rs} - \frac{5}{3}\alpha_{sr}\alpha_{rs}^2 \right)\left(v_i^2 w_i + v_i v_j w_j + v_i v_k w_k \right)$$
$$+ 2\left(\alpha_{sr}\alpha_{rs}^2 - \frac{5}{3}\alpha_{rs}^3 \right)\left(v_i w_i^2 + v_j w_i w_j + v_k w_i w_k \right) \Bigg]. \tag{A.10}$$

In the intra-species case we have $\alpha_{sr} = \alpha_{rs} = \frac{1}{2}$, hence (A.9) becomes

$$\int_{\mathbb{S}^2} v_i' v_j' d\omega = \pi \Big[v_i v_j + w_i w_j + v_i w_j + v_j w_i + \frac{\delta_{ij}}{3}(v^2 + w^2 - 2\boldsymbol{v}\cdot\boldsymbol{w}) \Big]. \tag{A.11}$$

and, analogously, (A.10) turns into

$$\int_{\mathbb{S}^2} v_i' \boldsymbol{v}'^2 d\omega = \frac{4}{3}\pi \left(v_i v^2 + w_i w^2 + v^2 w_i + v_i w^2 \right) \tag{A.12}$$
$$- \frac{2}{3}\pi \left(v_i^2 w_i + v_i w_i^2 + v_i v_j w_j + v_j w_i w_j + v_i v_k w_k + v_k w_i w_k \right).$$

Appendix B

Some Gaussian integrals

Starting from

$$\int_{\mathbb{R}} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}\,, \quad \int_{\mathbb{R}} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2a^{\frac{3}{2}}}\,, \quad \int_{\mathbb{R}} x^4 e^{-ax^2} dx = \frac{3\sqrt{\pi}}{4a^{\frac{5}{2}}}\,, \tag{B.1}$$

where $a > 0$, we compute

$$\begin{aligned}
&\frac{m_s}{2T}\int_{\mathbb{R}^3} c_i^4 f_s^{(0)}(\boldsymbol{v}) d\boldsymbol{v} = \left(\frac{m_s}{2T}\right)^{\frac{5}{2}} \pi^{-\frac{3}{2}} n_s \int_{\mathbb{R}^3} c_i^4 \exp\left\{-\frac{m_s}{2T}c^2\right\} d\boldsymbol{c} \\
&= \left(\frac{m_s}{2T}\right)^{\frac{5}{2}} \pi^{-\frac{3}{2}} n_s \int_{\mathbb{R}} c_i^4 \exp\left\{-\frac{m_s}{2T}c_i^2\right\} dc_i \int_{\mathbb{R}} \exp\left\{-\frac{m_s}{2T}c_j^2\right\} dc_j \int_{\mathbb{R}} \exp\left\{-\frac{m_s}{2T}c_k^2\right\} dc_k \\
&= \left(\frac{m_s}{2T}\right)^{\frac{5}{2}} \pi^{-\frac{3}{2}} n_s \frac{3}{2} \left(\frac{m_s}{2T}\right)^{-\frac{7}{2}} \pi^{\frac{3}{2}} = \frac{3n_sT}{2m_s}\,.
\end{aligned} \tag{B.2}$$

Analogously,

$$\begin{aligned}
&\frac{m_s}{2T}\int_{\mathbb{R}^3} c_i^2 c_j^2 f_s^{(0)}(\boldsymbol{v}) d\boldsymbol{v} \\
&= \left(\frac{m_s}{2T}\right)^{\frac{5}{2}} \pi^{-\frac{3}{2}} n_s \int_{\mathbb{R}} c_i^2 \exp\left\{-\frac{m_s}{2T}c_i^2\right\} dc_i \int_{\mathbb{R}} c_j^2 \exp\left\{-\frac{m_s}{2T}c_j^2\right\} dc_j \int_{\mathbb{R}} \exp\left\{-\frac{m_s}{2T}c_k^2\right\} dc_k \\
&= \frac{n_sT}{2m_s}\,.
\end{aligned} \tag{B.3}$$

Appendix C

Analytical computations of macroscopic fields

Analytical computations for the first-order approximation of the pressure tensor $\underline{\boldsymbol{P}}^{(1)}$ for the general mixed model

