



Study of Nonlocal Collisional Kinetic Models and Their Applications to Thick Sprays

Zhe Chen

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Study of Nonlocal Collisional Kinetic Models and Their Applications to Thick Sprays

**Étude de modèles cinétiques à collisions délocalisées et
applications aux sprays épais**

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COLOPHON

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Stories brought on the wind will bloom
into legend in due time.

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前面的路，以后再来探索吧!

Study of Nonlocal Collisional Kinetic Models and Their Applications to Thick Sprays Étude de modèles cinétiques à collisions délocalisées et applications aux sprays épais

Abstract

This thesis is devoted to the study of delocalized collision models and to the establishment of links between particle systems, delocalized kinetic models, and fluid–kinetic models for thick sprays.

Chapters 2 and 3 investigate the properties of several delocalized collision models. In Chapter 2, we present a unified framework from the revised Enskog model, Cercignani’s soft sphere model, and a modified Povzner model. Local conservative representations are established, from which the corresponding conservation laws are derived using the moment method, together with associated entropy inequalities. Chapter 3 applies the same method to the standard Enskog model and the original Povzner model, where conservative forms are obtained but the resulting entropy inequalities are weaker and of limited interest.

The second part of the thesis focuses on the formal derivation of the coupled Enskog and Vlasov–Euler equations for thick sprays. Chapter 4 derives the coupled Enskog equations from the underlying particle system, establishes conservation of mass, momentum, and energy, and proves an H-theorem. Chapter 5 studies the Eulerian–Lagrangian model as a hydrodynamic limit of the coupled Boltzmann–Enskog equations.

Keywords: kinetic models, fluid dynamics, aerosols, nonlocal collisions, Enskog model, conservation laws, entropy inequalities, moment method, particle systems, hydrodynamic limit, fluid–kinetic coupling, thick sprays

Résumé

Cette thèse est consacrée à l’étude de modèles cinétiques avec collisions délocalisées et à l’établissement de liens entre des systèmes de particules, des modèles cinétiques délocalisés et des modèles fluide-cinétiques pour les sprays épais.

La première partie étudie les propriétés de plusieurs modèles de collisions délocalisées. Le chapitre 2 analyse le modèle d’Enskog révisé, le modèle de sphères molles de Cercignani et un modèle modifié de Povzner, et montre qu’ils peuvent être unifiés dans un cadre commun. Des représentations conservatives locales sont établies, permettant de dériver les lois de conservation macroscopiques correspondantes par la méthode des moments, ainsi que les inégalités d’entropie associées. Le chapitre 3 applique la même approche méthodologique au modèle standard d’Enskog et au modèle original de Povzner ; bien que des formes conservatives soient obtenues, les inégalités d’entropie qui en résultent sont plus faibles et d’intérêt limité.

La seconde partie est consacrée à la dérivation formelle des équations couplées d’Enskog et d’un système de type Vlasov–Euler pour les sprays épais. Le chapitre 4 dérive les équations d’Enskog couplées à partir du système de particules, établit la conservation de la masse, de la quantité de mouvement et de l’énergie, et démontre un théorème H pour le système. Enfin, le chapitre 5 étudie le couplage fluide-cinétique comme limite hydrodynamique des équations couplées de Boltzmann–Enskog.

Mots clés : modèles cinétiques, mécanique des fluides, aérosols, collisions délocalisées, modèle d’Enskog, lois de conservation, inégalités d’entropie, méthode des moments, systèmes de particules, limite hydrodynamique, couplage fluide-cinétique, sprays épais

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Chapter 1

Introduction

1.1 The kinetic equations

The kinetic theory provides a statistical framework for describing systems with a large number of particles, serving as a bridge between the microscopic dynamics of individual molecules and macroscopic observables such as density, bulk velocity, and temperature. A central model in this theory is the Boltzmann equation [Bol72; Max67], which offers a classical collisional description of the dynamics of a monatomic dilute gas. This equation encodes both free transport and binary interactions of particles, and it plays a fundamental role in deriving hydrodynamic equations from first principles. For a more comprehensive treatment of classical kinetic theory, the reader is referred to standard textbooks such as [Vil02; Bou+00; Cer94; CC90]. In what follows, we first recall the Boltzmann equation and its main properties, before discussing several important variants and extensions, including models with modified collision operators and the Vlasov equation, which arises in the study of collisionless plasmas and self-consistent mean-field interactions.

1.1.1 The Boltzmann equation

Let $f \equiv f(t, x, w) \geq 0$ denote the number density distribution function of gas molecules at time $t \geq 0$, position $x \in \mathbb{R}^3$, and with velocity $w \in \mathbb{R}^3$. The evolution of f is then governed by the Boltzmann equation (1872):

$$\partial_t f(t, x, w) + w \cdot \nabla_x f(t, x, w) = \mathcal{C}_B[f](t, x, w), \quad (1.1.1)$$

where the Boltzmann collision integral is

$$\mathcal{C}_B[f](t, x, w) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left(f(t, x, 'w) f(t, x, 'w_*) - f(t, x, w) f(t, x, w_*) \right) b(w - w_*, \mathbf{n}) dw_* d\mathbf{n}. \quad (1.1.2)$$

Here $'w \equiv 'w(w, w_*, \mathbf{n})$ and $'w_* \equiv 'w_*(w, w_*, \mathbf{n})$ denote the velocities just before the collision, while w and w_* are the velocities immediately after the collision. For elastic collision between gas molecules, it's natural to require conservation of momentum and energy:

$$'w + 'w_* = w + w_*; \quad |'w|^2 + |'w_*|^2 = |w|^2 + |w_*|^2,$$

The system has 6 unknowns (3 component for each pre-collision velocity), and 4 constraints, which leaves 2-degree of freedom. In order to parametrize $'w$ and $'w_*$, we introduce additional variable $\mathbf{n}$, which belongs to the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$, and it's easy to show that the following representation satisfy the laws of conservation of momentum and energy:

$$\begin{cases} 'w \equiv 'w(w, w_*, \mathbf{n}) = w - (w - w_*) \cdot \mathbf{n} \mathbf{n}, \\ 'w_* \equiv 'w_*(w, w_*, \mathbf{n}) = w_* + (w - w_*) \cdot \mathbf{n} \mathbf{n}. \end{cases} \quad (1.1.3)$$

The representation of the pre-collision velocities $'w$ and $'w_*$ are not unique. The relationship between these vectors can be visualized in Figure 1.1.

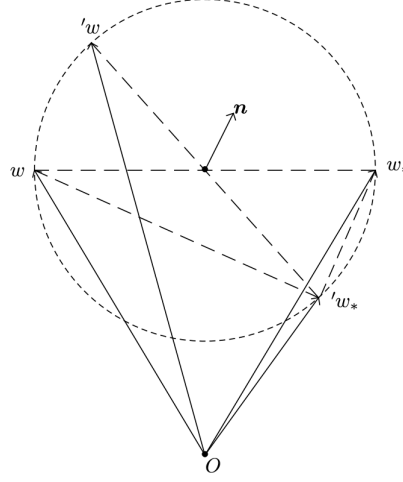


Figure 1.1: Geometric representation of pre-collision velocities $'w, 'w_*$ on a circle defined by conservation laws. The parameter $\mathbf{n}$ is normal vector in $\mathbb{S}^2$, and w, w_* are the post-collision velocities. O is the origin.

In addition, the collision kernel $b(z, \mathbf{n})$ takes the form

$$b(z, \mathbf{n}) = |z| \Sigma(|z|, \cos(\widehat{z, \mathbf{n}})) \quad \text{with } \Sigma > 0. \quad (1.1.4)$$

In most cases, the collision kernel is defined implicitly. Below, we list two important examples

- The hard sphere model corresponds to a potential $\phi(r) = \infty$ for $r \leq r_g$, and $\phi(r) = 0$ for $r > r_g$. The associated collision kernel is given by

$$b(z, \mathbf{n}) = (2r_g)^2 z \cdot \mathbf{n} H(z \cdot \mathbf{n}),$$

where $H : \mathbb{R} \rightarrow \{0, 1\}$ denotes the Heaviside step function is defined as

$$H(r) = \begin{cases} 1 & \text{for } r > 0 \\ 0 & \text{for } r \leq 0, \end{cases}$$

and where r_g is the radius of gas molecules, and m_g is the mass of each gas molecule.

- For inverse power law potential $\phi(r) = r^{-s}$: the collision kernel in dimension 3 is

$$b(z, \mathbf{n}) = \tilde{b}(\cos(\widehat{z, \mathbf{n}})) |z|^{(s-6)/s},$$

where $\tilde{b}$ is a positive function depending on the scattering angle.

Note that, due to the identities

$$|w - w_*| = |w - w_*|, \quad \text{and} \quad (w(w, w_*, \mathbf{n}) - w_*(w, w_*, \mathbf{n})) \cdot \mathbf{n} = -(w - w_*) \cdot \mathbf{n},$$

the collision kernel is invariant under collisions. In other words,

$$b(w - w_*, \mathbf{n}) = b(w(w, w_*, \mathbf{n}) - w_*(w, w_*, \mathbf{n}), \mathbf{n}). \quad (1.1.5)$$

Hence, during a collision, the term $f(w)f(w_*)d\mathbf{n}dw_*$ represents the number of molecules that gain velocity w after the collision, while $f(w)f(w_*)d\mathbf{n}dw_*$ accounts for the loss of molecules with velocity w . For this reason, we refer to the positive term as $\mathcal{C}_B^+$ (*gain term*), and the negative term as $\mathcal{C}_B^-$ (*loss term*), respectively.

In the absence of an external field, the left-hand side of (5.1.1), $\partial_t f + w \cdot \nabla_x f$, describes the variation of the distribution function within the infinitesimal phase space volume $f(t, x, w) dx dw$, capturing the evolution of number density.

The conservative form of collision integral

In [LP81], mathematically in [Vil99], they showed one possible expression for divergence form of Boltzmann collision kernel

Theorem 1.1.1. *In the sense of distributions, $\mathcal{C}_B[f] = -\text{div}_v \mathbf{J}[f]$ with*

$$\begin{aligned} \mathbf{J}_0[f](v) &:= - \int_{\langle v-w, \mathbf{n} \rangle > 0} \int_0^{\langle v-w, \mathbf{n} \rangle} B(v-w, \mathbf{n}) f(v+s\mathbf{n}) f(w+s\mathbf{n}) d\mathbf{n} dw ds \\ &= \int_{\langle w_*-v, w_o-v \rangle < 0} B\left(w_o - w_*, \frac{v-w_o}{|v-w_o|}\right) \frac{v-w_o}{|v-w_o|^3} f(w_o) f(w_*) d\mathbf{n} dw_* dw_o. \end{aligned} \quad (1.1.6)$$

Furthermore, the Boltzmann collision integral can be even written as a double divergence as

$$\mathcal{C}_B[f] = \sum_{1 \leq i, j \leq 3} \frac{\partial^2}{\partial v_i \partial v_j} \mathbf{A}_{ij}[f].$$

The explicit form of $\mathbf{A}$, together with the proof of Theorem 1.1.1, can be found in [Vil99]. The argument is based on the weak formulation of the Boltzmann collision integral (1.1.7), as well as on the structure of the Landau current associated with $\mathcal{C}_B[f](w)$ and its momentum-weighted counterpart $\mathcal{C}_B[f](w)w_i$ for $i = 1, 2, 3$. This provides an adaptation of Landau's original argument for passing from the Boltzmann collision integral to its grazing-collision limit, namely the Landau collision operator. Moreover, by invoking Stokes' theorem in velocity space, the collision term can be interpreted as the divergence of a flux, thereby

revealing collisions as a flux in velocity space. This viewpoint not only clarifies the conservative structure of the operator but also strengthens the analogy with transport phenomena in physical space, where fluxes across surfaces govern the evolution of conserved quantities.

Local conservation laws

From the conservative form of the collision integral, the conservation laws of the Boltzmann equation become evident. In a more convenient way, we can also be established through the following Lemma:

Lemma 1.1.1. *Let $f(w)$ and $\phi(w) \in L^\infty(\mathbb{R}^3)$, and assume that $f \in L^1(\mathbb{R}^3, (1 + |w|^2)^3 dw)$. The collision kernel $b(z, \mathbf{n}) > 0$ a.e., belongs to $L^1_{loc}(\mathbb{R}^3 \times \mathbb{S}^2)$ and is of the form (1.1.4). Then*

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{C}_B[f] \phi(w) dw \\ &= \frac{1}{4} \int_{\mathbb{R}^3 \times \mathbb{R}^2 \times \mathbb{S}^2} (f('w)f('w_*) - f(w)f(w_*)) (\phi('w)\phi('w_*) - \phi(w)\phi(w_*)) b(w-w, \mathbf{n}) dw dw_* d\mathbf{n}. \end{aligned} \quad (1.1.7)$$

As a corollary of the Lemma, if we take $\phi(w) = 1, w_1, w_2, w_3$ and $|w|^2$, then the collision integral mass, momentum, and energy locally (see, for instance, section 3.1 and section 3.3 in [Cer94])

Corollary 1.1.1. *Assume that $f \in L^1(\mathbb{R}^3, (1 + |w|^2)^3 dw)$. Then*

$$\int_{\mathbb{R}} \mathcal{C}_B[f](w) \begin{pmatrix} 1 \\ w_1 \\ w_2 \\ w_3 \\ |w|^2 \end{pmatrix} dw = \mathbf{0}. \quad (1.1.8)$$

This property implies that the Boltzmann collision integral does not contribute to the macroscopic equations *directly*, but only in an indirect way. In other words, we multiply equation (5.1.1) by 1, w , or $|w|^2/2$ and integrate it with respect to w . We obtain the following proposition.

Proposition 1.1.1. *Let $f \equiv f(t, x, w)$ be a classical solution of the Boltzmann equation (5.1.1). Besides, $f, \partial_t f$ and $\nabla_x f \in L^1(\mathbb{R}^3, (1 + |w|^2)^3 dw)$. Then we can write*

$$\begin{cases} \partial_t \int_{\mathbb{R}} f(t, x, w) dw + \operatorname{div}_x \int_{\mathbb{R}} w f(t, x, w) dw = 0, \\ \partial_t \int_{\mathbb{R}} w f(t, x, w) dw + \operatorname{div}_x \int_{\mathbb{R}} w^{\otimes 2} f(t, x, w) dw = 0, \\ \partial_t \int_{\mathbb{R}} \frac{|w|^2}{2} f(t, x, w) dw + \operatorname{div}_x \int_{\mathbb{R}} w \frac{|w|^2}{2} f(t, x, w) dw = 0, \end{cases}$$

where the divergence of a 2-tensor $\mathbf{B} \equiv (\mathbf{B}_{ij})$ with respect to variable x is defined componentwise by $(\operatorname{div}_x \mathbf{B})_i = (\sum_{j=1}^3 \partial_{x_j} \mathbf{B}_{ij})$.

Under the following definitions, we can establish the connection between kinetic description of gas and the framework of continuum mechanics. Let's introduce:

$$\begin{aligned}
R(t, x) &:= \int_{\mathbb{R}} f(t, x, w) dw, && \text{Local number density} \\
\mathbf{U}(t, x) &:= \frac{H(R(t, x))}{R(t, x)} \int_{\mathbb{R}} w f(t, x, w) dw, && \text{Bulk velocity} \\
\mathbf{P}(t, x) &:= \int_{\mathbb{R}} (w - \mathbf{U}(t, x))^{\otimes 2} f(t, x, w) dw, && \text{Stress tensor} \\
T(t, x) &:= \frac{H(R(t, x))}{2R(t, x)} \int_{\mathbb{R}} |w - \mathbf{U}(t, x)|^2 f(t, x, w) dw, && \text{Internal energy} \\
\mathbf{Q}(t, x) &:= \frac{1}{2} \int_{\mathbb{R}} (w - \mathbf{U}(t, x)) |w - \mathbf{U}(t, x)|^2 f(t, x, w) dw, && \text{Energy flux}
\end{aligned}$$

These definitions leads to the following fluid equations:

$$\begin{cases}
\partial_t R + \operatorname{div}_x (R\mathbf{U}) = 0, \\
\partial_t (R\mathbf{U}_i) + \sum_{j=1}^3 \partial_{x_j} (R\mathbf{U}_i \mathbf{U}_j + \mathbf{P}_{ij}) = 0, & i = 1, 2, 3 \\
\partial_t \left(R \left(\frac{1}{2} |\mathbf{U}|^2 + T \right) \right) + \operatorname{div}_x \left(R\mathbf{U} \left(\frac{1}{2} |\mathbf{U}|^2 + T \right) \right) + \sum_{i=1}^3 \partial_{x_i} \left[\sum_{j=1}^3 \mathbf{U}_j \mathbf{P}_{ij} + \mathbf{Q}_i \right] = 0.
\end{cases} \quad (1.1.9)$$

These equations represent, respectively, the conservation of mass, momentum, and energy in the fluid regime derived from the Boltzmann equation (5.1.1). By integrating (1.1.9) over $x \in \mathbb{R}^3$, and assuming that f vanishing at infinity, we obtain the following global conservation laws:

$$\begin{aligned}
\frac{d}{dt} \int_{\mathbb{R}^3} R(t, x) dx &= 0, \\
\frac{d}{dt} \int_{\mathbb{R}^3} R(t, x) \mathbf{U}(t, x) dx &= 0, \\
\frac{d}{dt} \int_{\mathbb{R}^3} R(t, x) T(t, x) dx &= 0.
\end{aligned} \quad (1.1.10)$$

However, this system is not closed, as the stress tensor $\mathbf{P}$ and heat flux $\mathbf{Q}$ still depend on the microscopic velocity distribution function $f(t, x, w)$, rather than solely on macroscopic quantities R , $\mathbf{U}$, and T .

The H-theorem

A central question in the fields of thermodynamics and statistical mechanics is how physical systems naturally evolve towards equilibrium. This presents a conceptual challenge: while microscopic dynamics are reversible, equilibration introduces a clear direction of time. This phenomenon is called the H-theorem:

Theorem 1.1.2 (H-Theorem). *Let $f(w) \in L^\infty(\mathbb{R}^3)$ satisfy*

- $f(w) > 0$ almost everywhere;

- As $|w| \rightarrow \infty$, $f(w)$ is rapidly decaying in w ;
- As $|w| \rightarrow \infty$, $\ln f(w)$ has at almost polynomial growth.

Then

$$\int_{\mathbb{R}^3} \mathcal{C}_B[f](w) \ln f(w) dw \leq 0, \quad (1.1.11)$$

with equality if and only if there exists $R, \mathbf{U}, T$ such that for almost everywhere $w \in \mathbb{R}^3$, f is a local Maxwellian

$$f(t, x, w) = \frac{R(t, x)}{(2\pi T(t, x))^{3/2}} e^{-\frac{|w - \mathbf{U}(t, x)|^2}{2T(t, x)}} \quad (1.1.12)$$

The proof of the theorem can be found in Section 2.1.3 in [Bou+00]. Another way to formulate the H-theorem is through the H-functional

$$H_B(t) := \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, x, w) \ln f(t, x, w) dx dw.$$

The theorem states that along the evolution governed by the Boltzmann equation, the functional $H(t)$ is a Lyapunov function, i.e. it is non-increasing¹ in time. In particular, this monotonicity reflects the emergence of time irreversibility at the kinetic level. This marks a fundamental distinction between the reversible dynamics of the underlying particle system and the irreversible behavior described by the Boltzmann equation. These correspond, respectively, to the Newtonian description of microscopic mechanics and to the second law of thermodynamics at the macroscopic level. Mathematically, we react it as the following corollary:

Corollary 1.1.2. *Let $f \in L^\infty(\mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3)$ be a solution of (5.1.1) in the sense of distribution, such that, f satisfies the conditions in Theorem 1.1.2. Then*

$$\frac{d}{dt} H_B(t) = - \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} D_B[f] b(w - w_*, \mathbf{n}) dw dw_* d\mathbf{n} \leq 0,$$

where $D[f]$ is the entropy production rate

$$D_B[f] := \frac{1}{4} (f'(w)f'(w_*) - f(w)f(w_*)) \ln \left(\frac{f'(w)f'(w_*)}{f(w)f(w_*)} \right).$$

This is also known to as the global entropy inequality for the Boltzmann equation. In the first part of this thesis, we investigate variants of this result, in particularly the local version, as well as corresponding variants of the Boltzmann equation. This perspective allows us to analyze the equilibrium states of the system and to quantify the rate at which solutions converge towards equilibrium. From a mathematical point of view, the global entropy inequality serves as a selection principle: it helps identify “good” weak solutions among the many possible weak solutions of the Boltzmann equation. However, the global entropy inequality alone does not guarantee that the selected solutions are entropic solutions, see [LS10].

¹The entropy in physics is a non-decreasing functional given by

$$S(t) = -k_B H(t),$$

where k_b denotes the Boltzmann constant.

The Hydrodynamic Limit

To derive the fluid system, we begin by nondimensionalizing the Boltzmann equation using the reference physical quantities listed in Table 1.1

Table 1.1: Scales

Parameter	Meaning
l_0	size of the container (periodic box)
t_0	time scale
θ_0	reference temperature
N_g	number of gas molecules $/l_0^3$
d_m	the diameter of the influence range of the intermolecular force
r_g	the radius of gas molecules
m_g	the mass of each gas molecule

We choose the *speed of sound* as the reference velocity:

$$v_s := \sqrt{\gamma \frac{k_B \theta_0}{m_g}},$$

where k_B is the Boltzmann constant, and γ is the adiabatic index. For monatomic gases, $\gamma = 5/3$. The dimensionless time, position and velocity variables are given by

$$\hat{t} := \frac{t}{t_0}, \quad \hat{x} = \frac{x}{l_0}, \quad \hat{w} = \frac{w}{v_s}.$$

Since $\int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, x, w) dx dw = N_g$, the corresponding dimensionless number density distribution function is

$$\hat{f}(\hat{t}, \hat{x}, \hat{w}) = \frac{l_0^3 v_s^3}{N_g} f(t, x, w)$$

We assume a constant collision frequency, meaning collisions are memoryless and independent of previous events. The *mean collision frequency* $\bar{\nu}_c$ is the reciprocal of the *mean free time*²:

$$\bar{\tau} = \frac{1}{\bar{\nu}_c}$$

Averaging the collision frequency over $w \in \mathbb{R}^3$ gives

$$\bar{\nu}_c = \frac{l_0^3}{N_g} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} f(w) f(w_*) B(w - w_*, \mathbf{n}) d\mathbf{n} dw_* dw.$$

²If we take $f(t, x, w)$ as a Maxwellian

$$f(t, x, w) = \frac{m_g N_g / l_0^3}{(2\pi k_B \theta_0)^{3/2}} e^{-\frac{m_g |w|^2}{2k_B \theta_0}},$$

we obtain the expression of mean collision frequency (one can refer Appendix A.8 in [Son07] for details)

$$\bar{\nu}_c = 4\sqrt{\pi} \theta_0 d_m^2 \frac{N_g}{l_0^3}$$

The Grad cutoff assumption ensures d_m is finite, and hence the mean free time is finite.

To nondimensionalize the collision kernel $B(z, \mathbf{n})$, note that

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \frac{N_g}{l_0^3 v_s^3} \hat{f}(\hat{w}) \frac{N_g}{l_0^3 v_s^3} \hat{f}(\hat{w}_*) B(w - w_*, \mathbf{n}) v_s^6 d\mathbf{n} d\hat{w}_* d\hat{w} = \frac{N_g}{l_0^3 \bar{\tau}}.$$

Normalizing this to unity, we define

$$\hat{B}(\hat{w} - \hat{w}_*, \mathbf{n}) = \frac{N_g \bar{\tau}}{l_0^3} B(w - w_*, \mathbf{n}).$$

The corresponding dimensionless collision integral is

$$\hat{\mathcal{C}}_B[\hat{f}](\hat{t}, \hat{x}, \hat{w}) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} [\hat{f}(\hat{t}, \hat{x}, \hat{w}_*) \hat{f}(\hat{t}, \hat{x}, \hat{w}) - \hat{f}(\hat{t}, \hat{x}, \hat{w}_*) \hat{f}(\hat{t}, \hat{x}, \hat{w})] \hat{B}(\hat{w} - \hat{w}_*, \mathbf{n}) d\hat{w}_* d\mathbf{n}$$

It is straightforward to verify that

$$' \hat{w}(w, w_*, \mathbf{n}) = ' w(\hat{w}, \hat{w}_*, \mathbf{n}), \quad ' \hat{w}_*(w, w_*, \mathbf{n}) = ' w_*(\hat{w}, \hat{w}_*, \mathbf{n}),$$

so that

$$\mathcal{C}_B[f](t, x, w) = \frac{N_g v_s^3}{l_0^3 \bar{\tau}} \hat{\mathcal{C}}_B[\hat{f}](\hat{t}, \hat{x}, \hat{w}) \quad (1.1.13)$$

For the transport term in (5.1.1), nondimensionalization yields

$$\partial_t f(t, x, w) + w \cdot \nabla_x f(t, x, w) = \frac{N_g v_s^3}{t_0 l_0^3} \partial_{\hat{t}} \hat{f}(\hat{t}, \hat{x}, \hat{w}) + \frac{N_g v_s^4}{l_0^4} \hat{w} \cdot \nabla_{\hat{x}} \hat{f}(\hat{t}, \hat{x}, \hat{w}). \quad (1.1.14)$$

Combining (1.1.14) and (1.1.13), we obtain the dimensionless Boltzmann equation

$$\frac{l_0}{t_0 v_s} \partial_{\hat{t}} \hat{f}(\hat{t}, \hat{x}, \hat{w}) + \hat{w} \cdot \nabla_{\hat{x}} \hat{f}(\hat{t}, \hat{x}, \hat{w}) = \frac{l_0}{\bar{\tau} v_s} \hat{\mathcal{C}}_B[\hat{f}](\hat{t}, \hat{x}, \hat{w})$$

To simplify these coefficients in terms of physical constants ³, we introduce the *Knudsen number*, which quantifies the degree of rarefaction, is defined as

$$\text{Kn} = \frac{\bar{\lambda}}{l_0},$$

where the *mean free path* is defined by

$$\bar{\lambda} = \bar{\tau} \bar{v}_{\text{rel}},$$

³This holds up to constant factors. For precise constant, one can refer to Section 1.9 in [Son07]. For instance, the average relative molecular speed for equipartition energy $3k_B \theta_0 / m_g$ is

$$\bar{v}_{\text{rel}} = \sqrt{\frac{6k_B \theta_0}{m_g}},$$

while the speed of sound is

$$v_s = \sqrt{\gamma \frac{k_B \theta_0}{m_g}}$$

where $\bar{v}_{\text{rel}}$ denotes the average relative molecular speed. And the *Mach number*, which measures the relative importance of compressibility effects, is given by

$$\text{Ma} = \frac{U_g}{v_s},$$

where the *bulk velocity*

$$U_g := \frac{l_0}{t_0}.$$

Dropping all the hats on variables and functions, the dimensionless form of the Boltzmann equation becomes

$$\text{Ma} \partial_t f + w \cdot \nabla_x f = \frac{1}{\text{Kn}} \mathcal{C}_B[f]. \quad (1.1.15)$$

To close the conservation laws (1.1.9), we consider the limit as the Knudsen number Kn tends to zero. This corresponds to strengthening the effect of collisions, meaning that a large number of collisions occur within a very short time interval.

We can use either the expansion method, which leads to, for example, the compressible Euler limit, the compressible Navier–Stokes asymptotics; or the moment closure method, which yields, for instance, the compressible Euler limit, as well as the incompressible Euler and Navier–Stokes limits.

The expansion method is based on representing the solution $f(t, x, w)$ as a series in powers of the Knudsen number Kn . A classical approach is the Hilbert expansion

$$f(t, x, w) = M[R_0, \mathbf{U}_0, T_0] + \sum_{k=1}^{\infty} \text{Kn}^k f_k(t, x, w),$$

where $M[R, \mathbf{U}, T]$ denotes the local Maxwellian distribution

$$M[R, \mathbf{U}, T](t, x, w) := \frac{R(t, x)}{(2\pi T(t, x))^{3/2}} \exp\left(-\frac{|w - \mathbf{U}(t, x)|^2}{2T(t, x)}\right).$$

Alternatively, one can use the Chapman–Enskog expansion

$$f(t, x, w) = M\left[R_0 + \sum_{k=1}^{\infty} \text{Kn}^k R_k, \mathbf{U}_0 + \sum_{k=1}^{\infty} \text{Kn}^k \mathbf{U}_k, T_0 + \sum_{k=1}^{\infty} \text{Kn}^k T_k\right].$$

Each order in the expansion corresponds to a different fluid equation at the macroscopic level.

The moment method, on the other hand, focuses on the zeroth, first, and second velocity moments of f , namely the density R , mean velocity $\mathbf{U}$, and temperature T . In regimes with larger Knudsen numbers, higher-order moments (such as the pressure tensor $\mathbf{P}$ or the heat flux) can be approximated by functions of the lower-order ones, using relations such as the equation of state or symmetry constraints on the stress tensor.

In this thesis, we mainly concentrate on the moment closure method. Nevertheless, the expansion method can also be used to derive other fluid equations; for instance, one obtains the Vlasov–Navier–Stokes system in the description of dense sprays.

Lastly, we introduce the Reynolds number Re , defined by

$$\text{Re} := \frac{\rho_g U_g l_0}{\mu},$$

where μ is the dynamic viscosity. The Reynolds number quantifies the relative importance of inertial forces to viscous forces in a flow. Equivalently, via the von Karman relation [Von63], it is proportional to the ratio of the Mach number Ma to the Knudsen number Kn , namely

$$\text{Re} \propto \frac{\text{Ma}}{\text{Kn}}.$$

This relation highlights the central role of Re in identifying the appropriate hydrodynamic regime.

- When $\text{Re} \ll 1$, inertial effects are negligible compared to viscous dissipation, leading to the Stokes (creeping) flow regime.
- When $\text{Re} = O(1)$, inertia and viscosity are of comparable magnitude, yielding the Navier–Stokes regime.
- When $\text{Re} \gg 1$, inertial effects dominate and viscous contributions are confined to thin boundary layers, so the macroscopic limit reduces to the Euler equations.

Thus, in the passage from kinetic theory to fluid dynamics, the Reynolds number serves as a key scaling parameter that determines which continuum model correctly captures the leading-order behavior of the system.

Here, we quote a diagram 1.2 from the book [Sai09] to explain the relation between the dimensionless Boltzmann equation and fluid equations. Further details on hydrodynamic limit can be found in [Sai09].

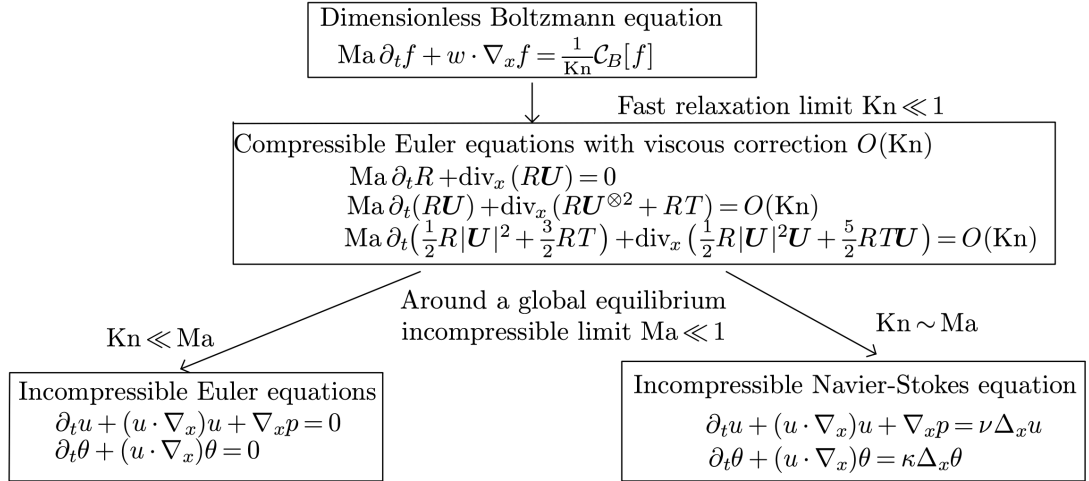


Figure 1.2: Diagram of hydrodynamic limits from the dimensionless Boltzmann equation to various fluid models under different scaling assumptions. Source: [Sai09]

The derivation of Boltzmann equation

The Boltzmann equation exhibits an arrow of time due to the H-theorem, because entropy is monotonically increasing. In contrast, the underlying particle system does not have this quantity. Therefore, it is of interest to understand why entropy emerges in the process of passing limit from particle systems to kinetic or fluid equations. This transition is closely related to Hilbert's sixth problem, which concerns the rigorous derivation of macroscopic equations from microscopic dynamics.

A seminal contribution to this field was made by Lanford [Lan75], who derived the Boltzmann equation for a system of hard spheres over short time. This proof was later refined by Gallagher, Saint-Raymond and Texier [GST14]. Subsequently, Illner and Pulvirenti [IP86] established the Boltzmann equation for long time, while in the near-vacuum regime. More recently still, Bodineau, Gallagher, Saint-Raymond and Simonella [Bod+24] have studied the long-time derivation of fluctuations around equilibrium.

For formal derivations of the Boltzmann equation, the reader is referred to Chapter 2 of [Cer94] and Appendix A of [Son07]. These techniques will also be presented in detail in Chapter 4.