In this appendix we report some technical computations useful to recover the closure of pressure tensor in Navier–Stokes equations derived from the general mixed Boltzmann-BGK model. More specifically, making use of (A.9), we compute

$$
\begin{aligned}
&m_s \lambda_{sr} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} v_i^{sr'} v_j^{sr'} \left[f_s^{(0)}(\boldsymbol{v}) f_r^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_r^{(0)}(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w} d\omega \\
&- 4\pi m_s \lambda_{sr} n_r \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v}
\end{aligned}
$$

$$
\begin{aligned}
&= 4\pi m_s \lambda_{sr} \Bigg\{ n_r \alpha_{sr}^2 \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + n_s \alpha_{rs}^2 \int_{\mathbb{R}^3} w_i w_j f_r^{(1)} d\boldsymbol{w} \\
&+ \alpha_{sr}\alpha_{rs} \Bigg[\int_{\mathbb{R}^3} v_i f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_j f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_i f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_j f_r^{(0)} d\boldsymbol{w} \\
&+ \int_{\mathbb{R}^3} v_j f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_j f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i f_r^{(0)} d\boldsymbol{w} \Bigg] \\
&+ \frac{\delta_{ij}}{3} \alpha_{rs}^2 \Bigg[n_r \int_{\mathbb{R}^3} v^2 f_s^{(1)} d\boldsymbol{v} + n_s \int_{\mathbb{R}^3} w^2 f_r^{(1)} d\boldsymbol{w} - 2 \int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} \boldsymbol{w} f_r^{(1)} d\boldsymbol{w} \\
&- 2 \int_{\mathbb{R}^3} \boldsymbol{v} f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} \boldsymbol{w} f_r^{(0)} d\boldsymbol{w} \Bigg] \Bigg\} - 4\pi m_s \lambda_{sr} n_r \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} \\
&= 4\pi m_s \lambda_{sr} \Bigg\{ n_r \underbrace{(\alpha_{sr}^2 - 1)}_{=-\alpha_{rs}(1+\alpha_{sr})} \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + n_s \alpha_{rs}^2 \int_{\mathbb{R}^3} v_i v_j f_r^{(1)} d\boldsymbol{v} \\
&+ \alpha_{sr}\alpha_{rs} n_s n_r \left(u_i u_j^{r^{(1)}} + u_j u_i^{s^{(1)}} + u_i u_j^{s^{(1)}} + u_j u_i^{r^{(1)}} \right) + \frac{\delta_{ij}}{3} \alpha_{rs}^2 n_s n_r \\
&\times \left[2\boldsymbol{u} \cdot (\boldsymbol{u}_s^{(1)} + \boldsymbol{u}_r^{(1)}) + \frac{3T_s^{(1)}}{m_s} - 2\boldsymbol{u} \cdot (\boldsymbol{u}_s^{(1)} + \boldsymbol{u}_r^{(1)}) + \frac{3T_r^{(1)}}{m_r} \right] \Bigg\} \\
&= 4\pi \lambda_{sr} \mu_{sr} \Bigg[n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + n_s \alpha_{rs} \int_{\mathbb{R}^3} v_i v_j f_r^{(1)} d\boldsymbol{v} \\
&+ \alpha_{sr} n_s n_r \left(u_i u_j^{r^{(1)}} + u_j u_i^{s^{(1)}} + u_i u_j^{s^{(1)}} + u_j u_i^{r^{(1)}} \right) + \delta_{ij} \alpha_{rs} n_s n_r \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r} \right) \Bigg].
\end{aligned}
\tag{C.1}
$$

Analytical computations for the first-order approximation of the heat flux vector $\boldsymbol{q}^{(1)}$ for the general mixed model