1.1.2 The variants of the Boltzmann equations—kinetic equation for dense gas

As discussed previously, the Boltzmann equation provides a powerful framework for modeling the dynamics of a *dilute gas*, where molecules are treated as point particles. However, this description becomes inadequate once the gas density increases and the finite size of molecules can no longer be neglected comparing to length scale. To extend kinetic theory into this finite-density regime, the Boltzmann equation was generalized by David Enskog in his pioneering 1922 work [Ens22], leading to what is now known as the *Standard Enskog theory*. This model accounts for the excluded volume effects and enhanced collision frequency arising from the finite molecular diameter, thereby offering a more accurate description of moderately dense gases. Building on Enskog's formulation, several important variants have been developed to refine or adapt the theory for different physical contexts. In the remainder of this section, we will present these generalizations, including the *Revised Enskog theory* [BE73a][BE73b], the *Povzner equation* [Pov65], and *Cercignani's soft-sphere model* [Cer83], highlighting their motivations and key features.

The Standard Enskog equation

We write the following so-called Standard Enskog equation

$$(\partial_t + v \cdot \nabla_x)F(t, x, v) = \mathcal{C}_{\text{SE}}[F](t, x, v), \quad (1.1.16)$$

where the standard Enskog collision integral is defined as

$$\begin{aligned} \mathcal{C}_{\text{SE}}[F](t, x, v) := & (2r_p)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left[\chi[F](x - r_p \mathbf{n}) F(t, x, v) F(t, x - r_p \mathbf{n}, v_*) \right. \\ & \left. - \chi[F](x + r_p \mathbf{n}) F(t, x, v) F(t, x + r_p \mathbf{n}, v_*) \right] (2r_p)^2 \langle v - v_*, \mathbf{n} \rangle_+ d\mathbf{n} dv_*, \quad (1.1.17) \end{aligned}$$

the pre-collision velocities ($'v(v, v_*, \mathbf{n}), 'v_*(v, v_*, \mathbf{n})$) are given by (1.1.3).

The Standard Enskog theory (SET) is a generalized Boltzmann equation aimed at modelling dense gases by no longer considering the particles as mass points when we formally derive the Boltzmann equation from Liouville equation. We distinguish between the collision point and the particle center. Its advantage is to describe two different kinds of particles collisions. More details can be found in Chapter 4 of this thesis. The correlation function arises from extending the assumption of molecular chaos (Stosszahlansatz) in the BBGKY hierarchy to include positional correlations. SET provides a more intuitive physical interpretation. In particular, the correlation function χ quantifies the extent to which finite particle size modifies collision frequencies, and it can be understood as depending on the ratio

$$\frac{\text{Impact of Volume Occupation}}{\text{Shielding Influence}}.$$

Roughly speaking, the finite volume of particles enhance the probability of multiple particles collision (comparing with dilute gas whose probability of ternary collision is 0). When analyzing a binary collision between two particles, we fix one particle center at origin and consider the possible positions of center of a second particle that could collide with it (subset of a sphere center at origin with radius $2r$). If a third particle is located such that the distance between its center and origin satisfies $2r < d < 4r$, it obstructs the region—specifically, the crown of the collision sphere—where the incoming particle would have otherwise approached. As a result, the presence of this third particle alters the effective collision probability by shielding certain directions, thereby influencing the two-body interaction through geometric exclusion. See Figure 1.3.

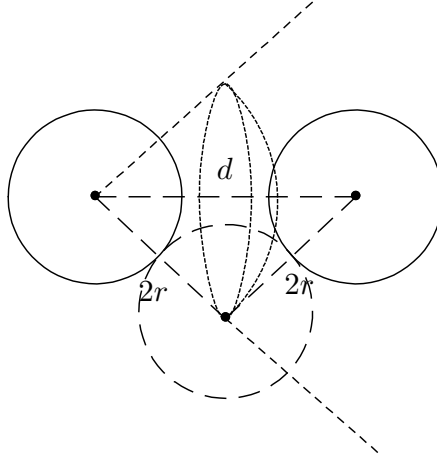


Figure 1.3: Schematic illustration of the shielding effect

Carnahan and Starling [CS69] proposed its asymptotic expression

$$\chi[\beta] = \frac{1 - \frac{1}{2}\beta}{(1 - \beta)^3},$$

where β denotes the packing fraction, i.e. the fraction of physical volume occupied by hard spheres, given explicitly by $\frac{\pi}{6}(2r_p)^3 R(t, x)$.

The revised Enskog equation

The literature on the SET is relative spare, since Van Beijeren and Ernst later proposed a revised model—the so-called the revised (or modified) Enskog theory (RET) in [BE73a][BE73b] which is now widely accepted.

$$(\partial_t + v_1 \cdot \nabla_x) f(t, x_1, v_1) = \mathcal{C}_{\text{RE}}[f, f](t, x_1, v_1), \quad (1.1.18)$$

where collision integral $\mathcal{C}_{\text{RE}}$ is given by

$$\begin{aligned} & \mathcal{C}_{\text{RE}}[\phi, \psi](x_1, v_1) \\ &:= \int_{\mathbb{R}^3 \times \mathbb{S}^2} (v_1 - v_*) \cdot \frac{x_1 - x_2}{|x_1 - x_2|} \varphi_{12} \left[g_2[\phi, \psi](x_1, x_2) \phi(x_1, v) \psi(x_2, v_*) H \left((v_1 - v_*) \cdot \frac{x_1 - x_2}{|x_1 - x_2|} \right) \right. \\ & \quad \left. - g_2[\phi, \psi](x_1, x_2) \phi(x_1, v_1) \psi(x_2, v_*) H \left((v_1 - v_*) \cdot \frac{x_2 - x_1}{|x_2 - x_1|} \right) \right] dx_2 dv_*. \end{aligned} \quad (1.1.19)$$

Here, $r_p > 0$ denotes the diameter of the particle, and $g_2 \equiv g_2[\phi, \psi](t, x, y)$ is the *pair correlation function* for the system of hard spheres in non-uniform equilibrium. To express the pair correlation function, we introduce the Mayer factors $\varphi_{ij}(x_i, x_j) \in \{0, -1\}^4$. The Mayer factor for hard sphere system is defined by

$$\varphi_{ij}(x_i, x_j) = H(|x_i - x_j| - 2r_p) - 1.$$

The irreducible cluster integral for the single-species case can then be written as

$$\begin{aligned} g_2[f, f](x_1, x_2) &= 1 + \int_{\mathbb{R}^3} V(12|3) R(x_3) dx_3 + \frac{1}{2} \int_{\mathbb{R}^3} V(12|34) R(x_3) R(x_4) dx_3 dx_4 + \dots \\ &+ \frac{1}{(k-2)!} \int_{\mathbb{R}^3} V(12|3 \dots k) R(x_3) \dots R(x_k) dx_3 \dots dx_k + \dots, \end{aligned} \quad (1.1.20)$$

where $R(t, x) := \int_{\mathbb{R}^3} F(t, x, v) dv$, and $V(12|3 \dots k)$ denotes the sum over all the graphs connecting particle-1 and particle-2, where each edge between nodes i and j is weighted by the Mayer factor φ_{ij} . For example, $V(12|3)$ consists of a single graph (see Figure 1.4)

$$V(12|3) = \varphi_{13}(x_1, x_3) \varphi_{23}(x_2, x_3).$$

This indicates that particle-1 and particle-2 are connected indirectly through particle-3. In other words, the three particles collide simultaneously. The second-order correction becomes more intricate. It consists of 5 cases with total 8 terms (see Figure 1.5).

$$\begin{aligned} V(12|34) &= [\varphi_{13} \varphi_{24} \varphi_{34} + \varphi_{14} \varphi_{23} \varphi_{34}] + [\varphi_{14} \varphi_{24} \varphi_{13} \varphi_{34} + \varphi_{13} \varphi_{23} \varphi_{14} \varphi_{34}] \\ &+ [\varphi_{13} \varphi_{23} \varphi_{34} \varphi_{24} + \varphi_{14} \varphi_{24} \varphi_{34} \varphi_{23}] + \varphi_{13} \varphi_{23} \varphi_{14} \varphi_{24} + \varphi_{13} \varphi_{23} \varphi_{14} \varphi_{24} \varphi_{34}. \end{aligned}$$

⁴The Mayer factor takes the values -1 and 0 , because, in higher-order terms, certain configurations are counted multiple times. For example, the case shown in Figure 1.4 is recomputed in several of the cases (II, III, IV, V) depicted in Figure 1.5. The value -1 is used to eliminate these redundant contributions through the principle of inclusion-exclusion.

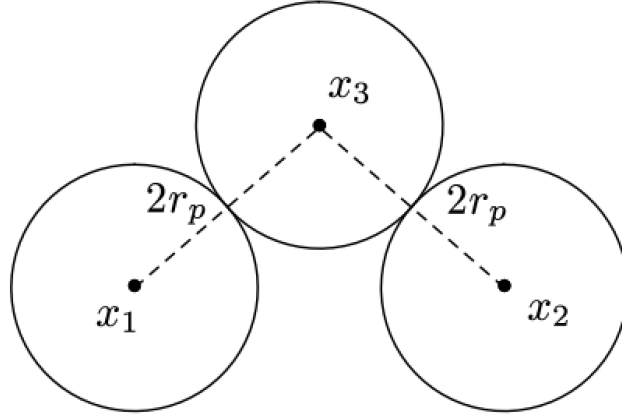
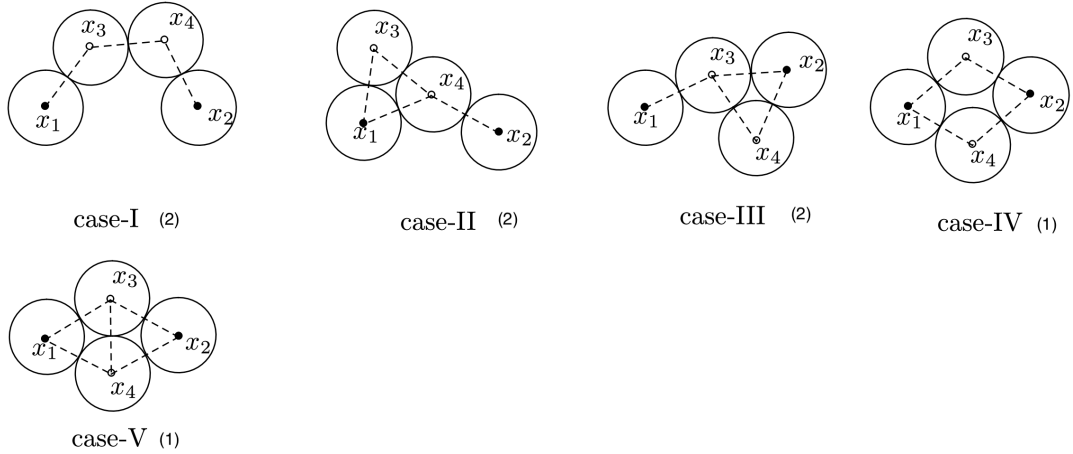
Figure 1.4: Configuration $V(12 | 3)$.

Figure 1.5: Configuration $V(12 | 34)$. In fact, particle-1 and particle-2 are in contact. However, in two dimensions it is impossible to arrange four balls such that each is tangent to the other three. Thus, the two-dimensional schematic is intended solely to illustrate the relations apart from the contact between particle-1 and particle-2.

Higher-order correction is very similar to this process by the Mayer graphs⁵. Convergence of the cluster expansion. For sufficiently small constant density R , the Mayer cluster expansion is known to converge [Rue99]. However, the question of convergence in the non-homogeneous case remains open [Pol01], to the best of the author's knowledge.

The H-theorem for the RET was first established in [R  s78], and later a local version of the H-theorem was obtained by Piasecki [Mar83]. When estimating the H-function of the Enskog equation, the associated inequality implies that equilibrium distributions must satisfy the following identity:

$$f(x, w)f(x + (2r_p)\mathbf{n}, w_*) = f(x, 'w)f(x + (2r_p)\mathbf{n}, 'w_*).$$

From another perspective, one finds that the finite-size collisions impose three additional constraints—the conservation of angular momentum:

$$x \times v + (x + 2r_p\mathbf{n}) \times v_* = x \times 'v + (x + 2r_p\mathbf{n}) \times 'v_*.$$

Consequently, the class of admissible local equilibrium states is more restrictive than in the Maxwellian case of the Boltzmann equation. In particular, the temperature T must be spatially homogeneous, while the velocity field $\mathbf{U}$ can only depend on position x through a rigid-body form. For instance, see [TT24] for further discussion. The corresponding local Maxwellian takes the form

$$\mu[R(t, x), \mathbf{U}(t, x) = \mathbf{U}_0(t) + x \times \omega(t), T(t)](v) := \frac{R}{(2\pi k_B T)^{3/2}} e^{-\frac{|v - \mathbf{U}|^2}{2k_B T}}$$

However, in contrast with the Boltzmann collision operator, this local equilibrium does not annihilate the Enskog collision term. That is, for a general non-homogeneous density field,

$$\mathcal{C}_{\text{RE}}[\mu[R, \mathbf{U}, T](v), \mu[R, \mathbf{U}, T](v)] \neq 0.$$

Comparing to SET, only RET can lead to the correct equilibrium distribution where SET not [Bei83a].

If we consider the hydrodynamic equations for an Enskog gas, the Enskog–Euler system can be derived from the first-order fluctuation in the Hilbert expansion, as shown in [Lac98]. Explicitly, the equations take the form

$$\begin{cases} \partial_t R + \operatorname{div}_x(R\mathbf{U}) = 0, \\ \partial_t(R\mathbf{U}) + \operatorname{div}_x(R\mathbf{U}^{\otimes 2}) + \operatorname{div}_x \left[RT \left(1 + \frac{2}{3}\pi(2r_p)R \right) \right] = 0, \quad j = 1, 2, 3, \\ \partial_t \left(R \left(\frac{3}{2}T + \frac{1}{2}|\mathbf{U}|^2 \right) \right) + \operatorname{div}_x \left[R\mathbf{U} \left(\frac{3}{2}T + \frac{1}{2}|\mathbf{U}|^2 \right) + R\mathbf{U}T \left(1 + \frac{2}{3}\pi(2r_p)R \right) \right] = 0. \end{cases} \quad (1.1.21)$$

A related hydrodynamic system was obtained via the Chapman–Enskog expansion in [JL04; JL05]. In the hydrodynamic limit, the pressure of a dense gas associated with the RET is

⁵In reality, the situation becomes more complex beyond the 12th order. As shown in [SW52], in three dimensions a ball can “kiss” at most 12 other balls. Consequently, each node can be incident to at most 13 edges.

modified according to the virial expansion

$$\frac{p_E}{k_B R T} = 1 + \sum_{k=1}^{\infty} R^k B_{k+1}.$$

where B_{k+1} are the virial coefficients. This expansion provides a systematic way to account for density-dependent corrections to the ideal gas law. In particular, the second virial coefficient is given by $B_2 = \frac{2}{3}\pi(2r_p)^3$. Intuitively, it corresponds to the contribution from three-particles collisions. If no correction is applied to the pair correlation function, i.e. $g_2 \equiv 1$, the resulting model is referred to as the *Boltzmann–Enskog equation*. In this simplified setting, the pressure law becomes

$$p_{BE} = k_B R T + \frac{2}{3}\pi(2r_p)^3 k_B R^2 T.$$

This expression makes explicit how the Enskog correction enhances the pressure relative to the ideal gas law, reflecting the reduced configurational entropy when particles occupy a finite volume.

A formal derivation on RET can be found in [Dom80], and some mathematical reviews on RET can be found in [EP91].

The Povzner equation

The Povzner collision integral was proposed to study the delocalized collision by Povzner in [Pov65]. The collision integral is of the following form

$$\mathcal{C}_P[\phi, \psi] := \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left(\phi(x, 'v) \psi(y, 'w) - \phi(x, v) \psi(y, w) \right) J(x - y, v - w) dw dy, \quad (1.1.22)$$

where the pre-collision velocities ($'v = 'v(v, w, \frac{y-x}{|y-x|})$, $'w = 'w(v, w, \frac{y-x}{|y-x|})$) are also given by (1.1.3) is assumed to satisfy the following four assumptions as showed in [Pov65]

- (i) J is continuous, and $|J(z, v)| \lesssim |v| + 1$, for any $z \in \mathbb{R}^3$
- (ii) Time reversibility: $J(-z, -v) = J(z, v)$.
- (iii) Invariance after collision⁶: $J(z, 'v - 'w) = J(z, v - w)$.
- (iv) Short-range interaction: There exists a constant C such that $J(z, v) = 0$ for $|z| > C$.

A possible expression of the Povzner collision kernel in [FHT11] is

$$J_{\epsilon_1, \epsilon_2}(z, v) := \frac{1}{2\epsilon_1^3} \frac{1}{\epsilon_2} H(\epsilon_1 - |z|) H(\epsilon_2 - |v|) \left| v \cdot \frac{z}{|z|} \right|, \text{ for some parameter } \epsilon_1, \epsilon_2 > 0.$$

From this example, we can find out more clearly that the Povzner collision integral allows for the possibility of a spatial smearing process with range of ϵ_2 and ϵ_1 of collisions as well as for the classically assumed process in which the molecules collide at a point. We point

⁶However, this assumption is not physically justified, as it doesn't distinguish the incoming and outgoing contributions. A detailed discussion is provided in Chapter 3.

out here that if we set $J(z, v) = \tilde{J}\left(|v|, \frac{z \cdot v}{|z||v|}\right) \delta_0(|z|)$ (here δ_0 is Dirac delta function centered at origin) in (3.1.15), then we can recover the Boltzmann collision kernel.

Cercignani's soft sphere model, first introduced in [Cer83], can be regarded as a special case of Povzner equation with the following mollifier

$$S_{\epsilon_1, \epsilon_2}(s) = K_{\epsilon_1, \epsilon_2}(s) \frac{\epsilon_2^2}{s^2 + \epsilon_1^2} C_{\epsilon_2/\epsilon_1},$$

where $K_{\epsilon_1, \epsilon_2}(s)$ serves as an approximation of the Dirac delta function. More precisely,

- $K_{\epsilon_1, \epsilon_2}$ is supported in $[\epsilon_2, \epsilon_2 + \epsilon_1]$

$$K_{\epsilon_1, \epsilon_2}(s) = \begin{cases} 0 & \text{if } 0 < s < \epsilon_2 \\ \frac{1}{\epsilon_1} & \text{if } \epsilon_2 \leq s \leq \epsilon_2 + \epsilon_1 \\ 0 & \text{if } \epsilon_2 + \epsilon_1 < s \end{cases}$$

- $K_{\epsilon_1, \epsilon_2}$ is normalized: $\int_{\mathbb{R}_+} K_{\epsilon_1, \epsilon_2}(s) ds = 1$ for all $\epsilon_1 > 0$;
- For any uniformly continuous test function ϕ , $\lim_{\epsilon_1 \rightarrow 0} \int_{\mathbb{R}_+} \phi(s) K_{\epsilon_1, \epsilon_2}(s) ds = \phi(\epsilon_2)$.

The factor $C_{\epsilon_2/\epsilon_1}$ aims make $S_{\epsilon_1, \epsilon_2}$ be of order ϵ_2^2 . Equivalently,

$$\int_{\mathbb{R}_+} S_{\epsilon_1, \epsilon_2}(s) s^2 ds = \epsilon_2^2.$$

This model extends the collision domain from a single point to a spherical shell of thickness ϵ_1 . In [Cer83], Cercignani proved the existence of solutions, established propagation of chaos for the soft-sphere model, and derived the corresponding conservation laws. However, the limits $\epsilon_1 \rightarrow 0$ and $\epsilon_2 \rightarrow 0$ are not interchangeable. Consequently, one cannot rigorously obtain the Boltzmann equation by first letting $\epsilon_1 \rightarrow 0$ and then $\epsilon_2 \rightarrow 0$ within this framework. This observation highlights that the Povzner equation enjoys improved analytic properties, thanks to the spatial mollification of collision kernel.

1.1.3 The Vlasov equation

The *Vlasov equation*, first proposed by Vlasov in 1938 [Vla68], is a fundamental model in kinetic theory describing the evolution of a collisionless particle system subject to a self-consistent mean-field interaction. If $f(t, x, w)$ denotes the number density distribution function of particles as before, the equation takes the form

$$\partial_t f(t, x, w) + w \cdot \nabla_x f(t, x, w) + \operatorname{div}_w \{ [f](t, x, w) f(t, x, w) \} = 0,$$

where the mean-field force field $[f]$ is typically determined by a potential generated through $f(t, x, w)$, usually via the Poisson equation (Vlasov–Poisson system) or the Maxwell equations (Vlasov–Maxwell system). Unlike the Boltzmann equation, which models collisions, the Vlasov equation describes a collisionless regime in which interactions between particles are weak but long-range, and the coupling occurs through the collective mean-field. From a

rigorous standpoint, Braun–Hepp [BH77] and Dobrushin [Dob79] derived the Vlasov equation from the Liouville equation in the mean-field limit, rather than in the Boltzmann–Grad scaling that leads to the Boltzmann equation.

When collisional effects are included, one obtains the *Boltzmann–Vlasov equation*:

$$\partial_t f(t, x, w) + w \cdot \nabla_x f(t, x, w) + \operatorname{div}_w \{ [f](t, x, w) f(t, x, w) \} = \mathcal{C}_B[f](t, x, w),$$

where $\mathcal{C}_B[f]$ denotes the Boltzmann collision operator. This equation can equivalently be interpreted as the Boltzmann equation augmented by a force term.

1.2 The two-species models

Beyond single-species models, many systems of practical interest involve multiple species. Examples include droplets suspended in air, sprays and aerosols in carrier fluids, dust particles in the atmosphere, water–oil mixtures, suspensions in engineering flows, and plasmas consisting of electrons and ions. To study such systems, it is necessary to generalize single-species models to multi-species settings through coupled equations. In this framework, one must account not only for self-interactions within each species but also for interactions between different species.

One way to classify these models is by the choice of equations used to describe the species. Depending on the scale of observation, one may employ Hamiltonian equations at the microscopic level, kinetic equations at the mesoscopic level, or fluid equations at the macroscopic level. There are two main approaches to coupling such equations: through boundary conditions or through external forces. Hamiltonian equations are typically coupled to other equations via boundary conditions, whereas kinetic and fluid equations are usually coupled through external forces.

When we consider Hamilton equations couple with other equations, after homogenization techniques, we can obtain the *Brinkman force* from the boundary condition. See, for instance, [DGR08].

This model always aims to model very dilute species suspended in a fluid bed. Mathematically, the number of one species N_p times its radius r_p is finite, i.e. $N_p r_p = O(1)$. The second part of the thesis focus on comparable binary mixture, in other words, $N_p r_p^3 = O(1)$. Thus in the following section, we do not mention much about the Hamilton equations. We focus on the mesoscopic and macroscopic levels, which are connected by external forces in this thesis.

Recent advances have been made in understanding the thin-particle regime from homogenization point of view. In this setting, several works have rigorously derived Vlasov–Stokes or Transport–Stokes type systems by starting from Hamiltonian particle dynamics coupled with fluid equations. These studies provide a systematic bridge between microscopic particle–fluid interactions and macroscopic fluid–fluid models (see, for instance, [Höf21; Mec21; HJ24; HS25]).

1.2.1 The fluid-fluid description

Travis, Harlow, and Amsden in [THa76] formulated the classical two-phase flow equations. The non-barotropic equations are given by

$$\left\{ \begin{array}{l} \partial_t(\alpha\rho_g) + \operatorname{div}_x(\alpha\rho_g\mathbf{u}_g) = 0 \\ \partial_t(\alpha\rho_g\mathbf{u}_g) + \operatorname{div}_x(\alpha\rho_g\mathbf{u}_g^{\otimes 2}) + \alpha\nabla_x p = - \\ \partial_t(\rho E_g) + \operatorname{div}_x(\rho_g\mathbf{u}_g E_g) + \operatorname{div}_x(\mathbf{u}_g p) = \quad \cdot \mathbf{u}_g, \\ \partial_t((1-\alpha)\rho_\ell) + \operatorname{div}_x((1-\alpha)\rho_\ell\mathbf{u}_\ell) = 0 \\ \partial_t((1-\alpha)\rho_\ell\mathbf{u}_\ell) + \operatorname{div}_x((1-\alpha)\rho_\ell\mathbf{u}_\ell^{\otimes 2}) + (1-\alpha)\nabla_x p = \\ \partial_t(\rho_\ell E_\ell) + \operatorname{div}_x(\rho_\ell\mathbf{u}_\ell E_\ell) + \operatorname{div}_x(\mathbf{u}_\ell p) = \quad \cdot \mathbf{u}_\ell, \\ p = n_g\theta_g, E_g = \frac{|\mathbf{u}_g|^2}{2} + \frac{3\theta_g}{2m_g}, n_g = \frac{\rho_g}{m_g}, E_\ell = \frac{|\mathbf{u}_\ell|^2}{2} + \frac{3\theta_\ell}{2m_\ell}, n_\ell = \frac{\rho_\ell}{m_\ell}, \end{array} \right. \quad (1.2.1)$$

where $n_g, \rho_g, \mathbf{u}_g, \theta_g, E_g$ denote, respectively, the number density, mass density, velocity, temperature, and internal energy of the gas phase, while $n_\ell, \rho_\ell, \mathbf{u}_\ell, \theta_\ell, E_\ell$ denote the corresponding quantities for the dispersed (liquid) phase. p is the hydrostatic pressure, and $\cdot$ is a given function describing the friction between the two species. $\alpha \equiv \alpha(t, x)$ denotes the volume fraction of gas, which prevents the spatial stacking of two species.

The traditional derivation of the system bases on averaging method see, Chapter 2 in [ORo81], also Part II of [IH11]. Put it simply, we introduce indicators

$$\chi(x) = \begin{cases} \frac{1}{L_1 L_2 L_3} & \text{if } x \in [0, L_1] \times [0, L_2] \times [0, L_3] \\ 0, & \text{otherwise.} \end{cases}$$

for each species, and define volume fraction via

$$\alpha(t, x) = \langle \chi \rangle = \frac{1}{N_E} \sum_{k=1}^{N_E} \int_{V_g(t, k)} \chi(y - x) dy,$$

where N_E is number of experiments, $V_g(t, k)$ denotes the volume occupied by the gas at time t in experiment k , and averaged quantity $\phi = \langle \chi \phi \rangle / \alpha$ (for example ϕ can take density, velocity, and internal energy). Finally, we multiply conservation laws for single species by χ , and take average.

Detailed discussions of the Eulerian–Eulerian model can be found in the classical review of Stewart and Wendroff [SW84] as well as in the recent doctoral thesis of Loison [Loi24].

1.2.2 The kinetic-kinetic description

Let $f \equiv f(t, x, w) \geq 0$ and $F \equiv F(t, x, v) \geq 0$ denote the number distribution functions of gas molecules and particles, respectively, depending on time $t \in \mathbb{R}_+$, position $x \in \mathbb{R}$, and velocities $w, v \in \mathbb{R}$. we can consider the following coupled Boltzmann equations for binary

mixture⁷:

$$\begin{cases} (\partial_t + w \cdot \nabla_x) f(t, x, w) &= \mathcal{R}[F, f](t, x, w) + \mathcal{C}[f, f](t, x, w), \\ (\partial_t + v \cdot \nabla_x) F(t, x, v) &= \mathcal{D}[f, F](t, x, v) + \mathcal{Q}[F, F](t, x, v). \end{cases} \quad (1.2.2)$$

Here, the collision integrals $\mathcal{R}, \mathcal{D}$ describe the interactions between two different species, while collision integrals $\mathcal{Q}, \mathcal{C}$ represent the self-collision within each species. Previous works are largely based on specific choices and modifications on the Boltzmann collision integral, for instance, [Cha09]. [CD09] considers the size of particles in the modeling. [CD25] and [CMS25] modified the Boltzmann collision integral via diffuse reflection.

In the kinetic theory of dense gases, van Beijeren [BE73b] extended the revised Enskog equation to the case of mixtures. Bisi, Cercignani, and Pulvirenti [BGP73] computed the associated mass, momentum, and kinetic energy fluxes, together with the corresponding transport coefficients. Subsequently, Garzó, Goldstein, and Sela [GG97a] established an H-theorem for binary hard-sphere mixtures, while in a complementary work [GG97b] they confirmed the validity of Onsager's reciprocal relations in this setting.

1.2.3 The kinetic-fluid description

In the Eulerian–Lagrangian description of sprays, the gaseous carrier phase is treated as a continuum governed by the Navier–Stokes, Euler equations, while the dispersed phase is described by tracking individual droplets or, more generally, by a number density function $F(t, x, v)$ satisfying a Vlasov-type transport equation. The interaction between the two phases is introduced through drag, heat, and mass-exchange terms that couple the particle dynamics to the fluid momentum and energy balances. Depending on the volume fraction of the dispersed phase, one distinguishes several modeling regimes: in the *very thin spray* limit, droplets do not influence the gas, and the gas evolves independently according to the Euler or Navier–Stokes equations; in the *thin spray* regime, the dispersed phase still has negligible volume but exerts a collective feedback on the carrier flow through drag, leading to the coupled Vlasov–Euler or Vlasov–Navier–Stokes systems; finally, in the *thick spray* regime, the liquid phase occupies a non-negligible volume fraction. Table 1.2 is a simple schematic of the categorization. Figure 1.6 shows the realistic scenarios corresponding to different spray models.

The Vlasov–Euler system

Beyond the kinetic description of collisions, an alternative framework involves coupling a fluid equation—such as the Navier–Stokes, Stokes, or Euler equations—with a kinetic equation, typically of Vlasov type. When the volume fraction of the dispersed phase is sufficiently small, the system is described by the so-called *thin sprays* model:

⁷The coupled kinetic model can be generalized to the case of multi-species, leading to the system

$$\partial_t f_i(t, x, w) + w \cdot \nabla_x f_i(t, x, w) = \sum_{1 \leq j \neq i \leq N} \mathcal{C}^{ij}[f_j, f_i] + \mathcal{C}^i[f_i]. \quad \text{for } i = 1, 2, \dots, N.$$

This formulation naturally corresponds to the multi-species fluid equations. A detailed discussion on connection between them, however, lies beyond the scope of the present thesis.

Reynolds number \ Volume fraction	Very thin spray $1 - \alpha < 10^{-3}$	Thin sprays $10^{-3} < 1 - \alpha < 10^{-1}$	Thick spray $1 - \alpha \sim 10^{-1}$
Inviscid (Euler)	Vf-E	Vf-Ef	Vfb-Efb
Viscous (Navier-Stokes)	Vf-NS	Vf-NSf	Vfb-NSfb
Very viscous (Stokes)	Vf-S	Vf-Sf	Vfb-Sfb

Table 1.2: Classification of sprays models. Here, V denotes the Vlasov equation, NS the Navier–Stokes equation, and S the Stokes equation. The notation “f” indicates the inclusion of an external friction force, while “fb” refers to the presence of both an external friction force and buoyancy effects.

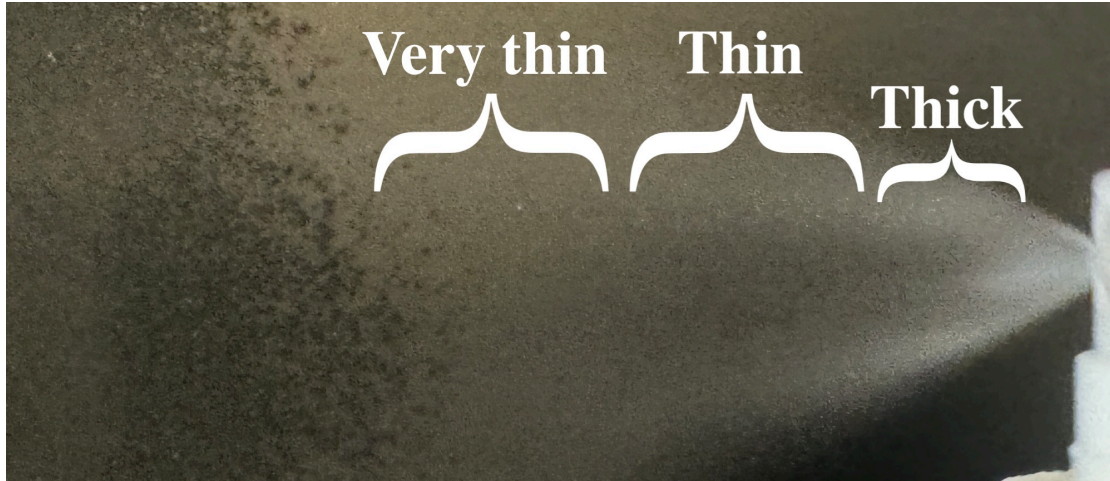


Figure 1.6: Spray pattern showing transitions from very thin to thick mist.

$$(\text{Vf} - \text{Ef}) \begin{cases} \partial_t \rho_g + \operatorname{div}_x(\rho_g \mathbf{u}_g) = 0, \\ \partial_t(\rho_g \mathbf{u}_g) + \operatorname{div}_x(\rho_g \mathbf{u}_g^{\otimes 2}) + \nabla_x p = m_g \int_{\mathbb{R}} F(v) (v - \mathbf{u}_g) dv, \\ \partial_t(\rho_g E_g) + \operatorname{div}_x(\rho_g \mathbf{u}_g E_g) + \operatorname{div}_x(\mathbf{u}_g p) = m_g \int_{\mathbb{R}} v \cdot (v - \mathbf{u}_g) F(v) dv, \\ \partial_t F + v \cdot \nabla_x F + \operatorname{div}_v[F(v) D(v - \mathbf{u}_g)] = 0, \\ p = n_g \theta_g, E_g = \frac{|\mathbf{u}_g|^2}{2} + \frac{3\theta_g}{2m_g}, n_g = \frac{\rho_g}{m_g} \end{cases} \quad (1.2.3)$$

A formal derivation of (5.2.1) (with quadratic friction force) from coupled Boltzmann equations has been presented in [DGR19].

To exclude overlapping of volume, we introduce the following so-call volume fraction (void) function α defined as

$$\alpha(t, x) := 1 - \frac{4\pi}{3} r_p^3 \int_{\mathbb{R}} F(t, x, v) dv,$$

Therefore, we can formally write the following Vlasov-Euler equations for thick sprays⁸ which is widely accepted:

$$(\text{Vfb} - \text{Efb}) \begin{cases} \partial_t(\alpha \rho_g) + \operatorname{div}_x(\alpha \rho_g \mathbf{u}_g) = 0, \\ \partial_t(\alpha \rho_g \mathbf{u}_g) + \operatorname{div}_x(\alpha \rho_g \mathbf{u}_g^{\otimes 2}) + \nabla_x p = m_g \int_{\mathbb{R}} F(v) \mathbf{D}(v - \mathbf{u}_g) dv, \\ \partial_t(\alpha \rho_g E_g) + \operatorname{div}_x(\alpha \rho_g \mathbf{u}_g E_g) + \operatorname{div}_x(\alpha \mathbf{u}_g p) + p \partial_t \alpha = m_g \int_{\mathbb{R}} \mathbf{D}(v - \mathbf{u}_g) \cdot v F(v) dv, \\ \partial_t F + v \cdot \nabla_x F + \operatorname{div}_v(F \mathbf{D}) = 0, \\ \mathbf{D}(v - \mathbf{u}_g) = \frac{4\pi}{3} r_p^3 \nabla_x p + (v - \mathbf{u}_g), \\ p = n_g \theta_g, E_g = \frac{|\mathbf{u}_g|^2}{2} + \frac{3\theta_g}{2m_g}, \rho_g = m_g n_g, \\ \alpha = 1 - \frac{4\pi}{3} r_p^3 \int_{\mathbb{R}} F(v) dv, \end{cases} \quad (1.2.4)$$

where $\mathbf{D}$ represents the drag force between gas and particle. Here the drag force includes not only the friction term, as in the case of thin sprays, but also an additional contribution

⁸The momentum equation of gas can be also written as

$$\partial_t(\alpha \rho_g \mathbf{u}_g) + \operatorname{div}_x(\alpha \rho_g \mathbf{u}_g^{\otimes 2}) + \alpha \nabla_x p = m_g \int_{\mathbb{R}} F(v) (v - \mathbf{u}_g) dv,$$

which reflects more clearly the influence of volume fraction on pressure.

accounting for pressure modification. The quadratic form of the friction force⁹ is given by

$$(t, x) = \frac{1}{2} \pi r_p^2 \rho_g(t, x) C_D |\mathbf{u}_g - v| (\mathbf{u}_g - v).$$

Here C_D is a dimensionless constant depending on Reynolds number Re . In the low Reynolds number regime, we can simplify this expression. When $\text{Re} \ll 1$, we have the following approximation (see equation (4.10.18) in [Bat00])

$$C_D = \frac{24}{\text{Re}} \left(1 + \frac{3}{16} \text{Re} \right) \sim \frac{24}{\text{Re}}.$$

and the Reynolds number for droplets is

$$\text{Re}_p = \frac{2r_p \rho_g |\mathbf{u}_g - v|}{\mu_g},$$

where $\mu_g = \rho_g \nu_g$ is dynamic viscosity of the fluid. Now plug Re_p into the quadratic friction force:

$$= 6\pi \mu_g r_p (\mathbf{u}_g - v).$$

This corresponds to the classical Stokes drag law in fluid mechanics (see also Brinkman [Bri49]). This transition (from quadratic to linear) is the hallmark of creeping flow. If we set $\alpha \equiv 1$ in equations (5.2.2), we recover the Vlasov-Euler system for thin sprays (5.2.1).

In the barotropic case, which means pressure p is a function depends only on density ρ_g , the governing system (5.2.2) simplifies through

$$\begin{cases} \partial_t(\alpha \rho_g) + \text{div}_x(\alpha \rho_g \mathbf{u}_g) = 0, \\ \partial_t(\alpha \rho_g \mathbf{u}_g) + \text{div}_x(\alpha \rho_g \mathbf{u}_g^{\otimes 2}) + \nabla_x p(\rho_g) = m_g \int_{\mathbb{R}} F(v) \mathbf{D}(v - \mathbf{u}_g) dv, \\ \partial_t F + v \cdot \nabla_x F + \text{div}_v(F \mathbf{D}) = 0, \\ \mathbf{D}(v - \mathbf{u}_g) = \frac{4\pi}{3} r_p^3 \nabla_x p(\rho_g) + (v - \mathbf{u}_g), \\ \alpha = 1 - \frac{4\pi}{3} r_p^3 \int_{\mathbb{R}} F(v) dv, \end{cases} \quad (1.2.5)$$

Besides, for the equation with internal energy variable can be found in Mathiaud's thesis [Mat06]

These models were originally proposed in [THa76], subsequently developed in a more systematic manner in [ORo81], and later implemented and extended within the KIVA code (see, e.g., [AOB89]). For a comprehensive overview of the subject, we refer the reader to the review by Ertzbischoff [Ert24]. A more detailed discussion of the relevant literature is provided in Chapter 5.

⁹Some authors absorb the $\frac{1}{2}$ into the definition of C_D . If that convention is used, the small Reynolds number asymptote becomes $C_D = \frac{12}{\text{Re}}$.

The Vlasov-Navier-Stokes system

If we consider the viscosity of the fluid themselves, we have the so-called incompressible Vlasov-Navier-Stokes equations

$$\begin{cases} \partial_t(\alpha\rho_g) + \operatorname{div}_x(\alpha\rho_g\mathbf{u}_g) \\ \partial_t(\alpha\rho_g\mathbf{u}_g) + \operatorname{div}_x(\alpha\rho_g\mathbf{u}_g^{\otimes 2}) + \alpha\nabla_x p(\rho_g) - \nu_g(\Delta_x u + \nabla_x \operatorname{div}_x u) = \int_{\mathbb{R}^3} F(v)(v - \mathbf{u}_g)dv \\ \partial_t F + v \cdot \nabla_x F + \operatorname{div}_v[F(\mathbf{u}_g - v) - F\nabla_x p(\rho)] = 0. \end{cases} \quad (1.2.6)$$

where ν_g denotes the viscosity of the gas. Setting $\nu_g = 0$ reduces the system to the Vlasov–Euler model. A version adapted to thin sprays ($\alpha = 1$) is also available. The well-posedness theory has been progressively developed: local-in-time classical solutions were obtained in [BD06], the existence of global weak solutions was established in [Bou+09; BGM17], while the existence of global strong solutions was recently proved in [Dan24]. In addition, the long-time behavior of solutions was investigated in [HMM20]. For a comprehensive overview, we refer the reader to the thesis of Ertzbischoff [Ert23].

The main focus of the present thesis will not be on viscous effects in the carrier fluid. Nevertheless, as a perspective, we intend in Chapter 5 to adapt the techniques developed here in order to derive the Vlasov–Navier–Stokes equations for non-barotropic thick sprays.

1.3 The outline of the thesis

The thesis is structured in two main parts. The first part focuses on delocalized collision models for single-species gases. This includes the Standard Enskog model, the original Povzner model, the Revised Enskog model, Cercignani’s soft sphere model, and the Modified Povzner model. Notably, the latter three models can be unified under a common framework using a general expression. **Chapter 2** is devoted to analyzing these three models. In particular, we establish their local conservative representations and derive the corresponding local conservation laws using the moment method. Furthermore, we investigate the local entropy inequalities associated with these models. In **Chapter 3**, we apply a similar methodology to study the remaining two models: the Standard Enskog and the original Povzner model. We derive their conservative forms. However, we observe that their local entropy inequalities are less interesting. This observation, along with explanations, is provided in the same chapter.

The second part of the thesis focuses on establishing the connections between microscopic, mesoscopic, and macroscopic models, as summarized in the schematic illustration (see Figure 1.7).

Chapter 4 presents the derivation that links the particle system (PS) to the coupled kinetic system (CKS). In addition, we examine the conservation laws of mass, momentum, and energy for each species, and establish the H-theorem for the CKS. **Chapter 5** is dedicated to deriving the macroscopic Eulerian-Lagrangian model (ELM) from the kinetic description provided by the CKS.

To make the framework more comprehensive, we highlight several directions and perspectives:

- (★) The passage from the Eulerian–Lagrangian model (ELM) to the Eulerian–Eulerian

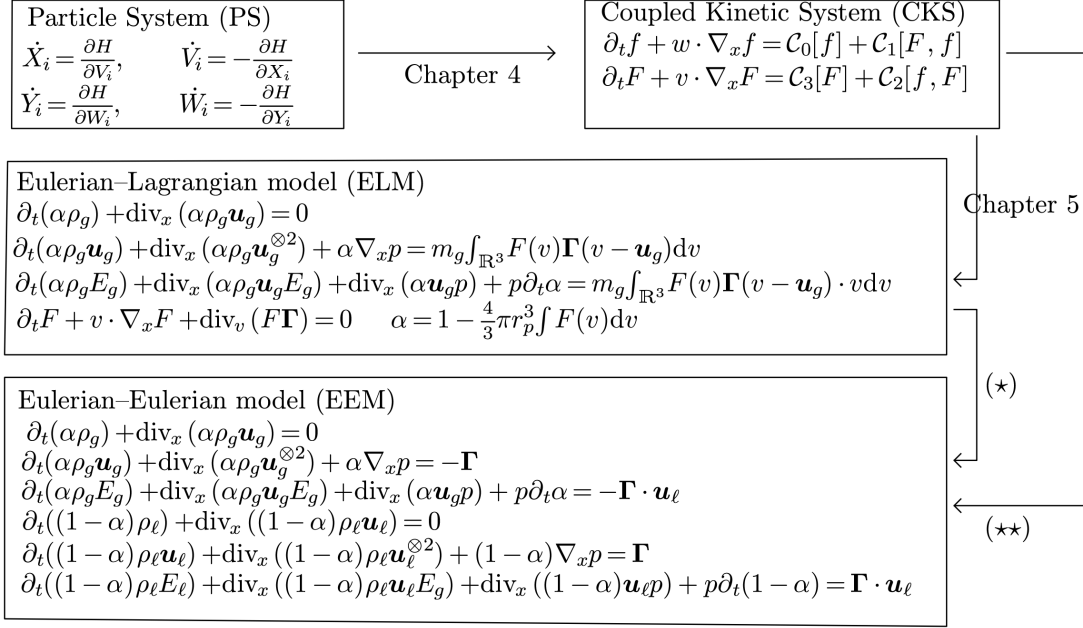


Figure 1.7: Flowchart of model derivations from particle system to continuum models.

model (EEM) has already been established, notably in [DM10].

- (**) As a future perspective, we expect that similar methodologies can be employed to derive the EEM directly from the coupled kinetic system (CKS), under alternative assumptions and scaling regimes. In particular, by no longer neglecting self-collisions between droplets, one may rigorously obtain effective fluid equations governing the droplet phase.

1.4 The strategy of the proofs

The strategy for deriving the local conservation laws for the variant of the Boltzmann equation (Chapters 2 and 3) is to insert a test function $\phi(x, w) \in C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ into the collision integral and carefully track each transformation applied to it. We then reorganize the resulting terms so that they appear entirely in the form $\nabla_x \phi(x, w)$ and $\nabla_v \phi(x, w)$. For certain remaining terms, we exploit the symmetry structure of the collision integral to rewrite them as differences. This approach is motivated by the notion of Landau currents for the Landau collision operator (see, e.g., §41 in [LP81]) and for the Boltzmann collision operator (see [Vil99]).

The main difficulty, in the case of delocalized collision integrals, lies in the fact that one must keep track not only of operations in the velocity variable but also in the position variable; in some cases, a single transformation acts on both variables simultaneously. Once the terms are fully organized, we integrate the kinetic equation against 1, w , and $|w|^2/2$ over $w \in \mathbb{R}^3$ to obtain the local conservation laws.

The same method can also be used to prove local entropy inequalities. In this case, the main difference is that in the expression $\int_{\mathbb{R}^3 \times \mathbb{R}^3} \phi(x, w) \mathcal{C}[f](x, w) \ln f(x, w) dw dx$, not all instances of ϕ can be organized as differences. One isolated term remains, which cannot be symmetrized on its own. However, this term can be interpreted as the time derivative of a quantity of the form $\int_{\mathbb{R}^3} [(\int_{\mathbb{R}^3} f(\cdot, w) dw) \star (\int_{\mathbb{R}^3} f(\cdot, w) dw)](x) \beta(x) dx$. We treat this as the “potential” part of the entropy, thereby obtaining the local entropy inequality for a suitably modified entropy functional.

We derive the CKS system from the PS system using the classical formal procedure for obtaining the Boltzmann equation from PS (see, for instance, [Cer94; Son07]), while retaining the delocalized effects and distinguishing between two species. The conservation laws and H-theorem for CKS follow from the results of Chapters 2 and 3, suitably generalized to the multi-species framework.

The technique employed in Chapters 5 and 6 is inspired by the approach of Desvillettes, Bernard, Golse, and Ricci, who developed a formal asymptotic derivation of coupled systems such as Vlasov–Navier–Stokes [Ber+17], Vlasov–Stokes [Ber+18], and Vlasov–Euler [DGR19], starting from a binary Boltzmann system for gas–particle mixtures. We first nondimensionalize the CKS system and choose an appropriate scaling, after which we verify that the resulting parameter functions satisfy the classical fluid equations. The main difficulty in such a derivation lies in the fact that, if one employs the classical Boltzmann equation—originally formulated for dilute gases—the contribution from the particle volume (of order $r^3 N$) is neglected. This is a consequence of the Boltzmann–Grad limit, where one fixes $r^2 N = O(1)$. However, for the derivation of models describing thick sprays, the particle volume must be taken into account. In this regime, the Boltzmann equation is no longer appropriate. To address this, we replace the Boltzmann collision integral in [DGR19] with the Enskog collision integral. Furthermore, by approximating the delocalization effect $f(x + a\mathbf{n}, w)$ as $f(x, w) + a\mathbf{n} \cdot \nabla_x f(x, w)$, we demonstrate that, at the macroscopic level, the latter term modifies the pressure.

Chapter 2

Local Conservation Laws and Entropy Inequality for revised Enskog equation, modified Povzner equation, and Cercignani's soft sphere model

This chapter is based on [CCG24] which is now accepted by *Math. Models and Methods in the Appl. Sci.*, in collaboration with Frédérique Charles and François Golse.

Introduction

We are concerned in this paper with the basic structure of some kinetic equations used to model non perfect monatomic gases. The classical kinetic theory of gases of Maxwell (1866) and Boltzmann (1872) is limited to perfect monatomic gases. It has been later generalized, in particular by Enskog (1922), to treat the case of dense gases (see chapter 16 of [CC70], for instance). Further generalizations of Enskog's theory — most notably Povzner's kinetic equation (1962), and Cercignani's model for the kinetic theory of soft spheres (1980) — are presented in section 2.1.

The classical kinetic theory of gases is intimately related to the Euler equations of (inviscid) gas dynamics through the local conservation laws of mass, momentum and energy, satisfied by classical solutions of the Boltzmann equation (see sections 3.1 and 3.3 in [Cer94], and the remarks in section 2.2). At the time of this writing, it would seem that these *local* conservation laws of mass, momentum and energy are not known to be verified by classical solutions of the Enskog equation or its variants presented in section 2.1.

For this reason, we propose in this work a systematic method for obtaining local conservation laws in the theory of kinetic models of Enskog type. Our arguments are based on writing the collision integrals of Enskog type as the divergence in the position and velocity

variables of mass, momentum and energy currents, following a little-known idea of Landau on the Boltzmann collision integral (see for instance §41 in [LP81] and [Vil99]).

In the case of the Boltzmann equation, the Friedrichs-Lax entropy condition used in the theory of the Euler system of (inviscid) gas dynamics (see sections 3.2, 4.5 and chapter V of [Daf10]) can be deduced from the local form of the Boltzmann H theorem [BG84]. For this reason, we also discuss the possibility of obtaining *local* entropy inequalities for classical solutions of Enskog-type kinetic equations.

The outline of this paper is as follows: various examples of kinetic models with delocalized collision integrals analogous to Enskog's are presented in section 2.1. Local conservation laws and its applications to fluid dynamics are briefly recalled in section 2.2. Our main results are presented in section 2.3. In particular, a general formulation of delocalized collision integrals is presented in section 2.3.1, and the corresponding global conservation laws of mass, momentum and energy in 2.3.2 are briefly recalled for these generalizations of Enskog's equation. The core of this paper is Theorem 2.3.1, in section 2.3.3, providing an analogue of Landau's representation of Boltzmann's collision integral as the divergence in v of a mass current, in the more complex case of delocalized collision integral. Our second main result is the local entropy inequality for a subclass of delocalized collision integrals presented in Theorem 2.3.3 of section 2.3.4. Applications of our results to the continuum mechanics of dense gases are discussed in section 2.4.

2.1 Examples of Delocalized Collision Integrals in the Kinetic Theory of Gases

Examples of Delocalized Collision Integrals
in the Kinetic Theory of Gases

All collisional kinetic models take the form

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \text{St}[f](t, x, v), \quad (2.1.1)$$

where $f \equiv f(t, x, v) \geq 0$ is the velocity distribution function, i.e. the number density of gas molecules at position $x \in \mathbf{R}^3$ and with velocity $v \in \mathbf{R}^3$ at time t , while St is the collision operator, usually a nonlinear integral operator acting on the velocity, and sometimes the position variables in f .

In the classical kinetic theory of gases due to Maxwell (1866) and Boltzmann (1872), the collision integral computes the variation in the number of gas molecules with velocity $v \in \mathbf{R}^3$ due to binary, elastic collisions with gas molecules at the same position with a velocity different from v . Specifically, if the gas molecules are hard spheres of radius $r > 0$, the Boltzmann collision integral is¹

$$\mathcal{B}[f, f](v) := \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (f(v')f(w') - f(v)f(w))(2r)^2(v - w|n)_+ dw dn, \quad (2.1.2)$$

where $f \geq 0$ is the velocity distribution function, while $(u|v)$ is the inner product of $u, v \in$

¹See in [Son07] the paragraph following equations (1.7) in chapter 1, especially footnote 6 on p. 4 in that chapter.

$\mathbf{R}^3$, and $z_+ := \max(z, 0)$ for all $z \in \mathbf{R}$ (see section 2.5 in [Cer94]). In the integrand above,

$$v' \equiv v'(v, w, n) := v - (v - w|n)n, \quad w' \equiv w'(v, w, n) := w + (v - w|n)n. \quad (2.1.3)$$

Notice that these transformations are invariant under the substitution $n \mapsto -n$.

One easily checks that $v'(v, w, n), w'(v, w, n)$ runs through the set of all the solutions of the system of equations

$$v' + w' = v + w, \quad |v'|^2 + |w'|^2 = |v|^2 + |w|^2 \quad (2.1.4)$$

as n runs through the unit sphere $\mathbf{S}^2$ of $\mathbf{R}^3$. The first equality above is the conservation of momentum for a pair of point particles with mass $m > 0$, while the second equality is the conservation of kinetic energy for the same particles in any elastic collision involving such particles located at the same position in $\mathbf{R}^3$, with velocities v, w immediately after the collision, and v', w' immediately before the collision. Without entering the details of the derivation of the Boltzmann collision integral, suffices it to say that, in that integral, one should think of the term $-f(v)f(w)$ as measuring the loss of gas molecules with velocity v due to an impending collision with another gas molecule at the same position with velocity w . Similarly, one should think of the term $f(v')f(w')$ as measuring the creation of gas molecules with velocity v resulting from the collision of a gas molecule with velocity v' with a gas molecule with velocity w' immediately before the collision. Thus all the pair of velocities involved in the Boltzmann collision integrand are always velocities of gas molecules *about to collide* (and never of gas molecules having just collided). This “justifies” the assumption of Maxwell and Boltzmann that such particle velocities are statistically independent, so that their joint distribution is $f(v')f(w')$ in the latter case, and $f(v)f(w)$ in the former.

Therefore, in the Boltzmann equation for the hard sphere gas, the molecular radius appears only as a scaling factor of the collision differential cross-section $(2r)^2(\cos(\widehat{v-w}, n))_+$, and never in the distribution function itself in the collision integral. This has been justified (for instance by Lanford [Lan75], see also chapters 2 and 4 in [Cer94] for a streamlined presentation of Lanford’s arguments) in the regime known as the “Boltzmann-Grad limit” of the classical mechanics of N -particle system, where $N \gg 1$ while $r \ll 1$ satisfy $Nr^2 \sim 1$. In particular $Nr^3 = O(r) \rightarrow 0$ in that limit, so that there is no excluded volume, and the resulting equations of state for the pressure and the internal energy correspond to a perfect gas.

Situations where the molecular radius is larger may fail to satisfy the Boltzmann-Grad assumption. Alternatively, one might also seek corrections in r to the perfect gas equation of state for the pressure and the internal energy. Whatever the motivation, one might be led to consider collision integrals involving a *delocalized* collision integrand, i.e. a collision integrand where gas molecules are not considered as point particles located at the same point, but are hard spheres of radius $r > 0$.

Perhaps the best known kinetic model with such delocalized collision integral is the Enskog-Boltzmann equation (see [Ark90; TB87]). In the hard sphere case, the Enskog-Boltzmann collision integral takes the form

$$\begin{aligned} \mathcal{E}[f, f](x, v) := & \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (f(x, v'(v, w, n))f(x - 2rn, w'(v, w, n)) \\ & - f(x, v)f(x + 2rn, w))4r^2(v - w|n)_+ dw dn. \end{aligned} \quad (2.1.5)$$

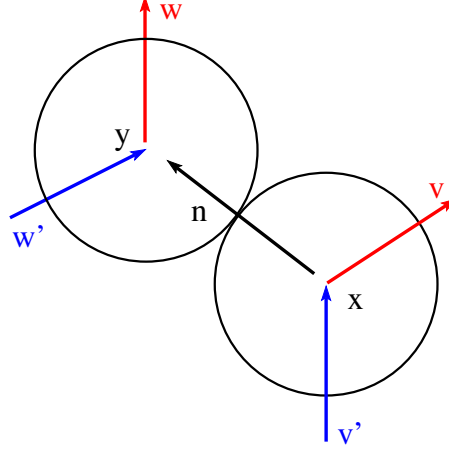


Figure 2.1: Two hard spheres centered at x and $y = x + rn$, with pre-collision velocities v' and w' , and post-collision velocities v and w . Observe that the post-collision velocities v and w satisfy the condition $(w - v|n) = (w - v|\frac{y-x}{|y-x|}) > 0$, while the pre-collision velocities satisfy $(w' - v'|n) = (w' - v'|\frac{y-x}{|y-x|}) < 0$.

This collision integral can be recast as

$$\begin{aligned} \mathcal{E}[f, f](x, v) := & \iint_{(\mathbf{R}^3)^2} (f(x, v'(v, w, n))f(x - z, w'(v, w, n)) \\ & - f(x, v)f(x + z, w))(v - w|\frac{z}{|z|})_+ \delta_{2r}(|z|)dw dz, \end{aligned}$$

where δ_{2r} is the Dirac “function” at $2r > 0$ on $\mathbf{R}$.

A first obvious generalization is based on the last formula for the Enskog-Boltzmann collision integral. Pick $\zeta \in C(\mathbf{R})$ satisfying

$$\zeta \geq 0, \quad \text{supp}(\zeta) = [-1, 1], \quad \int_{\mathbf{R}} \zeta(s)ds = 1,$$

and set

$$\zeta_\epsilon(s) := \frac{1}{\epsilon} \zeta\left(\frac{s}{\epsilon}\right), \quad \theta_{\epsilon, r}(|z|) = \zeta_\epsilon(|z| - 2r),$$

so that $\theta_{\epsilon, r} \rightarrow \delta_{2r}$ in $\mathcal{D}'(\mathbf{R})$ as $\epsilon \rightarrow 0^+$. If one replaces the Dirac measure $\delta_{2r}(|z|)$ with its regularized variant $\theta_{\epsilon, r}(|z|)$, one arrives at the expression

$$\begin{aligned} \mathcal{C}[f, f](x, v) := & \iint_{(\mathbf{R}^3)^2} \left(f(x, v'(v, w, \frac{z}{|z|}))f(x - z, w'(v, w, \frac{z}{|z|})) \right. \\ & \left. - f(x, v)f(x + z, w) \right) \theta_{\epsilon, r}(|z|) \left(v - w|\frac{z}{|z|} \right)_+ dw dz. \end{aligned} \quad (2.1.6)$$

One can think of this as a collision integral for “soft” spheres — soft meaning that the radius of the colliding balls is slightly distributed around $r > 0$, instead of being exactly equal to r ; otherwise the collision transformation of $(v, v_*) \mapsto (v', v'_*)$ is the same as above. In other words, these collisions are elastic. (It is unlikely that collisions between pairs of soft spherical

particles really behave in this manner, which is why the word *soft* is put between quotes.) See [Cer83] for a presentation of this model, which is derived from a large particle system in the style of Lanford's argument for the Boltzmann equation. In particular, Cercignani proposed a specific formula for $\theta_{\epsilon,r}$: see equations (2.1)-(2.5) on p. 481 in [Cer83].

The Cercignani soft-sphere collision integral can be recast as

$$\begin{aligned} \mathcal{C}[f, f](x, v) := & \iint_{(\mathbf{R}^3)^2} \left(f(x, v'(v, w, \frac{x-y}{|x-y|})) f(y, w'(v, w, \frac{x-y}{|x-y|})) \mathbf{1}_{(v-w|x-y|)>0} \right. \\ & \left. - f(x, v) f(y, w) \mathbf{1}_{(v-w|x-y|)<0} \right) \theta_{\epsilon,r}(|x-y|) \left| \left(v-w \frac{x-y}{|x-y|} \right) \right| dw dy. \end{aligned}$$

A last generalization consists in forgetting the specifics of the distribution $\theta_{\epsilon,r}$. This suggests considering instead the Povzner type collision integral

$$\begin{aligned} \mathcal{P}[f, f](x, v) := & \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \left(f(x, v'(v, w, \frac{x-y}{|x-y|})) f(y, w'(v, w, \frac{x-y}{|x-y|})) \mathbf{1}_{(v-w|x-y|)>0} \right. \\ & \left. - f(x, v) f(y, w) \mathbf{1}_{(v-w|x-y|)<0} \right) b(|x-y|) \left| \left(v-w \frac{x-y}{|x-y|} \right) \right| dw dy \end{aligned} \quad (2.1.7)$$

where $b \in C_c([0, +\infty))$ is a nonnegative function. See [Pov65], where this model² is introduced for the first time.

Along with the Enskog-Boltzmann collision integral above, one also finds in the literature the genuine Enskog equation (see chapter 16 of [CC70] or [BL88]) and a modified, or revised Enskog collision integral (see [Rés78], or [Bei83b] and [BE73a; BE73b]):

$$\begin{aligned} \tilde{\mathcal{E}}[f, f](x, v) := & \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (Y(\rho_f(x), \rho_f(x-2rn)) f(x, v'(v, w, n)) f(x-2rn, w'(v, w, n))) \\ & - Y(\rho_f(x), \rho_f(x+2rn)) f(x, v) f(x+2rn, w) 4r^2 (v-w|n)_+ dw dn, \end{aligned} \quad (2.1.8)$$

where the factor $Y : [0, +\infty)^2 \rightarrow [0, +\infty)$ is used to enhance the collision frequency, and where

$$\rho_f(x) := \int_{\mathbf{R}^3} f(x, v) dv. \quad (2.1.9)$$

²Povzner's original collision integral in [Pov65] is

$$\begin{aligned} \tilde{\mathcal{P}}[f, f](x, v) := & \iint_{(\mathbf{R}^3)^2} \left(f(x, v'(v, w, \frac{x-y}{|x-y|})) f(y, w'(v, w, \frac{x-y}{|x-y|})) \right. \\ & \left. - f(x, v) f(y, w) \right) b(|x-y|) \left| \left(v-w \frac{x-y}{|x-y|} \right) \right| dw dy. \end{aligned}$$

Since the transformation $(v, w) \mapsto (v'(v, w, n), w'(v, w, n))$ is invariant under the central symmetry $n \mapsto -n$,

$$\mathcal{B}[f, f](v) = \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (f(v') f(w') - f(v) f(w)) 2r^2 |(v-w|n)| dw dn.$$

Povzner's original definition of his delocalized collision integral is based on this last form of the Boltzmann integral instead of (2.1.2). Since $(v' - w'|x-y) = -(v-w|x-y) < 0$ for the gain part $f(x, v') f(y, w')$ and $(v-w|x-y) < 0$ for the loss part $f(x, v) f(y, w)$ of the collision integral $\mathcal{P}$, only particles about to collide are uncorrelated in (2.1.7), as in the case of (2.1.2). That this important feature of Boltzmann's theory is absent from [Pov65] may be an oversight. For this reason, we prefer considering $\mathcal{P}$ instead of $\tilde{\mathcal{P}}$.

2.2 Local Conservation Laws for the Boltzmann Collision Integral

Returning to the Boltzmann collision integral (2.1.2), it is well known that, for all $f \in L^1(\mathbf{R}^3, (1 + |v|)^3 dv)$,

$$\int_{\mathbf{R}^3} \mathcal{B}[f, f](v) \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} dv = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (2.2.1)$$

see for instance sections 3.1 and 3.3 in [Cer94]. These five identities correspond to the local conservation of mass (or particle number), of the three components of momentum, and of energy in the collision process described by the Boltzmann collision integral.

As a consequence of these identities, if f is a classical solution of the Boltzmann equation

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \mathcal{B}[f, f](t, x, v) (= \mathcal{B}[f(t, x, \cdot), f(t, x, \cdot)](v))$$

such that $f(t, x, \cdot), \partial_t f(t, x, \cdot)$ and $\nabla_x f(t, x, \cdot) \in L^1(\mathbf{R}^3, (1 + |v|)^3 dv)$, then

$$\partial_t \int_{\mathbf{R}^3} f(t, x, v) \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ \frac{1}{2}|v|^2 \end{pmatrix} dv + \nabla_x \cdot \int_{\mathbf{R}^3} v f(t, x, v) \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ \frac{1}{2}|v|^2 \end{pmatrix} dv = 0. \quad (2.2.2)$$

These five differential identities are of considerable importance in connecting the kinetic description of gases with continuum mechanics. Indeed, if one calls

$$\rho(t, x) := \int_{\mathbf{R}^3} f(t, x, v) dv \geq 0, \quad u(t, x) = \frac{\mathbf{1}_{\rho(t, x) > 0}}{\rho(t, x)} \int_{\mathbf{R}^3} v f(t, x, v) dv \in \mathbf{R}^3, \quad (2.2.3)$$

the first identity above takes the form of the equation of continuity of fluid mechanics

$$\partial_t \rho(t, x) + \nabla_x \cdot (\rho(t, x) u(t, x)) = 0, \quad (2.2.4)$$

while the second identity becomes

$$\partial_t (\rho(t, x) u(t, x)) + \nabla_x \cdot (\rho(t, x) u(t, x)^{\otimes 2}) + \nabla_x \cdot P(t, x) = 0, \quad (2.2.5)$$

where

$$P(t, x) := \int_{\mathbf{R}^3} (v - u(t, x))^{\otimes 2} f(t, x, v) dv. \quad (2.2.6)$$

Finally, the third identity takes the form

$$\begin{aligned} \partial_t \left(\frac{1}{2} \rho(t, x) |u(t, x)|^2 + \frac{1}{2} \text{tr} P(t, x) \right) + \nabla_x \cdot \left(u(t, x) \left(\frac{1}{2} \rho(t, x) |u(t, x)|^2 + \frac{1}{2} \text{tr} P(t, x) \right) \right) \\ + \nabla_x \cdot (P(t, x) \cdot u(t, x) + Q(t, x)) = 0, \end{aligned} \quad (2.2.7)$$

where Q is the time-dependent vector field defined by

$$Q(t, x) := \frac{1}{2} \int_{\mathbf{R}^3} (v - u(t, x)) |v - u(t, x)|^2 f(t, x, v) dv. \quad (2.2.8)$$

If $f(t, x, v)$ is an even function of $v - u(t, x)$ one easily checks (by a parity argument) that

$$Q(t, x) = 0,$$

These identities are obviously reminiscent of the Euler system of equations for compressible fluids (see (3.3.17) in chapter III of [Daf10]), and the tensor field $P(t, x)$ plays the role of the pressure. Specifically if f is a radial function of $v - u(t, x)$ — for instance if f is a local Maxwellian equilibrium in v centered at $u(t, x)$ — one finds that

$$P(t, x) = p(t, x)I, \quad \text{and hence} \quad \text{tr} P(t, x) = 3p(t, x)I.$$

Hence

$$\partial_t(\rho(t, x)u(t, x)) + \nabla_x \cdot (\rho(t, x)u(t, x)^{\otimes 2}) + \nabla_x p(t, x) = 0, \quad (2.2.9)$$

while

$$\partial_t(\frac{1}{2}\rho(t, x)|u(t, x)|^2 + \frac{3}{2}p(t, x)) + \nabla_x \cdot (u(t, x)(\frac{1}{2}\rho(t, x)|u(t, x)|^2 + \frac{5}{2}p(t, x))) = 0. \quad (2.2.10)$$

Setting $\theta(t, x) = p(t, x)/\rho(t, x)$, one finds that these are the Euler equation and local energy conservation law for a perfect gas with adiabatic index

$$\gamma = (5/2)/(3/2) = 5/3.$$

It is well known that the adiabatic index of a perfect gas is $\gamma = 1 + 2/n$, where n is the number of degrees of freedom of the gas molecule (see formulas (44.1-2) in [LL80]). For a monatomic gas, each molecule has $n = 3$ degrees of freedom (corresponding to translations in the directions of the coordinate axis), so that $\gamma = 5/3$ is the adiabatic index of a perfect monatomic gas. Thus the collision integral (2.1.2) can describe only perfect monatomic gases.