It holds that

$$
\begin{aligned}
&\int_{\mathbb{R}^3} v_i v^2 f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} = \int_{\mathbb{R}^3} \left[c_i c^2 + c_i u^2 + 2c_i \boldsymbol{u}\cdot\boldsymbol{c} + u_i c^2 + u_i u^2 + 2u_i \boldsymbol{u}\cdot(\boldsymbol{v}-\boldsymbol{u})\right] f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \\
&\int_{\mathbb{R}^3} \left[c_i c^2 + (v_i - u_i) u^2 + 2(v_i - u_i)\boldsymbol{u}\cdot(\boldsymbol{v}-\boldsymbol{u}) + u_i\left(v^2 + u^2 - 2\boldsymbol{v}\cdot\boldsymbol{u}\right) + 2u_i \boldsymbol{u}\cdot\boldsymbol{v}\right] f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \\
&= \int_{\mathbb{R}^3} \left[c_i c^2 + v_i u^2 + 2(v_i - u_i)\left(\boldsymbol{u}\cdot\boldsymbol{v} - u^2\right) + u_i v^2 - 2u_i \boldsymbol{u}\cdot\boldsymbol{v} + 2u_i \boldsymbol{u}\cdot\boldsymbol{v}\right] f_s^{(1)}(\boldsymbol{v}) d\boldsymbol{v} \\
&= \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} + n_s u^2 u_i^{s^{(1)}} + \int_{\mathbb{R}^3} \Big[2v_i\left(u_i v_i + u_j v_j + u_k v_k\right) - 2u_i\left(u_i v_i + u_j v_j + u_k v_k\right) \\
&- 2v_i u^2 + u_i v^2\Big] f_s^{(1)} d\boldsymbol{v} \\
&= \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} + 2u_i \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} + 2u_j \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + 2u_k \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} \\
&- n_s u^2 u_i^{s^{(1)}} - 2n_s\left(u_i^2 u_i^{s^{(1)}} + u_i u_j u_j^{s^{(1)}} + u_i u_k u_k^{s^{(1)}}\right) + n_s u_i \left(2\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s}\right) \\
&= \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} + 2u_i \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} + 2u_j \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + 2u_k \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} \\
&- n_s u^2 u_i^{s^{(1)}} + n_s u_i \frac{3T_s^{(1)}}{m_s}\,. \qquad \text{(C.2)}
\end{aligned}
$$

Making use of (3.40) and (3.51), for $q_i^{(1)}$ we compute

$$
\begin{aligned}
& m_s \int_{\mathbb{R}^3} \left[-u_i v^2 + u^2 v_i - 2(u_i v_i^2 + u_j v_i v_j + u_k v_i v_k) + 2u_i \boldsymbol{u}\cdot\boldsymbol{v}\right] \\
& \times \left[Q_{sr}(f_s^{(0)}, f_r^{(1)}) + Q_{rs}(f_s^{(1)}, f_r^{(0)})\right] d\boldsymbol{v} \\
& = m_s \Bigg\{ 4\pi\lambda_{sr} n_s n_r \alpha_{rs} u^2 \left[u_i^{r^{(1)}} - u_i^{s^{(1)}}\right] + 8\pi\lambda_{sr} n_s n_r \alpha_{rs} u_i \boldsymbol{u} \left[\boldsymbol{u}_r^{(1)} - \boldsymbol{u}_s^{(1)}\right] \\
& + 8\pi u_j \lambda_{sr}\alpha_{rs} \left[n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} dv + n_s \alpha_{rs} \int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v}\right] \\
& + 8\pi u_k \lambda_{sr}\alpha_{rs} \left[n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_i c_k f_s^{(1)} d\boldsymbol{v} + n_s \alpha_{rs} \int_{\mathbb{R}^3} c_i c_k f_r^{(1)} d\boldsymbol{v}\right] \\
& + 4\pi u_i \lambda_{sr}\alpha_{rs} \Bigg[3 \left(n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_i^2 f_s^{(1)} d\boldsymbol{v} + n_s\alpha_{rs} \int_{\mathbb{R}^3} c_i^2 f_r^{(1)} d\boldsymbol{v} + n_s n_r \alpha_{rs} \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r}\right)\right) \\
& + n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_j^2 f_s^{(1)} d\boldsymbol{v} + n_s\alpha_{rs} \int_{\mathbb{R}^3} c_j^2 f_r^{(1)} d\boldsymbol{v} + n_s n_r \alpha_{rs} \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r}\right) \\
& + n_r(-1-\alpha_{sr}) \int_{\mathbb{R}^3} c_k^2 f_s^{(1)} d\boldsymbol{v} + n_s\alpha_{rs} \int_{\mathbb{R}^3} c_k^2 f_r^{(1)} d\boldsymbol{v} + n_s n_r \alpha_{rs} \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r}\right) \Bigg] \\
& = 4\pi\lambda_{sr}\mu_{sr} \Bigg\{ n_s n_r u^2 \left[u_i^{r^{(1)}} - u_i^{s^{(1)}}\right] + 2n_s n_r u_i \boldsymbol{u}\cdot\left[\boldsymbol{u}_r^{(1)} - \boldsymbol{u}_s^{(1)}\right] \\
& + 2\Bigg[n_r(-1-\alpha_{sr}) \left(u_j \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + u_k \int_{\mathbb{R}^3} c_i c_k f_s^{(1)} d\boldsymbol{v}\right) \\
& + n_s\alpha_{rs} \left(u_j \int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v} + u_k \int_{\mathbb{R}^3} c_i c_k f_r^{(1)} d\boldsymbol{v}\right)\Bigg] \\
& + u_i \Bigg[n_r(-1-\alpha_{sr}) \left(3\int_{\mathbb{R}^3} c_i^2 f_s^{(1)} d\boldsymbol{v} + \int_{\mathbb{R}^3} c_j^2 f_s^{(1)} d\boldsymbol{v} + \int_{\mathbb{R}^3} c_k^2 f_s^{(1)} d\boldsymbol{v}\right) \\
& + n_s\alpha_{rs} \left(3\int_{\mathbb{R}^3} c_i^2 f_r^{(1)} d\boldsymbol{v} + \int_{\mathbb{R}^3} c_j^2 f_r^{(1)} d\boldsymbol{v} + \int_{\mathbb{R}^3} c_k^2 f_r^{(1)} d\boldsymbol{v}\right) \\
& + 5\alpha_{rs} n_s n_r \left(\frac{T_s^{(1)}}{m_s} + \frac{T_r^{(1)}}{m_r}\right)\Bigg].
\end{aligned}
\tag{C.3}
$$

Exchanging pre- and post-collision velocities and exploiting (A.10), we now derive

$$
\begin{aligned}
& m_s \lambda_{sr} \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i v^2 \left[f_s^{(0)}(\boldsymbol{v}'_{sr}) f_r^{(1)}(\boldsymbol{w}'_{sr}) + f_s^{(1)}(\boldsymbol{v}'_{sr}) f_r^{(0)}(\boldsymbol{w}'_{sr}) \right] d\boldsymbol{v} d\boldsymbol{w} d\omega \\
& - 4\pi m_s \lambda_{sr} n_r \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} \\
& = m_s \lambda_{sr} \int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i'^{sr} v_{sr}'^2 \left[f_s^{(0)}(\boldsymbol{v}) f_r^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_r^{(0)}(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w} d\omega \\
& - 4\pi m_s \lambda_{sr} n_r \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} \\
& = 4\pi m_s \lambda_{sr} \int_{\mathbb{R}^3\times\mathbb{R}^3} \Bigg[\left(\alpha_{sr}^3 + \frac{5}{3}\alpha_{sr}\alpha_{rs}^2 \right) v_i v^2 + \frac{8}{3}\alpha_{rs}^3 w_i w^2 + \frac{8}{3}\alpha_{sr}\alpha_{rs}^2 v_i w^2 \\
& + \left(\alpha_{sr}^2 \alpha_{rs} + \frac{5}{3}\alpha_{rs}^3 \right) v^2 w_i + 2\left(\alpha_{sr}^2\alpha_{rs} - \frac{5}{3}\alpha_{sr}\alpha_{rs}^2 \right) \left(v_i^2 w_i + v_i v_j w_j + v_i v_k w_k \right) \\
& + 2\left(\alpha_{sr}\alpha_{rs}^2 - \frac{5}{3}\alpha_{rs}^3 \right) \left(v_i w_i^2 + v_j w_i w_j + v_k w_i w_k \right) \Bigg] \\
& \times \left[f_s^{(0)}(\boldsymbol{v}) f_r^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_r^{(0)}(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w}
\end{aligned}
$$