All these considerations suggest studying the following question: compute

$$\int_{\mathbf{R}^3} \text{St}[f](t, x, v) \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} dv,$$

where $\text{St}[f]$ is any one of the delocalized collision integrals presented above, i.e. $\mathcal{E}[f, f]$ (Enskog-Boltzmann) or $\tilde{\mathcal{E}}[f, f]$ (revised Enskog), or $\mathcal{C}[f, f]$ (Cercignani's soft-sphere collision integral), or $\mathcal{P}[f, f]$ (Povzner-type collision integral).

In general, delocalization may prevent some of these quantities to be identically 0. However, it is certainly interesting to study these expressions in view of applications to fluid mechanics.

2.3 Main Results: Delocalized Collision Integrals in Conservative Form and Applications

In order to approach the question of local conservation laws for delocalized collision integrals, we shall make a small detour. While it may seem unnecessary, it sheds some light on the structure of these collision integrals.

Our approach finds its origin in a seemingly little-known property of the Boltzmann collision integral. The fact that the Boltzmann collision integral satisfies the local conservation of mass suggests seeking a mass current $J[f, f](v)$ such that

$$\mathcal{B}[f, f](v) = -\nabla_v \cdot J[f, f](v)$$

for all $f \in \mathcal{S}(\mathbf{R}^3)$ (the Schwartz space of smooth functions with rapidly decaying derivatives of all orders). This is the starting point of the derivation of the Landau collision integral from the Boltzmann collision integral in the grazing collisions regime (see §41 in [LP81]). A more systematic (and rigorous) discussion of this property can be found in [Vil99].

2.3.1 Delocalized Collision Integrals: a General Setting

In this section, we propose a common setting for the delocalized collision integrals $\mathcal{E}, \mathcal{C}, \mathcal{P}, \tilde{\mathcal{E}}$ presented in section 2.1.

The general form of delocalized collision integrals considered in this paper is

$$\begin{aligned} \text{St}[f, g](x, v) := & \int_{(\mathbf{R}^3)^2} (f(x, v'(v, w, n_{x,y}))g(y, w'(v, w, n_{x,y}))\mathbf{1}_{(v-w|n_{x,y})>0} \\ & - f(x, v)g(y, w)\mathbf{1}_{(v-w|n_{x,y})<0})B[\rho_f, \rho_g](x, y, v-w)dydw, \end{aligned} \quad (2.3.1)$$

where

$$\rho_f(x) := \int_{\mathbf{R}^3} f(x, v)dv, \quad \rho_g(y) := \int_{\mathbf{R}^3} g(y, w)dw$$

are the macroscopic densities of the distribution functions f and g , while

$$n_{x,y} := \frac{x-y}{|x-y|}, \quad x \neq y.$$

The collision kernel $B[\rho_f, \rho_g](x, y, v-w) \geq 0$ is in general a functional of the macroscopic densities ρ_f and ρ_g , and a function — or more generally a distribution — of the positions x, y , and of the relative velocity $v-w$. In addition, it satisfies

$$\begin{cases} (i) & B[\varpi, \rho](y, x, w-v) = B[\rho, \varpi](x, y, v-w), \\ (ii) & B[\rho, \varpi](x, y, v-w) = B[\rho, \varpi](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})), \\ (iii) & B[\rho, \varpi](x, y, v-w) = 0 \text{ if } |x-y| > R, \end{cases}$$

for some $R > 0$, a real parameter which can be thought of as being the radius of the sphere

of influence of a gas molecule³ of the gas molecules, together with the bound

$$(iv) \quad \sup_{v, w \in \mathbf{R}^3} \frac{1}{1 + |v - w|} \int_{(\mathbf{R}^3)^2} B[\rho, \varpi](x, y, v - w) \mathbf{1}_{|x| \leq A} dx dy < \infty.$$

Let us check that the examples of delocalized collision integrals considered in section 2.1 can be put in the form (2.3.1).

(1) Enskog-Boltzmann equation: in that case

$$B[\rho, \varpi](x, y, v - w) = (v - w | n_{x, y}) | \delta_{2r}(|x - y|),$$

(and of course, the collision kernel is independent of the macroscopic densities ρ, ϖ);

(2) Soft spheres: in that case

$$B[\rho, \varpi](x, y, v - w) = \theta_{\epsilon, r}(|x - y|) |(v - w | n_{x, y})|$$

(and of course, the collision kernel is independent of the macroscopic densities ρ, ϖ);

(3) Povzner-type equation: in that case

$$B[\rho, \varpi](x, y, v - w) = b(|x - y|) |(v - w | n_{x, y})|$$

(and of course, the collision kernel is independent of the macroscopic densities ρ, ϖ). This type of collision kernel will be used below in section 2.3.4 in connection with the H Theorem;

(4) Enskog equation: in that case

$$B[\rho, \varpi](x, y, v - w) = Y[\rho(x), \varpi(y)] |(v - w | n_{x, y})| \delta_{2r}(|x - y|).$$

2.3.2 Global Conservation Laws for Delocalized Collision Integrals

The following result is well-known in the case of the Enskog equation [Pol89; EP91]. We briefly sketch its proof in the more general setting considered here.

Proposition 2.3.1. *For all measurable, rapidly decaying f, g defined a.e. on $\mathbf{R}^3 \times \mathbf{R}^3$, the collision integral St satisfies the local mass conservation identity*

$$\int_{\mathbf{R}^3} \text{St}[f, g](x, v) dv = 0.$$

It also satisfies the global momentum and energy conservation identities

$$\int_{\mathbf{R}^3 \times \mathbf{R}^3} \text{St}[f, f](x, v) v_j dx dv = \int_{\mathbf{R}^3 \times \mathbf{R}^3} \text{St}[f, f](x, v) |v|^2 dx dv = 0, \quad j = 1, 2, 3.$$

³In other words, R is the distance beyond which a point particles is not affected by the presence of one gas molecule. Assuming short range molecular interactions, one can think of R as being of the order of a few van der Waals radii of the gas molecules.

Proof. For all measurable, rapidly decaying f, g defined a.e. on $\mathbf{R}^3 \times \mathbf{R}^3$,

$$\begin{aligned}
& \int_{\mathbf{R}^3} \text{St}[f, g](x, v) dv = \int_{(\mathbf{R}^3)^3} (f(x, v'(v, w, n))g(y, w'(v, w, n))\mathbf{1}_{(v-w|n_{x,y})>0} \\
& \quad - f(x, v)f(y, w)\mathbf{1}_{(v-w|n_{x,y})<0})B[\rho_f, \rho_g](x, y, v-w)dv dw dy \\
& = \int_{(\mathbf{R}^3)^3} (B[\rho_f, \rho_g](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y}))\mathbf{1}_{(v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})|n_{x,y})>0} \\
& \quad - B[\rho_f, \rho_g](x, y, v-w)\mathbf{1}_{(v-w|n_{x,y})<0})f(x, v)g(y, w)dv dw dy \\
& \quad \text{(with the change of variables } (v, w) \mapsto (v'(v, w, n), w'(v, w, n)) \text{ for each } n \\
& = \int_{(\mathbf{R}^3)^3} (B[\rho_f, \rho_g](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})) - B[\rho_f, \rho_g](x, y, v-w)) \\
& \quad \times \mathbf{1}_{(v-w|n_{x,y})<0} f(x, v)g(y, w)dv dw dy = 0. \\
& \quad \text{(since } (v'(v, w, n) - w'(v, w, n)|n) = -(v-w|n))
\end{aligned}$$

by assumption (ii) on B . Similarly

$$\begin{aligned}
& \int_{(\mathbf{R}^3)^2} \text{St}[f, f](x, v) v dv dx \\
& = \int_{(\mathbf{R}^3)^4} (f(x, v'(v, w, n_{x,y}))f(y, w'(v, w, n_{x,y}))\mathbf{1}_{(v-w|n_{x,y})>0} \\
& \quad - f(x, v)f(y, w)\mathbf{1}_{(v-w|n_{x,y})<0})B[\rho_f, \rho_f](x, y, v-w)v dx dv dy dw \\
& = \int_{(\mathbf{R}^3)^4} (B[\rho_f, \rho_f](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y}))v'(v, w, n_{x,y}) \\
& \quad - B[\rho_f, \rho_f](x, y, v-w)v)\mathbf{1}_{(v-w|n_{x,y})<0} f(x, v)f(y, w)dx dv dy dw \\
& \quad \text{(with the change of variables } (v, w) \mapsto (v'(v, w, n), w'(v, w, n)) \text{ for each } n \\
& \quad \text{since } (v'(v, w, n) - w'(v, w, n)|n) = -(v-w|n)) \\
& = \int_{(\mathbf{R}^3)^4} (B[\rho_f, \rho_f](y, x, v'(w, v, n_{y,x}) - w'(w, v, n_{y,x}))v'(w, v, n_{y,x}) \\
& \quad - B[\rho_f, \rho_f](y, x, w, v)w)\mathbf{1}_{(w-v|n_{y,x})<0} f(x, v)f(y, w)dx dv dy dw \\
& \quad \text{(exchanging the molecule at } x \text{ with velocity } v \\
& \quad \text{and the molecule at } y \text{ with velocity } w \text{ by assumption (i) on } B) \\
& = \int_{(\mathbf{R}^3)^4} (B[\rho_f, \rho_f](y, x, w'(v, w, n_{x,y}) - v'(v, w, n_{x,y}))w'(v, w, n_{x,y}) \\
& \quad - B[\rho_f, \rho_f](y, x, w, v)w)\mathbf{1}_{(w-v|n_{y,x})<0} f(x, v)f(y, w)dx dv dy dw \\
& \quad \text{(since } v'(w, v, n) = w'(v, w, n) = w'(v, w, -n) \\
& \quad \text{and } w'(w, v, n) = v'(v, w, n) = v'(v, w, -n)) \\
& = \int_{(\mathbf{R}^3)^4} (B[\rho_f, \rho_f](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y}))w'(v, w, n_{x,y}) \\
& \quad - B[\rho_f, \rho_f](x, y, v, w)w)\mathbf{1}_{(v-w|n_{x,y})<0} f(x, v)f(y, w)dx dv dy dw. \\
& \quad \text{(using assumption (i) on } B)
\end{aligned}$$

Summarizing, the first left-hand side is equal to the right-hand side of either the second or the sixth equality, and therefore to the mean of these expressions, i.e.

$$\begin{aligned} & \int_{\mathbf{R}^3 \times \mathbf{R}^3} \text{St}[f, f](x, v) v dv dx \\ &= \int_{(\mathbf{R}^3)^4} \left(B[\rho_f, \rho_f](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})) \frac{v'(v, w, n_{x,y}) + w'(v, w, n_{x,y})}{2} \right. \\ & \quad \left. - B[\rho_f, \rho_f](x, y, v - w) \frac{v+w}{2} \right) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) dx dv dy dw = 0 \end{aligned}$$

by assumption (ii) on B , and because of the first identity in (2.1.4).

Proceeding in exactly the same manner, we see that

$$\begin{aligned} & \int_{\mathbf{R}^3 \times \mathbf{R}^3} \text{St}[f, f](x, v) |v|^2 dv dx \\ &= \int_{(\mathbf{R}^3)^4} \left(B[\rho_f, \rho_f](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})) \frac{|v'(v, w, n_{x,y})|^2 + |w'(v, w, n_{x,y})|^2}{2} \right. \\ & \quad \left. - B[\rho_f, \rho_f](x, y, v - w) \frac{|v|^2 + |w|^2}{2} \right) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) dx dv dy dw = 0 \end{aligned}$$

again by assumption (ii) on B , and because of the second identity in (2.1.4). This concludes the proof. $\square$

2.3.3 Landau Currents for Delocalized Collision Integrals

By analogy with the arguments in §41 in [LP81] and in [Vil99] leading to a representation of the Boltzmann collision integral as the divergence of a “Landau” mass current in the velocity variable, our first main result in this paper is to represent delocalized collision integrals (2.3.1) in terms of divergences of Landau mass, momentum and energy currents. The main difference with the Boltzmann case is that only the global conservation laws of momentum and energy are known to be satisfied by delocalized collision integrals (2.3.1). As a result, one should seek representations in terms of divergences of Landau momentum and energy currents *in both the position and velocity variables*.

Definition 2.3.1. For each rapidly decaying $f, g \in C(\mathbf{R}^3 \times \mathbf{R}^3)$, and each rapidly decaying $\rho, \varpi \in C(\mathbf{R}^3)$, set

$$\begin{aligned} \mathfrak{J}_0[\rho, \varpi, f, g](x, y, v) &:= \int_{\mathbf{R}^3 \times \mathbf{R}} B[\rho, \varpi](x, y, v - w) \mathbf{1}_{0 < s < (v-w|n_{y,x})} \\ &\quad \times f(x, v + sn_{y,x}) g(y, w + sn_{y,x}) n_{y,x} dw ds. \end{aligned}$$

Our first main result in this paper is the following theorem, whose proof can be found in section 2.5.

Theorem 2.3.1. For each rapidly decaying $f \in C(\mathbf{R}^3 \times \mathbf{R}^3)$,

$$\text{St}[f, f] = \nabla_v \cdot \mathcal{J}_0[f], \quad \text{where } \mathcal{J}_0[f](x, v) := \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, f, f](x, y, v) dy. \quad (2.3.2)$$

For $i = 1, 2, 3$,

$$\text{St}[f, f]v_i = \nabla_x \cdot \mathcal{I}_i[f] + \nabla_v \cdot \mathcal{J}_i[f], \quad (2.3.3)$$

where

$$\begin{aligned} \mathcal{I}_i[f](x, v) := & -\frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\frac{\pi}{2}} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta})(v_{-\theta} - w_{-\theta} | n_{y_{-\theta}, x_{-\theta}})_+ \\ & \times f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta})(n_{y_{-\theta}, x_{-\theta}})_i y d\theta dy dw \end{aligned}$$

where

$$\begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} v_\theta \\ w_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix},$$

and

$$\begin{aligned} \mathcal{J}_i[f, f](x, v) := & \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, (v_i - (v | n_{x,y})(n_{x,y})_i) f, f](x, y, v) dy \\ & + \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, f, (w | n_{x,y})(n_{x,y})_i f](x, y, v) dy \\ & - \frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\frac{\pi}{2}} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta})(v_{-\theta} - w_{-\theta} | n_{y_{-\theta}, x_{-\theta}})_+ \\ & \times f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta})(n_{y_{-\theta}, x_{-\theta}})_i w d\theta dy dw. \end{aligned}$$

Finally

$$\text{St}[f, f]|v|^2 = \nabla_x \cdot \mathcal{I}_4[f] + \nabla_v \cdot \mathcal{J}_4[f], \quad (2.3.4)$$

where

$$\begin{aligned} \mathcal{I}_4[f](x, v) := & -\frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\frac{\pi}{2}} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta})(v_{-\theta} - w_{-\theta} | n_{y_{-\theta}, x_{-\theta}})_+ \\ & \times (v_{-\theta} + w_{-\theta} | n_{y_{-\theta}, x_{-\theta}}) f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) y d\theta dy dw, \end{aligned}$$

and

$$\begin{aligned} \mathcal{J}_4[f](x, v) := & \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, (|v|^2 - (v | n_{x,y})^2) f, f](x, y, v) dy \\ & + \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, f, (w | n_{x,y})^2 f](x, y, v) dy \\ & - \frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\frac{\pi}{2}} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta})(v_{-\theta} - w_{-\theta} | n_{y_{-\theta}, x_{-\theta}})_+ \\ & \times (v_{-\theta} + w_{-\theta} | n_{y_{-\theta}, x_{-\theta}}) f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) w d\theta dy dw. \end{aligned}$$

There is some arbitrariness in the choice of the currents $\mathcal{J}_0$ and $\mathcal{I}_i, \mathcal{J}_i$ for $i = 1, \dots, 4$. All these currents are obviously not unique, but defined up to arbitrary divergence-free vector fields. One can certainly try to eliminate this arbitrariness by means of some appropriate “gauge” condition, but the choice of such conditions is quite arbitrary, and we have chosen not to investigate this issue any further.

2.3.4 H Theorem

In general, delocalized collision integrals are not known to satisfy a property analogous to Boltzmann's H Theorem, which is well known in the case of the Boltzmann collision integral (2.1.2). However, variants of the H Theorem are known in some cases: see [R  s78; AC90; Pol89; BL91] for the Enskog case, or [Cer83] for the soft sphere case.

In this section, we shall assume that the collision kernel is of the form

$$B[\rho, \varpi](x, y, v - w) = b(|x - y|)(v - w|n_{x,y}|) \quad (2.3.5)$$

where

$$b \in C([0, +\infty)) \text{ satisfies } g \geq 0 \text{ on } [0, +\infty) \text{ and } \text{supp } b \subset [0, R].$$

We begin with a global Boltzmann type H Theorem — except that the analogue of Boltzmann's H function is modified to take into account delocalization effects in the collision integral.

Theorem 2.3.2. *Assume that $f(t, x, v)$ is a classical solution of*

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \text{St}[f, f](t, x, v),$$

with $(x, v) \mapsto f(t, x, v)$ rapidly decaying at infinity, while $(x, v) \mapsto \ln f(t, x, v)$ has at most polynomial growth at infinity. Then

$$\frac{d}{dt}(\mathbf{H}_B[f] + \mathbf{H}_\beta[\rho_f]) = -\Lambda[f] \leq 0,$$

where $\mathbf{H}_B[f]$ is the Boltzmann H functional

$$\mathbf{H}_B[f](t) := \int_{(\mathbf{R}^3)^2} f(t, x, v) \ln f(t, x, v) dx dv,$$

and $\mathbf{H}_\beta[\rho]$ the potential interaction energy

$$\mathbf{H}_\beta[\rho](t) := \frac{1}{2} \int_{(\mathbf{R}^3)^2} \rho_f(t, x) \rho_f(t, y) \beta(|x - y|) dx dy,$$

while

$$\begin{aligned} \Lambda[f](t) := \frac{1}{2} \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) \ell \left(\frac{f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x}))}{f(t, x, v) f(t, y, w)} \right) \\ \times b(|x - y|)(v - w|n_{y,x}|)_+ dx dv dy dw \end{aligned}$$

is the entropy production term. In these formulas, we have used the notations

$$\beta(r) := \int_r^\infty b(s) ds, \quad \ell(z) = z - 1 - \ln z \geq 0 \text{ for all } z > 0.$$

This result is not really original: it is a modest generalization of the inequality (2.9) in [AC90]. However, this generalization, especially the potential part $\mathbf{H}_\beta$, may have some important implications, to be discussed later.

The idea of conservative formulation of delocalized collision integral can be used in the context of the H Theorem. The idea is that the

Theorem 2.3.3. *Assume that $f(t, x, v)$ is a classical solution of*

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \text{St}[f, f](t, x, v),$$

with $(x, v) \mapsto f(t, x, v)$ rapidly decaying at infinity, while $(x, v) \mapsto \ln f(t, x, v)$ has at most polynomial growth at infinity. Then

$$\begin{aligned} \text{St}[f, f](t, x, v) \ln f(t, x, v) &\leq -\nabla_x \cdot \mathcal{K}[f](t, x, v) - \nabla_v \cdot \mathcal{L}[f](t, x, v) \\ &\quad - \frac{1}{2}(\partial_t + v \cdot \nabla_x) (f(t, x, v) \rho_f(t, \cdot) \star \beta(|\cdot|)(x)), \end{aligned} \quad (2.3.6)$$

in the sense of distributions. In this inequality, the notation $\star$ designates the convolution (in the variable x), viz.

$$\rho_f(t, \cdot) \star \beta(|\cdot|)(x) := \int_{\mathbf{R}^3} \rho_f(t, x - y) \beta(|y|) dy, \quad (2.3.7)$$

while

$$\begin{aligned} \mathcal{K}[f](t, x, v) &:= \frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\pi/2} (f(t, x_{-\theta}, v'(v, w, n_{y,x})_{-\theta}) f(t, y_{-\theta}, w'(v, w, n_{y,x})_{-\theta}) \\ &\quad - f(t, x_{-\theta}, v_{-\theta}) f(t, y_{-\theta}, w_{-\theta})) \ln f(t, y_{-\theta}, w_{-\theta}) b(|x_{-\theta} - y_{-\theta}|) \\ &\quad \times (v_{-\theta} - w_{-\theta} |n_{x_{-\theta}, y_{-\theta}})_+ y d\theta dy dw, \end{aligned}$$

while

$$\begin{aligned} \mathcal{L}[f](t, x, v) &:= \frac{1}{2} \mathcal{J}_0[f](t, x, v) (1 - \rho_f \star \beta(|\cdot|)(t, x)) \\ &\quad + \frac{1}{2} (\mathcal{J}_0[f \ln f, f](t, x, v) + \mathcal{J}_0[f, f \ln f](t, x, v)) \\ &\quad + \frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\pi/2} (f(t, x_{-\theta}, v'(v, w, n_{y,x})_{-\theta}) f(t, y_{-\theta}, w'(v, w, n_{y,x})_{-\theta}) \\ &\quad - f(t, x_{-\theta}, v_{-\theta}) f(t, y_{-\theta}, w_{-\theta})) \ln f(t, y_{-\theta}, w_{-\theta}) b(|x_{-\theta} - y_{-\theta}|) \\ &\quad \times (v_{-\theta} - w_{-\theta} |n_{x_{-\theta}, y_{-\theta}})_+ w d\theta dy dw. \end{aligned}$$

In this equality, the notation $\mathcal{J}_0[f, g]$ designates the current

$$\begin{aligned} \mathcal{J}_0[f, g](t, x, v) &:= \int_{(\mathbf{R}^3)^2 \times \mathbf{R}} b(|x - y|) (v - w |n_{y,x}) \mathbf{1}_{0 < s < (v-w|n_{y,x})} \\ &\quad \times f(t, x, v + sn_{y,x}) g(t, y, w + sn_{y,x}) n_{y,x} dy dw ds. \end{aligned}$$

In other words

$$\mathcal{J}_0[f, g](t, x, v) = \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_g, f, g](t, x, y, v) dy$$

with $\mathfrak{J}_0[\rho_f, \rho_g, f, g]$ as in Definition 2.3.1. However, here, the situation is much simpler, since

$$B[\rho_f, \rho_g](x, y, v - w) := b(|x - y|) |(v - w |n_{x,y})|$$

is independent of ρ_f and ρ_g , so that $\mathfrak{J}_0[\rho_f, \rho_g, f, g](t, x, y, v)$ is also independent of ρ_f and ρ_g .

The proofs of Theorems 3.4 and 3.5 can be found in section 2.6.

2.4 Applications to the Macroscopic Description of Dense Gases

2.4.1 Local Conservation of Mass, Momentum and Energy

The discussion in section 2.2 makes it very clear that the Boltzmann collision integral does not contribute to the stress tensor in (2.2.5), i.e. the pressure tensor P . This may seem somewhat disturbing, since one would expect that collisions between gas molecules should account for the acceleration driving the fluid.

This last point is of course not entirely true. Indeed, even in a gas of noninteracting point particles, i.e. if the distribution function satisfies

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = 0,$$

the pressure tensor P defined in (2.2.6) can be computed explicitly, and it is neither equal to zero (unless $f(t, x, v) = \rho(t, x) \delta(v - u(t, x))$), nor a constant in general. It can be computed explicitly for instance in the case where

$$f(0, x, v) = \exp(-(|x|^2 + |v|^2)).$$

One finds indeed that

$$f(t, x, v) = \exp\left(-\left(\frac{|x|^2}{1+t^2} + (1+t^2)|v - \frac{t}{1+t^2}x|^2\right)\right),$$

so that

$$P(t, x) = \frac{\pi^{3/2}}{2(1+t^2)^{5/2}} \exp\left(-\frac{|x|^2}{1+t^2}\right) I.$$

This elementary example shows that the force deriving from the pressure may be non trivial even in the absence of collisions.

In the case of the Boltzmann equation, the contribution of collisions to the pressure tensor is indirect: in the highly collisional regime, collisions induce a relaxation of the distribution function $f(t, x, v)$ to a local Maxwellian distribution, a radial function of $v - u(t, x)$, so that the current Q vanishes identically, and ρ, u defined in (2.2.3) and $p := \text{tr} P$ is a solution of the system of equations (2.2.4)-(2.2.9)-(2.2.10), i.e. the Euler system of gas dynamics for a perfect gas with adiabatic index $\gamma = 5/3$, as explained at the end of section 2.2. This follows from the approach of the hydrodynamic limit of the Boltzmann equation involving Hilbert's expansion, as in [CP79] or chapter 11 of [Cer94] — see also [BG84].

In the case of dense gases, the situation is completely different. The collision integral *directly* contributes to the stress tensor and energy flux in the local balance of momentum and energy in the gas, and this contribution is easily computed in terms of the momentum and energy currents in Theorem 2.3.1. See for instance [MGB18; Tak24] for other approaches to this issue.

Corollary 2.4.1. *Let f be a classical solution of the kinetic equation (2.1.1) with delocalized collision integral (2.3.1). Assume that the collision kernel B in (2.3.1) satisfies (i)-(iv), and that $(x, v) \mapsto f(t, x, v)$ is continuous on $\mathbf{R}^3 \times \mathbf{R}^3$ and rapidly decaying at infinity. Then*

$$\begin{cases} \partial_t \rho_f(t, x) + \nabla_x \cdot \int_{\mathbf{R}^3} v f(t, x, v) dv = 0, \\ \partial_t \int_{\mathbf{R}^3} v_i f(t, x, v) dv + \nabla_x \cdot \int_{\mathbf{R}^3} (v v_i f(t, x, v) - \mathcal{I}_i[f](t, x, v)) dv = 0, & i = 1, 2, 3, \\ \partial_t \int_{\mathbf{R}^3} \frac{1}{2} |v|^2 f(t, x, v) dv + \nabla_x \cdot \int_{\mathbf{R}^3} (v \frac{1}{2} |v|^2 f(t, x, v) - \frac{1}{2} \mathcal{I}_4[f](t, x, v)) dv = 0, \end{cases}$$

where $\mathcal{I}_i[f]$ and $\mathcal{I}_4[f]$ are respectively the projections of the momentum and energy phase-space currents involved in (2.3.3) and (2.3.4) on the space of positions.

With the definitions (2.1.9) for ρ_f and

$$u_f(t, x) := \frac{\mathbf{1}_{\rho_f(t, x) > 0}}{\rho_f(t, x)} \int_{\mathbf{R}^3} v f(t, x, v) dv,$$

and

$$P_f(t, x) := \int_{\mathbf{R}^3} (v - u_f(t, x))^{\otimes 2} f(t, x, v) dv,$$

while

$$Q_f(t, x) := \frac{1}{2} \int_{\mathbf{R}^3} (v - u_f(t, x)) |v - u_f(t, x)|^2 f(t, x, v) dv,$$

as in section 2.2, the identities obtained in the corollary above are recast as

$$\begin{cases} \partial_t \rho_f + \nabla_x \cdot (\rho_f u_f) = 0, \\ \partial_t (\rho_f u_f) + \nabla_x \cdot (\rho_f u_f^{\otimes 2} + P_f - \mathbb{I}[f]) = 0, \\ \partial_t (\frac{1}{2} (\rho_f |u_f|^2 + \text{tr} P_f)) + \nabla_x \cdot (\frac{1}{2} (\rho_f |u_f|^2 + \text{tr} P_f) u_f + P_f \cdot u_f + Q_f - \mathcal{I}_4[f]) = 0, \end{cases} \quad (2.4.1)$$

where $\mathbb{I}[f]$ is the square matrix whose rows are $\mathcal{I}_i[f] \in \mathbf{R}^3$, for $i = 1, 2, 3$, i.e.

$$\mathbb{I}[f] := \begin{bmatrix} \mathcal{I}_1[f] \\ \mathcal{I}_2[f] \\ \mathcal{I}_3[f] \end{bmatrix}.$$

Obviously the system (2.4.1) requires some closure relations — i.e. expressions of $\mathbb{I}[f]$, of Q_f and of $\mathcal{I}_4[f]$ in terms of ρ_f, u_f and P_f — before it can be considered as a bona fide system of equations for the dynamics of dense gases.

2.4.2 Local Entropy Inequality

It is a well-known fact that systems of conservation laws such as (2.4.1) with some appropriate closure assumptions may have infinitely many weak solutions corresponding to the same initial data: see for instance section 4.4 in chapter IV of [Daf10]. The example of loss of uniqueness given in section 4.4 in chapter IV of [Daf10] involves unphysical shock waves, which dissipate, instead of producing entropy. For that reason, systems of conserva-

tion laws often come with a Friedrichs-Lax entropy inequality used to qualify weak solutions of such systems: see section 4.5 and chapter V in [Daf10]. (Unfortunately this is in general not enough to guarantee uniqueness in space dimension 2 and higher: see [DS10].)

However, these considerations suggest seeking an entropy inequality for (2.4.1). By analogy with [BG84], we may think of using the local variant of the H Theorem reported in Theorem (2.3.3) to do so.

Corollary 2.4.2. *Let f be a classical solution of (2.1.1) with delocalized collision integral (2.3.1) and collision kernel of the form (2.3.5). Assume that $(x, v) \mapsto f(t, x, v)$ is rapidly decaying at infinity, while $(x, v) \mapsto \ln f(t, x, v)$ has at most polynomial growth at infinity. Then, the local conservation laws (2.4.1) are accompanied with the entropy inequality*

$$\begin{aligned} & \partial_t \left(\int_{\mathbf{R}^3} f \ln f(t, x, v) dv + \frac{1}{2} (\rho_f(t, \cdot) \star \beta(|\cdot|))(x) \rho_f(t, x) \right) \\ & + \nabla_x \cdot \left(\int_{\mathbf{R}^3} (f \ln f + \mathcal{K}[f])(t, x, v) dv + \frac{1}{2} (\rho_f(t, \cdot) \star \beta(|\cdot|))(x) \rho_f(t, x) u_f(t, x) \right) \leq 0 \end{aligned}$$

where

$$\rho_f(t, x) := \int_{\mathbf{R}^3} f(t, x, v) dv \geq 0, \quad u(t, x) = \frac{\mathbf{1}_{\rho(t, x) > 0}}{\rho(t, x)} \int_{\mathbf{R}^3} v f(t, x, v) dv \in \mathbf{R}^3,$$

while the functional $\mathcal{K}$ is defined in Theorem 2.3.3.

This is a straightforward consequence of Theorem 2.3.3, obtained by integrating in $v \in \mathbf{R}^3$ both sides of the inequality in that theorem. To be rigorous, one should observe that the inequality in Theorem 2.3.3, which is stated in the sense of distributions, holds true when applied to a more general class of test functions, including $(x, v) \mapsto \psi(x)$ where ψ belongs to $C_c^1(\mathbf{R}^3)$: see the beginning of the proof of Theorem 2.3.3.

The differential inequality obtained in Corollary 2.4.2 is not exactly an entropy inequality in the sense of Friedrichs and Lax, since the entropy

$$\eta(t, x) := \int_{\mathbf{R}^3} f \ln f(t, x, v) dv + \frac{1}{2} (\rho_f(t, \cdot) \star \beta(|\cdot|))(x) \rho_f(t, x),$$

even after some closure assumption specifying the v -dependence in f (e.g. a local Maxwellian distribution), is not a *local* function of the conserved densities in (2.4.1), since it involves the term $\frac{1}{2} (\rho_f(t, \cdot) \star \beta(|\cdot|))(x) \rho_f(t, x)$ which is nonlocal in ρ_f .

Therefore, the usual theory of Friedrichs-Lax extensions [FL71] of systems of conservation laws, and in particular the fact the convexity of η as a *local* function of the conserved density implies the hyperbolicity of the system of conservation laws, which can then be put in Godunov's form [God61], is unfortunately not available for us to handle the system (2.4.1). Nevertheless, even if one cannot apply directly the Godunov structure and the Friedrichs-Lax theory, the local entropy inequality reported in Corollary 2.4.2 may be of independent interest for studying (2.4.1). For instance, it could be interesting to connect the discussion of the fluid dynamic limit of the Enskog-Boltzmann equation in [Lac98] with the results presented in this paper. We hope to return to this question in more detail in the future.

2.5 Proof of Theorem 2.3.1

The proof of Theorem 2.3.1 involves rather intricate computations, and will be split in several steps.

2.5.1 Weak Forms of the Collision Integral

A first step in the representation of delocalized collision integrals in terms of divergences in (x, v) of momentum and energy currents is the weak formulation of these collision integrals.

Lemma 2.5.1. *Let $f, g \in C(\mathbf{R}^3 \times \mathbf{R}^3)$, rapidly decaying at infinity. For each test function $\phi \in C(\mathbf{R}^3 \times \mathbf{R}^3)$ with (at most) polynomial growth at infinity,*

$$\begin{aligned} \int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) dx dv &= \int_{(\mathbf{R}^3)^4} (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) f(x, v) g(y, w) \\ &\quad \times \mathbf{1}_{(v-w|n_{x,y}) < 0} B[\rho_f, \rho_g](x, y, v-w) dx dv dy dw. \end{aligned}$$

Proof. By definition of the collision integral $\text{St}[f, g]$,

$$\begin{aligned} &\int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) dx dv \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_g](x, y, v-w) (f(x, v'(v, w, n_{x,y})) g(y, w'(v, w, n_{x,y})) \mathbf{1}_{(v-w|n_{x,y}) > 0} \\ &\quad - f(x, v) g(y, w) \mathbf{1}_{(v-w|n_{x,y}) < 0}) \phi(x, v) dx dv dy dw. \end{aligned}$$

The gain term (positive part) of this collision integral satisfies the following symmetries:

$$\begin{aligned} &\int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_g](x, y, v-w) f(x, v'(v, w, n_{x,y})) g(y, w'(v, w, n_{x,y})) \\ &\quad \times \phi(x, v) \mathbf{1}_{(v-w|n_{x,y}) > 0} dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_g](x, y, v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})) f(x, v) g(y, w) \\ &\quad \times \phi(x, v'(v, w, n_{x,y})) \mathbf{1}_{(v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})|n_{x,y}) > 0} dx dv dy dw \\ &\quad (\text{integrating by substitution with } (v, w) \mapsto (v'(v, w, n_{x,y}), w'(v, w, n_{x,y}))) \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_g](x, y, v-w) f(x, v) g(y, v) \phi(x, v'(v, w, n_{x,y})) \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw \\ &\quad (\text{by (ii) and the equality } (v'(v, w, n_{x,y}) - w'(v, w, n_{x,y})|n_{x,y}) = -(v-w|n_{x,y})). \end{aligned}$$

Inserting this form of the gain term in the identity above implies the announced identity. $\square$

The preceding lemma gives a weak formulation of $\text{St}[f, g]$, where f and g may be different. In particular, the proof of this lemma does not involve property (i) of the collision kernel B . The next lemma gives a weak formulation of $\text{St}[f, f]$. Since $f = g$ in this case, property (i) of B is a key ingredient in the proof.

Lemma 2.5.2. *Let $f \in C(\mathbf{R}^3 \times \mathbf{R}^3)$ be rapidly decaying at infinity. For each test function $\phi \in C(\mathbf{R}^3 \times \mathbf{R}^3)$ with polynomial growth at infinity,*

$$\begin{aligned} & \int_{(\mathbf{R}^3)^2} \text{St}[f, f](x, v) \phi(x, v) dx dv \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\phi(x, v'(v, w, n_{x,y})) + \phi(y, w'(v, w, n_{x,y})) - \phi(x, v) - \phi(y, w)) \\ & \quad \times f(x, v) f(y, w) B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw. \end{aligned}$$

Proof. Starting from the identity in the preceding lemma

$$\begin{aligned} \int_{(\mathbf{R}^3)^2} \text{St}[f, f](x, v) \phi(x, v) dx dv &= \int_{(\mathbf{R}^3)^4} (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) f(x, v) f(y, w) \\ & \quad \times B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw. \end{aligned} \quad (2.5.1)$$

Integrating by substitution in the right-hand side with $(x, v, y, w) \mapsto (y, w, x, v)$,

$$\begin{aligned} & \int_{(\mathbf{R}^3)^2} \text{St}[f, f](x, v) \phi(x, v) dx dv \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](y, x, w - v) f(y, w) f(x, v) (\phi(y, v'(w, v, n_{y,x})) - \phi(y, w)) \\ & \quad \times \mathbf{1}_{(w-v|n_{y,x}) < 0} dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) f(x, v) f(y, w) (\phi(y, w'(v, w, n_{x,y})) - \phi(y, w)) \\ & \quad \times \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw, \end{aligned} \quad (2.5.2)$$

where the last equality follows from (i), while

$$v'(w, v, -n) = v'(w, v, n) = w'(v, w, n).$$

Since the last right-hand sides of (2.5.1) and (2.5.2) are equal, they are both equal to their average, i.e.

$$\begin{aligned} \int_{(\mathbf{R}^3)^2} \text{St}[f, f] \phi(x, v) dx dv &= \int_{(\mathbf{R}^3)^4} \frac{\phi(x, v'(v, w, n_{x,y})) - \phi(x, v) + \phi(y, w'(v, w, n_{x,y})) - \phi(y, w)}{2} \\ & \quad \times f(x, v) f(y, w) B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw, \end{aligned}$$

which is precisely the announced identity. $\square$

Lemma 2.5.1 will be used repeatedly in the proof of Theorem 2.3.1. Lemma 2.5.2, on the other hand, is used in the proofs of Theorems 2.3.2 and 2.3.3.

2.5.2 Mass Current: Proof of (2.3.2)

Observe that

$$\begin{aligned}\phi(x, v'(v, w, n)) - \phi(x, v) &= \int_0^{(v-w|n)} \frac{d}{ds} \phi(x, v - sn) ds \\ &= - \int_0^{(v-w|n)} n \cdot \nabla_v \phi(x, v - sn) ds.\end{aligned}$$

$$\begin{aligned}\int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) dx dv &= \int_{(\mathbf{R}^3)^4} (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) f(x, v) g(y, w) \\ &\quad \times \mathbf{1}_{(v-w|n_{x,y}) < 0} B[\rho_f, \rho_g](x, y, v - w) dx dv dy dw\end{aligned}$$

Inserting this expression in the right-hand side of the weak formulation of the collision integral $\text{St}[f, g]$ in Lemma 2.5.1 shows that

$$\begin{aligned}\int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) dx dv &= - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_g](x, y, v - w) f(x, v) g(y, w) \\ &\quad \times \left(\int_0^{(v-w|n_{y,x})} n_{y,x} \cdot \nabla_v \phi(x, v - sn_{y,x}) ds \right) \mathbf{1}_{(v-w|n_{y,x}) > 0} dx dv dy dw \\ &= - \int_{(\mathbf{R}^3)^4 \times \mathbf{R}} B[\rho_f, \rho_g](x, y, v - w) \mathbf{1}_{0 < s < (v-w|n_{y,x})} f(x, v) g(y, w) \\ &\quad \times n_{y,x} \cdot \nabla_v \phi(x, v - sn_{y,x}) dx dv dy dw ds.\end{aligned}$$

The last right-hand side above is recast as

$$\begin{aligned}&\int_{(\mathbf{R}^3)^4 \times \mathbf{R}} B[\rho_f, \rho_g](x, y, v - w) \mathbf{1}_{0 < s < (v-w|n_{y,x})} f(x, v) g(y, w) \\ &\quad \times n_{y,x} \cdot \nabla_v \phi(x, v - sn_{y,x}) dx dv dy dw ds \\ &= \int_{(\mathbf{R}^3)^4 \times \mathbf{R}} B[\rho_f, \rho_g](x, y, \bar{v} - \bar{w}) f(x, \bar{v} + sn_{y,x}) g(y, \bar{w} + sn_{y,x}) \\ &\quad \times \mathbf{1}_{0 < s < (\bar{v} - \bar{w}|n_{y,x})} n_{y,x} \cdot \nabla_v \phi(x, \bar{v}) dx d\bar{v} dy d\bar{w} ds,\end{aligned}$$

integrating by substitution with $\bar{v} := v - sn_{y,x}$ and $\bar{w} := w - sn_{y,x}$. Therefore

$$\int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) dx dv = - \int_{(\mathbf{R}^3)^3} \mathfrak{J}_0[\rho_f, \rho_g, f, g](x, y, \bar{v}) \cdot \nabla_v \phi(x, \bar{v}) dx dy d\bar{v},$$

which is the formulation in the sense of distributions of the identity (2.3.2). $\square$

2.5.3 Momentum Currents: Proof of (2.3.3)

Applying Lemma 2.5.1 to the test function $\phi(x, v)v_i$, we find that

$$\begin{aligned} \int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) v_i dx dv &= \int_{(\mathbf{R}^3)^4} (\phi(x, v'(v, w, n_{x,y})) v'_i(v, w, n_{x,y}) - \phi(x, v) v_i) \\ &\quad \times f(x, v) g(y, w) B[\rho_f, \rho_g](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw. \end{aligned}$$

Then we split the difference

$$\begin{aligned} &\phi(x, v'(v, w, n_{x,y})) v'_i(v, w, n_{x,y}) - \phi(x, v) v_i \\ &= (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) v'_i(v, w, n_{x,y}) \\ &\quad + (v'_i(v, w, n_{x,y}) - v_i) \phi(x, v) \\ &= (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) v_i \\ &\quad - (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) (v|n_{x,y})(n_{x,y})_i \\ &\quad + (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) (w|n_{x,y})(n_{x,y})_i \\ &\quad - \phi(x, v) (v - w|n_{x,y})(n_{x,y})_i \\ &= S_1 - S_2 + S_3 - S_4. \end{aligned}$$

Thus

$$\begin{aligned} &\int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_1 dx dv dy dw \\ &= - \int_{(\mathbf{R}^3)^3} \mathfrak{J}_0[\rho_f, \rho_f, v_i f, f](x, y, v) \cdot \nabla_v \phi(x, v) dx dy dv, \end{aligned}$$

while

$$\begin{aligned} &\int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_2 dx dv dy dw \\ &= - \int_{(\mathbf{R}^3)^3} \mathfrak{J}_0[\rho_f, \rho_f, (v|n_{x,y})(n_{x,y})_i f, f](x, y, v) \cdot \nabla_v \phi(x, v) dx dy dv, \end{aligned}$$

and

$$\begin{aligned} &\int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_3 dx dv dy dw \\ &= - \int_{(\mathbf{R}^3)^3} \mathfrak{J}_0[\rho_f, \rho_f, f, (w|n_{x,y})(n_{x,y})_i f](x, y, v) \cdot \nabla_v \phi(x, v) dx dy dv. \end{aligned}$$

We are left with the term

$$\begin{aligned} &\int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) (v - w|n_{y,x}) + (n_{y,x})_i \phi(x, v) f(x, v) f(y, w) dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](y, x, w - v) (v - w|n_{y,x}) + (n_{y,x})_i \phi(x, v) f(x, v) f(y, w) dx dv dy dw, \end{aligned}$$

where the last equality follows from assumption (i) on the collision kernel B . This last integral is transformed with the change of variables

$$(x, y, v, w) \mapsto (y, x, w, v)$$

so that

$$\begin{aligned} & \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](y, x, w-v)(v-w|n_{y,x})_+(n_{y,x})_i \phi(x, v) f(x, v) f(y, w) dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w)(w-v|n_{x,y})_+(n_{x,y})_i \phi(y, w) f(x, v) f(y, w) dx dv dy dw \\ &= - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w)(v-w|n_{y,x})_+(n_{y,x})_i \phi(y, w) f(x, v) f(y, w) dx dv dy dw. \end{aligned}$$

Thus

$$\begin{aligned} & \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w)(v-w|n_{y,x})_+(n_{y,x})_i \phi(x, v) f(x, v) f(y, w) dx dv dy dw \\ &= - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w)(v-w|n_{y,x})_+(n_{y,x})_i \phi(y, w) f(x, v) f(y, w) dx dv dy dw, \end{aligned}$$

so that, eventually,

$$\begin{aligned} & \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w)(v-w|n_{y,x})_+(n_{y,x})_i (\phi(x, v) - \phi(y, w)) \\ & \quad \times f(x, v) f(y, w) dx dv dy dw. \end{aligned}$$

Set

$$\begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} v_\theta \\ w_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}.$$

We shall express the difference $\phi(x, v) - \phi(y, w)$ as follows:

$$\phi(x, v) - \phi(y, w) = - \int_0^{\pi/2} \frac{d}{d\theta} \phi(x_\theta, v_\theta) d\theta.$$

Since

$$\frac{d}{d\theta} \phi(x_\theta, v_\theta) = y_\theta \cdot \nabla_x \phi(x_\theta, v_\theta) + w_\theta \cdot \nabla_v \phi(x_\theta, v_\theta),$$

we find that

$$\begin{aligned}
& \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\
&= -\frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\pi/2} B[\rho_f, \rho_f](x, y, v-w) (v-w|n_{y,x})_+ (n_{y,x})_i y_\theta \cdot \nabla_x \phi(x_\theta, v_\theta) \\
&\quad \times f(x, v) f(y, w) d\theta dx dv dy dw \\
&\quad -\frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\pi/2} B[\rho_f, \rho_f](x, y, v-w) (v-w|n_{y,x})_+ (n_{y,x})_i w_\theta \cdot \nabla_v \phi(x_\theta, v_\theta) \\
&\quad \times f(x, v) f(y, w) d\theta dx dv dy dw.
\end{aligned}$$

Since the Jacobian determinants

$$\det \frac{\partial(x_\theta, y_\theta)}{\partial(x, y)} = \det \frac{\partial(v_\theta, w_\theta)}{\partial(v, w)} = 1,$$

one can transform both integrals in the right-hand side of the identity above into

$$\begin{aligned}
& - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\
&= \frac{1}{2} \int_{(\mathbf{R}^3)^4} \nabla_x \phi(x, v) \cdot y \int_0^{\pi/2} B[\rho_f, \rho_f](x_\theta, y_\theta, v_\theta - w_\theta) (v_\theta - w_\theta | n_{y_\theta, x_\theta})_+ \\
&\quad \times (n_{y_\theta, x_\theta})_i f(x_\theta, v_\theta) f(y_\theta, w_\theta) d\theta dx dv dy dw \\
&\quad + \frac{1}{2} \int_{(\mathbf{R}^3)^4} \nabla_v \phi(x, v) \cdot w \int_0^{\pi/2} B[\rho_f, \rho_f](x_\theta, y_\theta, v_\theta - w_\theta) (v_\theta - w_\theta | n_{y_\theta, x_\theta})_+ \\
&\quad \times (n_{y_\theta, x_\theta})_i f(x_\theta, v_\theta) f(y_\theta, w_\theta) d\theta dx dv dy dw.
\end{aligned}$$

Summarizing, we have found that

$$\begin{aligned}
\int_{(\mathbf{R}^3)^2} \text{St}[f, f](x, v) \phi(x, v) v_k dx dv &= - \int_{(\mathbf{R}^3)^2} \mathcal{I}_i[f](x, v) \cdot \nabla_x \phi(x, v) dx dv \\
&\quad - \int_{(\mathbf{R}^3)^2} \mathcal{J}_i[f](x, v) \cdot \nabla_v \phi(x, v) dx dv,
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{I}_i[f](x, v) &:= -\frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\pi/2} B[\rho_f, \rho_f](x_\theta, y_\theta, v_\theta - w_\theta) (v_\theta - w_\theta | n_{y_\theta, x_\theta})_+ \\
&\quad \times f(x_\theta, v_\theta) f(y_\theta, w_\theta) (n_{y_\theta, x_\theta})_i y_\theta d\theta dy dw,
\end{aligned}$$

while

$$\begin{aligned} \mathcal{J}_i[f](x, v) &:= \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, (v_i - (v|n_{x,y})(n_{x,y})_i)f, f](x, y, v) dy \\ &\quad + \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, f, (w|n_{x,y})(n_{x,y})_i f](x, y, v) dy \\ &\quad - \frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\pi/2} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta})(v_{-\theta} - w_{-\theta}|n_{y_{-\theta}, x_{-\theta}})_+ \\ &\quad \times f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta})(n_{y_{-\theta}, x_{-\theta}})_i w d\theta dy dw. \end{aligned}$$

This is the weak formulation (in the sense of distributions) of (2.3.3). $\square$

2.5.4 Energy Currents: Proof of (2.3.4)

Applying Lemma 2.5.1 to the test function $\phi(x, v)|v|^2$, we find that

$$\begin{aligned} &\int_{(\mathbf{R}^3)^2} \text{St}[f, g](x, v) \phi(x, v) |v|^2 dx dv \\ &= \int_{(\mathbf{R}^3)^4} (\phi(x, v'(v, w, n_{x,y})) |v'(v, w, n_{x,y})|^2 - \phi(x, v) |v|^2) f(x, v) g(y, w) \\ &\quad \times B[\rho_f, \rho_g](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} dx dv dy dw \end{aligned}$$

Observe that

$$v'(v, w, n) = (v - (v|n)n) + (w|n)n \in (\mathbf{R}n)^\perp + \mathbf{R}n.$$

Hence

$$|v'(v, w, n)|^2 = |v - (v|n)n|^2 + (w|n)^2 = |v|^2 - (v|n)^2 + (w|n)^2.$$

Then we split the difference

$$\begin{aligned} &\phi(x, v'(v, w, n_{x,y})) |v'(v, w, n_{x,y})|^2 - \phi(x, v) |v|^2 \\ &= (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) |v'(v, w, n_{x,y})|^2 \\ &\quad + (|v'(v, w, n_{x,y})|^2 - |v|^2) \phi(x, v) \\ &= (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) |v|^2 \\ &\quad - (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) |(v|n_{x,y})|^2 \\ &\quad + (\phi(x, v'(v, w, n_{x,y})) - \phi(x, v)) |(w|n_{x,y})|^2 \\ &\quad - \phi(x, v) ((v|n_{x,y})^2 - (w|n_{x,y})^2) \\ &= S_1 - S_2 + S_3 - S_4. \end{aligned}$$

Proceeding as in the case of the momentum current, we find that

$$\begin{aligned}
& \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) \\
& \quad \times (S_1 - S_2 + S_3) dx dv dy dw \\
&= - \int_{(\mathbf{R}^3)^3} \mathfrak{I}_0[\rho_f, \rho_f, (|v|^2 - (v|n_{x,y})^2) f, f](x, y, v) \cdot \nabla_v \phi(x, v) dx dy dv \\
& \quad - \int_{(\mathbf{R}^3)^3} \mathfrak{I}_0[\rho_f, \rho_f, f, (w|n_{x,y})^2 f](x, y, v) \cdot \nabla_v \phi(x, v) dx dy dv.
\end{aligned}$$

Then we are left with the term

$$\begin{aligned}
& - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\
&= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} ((v|n_{x,y})^2 - (w|n_{x,y})^2) \phi(x, v) \\
& \quad \times f(x, v) f(y, w) dx dv dy dw \\
&= \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) (v-w|n_{y,x})_+ (v+w|n_{y,x}) \phi(x, v) \\
& \quad \times f(x, v) f(y, w) dx dv dy dw \\
&= - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](y, x, w-v) (w-v|n_{x,y})_+ (w+v|n_{x,y}) \phi(x, v) \\
& \quad \times f(x, v) f(y, w) dx dv dy dw.
\end{aligned}$$

by assumption (i) on the collision kernel B , observing that $n_{y,x} = -n_{x,y}$. With the change of variables

$$(x, v, y, w) \mapsto (y, w, x, v)$$

this last integral is transformed into

$$\begin{aligned}
& - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\
&= - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) (v-w|n_{y,x})_+ (v+w|n_{y,x}) \phi(y, w) \\
& \quad \times f(x, v) f(y, w) dx dv dy dw.
\end{aligned}$$

Therefore

$$\begin{aligned}
& - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw \\
&= \frac{1}{2} \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v-w) (v-w|n_{y,x})_+ (v+w|n_{y,x}) (\phi(x, v) - \phi(y, w)) \\
& \quad \times f(x, v) f(y, w) dx dv dy dw.
\end{aligned}$$

With the same notation as in the preceding section, i.e.

$$\begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} v_\theta \\ w_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix},$$

the difference $\phi(x, v) - \phi(y, w)$ is represented as

$$\phi(y, w) - \phi(x, v) = \int_0^{\pi/2} (y_\theta \cdot \nabla_x \phi + w_\theta \cdot \nabla_v \phi)(x_\theta, v_\theta) d\theta.$$

Substituting this expression in the identity above leads to

$$\begin{aligned} & - \int_{(\mathbf{R}^3)^4} B[\rho_f, \rho_f](x, y, v - w) \mathbf{1}_{(v-w|n_{x,y}) < 0} f(x, v) f(y, w) S_4 dx dv dy dw dn \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\pi/2} B[\rho_f, \rho_f](x, y, v - w) (y_\theta \cdot \nabla_x \phi + w_\theta \cdot \nabla_v \phi)(x_\theta, v_\theta) \\ & \quad \times (v - w|n_{y,x})_+ (v + w|n_{y,x}) f(x, v) f(y, w) d\theta dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} \int_0^{\pi/2} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta}) (y \cdot \nabla_x \phi + w \cdot \nabla_v \phi)(x, v) \\ & \quad \times (v_{-\theta} - w_{-\theta}|n_{y_{-\theta}, x_{-\theta}})_+ (v_{-\theta} + w_{-\theta}|n_{y_{-\theta}, x_{-\theta}}) f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) d\theta dx dv dy dw. \end{aligned}$$

Summarizing, we have proved that

$$\begin{aligned} \int_{(\mathbf{R}^3)^2} \text{St}[f, f](x, v) \phi(x, v) |v|^2 dx dv &= - \int_{(\mathbf{R}^3)^2} \mathcal{I}_4[f](x, v) \cdot \nabla_x \phi(x, v) dx dv \\ &\quad - \int_{(\mathbf{R}^3)^2} \mathcal{J}_4[f](x, v) \cdot \nabla_v \phi(x, v) dx dv, \end{aligned}$$

where

$$\begin{aligned} \mathcal{I}_4[f](x, v) &:= -\frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\pi/2} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta}) \\ &\quad \times (v_{-\theta} - w_{-\theta}|n_{y_{-\theta}, x_{-\theta}})_+ (v_{-\theta} + w_{-\theta}|n_{y_{-\theta}, x_{-\theta}}) f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) y d\theta dy dw. \end{aligned}$$

while

$$\begin{aligned} \mathcal{J}_4[f](x, v) &:= - \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, (|v|^2 - (v|n_{x,y})^2) f, f](x, y, v) dy \\ &\quad - \int_{\mathbf{R}^3} \mathfrak{J}_0[\rho_f, \rho_f, f, (w|n_{x,y})^2 f](x, y, v) dy \\ &\quad - \frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\pi/2} B[\rho_f, \rho_f](x_{-\theta}, y_{-\theta}, v_{-\theta} - w_{-\theta}) (v_{-\theta} - w_{-\theta}|n_{y_{-\theta}, x_{-\theta}})_+ \\ &\quad \times (v_{-\theta} + w_{-\theta}|n_{y_{-\theta}, x_{-\theta}}) f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) w d\theta dy dw. \end{aligned}$$

This is the weak formulation (in the sense of distributions) of (2.3.4). $\square$

2.6 Entropy Inequalities for Delocalized Collision Integrals

2.6.1 Proof of Theorem 2.3.2

Start from the weak formulation of the collision integral in Lemma 2.5.2, with test function $\phi := \ln f + 1$:

$$\begin{aligned} & \int_{(\mathbf{R}^3)^2} \text{St}[f, f](t, x, v) (\ln f(t, x, v) + 1) dx dv \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) \ln \frac{f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x}))}{f(t, x, v) f(t, y, w)} \\ & \quad \times b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw. \end{aligned}$$

Thus, in terms of the function ℓ ,

$$\begin{aligned} & \int_{(\mathbf{R}^3)^2} \text{St}[f, f](t, x, v) (\ln f(t, x, v) + 1) dx dv \\ &= -\frac{1}{2} \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) \ell \left(\frac{f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x}))}{f(t, x, v) f(t, y, w)} \right) \\ & \quad \times b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw \\ & \quad + \frac{1}{2} \int_{(\mathbf{R}^3)^4} (f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x})) - f(t, x, v) f(t, y, w)) \\ & \quad \times b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw \\ & \quad = S_1 + S_2. \end{aligned}$$

Obviously $S_1 \leq 0$, while

$$\begin{aligned} & \int_{(\mathbf{R}^3)^4} f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x})) b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) b(|x - y|)(v'(v, w, n_{y,x}) - w'(v, w, n_{y,x})|n_{y,x})_+ dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) b(|x - y|)(v - w|n_{x,y})_+ dx dv dy dw. \end{aligned}$$

Hence

$$\begin{aligned} S_2 &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) ((v - w|n_{x,y})_+ - (v - w|n_{x,y})_-) b(|x - y|) dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) (v - w|n_{x,y}) b(|x - y|) dx dv dy dw. \end{aligned}$$

The formula

$$\beta(r) := \int_r^\infty b(s) ds$$

implies that

$$\begin{aligned} (v \cdot \nabla_x + w \cdot \nabla_y) \beta(|x - y|) &= (v - w \frac{x-y}{|x-y|}) \beta'(|x - y|) \\ &= -(v - w |n_{x,y}|) b(|x - y|). \end{aligned} \quad (2.6.1)$$

Hence

$$\begin{aligned} & \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) (v - w |n_{x,y}|) b(|x - y|) dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} (v \cdot \nabla_x + w \cdot \nabla_y) (f(t, x, v) f(t, y, w)) \beta(|x - y|) dx dv dy dw \\ &= \int_{(\mathbf{R}^3)^4} (\text{St}[f, f](t, x, v) f(t, y, w) + f(t, x, v) \text{St}[f, f](t, y, w)) \beta(|x - y|) dx dv dy dw \\ &\quad - \int_{(\mathbf{R}^3)^4} (\partial_t f(t, x, v) f(t, y, w) + f(t, x, v) \partial_t f(t, y, w)) \beta(|x - y|) dx dv dy dw. \end{aligned}$$

Observing that the local mass conservation implies that

$$\int_{\mathbf{R}^3} \text{St}[f, f](t, x, v) dv = \int_{\mathbf{R}^3} \text{St}[f, f](t, y, w) dw = 0,$$

we conclude that

$$S_2 = -\frac{1}{2} \frac{d}{dt} \int_{(\mathbf{R}^3)^4} f(t, x, v) f(t, y, w) \beta(|x - y|) dx dv dy dw.$$

Summarizing, we have proved that

$$\frac{d}{dt} \int_{(\mathbf{R}^3)^2} f \ln f(t, x, v) dx dv = \int_{(\mathbf{R}^3)^2} \text{St}[f, f](t, x, v) (\ln f(t, x, v) + 1) dx dv = S_1 + S_2$$

and the conclusion follows from the expression of S_2 obtained above, after defining Λ by the formula $\Lambda := -S_1 \geq 0$. $\square$

2.6.2 Proof of Theorem 2.3.3

This proof involves somewhat lengthy computations, and will be split in six steps for the reader's convenience. Throughout this proof, ψ designates a test function satisfying the following conditions

$$\psi \in C^1(\mathbf{R}^3 \times \mathbf{R}^3) \cap L^\infty(\mathbf{R}^3 \times \mathbf{R}^3), \quad \psi(x, v) \geq 0 \text{ for all } x, v \in \mathbf{R}^3.$$

Step 1. Start from the weak formulation of the collision integral in Lemma 2.5.2, with test function $\phi := \psi \ln f$: observing that $v'(v, w, n) = v'(v, w, -n)$ and $w'(v, w, n) =$

$$w'(v, w, -n),$$

$$\begin{aligned} & \int_{(\mathbf{R}^3)^2} \text{St}[f, f](t, x, v) \ln f(t, x, v) \psi(x, v) dx dv \\ &= \int_{(\mathbf{R}^3)^4} \frac{(\psi \ln f)(t, x, v'(v, w, n_{y,x})) + (\psi \ln f)(t, y, w'(v, w, n_{y,x})) - (\psi \ln f)(t, x, v) - (\psi \ln f)(t, y, w)}{2} \\ & \quad \times f(t, x, v) f(t, y, w) b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw. \end{aligned}$$

Decompose

$$S := \frac{(\psi \ln f)(t, x, v'(v, w, n_{y,x})) + (\psi \ln f)(t, y, w'(v, w, n_{y,x})) - (\psi \ln f)(t, x, v) - (\psi \ln f)(t, y, w)}{2}$$

as

$$\begin{aligned} S &= \frac{1}{2} \psi(x, v'(v, w, n_{y,x})) \ln \frac{f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x}))}{f(t, x, v) f(t, y, w)} \\ &+ \frac{1}{2} (\psi(y, w'(v, w, n_{y,x})) - \psi(x, v'(v, w, n_{y,x}))) \ln f(t, y, w'(v, w, n_{y,x})) \\ &\quad - \frac{1}{2} (\psi(x, v) - \psi(x, v'(v, w, n_{y,x}))) \ln f(t, x, v) \\ &\quad - \frac{1}{2} (\psi(y, w) - \psi(x, v'(v, w, n_{y,x}))) \ln f(t, y, w) \\ &= S_1 + S_2 - S_3 - S_4. \end{aligned}$$

The term S_4 is decomposed further into

$$\begin{aligned} S_4 &= \frac{1}{2} (\psi(y, w) - \psi(x, v'(v, w, n_{y,x}))) \ln f(t, y, w) \\ &= \frac{1}{2} (\psi(y, w) - \psi(x, v)) \ln f(t, y, w) \\ &\quad + \frac{1}{2} (\psi(x, v) - \psi(x, v'(v, w, n_{y,x}))) \ln f(t, y, w) \\ &= S_{41} + S_{42}. \end{aligned}$$

Step 2. Similarly, with $\ell(z) := z - 1 - \ln z \geq 0$ for $z > 0$,

$$\begin{aligned} S_1 &= -\frac{1}{2} \psi(x, v'(v, w, n_{y,x})) \ell \left(\frac{f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x}))}{f(t, x, v) f(t, y, w)} \right) \\ &\quad + \frac{1}{2} \psi(x, v'(v, w, n_{y,x})) \left(\frac{f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x}))}{f(t, x, v) f(t, y, w)} - 1 \right) \\ &= -S_{11} + S_{12}. \end{aligned}$$

Thus

$$\begin{aligned} \int_{(\mathbf{R}^3)^2} \text{St}[f, f] \ln f(t, x, v) dx dv &= \int_{(\mathbf{R}^3)^4} (-S_{11} + S_{12} + S_2 - S_3 - S_{41} - S_{42}) \\ &\quad \times f(t, x, v) f(t, y, w) b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw. \end{aligned}$$

Set

$$\Lambda[\psi](t) := \int_{(\mathbf{R}^3)^4} S_{11} f(t, x, v) f(t, y, w) b(|x - y|)(v - w|n_{y,x})_+ dx dv dy dw;$$

clearly

$$\psi \geq 0 \implies \Lambda[\psi] \geq 0.$$

Step 3. Next

$$\begin{aligned} \Gamma_{12} &:= \int_{(\mathbf{R}^3)^4} S_{12} f(t, x, v) f(t, y, w) b(|x - y|) (v - w|n_{y,x})_+ dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} \psi(x, v'(v, w, n_{y,x})) (f(t, x, v'(v, w, n_{y,x})) f(t, y, w'(v, w, n_{y,x})) \\ &\quad - f(t, x, v) f(t, y, w)) b(|x - y|) (v - w|n_{y,x})_+ dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\psi(t, x, v) (v - w|n_{x,y})_+ - \psi(x, v'(v, w, n_{y,x})) (v - w|n_{y,x})_+) \\ &\quad \times f(t, x, v) f(t, y, w) b(|x - y|) dx dv dy dw \end{aligned}$$

where the change of variables $(v, w) \mapsto (v'(v, w, n_{y,x}), w'(v, w, n_{y,x}))$ leads to the last equality, upon observing that

$$(v - w|n_{y,x}) = (v'(v, w, n_{y,x}) - w'(v, w, n_{y,x})|n_{x,y}).$$

Since

$$\psi(t, x, v) (v - w|n_{x,y})_+ = \psi(t, x, v) (v - w|n_{x,y}) + \psi(t, x, v) (v - w|n_{y,x})_+,$$

the term Γ_{12} is recast as

$$\begin{aligned} \Gamma_{12} &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} \psi(x, v) b(|x - y|) (v - w|n_{x,y}) f(t, x, v) f(t, y, w) dx dv dy dw \\ &\quad + \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\psi(x, v) - \psi(x, v'(v, w, n_{y,x})) (v - w|n_{y,x})_+ \\ &\quad \times f(t, x, v) f(t, y, w) b(|x - y|) dx dv dy dw \\ &= \Gamma_{121} + \Gamma_{122}. \end{aligned}$$

Step 4. The term Γ_{121} is handled exactly as the potential term in the global entropy inequality: using the identity (2.6.1) leads to

$$\begin{aligned} \Gamma_{121} &= -\frac{1}{2} \int_{(\mathbf{R}^3)^4} \psi(x, v) f(t, x, v) f(t, y, w) (v \cdot \nabla_x + w \cdot \nabla_y) \beta(|x - y|) dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (v \cdot \nabla_x + w \cdot \nabla_y) [\psi(x, v) f(t, x, v) f(t, y, w)] \beta(|x - y|) dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} v \cdot \nabla_x \psi(x, v) f(t, x, v) f(t, y, w) \beta(|x - y|) dx dv dy dw \\ &\quad + \frac{1}{2} \int_{(\mathbf{R}^3)^4} \psi(x, v) \text{St}[f, f](t, x, v) f(t, y, w) \beta(|x - y|) dx dv dy dw \\ &\quad - \frac{1}{2} \frac{d}{dt} \int_{(\mathbf{R}^3)^4} \psi(x, v) f(t, x, v) f(t, y, w) \beta(|x - y|) dx dv dy dw. \end{aligned}$$

In the last equality above, we have used the equality

$$\begin{aligned}
(v \cdot \nabla_x + w \cdot \nabla_y)[\psi(x, v)f(t, x, v)f(t, y, w)] &= f(t, x, v)f(t, y, w)v \cdot \nabla_x \psi(x, v) \\
&\quad + \psi(x, v)f(t, y, w)(\text{St}[f, f](t, x, v) - \partial_t f(t, x, v)) \\
&\quad + \psi(x, v)f(t, x, v)(\text{St}[f, f](t, y, w) - \partial_t f(t, y, w)) \\
&= f(t, x, v)f(t, y, w)v \cdot \nabla_x \psi(x, v) \\
&\quad + \psi(x, v)(f(t, y, w)\text{St}[f, f](t, x, v) + f(t, x, v)\text{St}[f, f](t, y, w)) \\
&\quad - \psi(x, v)\partial_t(f(t, x, v)f(t, y, w)),
\end{aligned}$$

and the local conservation of mass (the first identity in Proposition 2.3.1)

$$\int_{\mathbf{R}^3} \text{St}[f, f](t, y, w)dw = 0$$

to dispose of the term $\psi(x, v)f(t, x, v)\text{St}[f, f](t, y, w)$ in the integral.