$$
\begin{aligned}
&= m_s 4\pi\lambda_{sr}\Bigg[\left(\alpha_{sr}^3 + \frac{5}{3}\alpha_{sr}\alpha_{rs}^2\right) n_r \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} + \frac{8}{3}\alpha_{rs}^3 n_s \int_{\mathbb{R}^3} v_i v^2 f_r^{(1)} d\boldsymbol{v} \\
&+ \frac{8}{3}\alpha_{sr}\alpha_{rs}^2 \left(\int_{\mathbb{R}^3} v_i f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w^2 f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_i f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w^2 f_r^{(0)} d\boldsymbol{w} \right) \\
&+ \left(\alpha_{sr}^2\alpha_{rs} + \frac{5}{3}\alpha_{rs}^3\right)\left(\int_{\mathbb{R}^3} v^2 f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v^2 f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i^2 f_s^{(0)} d\boldsymbol{w} \right) \\
&+ 2\left(\alpha_{sr}^2\alpha_{rs} - \frac{5}{3}\alpha_{sr}\alpha_{rs}^2\right)\Bigg(\int_{\mathbb{R}^3} v_i^2 f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i f_r^{(0)} d\boldsymbol{w} \\
&+ \int_{\mathbb{R}^3} v_i v_j f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_j f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_j f_r^{(0)} d\boldsymbol{w} \\
&+ \int_{\mathbb{R}^3} v_i v_k f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_k f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_k f_r^{(0)} d\boldsymbol{w} \Bigg) \\
&+ 2\left(\alpha_{sr}\alpha_{rs}^2 - \frac{5}{3}\alpha_{rs}^3\right)\Bigg(\int_{\mathbb{R}^3} v_i f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i^2 f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_i f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i^2 f_r^{(0)} d\boldsymbol{w} \\
&+ \int_{\mathbb{R}^3} v_j f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i w_j f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_j f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i w_j f_r^{(0)} d\boldsymbol{w} \\
&+ \int_{\mathbb{R}^3} v_k f_s^{(0)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i w_k f_r^{(1)} d\boldsymbol{w} + \int_{\mathbb{R}^3} v_k f_s^{(1)} d\boldsymbol{v} \int_{\mathbb{R}^3} w_i w_k f_r^{(0)} d\boldsymbol{w} \Bigg) \\
&= 4\pi m_s \lambda_{sr}\Bigg\{ \left(\alpha_{sr}^3 + \frac{5}{3}\alpha_{sr}\alpha_{rs}^2 - 1\right) n_r \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} + \frac{8}{3}\alpha_{rs}^3 n_s \int_{\mathbb{R}^3} v_i v^2 f_r^{(1)} d\boldsymbol{v} \\
&+ \frac{8}{3}\alpha_{sr}\alpha_{rs}^2 n_s n_r \left[u_i \left(2\boldsymbol{u}\cdot\boldsymbol{u}_r^{(1)} + \frac{3T_r^{(1)}}{m_r} \right) + u_i^{2^{(1)}} \left(u^2 + \frac{3T}{m_r} \right) \right] \\
&+ \left(\alpha_{sr}\alpha_{rs}^2 - \frac{5}{3}\alpha_{rs}^3\right) n_s n_r \left[u_i \left(2\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s} \right) + u_i^{2^{(1)}} \left(u^2 + \frac{3T}{m_s} \right) \right] \\
&+ 2\left(\alpha_{sr}^2\alpha_{rs} - \frac{5}{3}\alpha_{sr}\alpha_{rs}^2\right)\Bigg[n_s n_r \left(u_i \boldsymbol{u}\cdot\boldsymbol{u}_r^{(1)} + u_i^{r^{(1)}} \frac{T}{m_s} \right) \qquad \text{(C.4)} \\
&+ n_r \left(u_i \int_{\mathbb{R}^3} c_i^2 f_s^{(1)} d\boldsymbol{v} + u_j \int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v} + u_k \int_{\mathbb{R}^3} c_i c_k f_s^{(1)} d\boldsymbol{v} \right) \Bigg] \\
&+ 2\left(\alpha_{sr}\alpha_{rs}^2 - \frac{5}{3}\alpha_{rs}^3\right)\Bigg[n_s n_r \left(u_i \boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)} + u_i^{s^{(1)}} \frac{T}{m_r} \right) \\
&+ n_s \left(u_i \int_{\mathbb{R}^3} c_i^2 f_r^{(1)} d\boldsymbol{v} + u_j \int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v} + u_k \int_{\mathbb{R}^3} c_i c_k f_r^{(1)} d\boldsymbol{v} \right) \Bigg],
\end{aligned}
$$

where we used the moments of $f_s^{(0)}$, $f_s^{(1)}$, along with (3.50).
Now, taking advantage of (C.2) to explicit the integrals $\int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v}$, $\int_{\mathbb{R}^3} v_i v^2 f_r^{(1)} d\boldsymbol{v}$, (C.4) becomes