Representing $\text{St}[f, f](t, x, v)$ in terms of the Landau mass current $\mathcal{J}_0[f] = \mathcal{J}_0[f, f]$ (see (2.3.2), and the definition of $\mathcal{J}_0[f, g]$ in the statement of Theorem 2.3.3),

$$\begin{aligned}
\Gamma_{121} &= \frac{1}{2} \int_{(\mathbf{R}^3)^2} v \cdot \nabla_x \psi(x, v)f(t, x, v)\rho_f(t, \cdot) \star \beta(|\cdot|)(x)dx dv \\
&\quad - \frac{1}{2} \int_{(\mathbf{R}^3)^2} \nabla_v \psi(x, v) \cdot \mathcal{J}_0[f](t, x, v)\rho_f(t, \cdot) \star \beta(|\cdot|)(x)dx dv \\
&\quad - \frac{1}{2} \frac{d}{dt} \int_{(\mathbf{R}^3)^2} \psi(x, v)f(t, x, v)\rho_f(t, \cdot) \star \beta(|\cdot|)(x)dx dv.
\end{aligned}$$

Step 5. On the other hand

$$\begin{aligned}
\Gamma_{122} &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\psi(x, v) - \psi(x, v'(v, w, n_{y,x}))(v - w|n_{y,x})_+ \\
&\quad \times f(t, x, v)f(t, y, w)b(|x - y|)dx dv dy dw \\
&= -\frac{1}{2} \int_{(\mathbf{R}^3)^2} \psi(x, v)\text{St}[f, f](t, x, v)dx dv \\
&= \frac{1}{2} \int_{(\mathbf{R}^3)^2} \nabla_v \psi(x, v) \cdot \mathcal{J}_0[f](t, x, v)dx dv.
\end{aligned}$$

Next observe that

$$S_3 + S_{42} = \frac{1}{2}(\psi(x, v) - \psi(x, v'(v, w, n_{y,x})) \ln(f(t, x, v)f(t, y, w))),$$

so that

$$\begin{aligned}
\Gamma_{34} &:= \int_{(\mathbf{R}^3)^4} (S_3 + S_{42}) f(t, x, v) f(t, y, w) b(|x - y|) (v - w |n_{y,x})_+ dx dv dy dw \\
&= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\psi(x, v) - \psi(x, v'(v, w, n_{y,x}))) f(t, x, v) f(t, y, w) \ln(f(t, x, v) f(t, y, w)) \\
&\quad \times b(|x - y|) (v - w |n_{y,x})_+ dx dv dy dw \\
&= -\frac{1}{2} \int_{(\mathbf{R}^3)^2} \nabla_v \psi(x, v) \cdot (\mathcal{J}_0[f \ln f, f](t, x, v) + \mathcal{J}_0[f, f \ln f](t, x, v)) dx dv.
\end{aligned}$$

Step 6. While the terms Γ_{12} and Γ_{34} only contribute divergences in v and time derivatives, the two terms considered below contribute divergences in x .

First consider

$$\begin{aligned}
\Gamma_{41} &:= \int_{(\mathbf{R}^3)^4} S_{41} f(t, x, v) f(t, y, w) b(|x - y|) (v - w |n_{y,x})_+ dx dv dy dw \\
&= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\psi(y, w) - \psi(x, v)) f(t, x, v) f \ln f(t, y, w) b(|x - y|) (v - w |n_{y,x})_+ dx dv dy dw,
\end{aligned}$$

and express

$$\psi(y, w) - \psi(x, v) = \int_0^{\pi/2} \frac{d}{d\theta} \psi(x_\theta, v_\theta) d\theta,$$

where

$$\begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} v_\theta \\ w_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}.$$

Since

$$\frac{d}{d\theta} \psi(x_\theta, v_\theta) = y_\theta \cdot \nabla_x \psi(x_\theta, v_\theta) + w_\theta \cdot \nabla_v \psi(x_\theta, v_\theta),$$

one has

$$\begin{aligned}
\Gamma_{41} &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (y_\theta \cdot \nabla_x \psi(x_\theta, v_\theta) + w_\theta \cdot \nabla_v \psi(x_\theta, v_\theta)) f(t, x, v) f \ln f(t, y, w) \\
&\quad \times b(|x - y|) (v - w |n_{y,x})_+ dx dv dy dw \\
&= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (y \cdot \nabla_x \psi + w \cdot \nabla_v \psi)(x, v) \int_0^{\pi/2} f(t, x_\theta, v_\theta) f \ln f(t, y_\theta, w_\theta) \\
&\quad \times b(|x_\theta - y_\theta|) (v_\theta - w_\theta |n_{y_\theta, x_\theta})_+ d\theta dx dv dy dw
\end{aligned}$$

because

$$\det \frac{\partial(x_\theta, y_\theta)}{\partial(x, y)} = \det \frac{\partial(v_\theta, w_\theta)}{\partial(v, w)} = 1.$$

Step 7. Similarly, set

$$\begin{aligned}\Gamma_2 &:= \int_{(\mathbf{R}^3)^4} S_2 f(t, x, v) f(t, y, w) b(|x - y|) (v - w|n_{y,x})_+ dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (\psi(y, w) - \psi(x, v)) f(t, x, v'(v, w, n_{y,x})) \ln f(t, y, w) \\ &\quad \times f(t, y, w'(v, w, n_{y,x})) b(|x - y|) (v - w|n_{x,y})_+ dx dv dy dw.\end{aligned}$$

By the same change of variables as in Γ_2 , one finds that

$$\begin{aligned}\Gamma_2 &= \frac{1}{2} \int_{(\mathbf{R}^3)^4} (y \cdot \nabla_x \psi + w \cdot \nabla_v \psi)(x, v) \int_0^{\pi/2} f(t, x_{-\theta}, v'(v, w, n_{y,x})_{-\theta}) \\ &\quad \times f(t, y_{-\theta}, w'(v, w, n_{y,x})_{-\theta}) \ln f(t, y_{-\theta}, w_{-\theta}) b(|x_{-\theta} - y_{-\theta}|) \\ &\quad \times (v_{-\theta} - w_{-\theta}|n_{x_{-\theta}, y_{-\theta}})_+ d\theta dx dv dy dw.\end{aligned}$$

Conclusion. Gathering all these terms together, we arrive at the following identity:

$$\begin{aligned}&\int_{(\mathbf{R}^3)^2} \text{St}[f, f](t, x, v) \ln f(t, x, v) \psi(x, v) dx dv = -\Lambda[\psi](t) \\ &+ \int_{(\mathbf{R}^3)^2} (\mathcal{K}[f](t, x, v) \cdot \nabla_x \psi(x, v) + \mathcal{L}[f](t, x, v) \cdot \nabla_v \psi(x, v)) dx dv \\ &\quad - \frac{1}{2} \frac{d}{dt} \int_{(\mathbf{R}^3)^2} \psi(x, v) f(t, x, v) \rho_f(t, \cdot) \star \beta(|\cdot|)(x) dx dv,\end{aligned}$$

where

$$\begin{aligned}\mathcal{L}[f](t, x, v) &:= -\frac{1}{2} \mathcal{J}_0[f, f](t, x, v) (1 - \rho_f \star \beta(|\cdot|)(t, x)) \\ &\quad - \frac{1}{2} (\mathcal{J}_0[f \ln f, f](t, x, v) + \mathcal{J}_0[f, f \ln f](t, x, v)) \\ &+ \frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\pi/2} (f(t, x_{-\theta}, v'(v, w, n_{y,x})_{-\theta}) f(t, y_{-\theta}, w'(v, w, n_{y,x})_{-\theta}) \\ &\quad - f(t, x_{-\theta}, v_{-\theta}) f(t, y_{-\theta}, w_{-\theta})) \ln f(t, y_{-\theta}, w_{-\theta}) b(|x_{-\theta} - y_{-\theta}|) \\ &\quad \times (v_{-\theta} - w_{-\theta}|n_{x_{-\theta}, y_{-\theta}})_+ w d\theta dy dw,\end{aligned}$$

where the notation $\rho_f(t, \cdot) \star \beta(|\cdot|)$ has been defined in (2.3.7), while

$$\begin{aligned}\mathcal{K}[f](t, x, v) &:= \frac{1}{2} \int_{(\mathbf{R}^3)^2} \int_0^{\pi/2} (f(t, x_{-\theta}, v'(v, w, n_{y,x})_{-\theta}) f(t, y_{-\theta}, w'(v, w, n_{y,x})_{-\theta}) \\ &\quad - f(t, x_{-\theta}, v_{-\theta}) f(t, y_{-\theta}, w_{-\theta})) \ln f(t, y_{-\theta}, w_{-\theta}) b(|x_{-\theta} - y_{-\theta}|) \\ &\quad \times (v_{-\theta} - w_{-\theta}|n_{x_{-\theta}, y_{-\theta}})_+ y d\theta dy dw.\end{aligned}$$

2.7 Conclusion

Summarizing, we have seen that delocalized collision integrals in the style of the Enskog, Povzner or soft sphere integrals can be expressed in terms of momentum and energy currents which have nontrivial components in the space of positions. For that reason, such delocalized

collision integrals contribute to the local conservation laws of momentum and energy which appear in the Euler system of gas dynamics in the case of dense gases. This effect has been analyzed at the level of asymptotic analysis in [Lac98] by means of the Hilbert expansion method, along with the resulting virial expansion of the pressure. One can also find in chapter 16 of [CC70] (see in particular §16.32) a variant of the discussions in the present paper limited to an asymptotic expansion in terms of the molecular radius. What is proposed in the present article is a non-asymptotic discussion which parallels that of §16.32 in [CC70], along with a discussion of a local variant of the Boltzmann H Theorem in Theorem 2.3.3. All our discussions are based on Landau's formulation of the Boltzmann collision integral in terms of a mass current in the space of molecular velocities, to be found in §41 of [LP81], and discussed in [Vil99] in full detail.

Chapter 3

Conservative form of Standard Enskog equation and Povzner equation

This chapter is based on the preprint [Che25b], which has been submitted to a journal for publication.

Introduction

This paper focuses on collisional kinetic models designed to describe the dynamics of monatomic gases. The most classical example is the Boltzmann equation, introduced by Ludwig Boltzmann in 1872, which models the statistical behavior of dilute gas particles through binary collisions. The Standard Enskog equation, proposed by David Enskog in 1921, extends Boltzmann's framework to dense gases by accounting for particle size and excluded volume. The Povzner collision integral, introduced in 1965, generalizes the model by allowing collisions between molecules to be elastic or soft. Roughly speaking, Enskog's model permits collisions on a sphere, while Povzner's model extends this to collisions within a spherical shell.

The kinetic equation is connected to the conservation laws of mass, momentum, and energy through the definition of macroscopic quantities via the particle distribution function; see Section 3.3 in [Cer94], for example. At the time of this writing, the direct verification of local conservation laws for mass, momentum, and energy by classical solutions of the Standard Enskog equation or the Povzner equation, as discussed in Section 3.1, does not seem to have been studied systematically. To address this gap, we propose a systematic method for deriving local conservation laws in the framework of kinetic models for these two equations. Our approach is based on expressing the collision integrals as divergences in the position and velocity variables of mass, momentum, and energy currents, drawing inspiration from a lesser-known idea by Landau regarding the Boltzmann collision integral; see, for instance, [Vil99; LP81].

The outline of this paper is as follows: In Section 3.1, we first revisit the classical

Boltzmann equation and introduce the motivation behind this work. We then present the two models under consideration—the Standard Enskog equation and the Povzner equation. Section 5.4 is dedicated to the main results of the paper. Subsequently, in Section 3.3, we explore the application of these results to macroscopic dynamics and local conservation laws. Finally, the proofs of the main results are provided in Section 3.4 and Section 3.5, respectively. Similar results for a class of delocalized collision integrals which does not include the Standard Enskog and the Povzner collision integrals have been obtained in [CCG24].

3.1 Collisional kinetic Models

3.1.1 The Boltzmann equation

We begin with considering the following collisional kinetic equation

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \mathcal{C}(f, f)(t, x, v), \quad (3.1.1)$$

where $f(t, x, v) \in \mathbb{R}_+$ is a single particle distribution depending on time $t \in \mathbb{R}_+$ space $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, and velocity $v = (v_1, v_2, v_3) \in \mathbb{R}^3$. The most classical example is the hard sphere Boltzmann collision operator defined by

$$B(f, g) := \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} (f(x, v') g(x, w') - f(x, v) g(x, w)) \langle v - w, n \rangle_+ \mathrm{d}n \mathrm{d}w, \quad (3.1.2)$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product in Euclidean space, and $\langle \cdot, \cdot \rangle_+ := \max\{0, \langle \cdot, \cdot \rangle\}$. The pre-collision velocities (v', w') are determined by the unit vector $n \in \mathbb{S}^2$

$$\begin{cases} v'(v, w, n) = v - n \langle n, v - w \rangle \\ w'(v, w, n) = w + n \langle n, v - w \rangle, \end{cases} \quad (3.1.3)$$

Here we list some basic properties of the collision transform;

- The collision transform is reversible:

$$v''(v'(v, w, n), w'(v, w, n), n) = v; \quad w''(v'(v, w, n), w'(v, w, n), n) = w. \quad (3.1.4)$$

- The collision transform is symmetric:

$$v'(w, v, n) = w'(v, w, n); \quad w'(w, v, n) = v'(v, w, n). \quad (3.1.5)$$

- The collision transform is even with respect to n :

$$v'(w, v, -n) = v'(v, w, n); \quad w'(w, v, -n) = w'(v, w, n). \quad (3.1.6)$$

- collision transform has Jacobian determinant:

$$\det \left(\frac{\partial(v', w')}{\partial(v, w)} \right) = -1. \quad (3.1.7)$$

- The collision transform conserves momentum and energy:

$$v'(w, v, n) + w'(v, w, n) = v + w; \quad |v'(x, w, n)|^2 + |w'(v, w, n)|^2 = |v|^2 + |w|^2. \quad (3.1.8)$$

- The collision transform reverses the direction with respect to n :

$$\langle v'(v, w, n) - w'(v, w, n), n \rangle = -\langle v - w, n \rangle \quad (3.1.9)$$

The two particles collide at the same position x . Due to the pre-to-post transformation (3.1.3), the Boltzmann collision operator locally conserves the mass, momentum, and energy respectively, namely for classical solution with rapidly decaying of (3.1.1) with Boltzmann collision integrals,

$$\frac{d}{dt} \int_{\mathbb{R}^3} f(t, x, v) \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} dv = \int_{\mathbb{R}^3} B[f, f] \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} dv = \mathbf{0}. \quad (3.1.10)$$

This result is given by the weak formula for the Boltzmann collision interal which can be found in every textbook in kinetic theory, such as section 3.1 in [Cer94]. If we generalize the model to dense gases, which means the molecular radius cannot be neglected. In that case, the centers of two colliding particles are no longer at the same position in space.

For Enskog's model and Povzner's model, it is easily seen that one cannot arrive the same local result as in (3.1.10). In other words, the quantities shown in (3.1.10) do not always vanish. On the other hand, we have the global conservation

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} E[f, f] \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} dv dx = \int_{\mathbb{R}^3 \times \mathbb{R}^3} P[f, f] \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} dv dx = 0. \quad (3.1.11)$$

This result for the Povzner collision operator can be found in [FHT11]. For the Enskog version, the reader can read Chapter 16 in [CC90]. In [LP81] (see [Vil99] for a rigorous discussion), it was found that the Boltzmann collision integral can be expressed as the divergence in v of a mass current, $B[f, f] = -\nabla_v \cdot \mathcal{J}_0(f, f)$ where

$$\mathcal{J}_0(f, f) := - \int_{\langle v-w, n \rangle > 0} \int_0^{\langle v-w, n \rangle} \langle v-w, n \rangle f(x, v+sn) f(x, w+sn) n dn dw ds.$$

In [PL12], this formula is used to derive the Landau equation from the Boltzmann equation. Comparing to the delocalized collision operator, a natural question comes from (3.1.11) :

can we express delocalized collision operator as the following conservative form

$$\mathcal{C}(f, f) \begin{pmatrix} 1 \\ v_1 \\ v_2 \\ v_3 \\ |v|^2 \end{pmatrix} = \nabla_v \cdot \mathbf{J} + \nabla_x \cdot \mathbf{I} \quad (3.1.12)$$

3.1.2 The Standard Enskog equation

We write the following so-called Standard Enskog equation

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = E[f, f](t, x, v), \quad (3.1.13)$$

where Enskog collision integral is defined as

$$E[f, g](t, x, v) := \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left[\chi(x - \frac{1}{2}\sigma n) f(t, x, v') g(t, x - \sigma n, w') - \chi(x + \frac{1}{2}\sigma n) f(t, x, v) g(t, x + \sigma n, w) \right] \sigma^2 \langle v - w, n \rangle_+ dn dw, \quad (3.1.14)$$

the pre-collision velocities (v', w') are given by (3.1.3).

We have to say that it seems nonsensical to define Standard Enskog collision integral as a bilinear functional of distribution functions, since one always assumes that the correlation function χ depends on one of the distribution function f . In that case, the two functions don't share the symmetry structure anymore. Here, we write the collision integral in this way only for mathematical convenience.

In addition to Standard Enskog equation, some people have also proposed a Revised Enskog equation. It has more mathematical structure. For example, it has the symmetry between two colliding particles, and it is more easily generalized to the case of mixtures. (The standard Enskog equation can also be generated to mixture case, see Chapter 16 of [CC90] for instance.) The Revised Enskog collision operator is

$$\tilde{E}[f, g] := \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left(Y(\rho_f(x), \rho_g(x - \sigma n)) f(x, v') g(x - \sigma n, w') - Y(\rho_f(x), \rho_g(x + \sigma n)) f(x, v) g(x + \sigma n, w) \right) \langle n, v - w \rangle_+ dw dn,$$

where the correlation function Y satisfies $Y(x, y) = Y(y, x)$. The Enskog equation is a generalized Boltzmann equation aimed at modelling dense gases. When we formally derive the Boltzmann equation from Liouville equation, we no longer consider the particles as mass points. We distinguish between the collision point and the particle center. Its advantage is to describe two different kinds of particles collisions. The Enskog equation was first proposed by David Enskog in 1922 [Ens22]. [BE73a][BE73b] proposed the modified Enskog equation. More research has been conducted on the revised Enskog equation due to its improved mathematical structure, particularly its symmetry, which makes it easier to establish properties

such as the H-theorem [R  s78], and consistent with irreversible thermodynamics– leads to the correct equilibrium [Bei83a]. Nevertheless, the standard Enskog equation remains equally valuable for study because of its more intuitive physical interpretation. Specifically, the correlation function in the standard Enskog equation depends on the ratio:

$$\frac{\text{Impact of Volume Occupation}}{\text{Shielding Influence}}.$$

Hence, we have a more explicit formula for analyzing the equation. For example, asymptotically, one can assume $\chi(t, x) = 1 + \frac{5}{8} \frac{2}{3} \pi \sigma^3 \rho_f(t, x)$ where $\rho_f(t, x) := \int_{\mathbb{R}^3} f(t, x, v) dv$: see for instance Chapter 16 in [CC90].

In the following discussion, we focus on the Standard Enskog model. For details regarding the revised/modified Enskog model, is referred to [CCG24]. It is important to emphasize that the results presented in [CCG24] do not include those in Section 5.4, despite the similarities in the approaches. This is because, in the proofs of [CCG24], the collision integral $\text{St}[\cdot, \cdot]$ is assumed to be in a symmetric form, i.e., $\text{St}[f, g] = \text{St}[g, f]$.

3.1.3 The Povzner equation

The Povzner collision integral was proposed to study the delocalized collision by Povzner in [Pov65]. The collision integral is of the following form

$$P[f, g] := \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left(f(x, v') g(y, w') - f(x, v) g(y, w) \right) J(x - y, v - w) dw dy, \quad (3.1.15)$$

where the pre-collision velocities (v', w') are also given by (3.1.3) with $n = \frac{y-x}{|y-x|}$. $J(\xi, v)$ is assumed to satisfy the following four assumptions as showed in [Pov65]

(i) J is continuous, and $|J(\xi, v)| \lesssim |v| + 1$.

(ii) Time reversibility:

$$J(-\xi, -v) = J(\xi, v). \quad (3.1.16)$$

(iii) Invariance after collision:

$$J(\xi, v' - w') = J(\xi, v - w). \quad (3.1.17)$$

(iv) Short-range interaction: There exists a constant R such that $J(\xi, v) = 0$ for $|\xi| > R$.

An example of Povzner kernel in [FHT11] is

$$J_{\epsilon_1, \epsilon_2}(\xi, v) := \frac{1}{2\epsilon_1^3} \frac{1}{\epsilon_2} H(\epsilon_1 - |\xi|) H(\epsilon_2 - |v|) \left| v \cdot \frac{\xi}{|\xi|} \right|,$$

where H is the Heaviside step function. From this example, we can find out more clearly that the Povzner collision integral allows for the possibility of a spatial smearing process with range of ϵ_2 and ϵ_1 of collisions as well as for the classically assumed process in which the molecules collide at a point. We point out here that if we set $J(\xi, v) = \tilde{J}(|v|, \frac{\langle \xi, v \rangle}{|\xi||v|}) \delta(|\xi|)$ in (3.1.15), then we can recover the Boltzmann collision kernel. However, the Povzner collision integral generalizes the following form of the Boltzmann collision integral:

$$\frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{S}^2} [f(x, v')f(x, w') - f(x, v)f(x, w)] |\langle v - w, n \rangle| dn dw,$$

which corresponds to (3.1.2) after changing n into $-n$ and symmetrizing (3.1.2). In the Boltzmann collision operator, the direction of the unit vector n is inconsequential, as it cancels out when taking the Boltzmann-Grad limit. However, in the case of dense gases, the locations of the gain term and the loss term differ. Consequently, a more physically meaningful assumption would be:

$$J(\xi, v' - w') = J(-\xi, v - w), \quad (3.1.18)$$

instead of (3.1.17). Nevertheless, in the following discussion, we adhere to Povzner's original assumption (3.1.17). For results derived under the new assumption (3.1.18), we refer the reader to [CCG24].

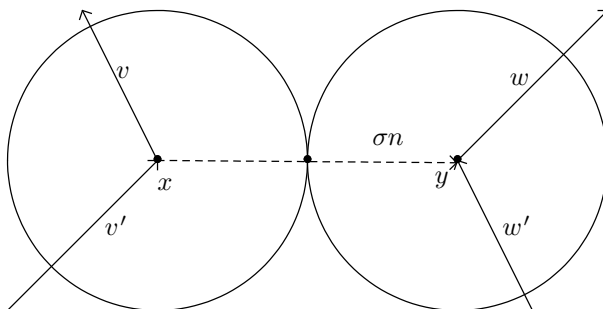


Figure 3.1: Schematic diagram of ingoing and outgoing processes

3.2 Main results

As mentioned in section 3.1, we seek a representation of a form of (3.1.12). Before stating the main result, we introduce the general Landau mass current

Definition 3.2.1 (Landau mass current for the Standard Enskog collision integral). *For*

each $f, g \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ with rapidly decaying, we define

$$\mathfrak{J}_0^E[f, g](x, n, v) := \int_{\mathbb{R}^3} \int_0^{\langle v-w, n \rangle} \chi(x + \frac{1}{2}\sigma n) f(x, v + sn) g(x + \sigma n, w + sn) n ds dw \quad (3.2.1)$$

Definition 3.2.2 (Landau mass current for the Povzner collision integral). *For each $f, g \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ with rapidly decay, we define*

$$\begin{aligned} \mathfrak{J}_0^P[f, g](x, y, v) := \int_{\mathbb{R}^3} \int_0^{\langle v-w, n \rangle} f(x, v + s \frac{y-x}{|y-x|}) g\left(y, w + s \frac{y-x}{|y-x|}\right) \\ \times J(x-y, v-w) \frac{y-x}{|y-x|} ds dw \end{aligned} \quad (3.2.2)$$

For Enskog collision integral, we have the following result

Theorem 3.2.1. *For each rapidly decaying function $f \in C(\mathbb{R}^3 \times \mathbb{R}^3)$, we have*

$$E[f, f] = \nabla_v \cdot \mathcal{J}_0^E[f, f] \quad (3.2.3)$$

$$E[f, f]v_1 = \nabla_v \cdot \mathcal{J}_1^E[f, f] + \nabla_x \cdot \mathcal{I}_1^E[f, f] \quad (3.2.4)$$

$$E[f, f]v_2 = \nabla_v \cdot \mathcal{J}_2^E[f, f] + \nabla_x \cdot \mathcal{I}_2^E[f, f] \quad (3.2.5)$$

$$E[f, f]v_3 = \nabla_v \cdot \mathcal{J}_3^E[f, f] + \nabla_x \cdot \mathcal{I}_3^E[f, f] \quad (3.2.6)$$

$$E[f, f]|v|^2 = \nabla_v \cdot \mathcal{J}_4^E[f, f] + \nabla_x \cdot \mathcal{I}_4^E[f, f] \quad (3.2.7)$$

where vectors fields $\mathcal{I}_k^E(x, v), \mathcal{J}_l^E(x, v)$, $k = 1, 2, 3, 4$, $l = 0, 1, 2, 3, 4$ are defined by

$$\mathcal{J}_0^E = \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, f](x, n, v) dn, \quad (3.2.8)$$

for $k = 1, 2, 3$:

$$\begin{aligned} \mathcal{J}_k^E[f, f] \\ = \mathcal{J}_0^E[v_k f, f] - \int_{\mathbb{S}^2} \mathfrak{J}_0^E[\langle v, n \rangle n_k f, f] dn + \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, \langle w, n \rangle n_k f] dn \\ - \frac{1}{2} \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} \chi(x - \frac{1}{2}\sigma n) f(x - \sigma n, v_{-\theta}) f(x, w_{-\theta}) \langle v_{-\theta} - w_{-\theta}, n \rangle_+^2 n_k \\ \times w dn dw d\theta, \end{aligned} \quad (3.2.9)$$

and $l = 1, 2, 3$

$$\begin{aligned} \mathcal{I}_l^E[f, f] = \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{S}^2} \int_0^\sigma \chi\left(x + \left(\frac{1}{2}\sigma - s\right)n\right) f(x - sn, v) f(x + (\sigma - s)n, w) \\ \times \langle v - w, n \rangle_+^2 n_l n dw dn ds, \end{aligned} \quad (3.2.10)$$

finally,

$$\mathcal{J}_4^E[f, f] \quad (3.2.11)$$

$$\begin{aligned}
&= \mathcal{J}_0^E[|v|^2 f, f] - \int_{\mathbb{S}^2} \mathfrak{J}_0^E[\langle v, n \rangle^2 f, f] dn + \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, \langle w, n \rangle^2 f] dn \\
&\quad - \frac{1}{2} \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} \chi(x - \frac{1}{2}\sigma n) f(x - \sigma n, v_{-\theta}) f(x, w_{-\theta}) \langle v_{-\theta} - w_{-\theta}, n \rangle_+^2 \\
&\quad \times \langle v_{-\theta} + w_{-\theta}, n \rangle w dn dw d\theta,
\end{aligned}$$

while

$$\begin{aligned}
\mathcal{I}_4^E[f, f] &= \frac{1}{2} \int_{\mathbb{R}^3 \times \mathbb{S}^2} \int_0^\sigma \chi\left(x + \left(\frac{1}{2}\sigma - s\right)n\right) f(x - sn, v) f(x + (\sigma - s)n, w) \\
&\quad \times \langle v - w, n \rangle_+^2 \langle v + w, n \rangle n dw dn ds, \quad (3.2.12)
\end{aligned}$$

For Povzner collision integral, we have the following parallel result

Theorem 3.2.2. *For each rapidly decaying function $f \in C(\mathbb{R}^3 \times \mathbb{R}^3)$, we have*

$$P[f, f] = \nabla_v \cdot \mathcal{J}_0^P[f, f] \quad (3.2.13)$$

$$P[f, f]v_1 = \nabla_v \cdot \mathcal{J}_1^P[f, f] + \nabla_x \cdot \mathcal{I}_1^P[f, f] \quad (3.2.14)$$

$$P[f, f]v_2 = \nabla_v \cdot \mathcal{J}_2^P[f, f] + \nabla_x \cdot \mathcal{I}_2^P[f, f] \quad (3.2.15)$$

$$P[f, f]v_3 = \nabla_v \cdot \mathcal{J}_3^P[f, f] + \nabla_x \cdot \mathcal{I}_3^P[f, f] \quad (3.2.16)$$

$$P[f, f]|v|^2 = \nabla_v \cdot \mathcal{J}_4^P[f, f] + \nabla_x \cdot \mathcal{I}_4^P[f, f] \quad (3.2.17)$$

where vector fields $\mathcal{I}_k^P(x, v), \mathcal{J}_l^P(x, v)$, $k = 1, 2, 3, 4$, $l = 0, 1, 2, 3, 4$ are defined by

$$\mathcal{J}_0^P = \int_{\mathbb{R}^3} \mathfrak{J}_0^P[f, f](x, y, v) dy, \quad (3.2.18)$$

for $k = 1, 2, 3$:

$$\begin{aligned}
&\mathcal{J}_0^P[v_i f, f] \quad (3.2.19) \\
&\quad - \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[\left\langle v, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i f, f \right] dy \\
&\quad + \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[f, \left\langle w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i f \right] dy \\
&\quad - \frac{1}{2} \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \\
&\quad \times \left\langle v - w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{x_{-\theta} - y_{-\theta}}{|x-y|} \right)_i w dn dw d\theta,
\end{aligned}$$

and $l = 1, 2, 3$

$$\begin{aligned}
\mathcal{I}_l^P[f, f] &= -\frac{1}{2} \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \\
&\quad \times \left\langle v - w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{x_{-\theta} - y_{-\theta}}{|x-y|} \right)_i y dn dw d\theta, \quad (3.2.20)
\end{aligned}$$

finally,

$$\mathcal{J}_4^P[f, f] \quad (3.2.21)$$

$$\begin{aligned} &= \mathcal{J}_0^P[|v|^2 f, f] - \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[\left\langle v, \frac{y-x}{|y-x|} \right\rangle^2 f, f \right] dy + \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[f, \left\langle w, \frac{y-x}{|y-x|} \right\rangle^2 f \right] dy \\ &\quad - \frac{1}{2} \int_{(\mathbb{R}^3)^2} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \\ &\quad \times \left\langle v - w, \frac{y-x}{|y-x|} \right\rangle \left\langle v + w, \frac{y-x}{|y-x|} \right\rangle w dy dw d\theta, \end{aligned} \quad (3.2.22)$$

while

$$\begin{aligned} \mathcal{I}_4^P[f, f] &= -\frac{1}{2} \int_{(\mathbb{R}^3)^2} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \\ &\quad \times \left\langle v - w, \frac{y-x}{|y-x|} \right\rangle \left\langle v + w, \frac{y-x}{|y-x|} \right\rangle y dy dw d\theta, \end{aligned} \quad (3.2.23)$$

3.3 Application to local conservation laws and H theorem

To build up the connection with macroscopic equation, we need to define some macroscopic quantities

$$\begin{cases} \rho_f(t, x) := \int_{\mathbb{R}^3} f(t, x, v) dv \\ u_f(t, x) := \frac{1_{\rho_f > 0}}{\rho_f(t, x)} \int_{\mathbb{R}^3} v f(t, x, v) dv \\ P_f(t, x) := \int_{\mathbb{R}^3} (v - u_f(t, x))^{\otimes 2} f(t, x, v) dv \\ q_f(t, x) := \frac{1}{2} \int_{\mathbb{R}^3} (v - u_f(t, x)) |v - u_f(t, x)|^2 f(t, x, v) dv, \end{cases}$$

where ρ_f, u_f, P_f , and q_f represent the mass density, bulk velocity, stress tensor, and heat-flow of the gas. If f is a classical solution of the Boltzmann equation (3.1.1) with the collision integral given by (3.1.2), the following macroscopic equations for dilute gases can be derived:

$$\begin{cases} \partial_t \rho_f + \nabla_x \cdot (\rho_f u_f) = 0, \\ \partial_t (\rho_f u_f) + \nabla_x \cdot (\rho_f u_f^{\otimes 2}) + \nabla_x \cdot (P_f) = 0, \\ \partial_t \left(\frac{1}{2} |u_f|^2 + \text{tr} P_f \right) + \nabla_x \cdot \left[\left(\frac{1}{2} |u_f|^2 + \text{tr} P_f \right) u_f + P_f \cdot u_f + q_f \right] = 0. \end{cases} \quad (3.3.1)$$

However, the situation changes significantly when dealing with the Enskog equation.

Corollary 3.3.1. *Let f^E be a classical solution of the kinetic equation (3.1.1) with collision*

integral (3.1.14). Moreover $f^E \in C(\mathbb{R}_x^3 \times \mathbb{R}_v^3)$ rapidly decaying with respect to x and v . Then

$$\begin{cases} \partial_t \rho_{f^E} + \nabla_x \cdot (\rho_{f^E} u_{f^E}) = 0 \\ \partial_t (\rho_{f^E} u_{f^E}) + \nabla_x \cdot (\rho_{f^E} u_{f^E}^{\otimes 2}) + \nabla_x \cdot (P_{f^E} - \mathbb{I}^E) = 0 \\ \partial_t (\frac{1}{2} |u_{f^E}|^2 + \text{tr} P_{f^E}) \\ \quad + \nabla_x \cdot [(\frac{1}{2} |u_{f^E}|^2 + \text{tr} P_{f^E}) u_{f^E} + P_{f^E} \cdot u_{f^E} + q_{f^E} - \mathcal{I}_4^E] = 0, \end{cases} \quad (3.3.2)$$

where $\mathcal{I}_i^E, i = 1, 2, 3$ are components of $\mathbb{I}^E$, namely

$$\mathbb{I}^E(t, x, v) = \begin{pmatrix} \mathcal{I}_1^E \\ \mathcal{I}_2^E \\ \mathcal{I}_3^E \end{pmatrix}$$

Correspondingly, we have the similar result for the Povzner equation.