$$
\begin{aligned}
& m_s\lambda_{sr}\int_{\mathbb{R}^3\times\mathbb{R}^3\times\mathbb{S}^2} v_i v^2\Big[f_s^{(0)}(\boldsymbol{v}'_{sr})f_r^{(1)}(\boldsymbol{w}'_{sr})+f_s^{(1)}(\boldsymbol{v}'_{sr})f_r^{(0)}(\boldsymbol{w}'_{sr})\Big]d\boldsymbol{v}d\boldsymbol{w}d\omega \\
& -4\pi m_s\lambda_{sr}n_r\int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} \\
& =4\pi m_s\lambda_{sr}\Bigg\{\left(\alpha_{sr}^3+\frac{5}{3}\alpha_{sr}\alpha_{rs}^2-1\right)n_r\Bigg[\int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v}+2\Bigg(u_i\int_{\mathbb{R}^3} c_i^2 f_s^{(1)} d\boldsymbol{v} \\
& +u_j\int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v}+u_k\int_{\mathbb{R}^3} c_i c_k f_s^{(1)} d\boldsymbol{v}\Bigg)+n_s u^2 u_i^{s^{(1)}}+n_s u_i\left(2\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)}+\frac{3T_s^{(1)}}{m_s}\right)\Bigg] \\
& +\frac{8}{3}\alpha_{rs}^3 n_s\Bigg[\int_{\mathbb{R}^3} c_i c^2 f_r^{(1)} d\boldsymbol{v}+2\Bigg(u_i\int_{\mathbb{R}^3} c_i^2 f_r^{(1)} d\boldsymbol{v}+u_j\int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v} \\
& +u_k\int_{\mathbb{R}^3} c_i c_k f_r^{(1)} d\boldsymbol{v}\Bigg)+n_s u^2 u_i^{r^{(1)}}+n_s u_i\left(2\boldsymbol{u}\cdot\boldsymbol{u}_r^{(1)}+\frac{3T_r^{(1)}}{m_r}\right)\Bigg] \\
& +\frac{8}{3}\alpha_{sr}\alpha_{rs}^2 n_s n_r\left[u_i\left(2\boldsymbol{u}\cdot\boldsymbol{u}_r^{(1)}+\frac{3T_r^{(1)}}{m_r}\right)+u_i^{2^{(1)}}\left(u^2+\frac{3T}{m_r}\right)\right] \qquad\qquad (C.5) \\
& +\left(\alpha_{sr}\alpha_{rs}^2-\frac{5}{3}\alpha_{rs}^3\right)n_s n_r\left[u_i\left(2\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)}+\frac{3T_s^{(1)}}{m_s}\right)+u_i^{2^{(1)}}\left(u^2+\frac{3T}{m_s}\right)\right] \\
& +2\left(\alpha_{sr}^2\alpha_{rs}-\frac{5}{3}\alpha_{sr}\alpha_{rs}^2\right)\Bigg[n_s n_r\left(u_i\boldsymbol{u}\cdot\boldsymbol{u}_r^{(1)}+u_i^{r^{(1)}}\frac{T}{m_s}\right) \\
& +n_r\left(u_i\int_{\mathbb{R}^3} c_i^2 f_s^{(1)} d\boldsymbol{v}+u_j\int_{\mathbb{R}^3} c_i c_j f_s^{(1)} d\boldsymbol{v}+u_k\int_{\mathbb{R}^3} c_i c_k f_s^{(1)} d\boldsymbol{v}\right)\Bigg] \\
& +2\left(\alpha_{sr}\alpha_{rs}^2-\frac{5}{3}\alpha_{rs}^3\right)\Bigg[n_s n_r\left(u_i\boldsymbol{u}\cdot\boldsymbol{u}_s^{(1)}+u_i^{s^{(1)}}\frac{T}{m_r}\right) \\
& +n_s\left(u_i\int_{\mathbb{R}^3} c_i^2 f_r^{(1)} d\boldsymbol{v}+u_j\int_{\mathbb{R}^3} c_i c_j f_r^{(1)} d\boldsymbol{v}+u_k\int_{\mathbb{R}^3} c_i c_k f_r^{(1)} d\boldsymbol{v}\right)\Bigg].
\end{aligned}
$$

Analytical computations for the first-order approximation of the heat flux vector $\boldsymbol{q}^{(1)}$ under the assumption $\chi_{sr} = \delta_{sr}$

Recalling (4.4) and setting $\boldsymbol{v}'_s = \boldsymbol{v}'$, we compute $m_s \int_{\mathbb{R}^3} c_i c^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v}$,

$$
\begin{aligned}
&\frac{1}{2} m_s \int_{\mathbb{R}^3} c_i c^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \\
&= \frac{1}{2} m_s \int_{\mathbb{R}^3} (v_i - \underbrace{u_i}_{=0}) \left(v^2 + w^2 - 2v_i u_i - 2v_j u_j - 2v_k u_k\right) f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \\
&= \frac{1}{2} m_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} - m_s \int_{\mathbb{R}^3} \left(u_i v_i^2 + u_j v_i v_j + u_k v_i v_k\right) f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} \\
&= \frac{1}{2} m_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} - 2\pi u_i m_s \lambda_s n_s \Big\{ - \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} + 2 n_s u_i u_i^{s^{(1)}} + n_s \frac{T_s^{(1)}}{m_s} \Big\} \\
&- 2\pi u_j m_s \lambda_s n_s \Big\{ - \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} + n_s \left(u_i u_j^{s^{(1)}} + u_j u_i^{s^{(1)}} \right) \Big\} \qquad \text{(C.6)} \\
&- 2\pi u_k m_s \lambda_s n_s \Big\{ - \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} + n_s \left(u_i u_k^{s^{(1)}} + u_k u_i^{s^{(1)}} \right) \Big\}.
\end{aligned}
$$

Now, making use of (A.12) and the symmetry with respect to the variables $\boldsymbol{v}$ and $\boldsymbol{w}$ of the linearized intra-species operator, we obtain

$$
\begin{aligned}
&\frac{1}{2} m_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} = \frac{1}{2} m_s \lambda_s \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} v'_i v'^2 \\
&\times \left[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_s^{(0)}(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w} d\omega - 2\pi m_s \lambda_s n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} \\
&= \frac{\pi}{2} m_s \lambda_s \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left(\frac{8}{3} v_i v^2 + \frac{8}{3} v^2 w_i - \frac{4}{3} v_i^2 w_i - \frac{4}{3} v_i v_j w_i - \frac{4}{3} v_i v_k w_k \right) \\
&\times \left[f_s^{(0)}(\boldsymbol{v}) f_s^{(1)}(\boldsymbol{w}) + f_s^{(1)}(\boldsymbol{v}) f_s^{(0)}(\boldsymbol{w}) \right] d\boldsymbol{v} d\boldsymbol{w} - 2\pi m_s \lambda_s n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} \\
&= \frac{\pi}{2} m_s \lambda_s \Bigg[- \frac{4}{3} n_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} + \frac{8}{3} n_s^2 \left(u^2 + \frac{3T}{m_s} \right) u_i^{s^{(1)}} + \frac{16}{3} n_s^2 u_i \boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} \\
&- \frac{4}{3} n_s u_i \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} - \frac{4}{3} n_s^2 \left(u_i^2 + \frac{T}{m_s} \right) u_i^{s^{(1)}} - \frac{4}{3} n_s u_j \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} \\
&- \frac{4}{3} n_s u_k \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} - \frac{4}{3} n_s^2 \left(u_i u_j u_j^{s^{(1)}} + u_i u_k u_k^{s^{(1)}} \right) \Bigg]
\end{aligned}
$$

$$= \frac{2}{3}\pi m_s \lambda_s n_s \Bigg\{ - \int_{\mathbb{R}^3} v_i v^2 f_s^{(1)} d\boldsymbol{v} - u_i \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} - u_j \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v}$$

$$- u_k \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} + 2 n_s u_i^{s^{(1)}} \left(u^2 + \frac{3T}{m_s} \right) + 2 n_s u_i \left(2\boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s} \right)$$

$$- n_s \left[u_i^{s^{(1)}} \left(u_i^2 + \frac{T}{m_s} \right) + u_i u_j u_j^{s^{(1)}} + u_i u_k u_k^{s^{(1)}} \right]$$

$$= \frac{2}{3}\pi m_s \lambda_s n_s \Bigg\{ - \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} - 3u_i \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v} - 3u_j \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v}$$

$$- 3u_k \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} + n_s u^2 u_i^{s^{(1)}} + 2 n_s u_i \boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} - n_s u_i \left(2\boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s} \right)$$

$$+ 2 n_s u_i^{s^{(1)}} \left(u^2 + \frac{3T}{m_s} \right) + 2 n_s u_i \left(2\boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s} \right)$$

$$- n_s \left[u_i^{s^{(1)}} \left(u_i^2 + \frac{T}{m_s} \right) + u_i \left(u_j u_j^{s^{(1)}} + u_k u_k^{s^{(1)}} \right) \right] \Bigg\},$$