To conclude the corollary, we only need to integrate (3.2.3)–(3.2.7) with respect to v over $\mathbb{R}^3$. However, it is important to note that the equations in (3.3.2) are not closed. Closure is achieved only after solving the general kinetic equation (3.1.1) and computing $\mathcal{I}_4^E$, $\mathbb{I}^E$, and q_{f^E} . Furthermore, a closure relation is necessary. For example, to derive the Euler system, the distribution function f should approximate a Maxwellian such that q_{f^E} and the anisotropic part of P_{f^E} become negligible, i.e.,

$$q_{f^E} = \mathbf{0}, \quad P_{f^E} = p \text{Id}_3.$$

This reduction allows us to solve the equations with four unknowns (ρ, u, p) , instead of handling ten unknowns with only four constraints.

The corollary not only clarifies the influence of molecular volume occupation on macroscopic equations but also highlights a key distinction: the Boltzmann collision integral does not contribute to the stress tensor P_f —even a free transport equation can generate a stress tensor. In contrast, the Enskog and Povzner collision integrals have a direct impact on the pressure tensor. This distinction is significant because the coefficient of pressure depends on the adiabatic index, indicating that the gas governed by equations (3.3.2) no longer behaves as a perfect gas. This observation provides an alternative perspective on the limitations of the perfect gas assumption for such systems.

It is straightforward to establish the local entropy inequality, as demonstrated in [CCG24], due to the availability of a stronger weak formulation for the Povzner collision integral:

$$\begin{aligned} (P[f, f], \phi)_{x,v} &= \frac{1}{2} \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \\ &\quad \times [\phi(x, v') + \phi(y, w') - \phi(x, v) - \phi(y, w)] dx dy dv dw, \end{aligned}$$

as given in equation (10) of [Pov65]. If we choose $\phi(x, v) = \ln f(x, v)$, the following entropy inequality is obtained:

$$\frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, x, v) \ln f(t, x, v) dx dv$$

$$= \frac{1}{2} \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \ln \left(\frac{f(x, v') f(y, w')}{f(x, v) f(y, w)} \right) dx dy dv dw \leq 0,$$

which follows from the basic inequality: for $a, b > 0$,

$$a \ln \frac{b}{a} \leq b - a.$$

However, this result is less remarkable for the Povzner equation because the entropy inequality is identical to the original Boltzmann's entropy. As such, we do not discuss it further here. As for the Standard Enskog equation, the local and global entropy inequality are studied in [GG97a].

3.4 Proof of Theorem 3.2.1

The following proof is based on multiplying the collision kernel by a test function. Before we prove the theorem, we begin with a lemma which will be used repeatedly.

Lemma 3.4.1. *Let $f, g \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ with rapid decay at infinity. For each test function $\phi \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ with at most polynomial growth at infinity,*

$$\begin{aligned} (E[f, g], \phi)_{x, v} &:= \int_{\mathbb{R}^3 \times \mathbb{R}^3} E[f, g](x, v) \phi(x, v) dx dv \\ &= \int_{(\mathbb{R}^3)^4} \chi(x + \frac{1}{2}\sigma n) f(x, v) g(x + \sigma n, w) \langle v - w, n \rangle_+ \\ &\quad \times [\phi(x, v') - \phi(x, v)] dx dn dv dw \end{aligned} \quad (3.4.1)$$

Proof. For the gain term of the Standard Enskog collision integral defined in 3.1.14, we apply the transform $(v, w, n) \mapsto (v', w', -n)$. Since the absolute value of the Jacobian determinate is 1 (3.1.7), the gain term becomes

$$\begin{aligned} \int_{(\mathbb{R}^3)^4} \chi(x + \frac{1}{2}\sigma n) f(x, v'') g(x + \sigma n, w'') \langle v' - w', -n \rangle_+ \\ \times \phi(x, v'(v, w, -n)) dx dn dv dw. \end{aligned}$$

The properties (3.1.4), (3.1.9) and (3.1.6) show that this term is equal to

$$\int_{(\mathbb{R}^3)^4} \chi(x + \frac{1}{2}\sigma n) f(x, v) g(x + \sigma n, w) \langle v - w, n \rangle_+ \phi(x, v'(v, w, n)) dx dn dv dw.$$

Summing with the loss term leads to the sought result. $\square$

For brevity, $(A(x, v), b(x, v))_{x, v}$ is designated to $\int_{\mathbb{R}^3 \times \mathbb{R}^3} \langle A(x, v), b(x, v) \rangle dx dv$. Indeed, in the standard Enskog equation, the correlation function χ depends on the distribution function f , whereas the following proof does not rely on this dependence. For clarity, throughout the proof, whenever we introduce the bilinear operator for the Enskog collision

integral—for instance, $\mathfrak{J}_i^E[\cdot, \cdot]$ and $\mathcal{J}_i^E[\cdot, \cdot]$ —we assume that the function χ is independent of its functional argument.

3.4.1 Mass current for Enskog collision integral: Proof of (3.2.3)

Proof. As the first step, we apply the Lemma 3.4.1, then note the following identity

$$\begin{aligned} \phi(x, v') - \phi(x, v) &= \int_0^{\langle v-w, n \rangle} \frac{d}{ds} \phi(x, v - sn) ds \\ &= - \int_0^{\langle v-w, n \rangle} \langle n, \nabla_v \phi(x, v - sn) \rangle ds, \end{aligned} \quad (3.4.2)$$

hence we can write $(E[f, g], \phi)_{x, v}$ as

$$\begin{aligned} - \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\langle v-w, n \rangle} \chi(x + \frac{1}{2}\sigma n) f(x, v) g(x + \sigma n, w) \langle v - w, n \rangle_+ \\ \times \langle n, \nabla_v \phi(x, v - sn) \rangle ds dn dw dx dv. \end{aligned}$$

Subsequently, we translate v and w along n by s , namely

$$\begin{aligned} - \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\langle v-w, n \rangle} \chi(x + \frac{1}{2}\sigma n) f(x, v + sn) g(x + \sigma n, w + sn) \langle v - w, n \rangle_+ \\ \times \langle n, \nabla_v \phi(x, v) \rangle ds dn dw dx dv. \end{aligned}$$

With the notation of the Landau mass current of the Enskog collision integral (3.2.1), we may represent $(E[f, g], \phi)_{x, v}$ as

$$\left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, g] dn, \nabla_v \phi(x, v) \right)_{x, v}$$

We merely need to let $f = g$ to deduce the result in the sense of distributions. $\square$

In fact, we established a stronger result than (3.2.3), allowing for different distribution functions in the collision integral. We will utilize this stronger result later to express the momentum and energy current.

3.4.2 Momentum current for Enskog collision integral: Proof of (3.2.4)(3.2.5)(3.2.6)

Proof. Again, we apply Lemma 3.4.1 to test function $v_i \phi(x, v)$ for $i = 1, 2, 3$. We reformulate $(E[f, f]v_i, \phi)$ as

$$\begin{aligned} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \\ \times [v'_i \phi(x, v') - v_i \phi(x, v)] dx dv dn dw. \end{aligned}$$

Then we split the difference $v'\phi(x, v') - v\phi(x, v)$ into two parts,

$$v'_i[\phi(x, v') - \phi(x, v)] + [v'_i - v_i]\phi(x, v)$$

Thereafter, we use the i -th component of (3.1.3) to replace v'_i , hence

$$\begin{aligned} & \underbrace{v_i[\phi(x, v') - \phi(x, v)]}_{=:\phi_1} - \underbrace{\langle v, n \rangle n_i [\phi(x, v') - \phi(x, v)]}_{=:\phi_2} \\ & \quad + \underbrace{\langle w, n \rangle n_i [\phi(x, v') - \phi(x, v)]}_{=:\phi_3} - \underbrace{\langle v - w, n \rangle n_i \phi(x, v)}_{=:\phi_4}. \end{aligned}$$

We use Lemma 3.4.1 for ϕ_1 , then it shows

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \phi_1 dx dv dn dw \\ & \quad = (E[v_i f, f], \phi)_{x, v}. \end{aligned}$$

Following this, we use the result (3.2.3) obtained in the last section. It shows that

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \phi_1 dx dv dn dw \\ & \quad = (-\mathcal{J}_0^E[v_i f, f], \nabla_v \phi)_{x, v}. \end{aligned}$$

By the same reasoning, we can deal with ϕ_2 and ϕ_3 ,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \phi_2 dx dv dn dw \\ & \quad = \left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[\langle v, n \rangle n_i f, f] dn, \nabla_v \phi \right)_{x, v}, \end{aligned}$$

and

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \phi_3 dx dv dn dw \\ & \quad = \left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, \langle w, n \rangle n_i f] dn, \nabla_v \phi \right)_{x, v}. \end{aligned}$$

Regarding ϕ_4 , we change of variables from (v, w, x, n) to $(w, v, x + \sigma n, -n)$,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \phi_4 dx dv dn dw \\ & \quad = - \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \phi(x + \sigma n, w) \\ & \quad \quad \quad dx dv dn dw. \end{aligned}$$

Therefore, we symmetrize it,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \phi_4 dx dv dn dw \\ &= \frac{1}{2} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \\ & \quad \times [\phi(x, v) - \phi(x + \sigma n, w)] dx dv dn dw. \end{aligned}$$

Subsequently, we decompose $\phi(x, v) - \phi(x + \sigma n, w)$ into

$$\underbrace{\phi(x, v) - \phi(x + \sigma n, v)}_{=: \phi_{41}} + \underbrace{\phi(x + \sigma n, v) - \phi(x + \sigma n, w)}_{=: \phi_{42}}.$$

Consider the following two identities

$$\phi(x, v) - \phi(x + \sigma n, v) = \int_0^\sigma \frac{d}{ds} \phi(x + sn, v) ds = \int_0^\sigma \langle n, \nabla_x \phi(x + sn, v) \rangle ds, \quad (3.4.3)$$

and

$$\begin{aligned} \phi(x + \sigma n, v) - \phi(x + \sigma n, w) &= - \int_0^{\pi/2} \frac{d}{d\theta} \phi(x + \sigma n, v_\theta) d\theta \\ &= - \int_0^{\pi/2} \langle w_\theta, \nabla_v \phi(x + \sigma n, v_\theta) \rangle d\theta, \end{aligned} \quad (3.4.4)$$

where (v_θ, w_θ) are defined by

$$\begin{pmatrix} v_\theta \\ w_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} v \\ w \end{pmatrix}. \quad (3.4.5)$$

since

$$\frac{d}{d\theta} \phi(x, v_\theta) = \langle w_\theta, \nabla_v \phi(x, v_\theta) \rangle.$$

The reason for choosing these variables is to ensure that the determinant of the Jacobian equals 1, namely,

$$\det \left(\frac{\partial(v_\theta, w_\theta)}{\partial(v, w)} \right) = 1.$$

Hence we plug (3.4.3) into ϕ_{41} term,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \phi_{41} dx dv dn dw \\ &= \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^\sigma \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \\ & \quad \times \langle n, \nabla_x \phi(x + sn, v) \rangle dx dv dn dw ds. \end{aligned}$$

Then we replace x by $x - sn$, it becomes

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \phi_{41} dx dv dn dw \\ &= \left(\int_{\mathbb{R}^3 \times \mathbb{S}^2} \int_0^\sigma \chi(x + (\frac{1}{2}\sigma - s)n) f(x - sn, v) f(x + (\sigma - s)n, w) \right. \\ & \quad \left. \times \langle v - w, n \rangle_+^2 n_i n dw dn ds, \nabla_x \phi(x, v) \right)_{x, v}. \end{aligned}$$

In an analogous fashion, we can substitute (3.4.4) into ϕ_{42} term,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \phi_{42} dx dv dn dw \\ &= - \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\pi/2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \\ & \quad \times \langle w_\theta, \nabla_v \phi(x + \sigma n, v_\theta) \rangle dx dv dn dw d\theta. \end{aligned}$$

Then we rotate the velocities by $-\theta$, and translate x along n by σ ,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \phi_{42} dx dv dn dw \\ &= \left(- \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\pi/2} \chi(x - \frac{1}{2}\sigma n) f(x - \sigma n, v_{-\theta}) f(x, w_{-\theta}) \langle v_{-\theta} - w_{-\theta}, n \rangle_+^2 n_i \right. \\ & \quad \left. \times w dn dw d\theta, \nabla_v \phi(x, v) \right)_{x, v}. \end{aligned}$$

For $i = 1, 2, 3$, sum them all together, we arrive the weak formulation of (3.2.4)-(3.2.6):

$$\begin{aligned} (v_i E[f, f](x, v), \phi(x, v))_{x, v} &= (-\mathcal{J}_0^E[v_i f, f], \nabla_v \phi)_{x, v} - \left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[\langle v, n \rangle n_i f, f] dn, \nabla_v \phi \right)_{x, v} \\ & \quad + \left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, \langle w, n \rangle n_i f] dn, \nabla_v \phi \right)_{x, v} \\ & - \frac{1}{2} \left(\int_{\mathbb{R}^3 \times \mathbb{S}^2} \int_0^\sigma \chi(x + (\frac{1}{2}\sigma - s)n) f(x - sn, v) f(x + (\sigma - s)n, w) \langle v - w, n \rangle_+^2 n_i n dw dn ds, \nabla_x \phi(x, v) \right)_{x, v} \\ & - \frac{1}{2} \left(- \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} \chi(x - \frac{1}{2}\sigma n) f(x - \sigma n, v_{-\theta}) f(x, w_{-\theta}) \langle v_{-\theta} - w_{-\theta}, n \rangle_+^2 n_i w dn dw d\theta, \nabla_v \phi(x, v) \right)_{x, v}. \end{aligned}$$

□

3.4.3 Energy current for Enskog collision integral: Proof of (3.2.7)

Proof. Substituting $\phi(x, v) = |v|^2 \varphi(x, v)$ into Lemma 3.4.1, we obtain:

$$\int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \times [|v'|^2 \varphi(x, v') - |v|^2 \varphi(x, v)] dx dv dn dw.$$

Then, with the help of (3.1.3), we split the difference $|v'|^2 \varphi(x, v') - |v|^2 \varphi(x, v)$ into four parts,

$$\underbrace{|v|^2 [\varphi(x, v') - \varphi(x, v)]}_{=:\varphi_1} - \underbrace{\langle v, n \rangle^2 [\varphi(x, v') - \varphi(x, v)]}_{=:\varphi_2} + \underbrace{\langle w, n \rangle^2 [\varphi(x, v') - \varphi(x, v)]}_{=:\varphi_3} - \underbrace{(\langle v, n \rangle^2 - \langle w, n \rangle^2) \varphi(x, v)}_{=:\varphi_4},$$

since

$$|v'|^2 = |v - \langle v - w, n \rangle n|^2 = |v|^2 - \langle v, n \rangle^2 + \langle w, n \rangle^2.$$

Following this, we use the result (3.2.3), which we obtained in the last section. We find that

$$\int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ (\varphi_1 - \varphi_2 + \varphi_3) dx dv dn dw = \left(- \int_{\mathbb{S}^2} \mathfrak{I}_0^E[(|v|^2 - \langle v, n \rangle^2) f, f] + \mathfrak{I}_0^E[f, \langle w, n \rangle^2 f] dn, \nabla_v \phi \right)_{x, v}.$$

By the same process showed as above, we perform the change of variables $(v, w, x, n) \mapsto (w, v, x + \sigma n, -n)$ in the φ_4 term, then symmetrize it,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+ \varphi_4 dx dv dn dw \\ &= \frac{1}{2} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 \langle v + w, n \rangle \\ & \quad \times [\varphi(x, v) - \varphi(x + \sigma n, w)] dx dv dn dw. \end{aligned}$$

Therefore, we replace $\varphi(x, v) - \varphi(x + \sigma n, w)$ by (3.4.4) and (3.4.3)

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 n_i \varphi_4 dx dv dn dw \\ &= \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^\sigma \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 \langle v + w, n \rangle \\ & \quad \times \langle n, \nabla_x \phi(x + sn, v) \rangle dx dv dn dw ds \\ & - \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\pi/2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 \langle v + w, n \rangle \\ & \quad \times \langle w_\theta, \nabla_v \phi(x + \sigma n, v_\theta) \rangle dx dv dn dw d\theta. \end{aligned}$$

Finally, we perform the change of variables to ensure the variables of φ is exact x and v ,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 \langle v + w, n \rangle \varphi_4 dx dv dn dw \\ &= - \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\pi/2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 \langle v + w, n \rangle \\ & \quad \times \langle w_\theta, \nabla_v \varphi(x + \sigma n, v_\theta) \rangle dx dv dn dw d\theta. \end{aligned}$$

Then we rotate the velocities by $-\theta$, and translate x along n by σ ,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \chi(x + \frac{1}{2}\sigma n) f(x, v) f(x + \sigma n, w) \langle v - w, n \rangle_+^2 \langle v + w, n \rangle \varphi_4 dx dv dn dw \\ &= \left(- \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} \int_0^{\pi/2} \chi(x - \frac{1}{2}\sigma n) f(x - \sigma n, v_{-\theta}) f(x, w_{-\theta}) \langle v_{-\theta} - w_{-\theta}, n \rangle_+^2 \right. \\ & \quad \left. \times \langle v_{-\theta} + w_{-\theta}, n \rangle w dn dw d\theta, \nabla_v \varphi(x, v) \right)_{x,v}. \end{aligned}$$

In summary, we have

$$\begin{aligned} & (|v|^2 E[f, f](x, v), \varphi(x, v))_{x,v} = (-\mathcal{J}_0^E[|v|^2 f, f], \nabla_v \phi)_{x,v} \\ & - \left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[\langle v, n \rangle^2 f, f] dn, \nabla_v \varphi \right)_{x,v} + \left(- \int_{\mathbb{S}^2} \mathfrak{J}_0^E[f, \langle w, n \rangle^2 f] dn, \nabla_v \varphi \right)_{x,v} \\ & - \frac{1}{2} \left(\int_{\mathbb{R}^3 \times \mathbb{S}^2} \int_0^\sigma \chi(x + (\frac{1}{2}\sigma - s)n) f(x - sn, v) f(x + (\sigma - s)n, w) \right. \\ & \quad \left. \times \langle v - w, n \rangle_+^2 \langle v + w, n \rangle n dw dn ds, \nabla_x \varphi(x, v) \right)_{x,v} \\ & - \frac{1}{2} \left(- \int_{\mathbb{R}^3 \times \mathbb{S}^2} \int_0^{\pi/2} \chi(x - \frac{1}{2}\sigma n) f(x - \sigma n, v_{-\theta}) f(x, w_{-\theta}) \langle v_{-\theta} - w_{-\theta}, n \rangle_+^2 \right. \\ & \quad \left. \times \langle v_{-\theta} + w_{-\theta}, n \rangle w dn dw d\theta, \nabla_v \varphi(x, v) \right)_{x,v}, \end{aligned}$$

which is the weak formulation of (3.2.7). $\square$

3.5 Proof of Theorem 3.2.2

We have analogous results for Povzner collision integral.

Lemma 3.5.1. *Let $f, g \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ with rapidly decay at infinity. For each test function $\phi \in C(\mathbb{R}^3 \times \mathbb{R}^3)$ with at most polynomial growth at infinity,*

$$(P[f, g], \phi)_{x,v} := \int_{\mathbb{R}^3 \times \mathbb{R}^3} P[f, g](x, v) \phi(x, v) dx dv$$

$$= \int_{(\mathbb{R}^3)^4} f(x, v) g(y, w) J(x - y, v - w) [\phi(x, v') - \phi(x, v)] dx dy dv dw. \quad (3.5.1)$$

Proof. We do the transformation $(v, w) \mapsto (v', w')$ for the gain term in (3.1.15), then the left-hand side of (3.5.1) becomes

$$\int_{(\mathbb{R}^3)^4} f(x, v) g(y, w) J(x - y, v' - w') \phi(x, v') dx dy dv dw.$$

We can conclude with the help of assumption (3.1.17). $\square$

3.5.1 Mass current for Povzner collision integral: Proof of (3.2.13)

Proof. Note that

$$\begin{aligned} \phi(x, v') - \phi(x, v) &= \int_0^{\langle v-w, \frac{y-x}{|y-x|} \rangle} \frac{d}{ds} \phi \left(x, v - s \frac{y-x}{|y-x|} \right) ds \\ &= - \int_0^{\langle v-w, \frac{y-x}{|y-x|} \rangle} \left\langle \frac{y-x}{|y-x|}, \nabla_v \phi \left(x, v - s \frac{y-x}{|y-x|} \right) \right\rangle ds, \end{aligned}$$

We substitute the identity above into (3.5.1). Subsequently, we translate v and w in the direction $\frac{y-x}{|y-x|}$ by s , then we can rewrite $(P[f, g], \phi)_{x,v}$ by

$$\begin{aligned} & - \int_{(\mathbb{R}^3)^4} \int_0^{\langle v-w, \frac{y-x}{|y-x|} \rangle} f \left(x, v + s \frac{y-x}{|y-x|} \right) g \left(y, w + s \frac{y-x}{|y-x|} \right) \\ & \quad \times J(x - y, v - w) \left\langle \frac{y-x}{|y-x|}, \nabla_v \phi(x, v) \right\rangle ds dy dw dx dv. \end{aligned}$$

Using the notation of Landau mass current for the Povzner collision integral (3.2.2), we may represent $(P[f, g], \phi)_{x,v}$ by

$$\left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P[f, g] dy, \nabla_v \phi(x, v) \right)_{x,v}$$

We merely need to let $f = g$ to deduce the desired result in the sense of distributions. $\square$

3.5.2 Momentum current for Povzner collision integral: Proof of (3.2.14)(3.2.15)(3.2.16)

Proof. We apply Lemma 3.5.1 to the test function $v_i \phi(x, v)$ for $i = 1, 2, 3$. We reformulate $(P[f, f] v_i, \phi)$ by

$$\int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) [v'_i \phi(x, v') - v_i \phi(x, v)] dx dy dv dw.$$

Then we split the difference $v'\phi(x, v') - v\phi(x, v)$ into two parts,

$$v'_i[\phi(x, v') - \phi(x, v)] + [v'_i - v_i]\phi(x, v)$$

Thereafter, we use the i -th component of (3.1.3) to replace v'_i , hence

$$\begin{aligned} & \underbrace{v_i[\phi(x, v') - \phi(x, v)]}_{=:\phi_1} - \underbrace{\left\langle v, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i [\phi(x, v') - \phi(x, v)]}_{=:\phi_2} \\ & + \underbrace{\left\langle w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i [\phi(x, v') - \phi(x, v)]}_{=:\phi_3} \\ & - \underbrace{\left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i \phi(x, v)}_{=:\phi_4}. \end{aligned}$$

We use Lemma 3.5.1 for ϕ_1 , which shows

$$\int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \phi_1 dx dv dy dw = (P[v_i f, f], \phi)_{x, v}.$$

Following this, we use (3.2.13), which we obtained in the last section. It shows that

$$\int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \phi_1 dx dv dy dw = (-\mathcal{J}_0^P[v_i f, f], \nabla_v \phi)_{x, v}.$$

By the same token, we can deal with ϕ_2 and ϕ_3 ,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \phi_2 dx dv dy dw \\ & = \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[\left\langle v, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i f, f \right] dy, \nabla_v \phi \right)_{x, v}, \end{aligned}$$

and

$$\begin{aligned} & \int_{(\mathbb{R}^3)^4} f(x, v) f(x + \sigma n, w) J(x-y, v-w) \phi_3 dx dv dy dw \\ & = \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[f, \left\langle w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i f \right] dy, \nabla_v \phi \right)_{x, v}. \end{aligned}$$

Thanks to (3.1.16), we change variables from (v, w, x, y) to (w, v, y, x) ,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \phi_4 dx dv dn dw \\ & = - \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left(\frac{y-x}{|y-x|} \right)_i \end{aligned}$$

$$\times \phi(y, w) dx dv dn dw,$$

Symmetrizing the identity above

$$\begin{aligned} & \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \phi_4 dx dv dy dw \\ &= \frac{1}{2} \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{y - x}{|y - x|} \right)_i \\ & \quad \times [\phi(x, v) - \phi(y, w)] dx dv dy dw. \end{aligned}$$

Notice that

$$\begin{aligned} \phi(x, v) - \phi(y, w) &= - \int_0^{\pi/2} \frac{d}{d\theta} \phi(x_\theta, v_\theta) d\theta \\ &= - \int_0^{\pi/2} \langle y_\theta, \nabla_x \phi(x_\theta, v_\theta) \rangle + \langle w_\theta, \nabla_v \phi(x_\theta, v_\theta) \rangle d\theta, \end{aligned} \quad (3.5.2)$$

where (v_θ, w_θ) are defined in (3.4.5), and (x_θ, y_θ) are determined by

$$\begin{pmatrix} x_\theta \\ y_\theta \end{pmatrix} := \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \quad (3.5.3)$$

Hence we plug (3.5.2) into the ϕ_4 term,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{y - x}{|y - x|} \right)_i \phi_4 dx dv dn dw \\ &= \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x, v) f(y, w) J(x - y, v - w) \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{y - x}{|y - x|} \right)_i \\ & \quad \times [\langle y_\theta, \nabla + \phi(x_\theta, v_\theta) \rangle + \langle w_\theta, \nabla_v \phi(x_\theta, v_\theta) \rangle] dx dv dn dw ds. \end{aligned}$$

Then we rotate both the positions and velocities by $-\theta$,

$$\begin{aligned} & \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{y - x}{|y - x|} \right)_i \phi_4 dx dv dn dw \\ &= \left(- \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \right. \\ & \quad \times \left(\frac{x_{-\theta} - y_{-\theta}}{|x - y|} \right)_i w dn dw d\theta, \nabla_v \phi(x, v) \Big)_{x, v} \\ &+ \left(- \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \right. \\ & \quad \times \left(\frac{x_{-\theta} - y_{-\theta}}{|x - y|} \right)_i y dn dw d\theta, \nabla_x \phi(x, v) \Big)_{x, v}, \end{aligned}$$

since

$$\left\langle v - w, \frac{y - x}{|y - x|} \right\rangle = \left\langle v_{-\theta} - w_{-\theta}, \frac{y_{-\theta} - x_{-\theta}}{|y_{-\theta} - x_{-\theta}|} \right\rangle,$$

and

$$|y_{-\theta} - x_{-\theta}| = |y - x|.$$

For $i = 1, 2, 3$, sum them all together, we arrive the weak formulation of (3.2.14)-(3.2.16):

$$\begin{aligned} (v_i P[f, f](x, v), \phi(x, v))_{x, v} &= (-\mathcal{J}_0^P[v_i f, f], \nabla_v \phi)_{x, v} \\ &\quad - \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[\left\langle v, \frac{y - x}{|y - x|} \right\rangle \left(\frac{y - x}{|y - x|} \right)_i f, f \right] dy, \nabla_v \phi \right)_{x, v} \\ &\quad + \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[f, \left\langle w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{y - x}{|y - x|} \right)_i f \right] dy, \nabla_v \phi \right)_{x, v} \\ &\quad - \frac{1}{2} \left(- \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \right. \\ &\quad \times \left. \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{x_{-\theta} - y_{-\theta}}{|x_{-\theta} - y_{-\theta}|} \right)_i w dn dw d\theta, \nabla_v \phi(x, v) \right)_{x, v} \\ &\quad - \frac{1}{2} \left(- \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \right. \\ &\quad \times \left. \left\langle v - w, \frac{y - x}{|y - x|} \right\rangle \left(\frac{x_{-\theta} - y_{-\theta}}{|x_{-\theta} - y_{-\theta}|} \right)_i y dn dw d\theta, \nabla_x \phi(x, v) \right)_{x, v}. \end{aligned}$$

□

If we additionally assume $\widehat{J(x - y, v - w)}$ is radially symmetric, i.e. $J(x - y, v - w) = J(|x - y|, |v - w|, \cos(x - y, v - w))$, which is true for Boltzmann collision kernel. $J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta})$ can be further simplified by $J(x - y, v - w)$.

3.5.3 Energy current for Povzner collision integral: Proof of (3.2.17)

Proof. Using the test function $\phi(x, v) = |v|^2 \varphi(x, v)$ in the statement of Lemma 3.5.1, we obtain:

$$\begin{aligned} &\int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x - y, v - w) \\ &\quad \times [|v'|^2 \varphi(x, v') - |v|^2 \varphi(x, v)] dx dv dy dw. \end{aligned}$$

Then, with the help of (3.1.3), we split the difference $|v'|^2 \varphi(x, v') - |v|^2 \varphi(x, v)$ into four parts,

$$\underbrace{|v|^2 [\varphi(x, v') - \varphi(x, v)]}_{=:\varphi_1} - \underbrace{\left\langle v, \frac{y - x}{|y - x|} \right\rangle^2 [\phi(x, v') - \phi(x, v)]}_{=:\varphi_2}$$

$$\begin{aligned}
& + \underbrace{\left\langle w, \frac{y-x}{|y-x|} \right\rangle^2}_{=:\varphi_3} [\varphi(x, v') - \varphi(x, v)] \\
& \quad - \underbrace{\left(\left\langle v, \frac{y-x}{|y-x|} \right\rangle^2 - \left\langle w, \frac{y-x}{|y-x|} \right\rangle^2 \right)}_{=:\varphi_4} \varphi(x, v),
\end{aligned}$$

since

$$\begin{aligned}
|v'|^2 &= \left| v - \left\langle v - w, \frac{y-x}{|y-x|} \right\rangle \frac{y-x}{|y-x|} \right|^2 \\
&= |v|^2 - \left\langle v, \frac{y-x}{|y-x|} \right\rangle^2 + \left\langle w, \frac{y-x}{|y-x|} \right\rangle^2.
\end{aligned}$$

Following this, we use the result (3.2.13), which we obtained in the last section. It shows that

$$\begin{aligned}
& \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) (\varphi_1 - \varphi_2 + \varphi_3) dx dv dy dw \\
&= \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[(|v|^2 - \left\langle v, \frac{y-x}{|y-x|} \right\rangle^2) f, f \right] \right. \\
& \quad \left. + \mathfrak{J}_0^E \left[f, \left\langle w, \frac{y-x}{|y-x|} \right\rangle^2 f \right] dy, \nabla_v \phi \right)_{x,v}.
\end{aligned}$$

By the same process showed before, We perform the change of variables $(v, w, x, y) \mapsto (w, v, y, x)$ in φ_4 term, then symmetrize it,

$$\begin{aligned}
& \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \varphi_4 dx dv dy dw \\
&= \frac{1}{2} \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle \\
& \quad \times [\varphi(x, v) - \varphi(y, w)] dx dv dy dw.
\end{aligned}$$

Therefore, we replace $\varphi(x, v) - \varphi(y, w)$ by (3.5.2),

$$\begin{aligned}
& \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \varphi_4 dx dv dy dw \\
&= - \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} J(x-y, v-w) \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle \\
& \quad \times f(x, v) f(y, w) \langle y_\theta, \nabla_x \phi(x_\theta, v_\theta) \rangle dx dv dy dw d\theta
\end{aligned}$$

$$\begin{aligned}
& - \int_{(\mathbb{R}^3)^4} \int_0^{\pi/2} J(x-y, v-w) \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle \\
& \quad \times f(x, v) f(y, w) \langle w_\theta, \nabla_v \phi(x_\theta, v_\theta) \rangle dx dv dy dw d\theta.
\end{aligned}$$

Finally, we rotate both the positions and velocities by $-\theta$,

$$\begin{aligned}
& \int_{(\mathbb{R}^3)^4} f(x, v) f(y, w) J(x-y, v-w) \varphi_4 dx dv dy dw \\
& = \left(- \int_{(\mathbb{R}^3)^2} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \right. \\
& \quad \times \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle dy dw d\theta, \nabla_x \phi(x, v) \Bigg)_{x,v} \\
& + \left(- \int_{(\mathbb{R}^3)^2} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \right. \\
& \quad \times \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle w dy dw d\theta, \nabla_v \phi(x, v) \Bigg)_{x,v}.
\end{aligned}$$

In summary, we have

$$\begin{aligned}
& (|v|^2 P[f, f](x, v), \varphi(x, v))_{x,v} = (-\mathcal{J}_0^P[|v|^2 f, f], \nabla_v \phi)_{x,v} \\
& - \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P \left[\left\langle v, \frac{y-x}{|y-x|} \right\rangle^2 f, f \right] dy, \nabla_v \varphi \right)_{x,v} \\
& + \left(- \int_{\mathbb{R}^3} \mathfrak{J}_0^P [f, \left\langle w, \frac{y-x}{|y-x|} \right\rangle^2 f] dy, \nabla_v \varphi \right)_{x,v} \\
& - \frac{1}{2} \left(- \int_{(\mathbb{R}^3)^2} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \right. \\
& \quad \times \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle dy dw d\theta, \nabla_x \phi(x, v) \Bigg)_{x,v} \\
& - \frac{1}{2} \left(- \int_{(\mathbb{R}^3)^2} \int_0^{\pi/2} f(x_{-\theta}, v_{-\theta}) f(y_{-\theta}, w_{-\theta}) J(x_{-\theta} - y_{-\theta}, v_{-\theta} - w_{-\theta}) \right. \\
& \quad \times \left\langle v-w, \frac{y-x}{|y-x|} \right\rangle \left\langle v+w, \frac{y-x}{|y-x|} \right\rangle w dy dw d\theta, \nabla_v \phi(x, v) \Bigg)_{x,v},
\end{aligned}$$

which is the weak formulation of (3.2.7). $\square$

3.6 Conclusion

This paper serves as a complement to [CCG24]. While the general framework developed there does not cover all delocalized collision models, we have here established conservative formulations for two cases that fall outside the framework given in [CCG24], namely the

original Povzner and standard Enskog collision integrals. A key feature of our result is that it does not rely on asymptotic expansions around equilibrium: the conservative form remains valid for distributions far from equilibrium, thereby extending its mathematical and physical relevance. This provides new insight into the structure of kinetic models where standard perturbative approaches fail, and reinforces the role of conservation and entropy principles in non-equilibrium regimes.