where in the last equality we exploited (C.2). Hence,

$$\frac{1}{2} m_s \int_{\mathbb{R}^3} v_i v^2 f_s^{(0)} \mathcal{L}(h_s^{(1)}) d\boldsymbol{v} = \frac{2}{3}\pi m_s \lambda_s n_s \Bigg\{ - \int_{\mathbb{R}^3} c_i c^2 f_s^{(1)} d\boldsymbol{v} - 3u_i \int_{\mathbb{R}^3} v_i^2 f_s^{(1)} d\boldsymbol{v}$$

$$- 3u_j \int_{\mathbb{R}^3} v_i v_j f_s^{(1)} d\boldsymbol{v} - 3u_k \int_{\mathbb{R}^3} v_i v_k f_s^{(1)} d\boldsymbol{v} + n_s u^2 u_i^{s^{(1)}} - n_s u_i \frac{3T_s^{(1)}}{m_s} \tag{C.7}$$

$$+ 2 n_s u_i^{s^{(1)}} \left(u^2 + \frac{3T}{m_s} \right) + 2 n_s u_i \left(2\boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + \frac{3T_s^{(1)}}{m_s} \right) - n_s \left(u_i \boldsymbol{u} \cdot \boldsymbol{u}_s^{(1)} + u_i^{s^{(1)}} \frac{T}{m_s} \right) \Bigg\}.$$

Appendix D

Ciszar-Kullback inequality

Theorem 5. *Let $\Omega \subset \mathbb{R}^d$ and $f_\infty : \Omega \to \mathbb{R}^+$ be a strictly probability density on Ω. Assume that $\phi : \mathbb{R}^+ \to \mathbb{R}$ is a smooth and strictly convex function with $\phi^{"}(1) \geq c > 0$ for all $0 \leq x \leq 1$.*
For the relative enthropy functional

$$H_\phi[f] := \int_\Omega \phi\left(\frac{f}{f_\infty}\right) f_\infty dx \ ,$$

the following ineqaulity holds

$$||f - f_\infty||_{L^1(\Omega)} \leq C\left(H_\phi[f] - H_\phi[f_\infty]\right)^{\frac{1}{2}} \ ,$$

for all probability densities $f \in P(\Omega)$.

Proof. The proof is given in [38].
Since ϕ is assumed to be smooth, we can write the Taylor expansion of ϕ as

$$\phi(s) = \phi(1) + \phi'(1)(s-1) + \frac{\phi^{"}(\tau)}{2}(1-s)^2 \ ,$$

for $s > 0$ and τ between s and 1. Since ϕ is convex with $\phi^{"}(x) \geq 2c > 0$ for all $x \in [0,1]$, we obtain

$$\phi(s) - \phi(1) \geq \phi'(1)(s-1) + c(1-s)^2 \mathbf{1}_{\{s<1\}},$$

for all $s > 0$, where $\mathbf{1}_A$ denotes the characteristic function of the set A. Since $f_\infty(x)dx$ defines a probability measure on Ω, we have

$$\begin{aligned} H_\phi[f] - H_\phi[f_\infty] &= \int_\Omega \left[\phi\left(\frac{f}{f_\infty}\right) - \phi(1)\right] f_\infty dx \\ &\geq \phi'(1)\int_\Omega (f - f_\infty)dx + c\int_{f<f_\infty}\left(\frac{f}{f_\infty} - 1\right)^2 f_\infty dx. \end{aligned} \tag{D.1}$$

The integral $\int_\Omega (f - f_\infty)dx$ vanishes because fdx and $f_\infty dx$ are both probability measures meaning the integrals of both function are 1. So the previous inequality reduces to

$$H_\phi[f] - H_\phi[f_\infty] \geq c \int_{f<f_\infty} \left(\frac{f}{f_\infty} - 1 \right)^2 f_\infty dx \ . \tag{D.2}$$

Another consequence for the probability measures is that

$$\begin{aligned} ||f - f_\infty||_{L^1(\Omega)} &= 2 \int_{f<f_\infty} |f - f_\infty| dx = 2 \int_{f<f_\infty} f_\infty \left| \frac{f}{f_\infty} - 1 \right| dx \\ &\geq 2 \left(\int_{f<f_\infty} \left(\frac{f}{f_\infty} - 1 \right)^2 f_\infty dx \right)^{\frac{1}{2}} \ , \end{aligned} \tag{D.3}$$

where the last inequality uses the Hölder inequality for the functions $(f_\infty)^{\frac{1}{2}}$ and $(f_\infty)^{\frac{1}{2}} |\frac{f}{f_\infty} - 1|$.
A combination of (D.2) and (D.3) leads to the result. □

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