As a perspective, and in analogy with [CCG24], we plan to extend these results to multispecies systems. In particular, we aim to investigate how the delocalized collision framework can be adapted to the study of dense gases.

Chapter 4

Derive the Enskog-Enskog system from particle system

Introduction

Multicomponent gas systems play a central role in various physical and engineering applications, ranging from astrophysics to industrial processes involving particulate suspensions and granular materials. Many models have been proposed to describe such systems. For binary mixtures, the most common modelling approaches include:

- A fluid equation coupled with another fluid equation, such as the Euler, Navier–Stokes, or Stokes equations;
- A fluid equation coupled with a kinetic equation, such as the Vlasov or Boltzmann equation;
- Two coupled kinetic equations.

This paper focuses on the third type of model—two coupled kinetic equations. Specifically, if we denote by $f \equiv f(t, x, w) \geq 0$ and $F \equiv F(t, x, v) \geq 0$ the velocity distribution functions of gas molecules and particles, respectively, at time t , position $x \in \mathbb{R}^3$, and velocities $w, v \in \mathbb{R}^3$, then f and F satisfy the following partial differential equations:

$$\begin{cases} \partial_t f + w \cdot \nabla_x f = \mathcal{R}[F, f] + \mathcal{C}[F]; \\ \partial_t F + v \cdot \nabla_x F = \mathcal{D}[f, F] + \mathcal{P}[f], \end{cases}$$

where $\mathcal{R}, \mathcal{C}, \mathcal{D}$ and $\mathcal{P}$ stand for collision operators. For dilute binary gas mixtures, the classical Boltzmann equation offers a well-established framework for capturing the dynamics of particle interactions.

However, as the system becomes denser—particularly with an increasing concentration of one component—the assumptions underlying the Boltzmann equation become inadequate. It is essential to retain the delocalization effect, which reflects the spatial correlation between particles during collisions. In regimes where interparticle correlations due to finite density

are significant, the Enskog equation provides a more accurate description. Originally developed by D. Enskog [Ens22] as an extension of the Boltzmann equation for dense gases, the Enskog framework accounts for the increased frequency of collisions and spatial correlations between particles. To model a multicomponent gas-particle system in such dense regimes, we employ a set of coupled Enskog equations that capture the interactions between gas molecules and dispersed particles more faithfully than dilute-limit approximations.

This paper is devoted to the formulation and properties of a coupled kinetic model based on the Enskog equation for a binary mixture. Our goal is to establish a framework for describing the dynamics of dense gas-particle systems, with particular attention to the effects of composition and particle interactions on transport properties and evolution. This derivation is grounded in the BBGKY (Bogoliubov–Born–Green–Kirkwood–Yvon) hierarchy, a fundamental tool in nonequilibrium statistical mechanics for describing the evolution of marginal distributions in a many-particle system. This work also establishes the basis for mathematically deriving the thick sprays model.

In addition to deriving the coupled kinetic equations, we also establish the macroscopic conservation laws governing mass, momentum, and energy for both species. These equations form the basis for continuum descriptions of multicomponent flows and are critical for applications in fluid dynamics and thermodynamics. Furthermore, we introduce an appropriate entropy functional for the coupled Enskog system and prove an H-theorem, demonstrating that the entropy is non-increasing in time. This provides a fundamental link between the microscopic reversibility of Newtonian dynamics and the macroscopic irreversibility observed in thermodynamic systems.

The outline of this paper is as follows: In Section 4.1, we review the classical derivation of the Boltzmann equation from a microscopic perspective, and we show the conservation laws of mass, momentum and energy for each species, and the entropy inequality for coupled Boltzmann system. Our main results are presented in Section 4.2. In particular, the target system is introduced in Section 4.2.1, followed by the derivation of the corresponding conservation laws in Section 4.2.2, and the entropy inequality for the coupled Enskog system is established in Section 4.2.3. Section 4.3 is devoted to the formal derivation of the coupled Enskog equations from Newtonian mechanics.

4.1 The classical model

4.1.1 Derivation of Boltzmann equation

Consider a system governed by Newtonian mechanics, consisting of N identical particles of a single species. Let the position and velocity of the i -th particle at time t be denoted by $X_i(t), V_i(t) \in \mathbb{R}^3$, respectively, for $1 \leq i \leq N$. Each particle is assumed to be a rigid sphere of fixed radius $r > 0$. The time evolution of the system is determined by the following Hamilton's equations:

$$\begin{cases} \frac{dX_i}{dt} = \frac{\partial \mathcal{H}}{\partial V_i}, \\ \frac{dV_i}{dt} = -\frac{\partial \mathcal{H}}{\partial X_i}, \end{cases} \quad \text{for } 1 \leq i \leq N, \text{ in } \Omega \quad (4.1.1)$$

where the Hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H}(t) = \sum_{i=1}^N \frac{|V_i(t)|^2}{2},$$

with the admissible phase space domain Ω is defined as

$$\Omega := \{(X_1, \dots, X_N) \in \mathbb{R}^{6N} : |X_i - X_j| \geq 2r\}.$$

On the boundary, we impose the specular reflection condition, whose explicit formulation will be provided in Section 4.3.

Grad [Gra49] derived the Boltzmann equation for velocity distribution function $f(t, x, v)$ by BBGKY hierachy under the Boltzmann-Grad limit

$$\partial_t f(t, x, w) + w \cdot \nabla_x f(t, x, w) = \mathcal{B}[f](t, x, w),$$

where the Boltzmann collision integral is defined by

$$\mathcal{B}[f](t, x, w) := \int_{\mathbb{R}^3 \times \mathbb{S}^2} (f(t, x, w^o) f(t, x, w_1^o) - f(t, x, w) f(t, x, w_1)) b(w - w_1, n) dw_1 dn. \quad (4.1.2)$$

Here $b \equiv b(z, \xi)$ denotes collision kernel, and pre-collision velocities (w^o, w_1^o) are given by

$$\begin{cases} w^o(w, w_1, n) = w - (w - w_1) \cdot nn \\ w_1^o(w, w_1, n) = w_1 - (w - w_1) \cdot nn. \end{cases} \quad (4.1.3)$$

Furthermore, for a system consisting of particles with mass m_p and gas molecules with mass m_g , let $f \equiv f(t, x, w)$ and $F \equiv F(t, x, w)$ denote the respective distribution functions of gas molecules and particles. We can obtain the following coupled Boltzmann equations of binary mixture by a similar technique:

$$\begin{cases} \partial_t f + w \cdot \nabla_x f = \mathcal{B}[f] + \mathcal{B}_1[f, F] \\ \partial_t F + v \cdot \nabla_x F = \mathcal{B}_2[F, f] + \mathcal{B}[F], \end{cases} \quad (4.1.4)$$

where Boltzmann collision integrals $\mathcal{B}_1, \mathcal{B}_2$ are defined by

$$\begin{aligned} \mathcal{B}_1[f, F](w) &= \int_{\mathbb{R}^3 \times \mathbb{S}^2} (f(w') F(v') - f(w) F(v)) b(v - w, n) dv dn \\ \mathcal{B}_2[F, f](v) &= \int_{\mathbb{R}^3 \times \mathbb{S}^2} (f(w') F(v') - f(w) F(v)) b(v - w, n) dw dn, \end{aligned}$$

with the pre-collision velocities

$$\begin{cases} w'(v, w, n, \eta) = w + \frac{2}{1 + \eta} (v - w) \cdot nn \\ v'(v, w, n, \eta) = v - \frac{2\eta}{1 + \eta} (v - w) \cdot nn, \end{cases} \quad (4.1.5)$$

where $\eta := m_g/m_p \leq 1$ represents the mass ratio between different species. And $\mathcal{B}_0$ is classical Boltzmann collision integral defined in (4.1.2). For a detailed treatment of the two-species case in the context of coupled Boltzmann equations, we refer the reader to Chapter 8 in [CC70], rigorously in [AMP22]. At the end of this subsection, we state several properties of pre-collision velocities given by (4.1.3) and (4.1.5), whose verification is straightforward:

- Pre-collision velocities are even function with respect to n

$$\begin{aligned} v'(v, w, n) &= v'(v, w, -n); & w'(v, w, n) &= w'(v, w, -n) \\ v^o(v, v_*, n) &= v^o(v, v_*, -n); & v_*^o(v, v_*, n) &= v_*^o(v, v_*, -n) \end{aligned} \quad (4.1.6)$$

- The collision process is reversible

$$\begin{aligned} v'(v', w', n) &= v; & w'(v', w', n) &= w \\ v^o(v^o, v_*^o, n) &= v; & v_*^o(v^o, v_*^o, n) &= v_* \end{aligned} \quad (4.1.7)$$

- The result above gives the absolute value the determinant of the Jacobian of the change of variable is 1

$$\left| \det \frac{\partial(v', w')}{\partial(v, w)} \right| = \left| \det \frac{\partial(v^o, v_*^o)}{\partial(v, v_*)} \right| = 1 \quad (4.1.8)$$

- The collision is specular reflection with respect to norm vector n

$$\begin{aligned} (v'(v, w, n) - w'(v, w, n)) \cdot n &= -(v - w) \cdot n \\ (v^o(v, v_*, n) - v_*^o(v, v_*, n)) \cdot n &= -(v - v_*) \cdot n \end{aligned} \quad (4.1.9)$$

4.1.2 Conservation laws for Boltzmann-Boltzmann system

We can naturally establish conservation laws from coupled Boltzmann equations with the following definitions

$$\begin{aligned} \rho_g(t, x) &:= \int_{\mathbb{R}^3} f(t, x, w) dw \\ u_g(t, x) &:= \frac{\mathbb{1}_{\rho_g(t, x) > 0}}{\rho_g(t, x)} \int_{\mathbb{R}^3} w f(t, x, w) dw \\ P_g(t, x) &:= \int_{\mathbb{R}^3} (w - u_g(t, x))^{\otimes 2} f(t, x, w) dw \\ \theta_g(t, x) &:= \frac{\mathbb{1}_{\rho_g(t, x) > 0}}{\rho_g(t, x)} \int_{\mathbb{R}^3} \frac{|w - u_g(t, x)|^2}{2} f(t, x, w) dw \\ q_g(t, x) &:= \frac{1}{2} \int_{\mathbb{R}^3} (w - u_g(t, x)) |w - u_g(t, x)|^2 f(t, x, w) dw \end{aligned} \quad (4.1.10)$$

$$\begin{aligned}
\rho_\ell(t, x) &:= \int_{\mathbb{R}^3} F(t, x, v) dv \\
u_\ell(t, x) &:= \frac{\mathbb{1}_{\rho_\ell(t, x) > 0}}{\rho_\ell(t, x)} \int_{\mathbb{R}^3} v F(t, x, v) dv \\
P_\ell(t, x) &:= \int_{\mathbb{R}^3} (v - u_\ell(t, x))^{\otimes 2} F(t, x, v) dv \\
\theta_\ell(t, x) &:= \frac{\mathbb{1}_{\rho_\ell(t, x) > 0}}{\rho_\ell(t, x)} \int_{\mathbb{R}^3} \frac{|v - u_\ell(t, x)|^2}{2} F(t, x, v) dv \\
q_\ell(t, x) &:= \frac{1}{2} \int_{\mathbb{R}^3} (v - u_\ell(t, x)) |v - u_\ell(t, x)|^2 F(t, x, v) dv.
\end{aligned} \tag{4.1.11}$$

We multiply the coupled Boltzmann equations (4.1.4) by $1, w, \frac{1}{2}|w|^2$ for the gas molecules and $1, v, \frac{1}{2}|v|^2$ for the particles, and then integrate with respect to the velocity variables w or v , respectively. Moreover, with the help of the following proposition, we obtain the interaction between two species:

Proposition 4.1.1. *For any test function $\varphi(v) \in C^\infty(\mathbb{R}^3)$, we have the following identity,*

$$\begin{aligned}
&\eta \int_{\mathbb{R}^3} \mathcal{B}_1[f, F](w) \varphi(w) dw + \int_{\mathbb{R}^3} \mathcal{B}_2[F, f](v) \varphi(v) dv \\
&= \int_{\mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} f(w) F(v) b(v - w, n) [\eta \varphi(w') + \varphi(v') - \eta \varphi(w) - \varphi(v)] dn dv dw. \tag{4.1.12}
\end{aligned}$$

The proof of the proposition follows directly by performing the pre-to-post transformation on the gain terms of both collision integrals. One can also refer to [DGR19] for details. Because momentum and energy are conserved during the collisions (4.3.2), taking $\varphi(v) = v$ or $|v|^2$ in the weak formulation (4.1.12) implies the right-hand side of equation (4.1.12) vanishes. Consequently, the force and energy are balanced between two phases.

Hence, we obtain the equations for the dispersed phase (fluid bed)

$$\begin{cases} \partial_t \rho_g + \operatorname{div}_x(\rho_g u_g) = 0 \\ \partial_t(\rho_g u_g) + \operatorname{div}_x(\rho_g u_g^{\otimes 2}) + \operatorname{div}_x P_g = F_B^{\text{int}} \\ \partial_t \left(\rho_g \frac{1}{2} |u_g|^2 + \rho_g \theta_g \right) + \operatorname{div}_x \left(\rho_g \frac{1}{2} u_g |u_g|^2 + \rho_g u_g \theta_g \right) + \operatorname{div}_x(P_g u_g + q_g) = E_B^{\text{int}}, \end{cases} \tag{4.1.13}$$

and the equations for the continuous phase (droplets)

$$\begin{cases} \partial_t \rho_\ell + \operatorname{div}_x(\rho_\ell u_\ell) = 0 \\ \partial_t(\rho_\ell u_\ell) + \operatorname{div}_x(\rho_\ell u_\ell^{\otimes 2}) + \operatorname{div}_x P_\ell = -\eta F_B^{\text{int}} \\ \partial_t \left(\rho_\ell \frac{1}{2} |u_\ell|^2 + \rho_\ell \theta_\ell \right) + \operatorname{div}_x \left(\rho_\ell \frac{1}{2} u_\ell |u_\ell|^2 + \rho_\ell u_\ell \theta_\ell \right) + \operatorname{div}_x(P_\ell u_\ell + q_\ell) = -\eta E_B^{\text{int}}, \end{cases} \tag{4.1.14}$$

where interaction force F_B^{int} , and energy exchange E_B^{int} are given by

$$F_B^{\text{int}}(t, x) := \int_{\mathbb{R}^3} \mathcal{B}_1[f, F](t, x, w) w dw, \quad E_B^{\text{int}}(t, x) := \int_{\mathbb{R}^3} \mathcal{B}_1[f, F](t, x, w) \frac{|w|^2}{2} dw. \tag{4.1.15}$$

We define the total mass, momentum, and energy for each species are

$$\begin{aligned} M_g(t) &:= \int_{\mathbb{R}^3} \rho_g dx & M_\ell(t) &:= \int_{\mathbb{R}^3} \rho_\ell dx \\ Q_g(t) &:= \int_{\mathbb{R}^3} \rho_g u_g dx & Q_\ell(t) &:= \int_{\mathbb{R}^3} \rho_\ell u_\ell dx \\ E_g(t) &:= \int_{\mathbb{R}^3} \rho_g \frac{|u_g|^2}{2} + \rho_g \theta_g dx & E_\ell(t) &:= \int_{\mathbb{R}^3} \rho_\ell \frac{|u_\ell|^2}{2} + \rho_\ell \theta_\ell dx \end{aligned} \quad (4.1.16)$$

From these equations, we can observe that both species conserves mass individually

$$\frac{d}{dt} M_g = \frac{d}{dt} M_\ell = 0. \quad (4.1.17)$$

Although, each species does not conserve momentum, the total momentum of the system is conserved

$$\frac{d}{dt} (\eta Q_g + Q_\ell) = 0. \quad (4.1.18)$$

A similar conservation law holds for the total energy:

$$\frac{d}{dt} (\eta E_g + E_\ell) = 0. \quad (4.1.19)$$

4.1.3 Entropy for Boltzmann-Boltzmann system

Studying the entropy of coupled Boltzmann equations is essential for understanding the thermodynamic behavior and convergence dynamics of multi-component kinetic systems. Entropy functionals enable one to rigorously analyze the H-theorem in the coupled context, quantify dissipation rates, and derive convergence to equilibrium with explicit rates under appropriate conditions. These methods are instrumental in establishing well-posedness, long-time stability, and macroscopic limits for interacting species. Building on foundational entropy frameworks in kinetic theory—such as Villani’s review on collisional kinetic theory [Vil02] and the quantitative approach to trend to equilibrium [DV05]—entropy-based techniques have also been applied in multi-species and reaction-diffusion settings (e.g. [DFT17]). Extending these methods to truly coupled Boltzmann systems allows the derivation of entropy-entropy dissipation inequalities tailored to inter-species interactions, enabling the study of exponential return to equilibrium, propagation of regularity, and robust numerical schemes that preserve structural properties.

The entropy of the system (4.1.4) is simply the sum of the two Boltzmann entropies:

$$S_{\text{BB}}(t) := \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, x, w) \ln f(t, x, w) dx dw + \int_{\mathbb{R}^3 \times \mathbb{R}^3} F(t, x, v) \ln F(t, x, v) dx dv. \quad (4.1.20)$$

Then we can propose the following proposition:

Proposition 4.1.2. *Let f and F be classical solution of (4.1.4). Assume that $(x, v) \mapsto F(t, x, v)$ and $(x, w) \mapsto f(t, x, w)$ rapidly decaying at infinity, while $(x, w) \mapsto \ln f(t, x, w)$*

and $(x, v) \mapsto \ln F(t, x, v)$ have at most polynomial growth at infinity. Then

$$\frac{d}{dt} S_{\text{BB}} \leq 0. \quad (4.1.21)$$

Proof.

$$\begin{aligned} \frac{d}{dt} S_{\text{BB}} &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \partial_t f(t, x, w) \ln f(t, x, w) dx dw + \frac{d}{dt} M_g \\ &\quad + \int_{\mathbb{R}^3 \times \mathbb{R}^3} \partial_t F(t, x, v) \ln F(t, x, v) dx dv + \frac{d}{dt} M_\ell. \end{aligned}$$

We have already shown that both of the species conserves its mass. Since f and F satisfy equations (4.1.4), it follows that

$$\begin{aligned} \frac{d}{dt} S_{\text{BB}} &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} (-w \cdot \nabla_x f + \mathcal{B}_0[f] + \mathcal{B}_1[f, F]) \ln f dx dw \\ &\quad + \int_{\mathbb{R}^3 \times \mathbb{R}^3} (-v \cdot \nabla_x F + \mathcal{B}_0[F] + \mathcal{B}_2[F, f]) \ln F dx dv. \end{aligned}$$

Noting that

$$w \cdot \nabla_x f \ln f = \text{div}_x(w f \ln f) - \text{div}_x(w f),$$

and the classical H-theorem for Boltzmann collision integral shows

$$\int_{\mathbb{R}^3} \mathcal{B}_0[f] \ln f dw \leq 0,$$

we obtain

$$\frac{d}{dt} S_{\text{BB}} \leq \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{B}_1[f, F] \ln f dx dw + \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{B}_2[F, f] \ln F dx dv.$$

Performing the pre-to-post transformation on the gain term of collision integral $\mathcal{B}_1$ and $\mathcal{B}_2$, we find

$$\int_{\mathbb{R}^3} \mathcal{B}_1[f, F] \ln f dw + \int_{\mathbb{R}^3} \mathcal{B}_2[F, f] \ln F dv = \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} f(w) F(v) \ln \frac{f(w') F(v')}{f(w) F(v)} b(v-w, n) dn dv dw.$$

Thanks to the following fundamental inequality

$$\lambda(z) := z - 1 - \ln z \geq 0, \text{ for } z > 0 \quad (4.1.22)$$

we deduce

$$\frac{d}{dt} S_{\text{BB}} \leq \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} [f(w') F(v') - f(w) F(v)] b(v-w, n) dn dv dw dx = 0,$$

where the last equality follows from the change of variables $(v, w) \mapsto (v', w')$ given by (4.1.5) and the invariance of collision kernel b . $\square$

4.2 Main results

4.2.1 The coupled Enskog equations

Our first main result is formally deriving the following coupled Enskog equations:

$$\begin{cases} \partial_t f + w \cdot \nabla_x f = \mathcal{E}_0[f] + \mathcal{E}_1[f, F], \\ \partial_t F + v \cdot \nabla_x F = \mathcal{E}_2[F, f] + \mathcal{E}_3[F], \end{cases} \quad (4.2.1)$$

where Enskog collision integrals $\mathcal{E}_i$ with $i = 0, 1, 2, 3$ are defined by

$$\begin{aligned} \mathcal{E}_0[f] := & \frac{(2r_g)^2}{m_g} \int_{(w-w_*) \cdot n > 0} |(w-w_*) \cdot n| \left[Y^{(0,2)}[f, f](x, x-2r_g n) \right. \\ & \left. \times f(x, w^o) f(x-2r_g n, w_*^o) - Y^{(0,2)}[f, f](x, x+2r_g n) f(x, w) f(x+2r_g n, w_*) \right] \mathrm{d}n \mathrm{d}w_*, \end{aligned} \quad (4.2.2)$$

$$\begin{aligned} \mathcal{E}_1[f, F] := & \frac{(r_g+r_p)^2}{m_p} \int_{(v-w) \cdot n > 0} |(v-w) \cdot n| \left[Y^{(1,1)}[f, F](x, x+(r_g+r_p)n) \right. \\ & \left. \times f(x, w') F(x+(r_g+r_p)n, v') - Y^{(1,1)}[f, F](x, x-(r_g+r_p)n) f(x, w) F(x-(r_g+r_p)n, v) \right] \mathrm{d}n \mathrm{d}v. \end{aligned} \quad (4.2.3)$$

$$\begin{aligned} \mathcal{E}_2[F, f] := & \frac{(r_g+r_p)^2}{m_g} \int_{(v-w) \cdot n > 0} |(v-w) \cdot n| \left[Y^{(1,1)}[F, f](x, x-(r_g+r_p)n) \right. \\ & \left. \times F(x, v') f(x-(r_g+r_p)n, w') - Y^{(1,1)}[F, f](x, x+(r_g+r_p)n) F(x, v) f(x+(r_g+r_p)n, w) \right] \mathrm{d}n \mathrm{d}w, \end{aligned} \quad (4.2.4)$$

and

$$\begin{aligned} \mathcal{E}_3[F] := & \frac{(2r_p)^2}{m_p} \int_{(v-v_*) \cdot n > 0} |(v-v_*) \cdot n| \left[Y^{(2,0)}[F, F](x, x-2r_p n) \right. \\ & \left. \times F(x, v^o) F(x-2r_p n, v_*^o) - Y^{(2,0)}[F, F](x, x+2r_p n) F(x, v) F(x+2r_p n, v_*) \right] \mathrm{d}n \mathrm{d}v_*, \end{aligned} \quad (4.2.5)$$

where the pre-collision velocities are given by (4.1.3) and (4.1.5), and correlation pair functions $Y^{(i,j)}$ for $i, j \in \{0, 1, 2\}$ are defined later in (4.3.19).

The derivation process is presented in Section 4.3. A key insight in our approach is to correctly identify the direction of delocalization, a structural feature that is typically neglected in the classical Boltzmann hierarchy. By revisiting the BBGKY hierarchy for two interacting species and incorporating this directional dependence, we uncover the correct

formulation of the Enskog collision operators and provide a physically meaningful kinetic model that accounts for the anisotropy introduced by particle interactions at short distances.

Please note that in this context, f and F represent the *mass density* distribution functions of gas molecules and particles, respectively. If instead we wish to interpret $f_{\text{num}} := \frac{f}{m_g}$ and $F_{\text{num}} := \frac{F}{m_p}$ as *number density* distribution functions, then the prefactors $1/m_g$ or $1/m_p$ in front of each collision integral should be removed accordingly.

4.2.2 Conservation laws for Enskog-Enskog system

Unlike the classical Boltzmann collision integral, it conserves mass, momentum, and energy. In other words,

$$\int_{\mathbb{R}^3} \mathcal{B}[f](w) \begin{pmatrix} 1 \\ w_1 \\ w_2 \\ w_3 \\ |w|^2 \end{pmatrix} dw = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (4.2.6)$$

For the system governed by Enskog-Enskog equations (4.2.1), although the corresponding system will conserve mass, total momentum, and total energy globally, the system does not satisfy the same local conservation laws as in (4.1.13) and (4.1.14). We adopt the same notations defined in (4.1.10), (4.1.11), (4.2.10) and (4.1.16). From [CCG24]. We know that the Boltzmann-Enskog collision integral can be expressed in the following conservative form:

$$\mathcal{E}_0[f](w) \begin{pmatrix} 1 \\ w_1 \\ w_2 \\ w_3 \\ |w|^3 \end{pmatrix} = \begin{pmatrix} \text{div}_v \mathbb{J}_0 \\ \text{div}_x \mathbb{I}_1 + \text{div}_v \mathbb{J}_1 \\ \text{div}_x \mathbb{I}_2 + \text{div}_v \mathbb{J}_2 \\ \text{div}_x \mathbb{I}_3 + \text{div}_v \mathbb{J}_3 \\ \text{div}_x \mathbb{I}_4 + \text{div}_v \mathbb{J}_4 \end{pmatrix}, \quad (4.2.7)$$

where the explicit definitions of quantities $\mathbb{I}_k$ and $\mathbb{J}_k$ for $k = 0, 1, 2, 3, 4$ are given in the [CCG24]. The remaining question is how to handle the interaction terms $\mathcal{E}_1$ and $\mathcal{E}_2$. Considering this, we introduce the following proposition:

Proposition 4.2.1. *For Boltzmann-Enskog collision integrals defined in (4.2.3), (4.2.4) obeys the collision laws (4.3.4). Let $Y^{(1,1)} \equiv 1$. v', w' are given by (4.1.5). For any test function $\varphi(x, v) \in C^\infty(\mathbb{R} \times \mathbb{R})$, we have the following identity*

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{E}_1[f, F](w) \varphi(x, w) dw + \int_{\mathbb{R}^3} \mathcal{E}_2[F, f](v) \varphi(x, v) dv + \eta \text{div}_x I[f, F; \varphi] \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} a^2 f(x, w) F(x - an, v) (v - w) \cdot n H((v - w) \cdot n) \left[\eta \varphi(x - an, w') + \varphi(x, v') \right. \\ & \quad \left. - \eta \varphi(x - an, w) - \varphi(x, v) \right] dndvdw, \quad (4.2.8) \end{aligned}$$

where

$$I[f, F; \varphi] := \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \int_0^a a^2 n (v - w) \cdot n H((v - w) \cdot n) (\varphi(x + sn, w') - \varphi(x + sn, w))$$

$$f(x + sn, w)F(x - (a - s)n, v)dn dv dw ds.$$

Proof. We do the change of variables $(v, w, n) \mapsto (v', w', -n)$ for the gain terms of $\int_{\mathbb{R}^3} \mathcal{E}_1[f, F]\varphi(x, w)dw$ and $\int_{\mathbb{R}^3} \mathcal{E}_2[F, f]\varphi(x, v)dv$, the properties (5.3.9)-(5.3.12) show

$$\int_{\mathbb{R}^3} \mathcal{E}_1[f, F]\varphi(x, w)dw = \frac{a^2}{m_p} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \mathbb{S}^2} (\varphi(x, w') - \varphi(x, w)) f(x, w) F(x - an, v) (v - w) \cdot n H((v - w) \cdot n) dn dv dw,$$

and

$$\int_{\mathbb{R}^3} \mathcal{E}_2[F, f]\varphi(x, v)dv = \frac{a^2}{m_g} \int_{\mathbb{R}^3 \times \mathbb{R}^3 \mathbb{S}^2} (\varphi(x, v') - \varphi(x, v)) f(x + an, w) F(x, v) (v - w) \cdot n H((v - w) \cdot n) dn dv dw.$$

Therefore, we have

$$\begin{aligned} & \eta \int_{\mathbb{R}^3} \mathcal{E}_1[f, F]\varphi(x, w)dw + \int_{\mathbb{R}^3} \mathcal{E}_2[F, f]\varphi(x, v)dv \\ &= a^2 \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3} f(x + an, w) F(x, v) (v - w) \cdot n H((v - w) \cdot n) \left[\varphi(x, w') + \varphi(x + an, v') \right. \\ & \quad \left. - \eta \varphi(x, w) - \eta \varphi(x + an, v) \right] dn dv dw \\ & \quad + \eta \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} a^2 (v - w) \cdot n H((v - w) \cdot n) \left[(\varphi(x, w') - \varphi(x, w)) f(x, w) F(x - an, v) \right. \\ & \quad \left. - (\varphi(x + an, w') - \varphi(x + an, w)) f(x + an, w) F(x, v) \right] dn dv dw. \end{aligned}$$

The fundamental theorem of calculus shows

$$\Phi(x + an) - \Phi(x) = \int_0^a \frac{d}{ds} \Phi(x + sn) ds = \int_0^a n \cdot \nabla_x \Phi(x + sn) ds.$$

Since φ is smooth, and furthermore if $f(\cdot, w)F(\cdot, w)$ is smooth, then the last line of the right-hand side can be rewritten as

$$\begin{aligned} & -\eta \operatorname{div}_x \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} \int_0^a a^2 n (v - w) \cdot n H((v - w) \cdot n) (\varphi(x + sn, w') - \varphi(x + sn, w)) \\ & \quad f(x + sn, w) F(x - (a - s)n, v) dn dv dw ds. \end{aligned}$$

□

When we take test function $\varphi(x, v) = v$ or $\frac{|v|^2}{2}$ in (4.2.8), the right-hand side will still vanish due to (4.3.2). However, the drift term $I[f, F; \varphi]$ remains. This term introduces corrections to the macroscopic equations, leading to modifications in the momentum and

energy balances compared to Boltzmann-Boltzmann system:

$$\begin{cases} \partial_t \rho_g + \operatorname{div}_x(\rho_g u_g) = 0 \\ \partial_t(\rho_g u_g) + \operatorname{div}_x(\rho_g u_g^{\otimes 2}) + \operatorname{div}_x P_g = F_E^{\text{int}} \\ \partial_t \left(\rho_g \frac{1}{2} |u_g|^2 + \rho_g \theta_g \right) + \operatorname{div}_x \left(\rho_g \frac{1}{2} u_g |u_g|^2 + \rho_g u_g \theta_g \right) + \operatorname{div}_x(P_g u_g + q_g) = E_E^{\text{int}}, \\ \partial_t \rho_\ell + \operatorname{div}_x(\rho_\ell u_\ell) = 0 \\ \partial_t(\rho_\ell u_\ell) + \operatorname{div}_x(\rho_\ell u_\ell^{\otimes 2}) + \operatorname{div}_x P_\ell + \eta \operatorname{div}_x P^{\text{imb}} = -\eta F_E^{\text{int}} \\ \partial_t \left(\rho_\ell \frac{1}{2} |u_\ell|^2 + \rho_\ell \theta_\ell \right) + \operatorname{div}_x \left(\rho_\ell \frac{1}{2} u_\ell |u_\ell|^2 + \rho_\ell u_\ell \theta_\ell \right) + \operatorname{div}_x(P_\ell u_\ell + q_\ell) + \eta \operatorname{div}_x Q^{\text{imb}} = -\eta E_E^{\text{int}}, \end{cases} \quad (4.2.9)$$

where interaction force F_E^{int} , and energy exchange E_E^{int} are given by

$$F_E^{\text{int}}(t, x) := \int_{\mathbb{R}^3} \mathcal{E}_1[f, F](t, x, w) w dw, \quad E_E^{\text{int}}(t, x) := \int_{\mathbb{R}^3} \mathcal{E}_1[f, F](t, x, w) \frac{|w|^2}{2} dw, \quad (4.2.10)$$

and the imbalanced pressure P^{imb} and energy flux S^{imb} are give by

$$P^{\text{imb}}(t, x) := I[f, F; \varphi(x, v) = v], \quad Q^{\text{imb}}(t, x) := I \left[f, F; \varphi(x, v) = \frac{|v|^2}{2} \right]. \quad (4.2.11)$$

Fortunately, we still retain global conservation laws (4.1.17), (4.1.18), and (4.1.19) by integrating equation (4.2.9) over the spatial domain $x \in \mathbb{R}^3$. Although the corresponding macroscopic equations lack local force and energy balance, this phenomenon is expected when the system is out of equilibrium; see, for instance, [GHS04; DM10].

Obviously, the system (4.2.9) is not closed and requires additional assumptions to become so. To address this issue, one typically needs to be rescaled the coupled kinetic equation (4.2.1). As a result, the interaction force F_E^{int} and energy exchange E_E^{int} admit more explicit expressions. However, such an analysis is beyond the scope of this paper.

4.2.3 Entropy for Enskog-Enskog system

The entropy for Enskog-Enskog system becomes more intricate. In this section, we still restrict our attention to the Boltzmann-Enskog collision integral, which means that the correlation functions $Y^{(i,j)}$ for $i, j \in \{0, 1, 2\}$ are set to be 1. In addition to the kinetic part, there is potential part in the entropy. With this in mind, we define the entropy of the Enskog-Enskog system as follows:

$$\begin{aligned} S_{\text{EE}}(t) &:= \frac{1}{m_g} \int_{\mathbb{R}^3 \times \mathbb{R}^3} f(t, x, w) \ln f(t, x, w) dx dw + \frac{1}{m_p} \int_{\mathbb{R}^3 \times \mathbb{R}^3} F(t, x, v) \ln F(t, x, v) dx dv \\ &+ \frac{1}{2m_g^2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{2r_p}(|x-y|) \rho_\ell(t, x) \rho_\ell(t, y) dx dy + \frac{1}{2m_p^2} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{2r_g}(|x-y|) \rho_g(t, x) \rho_g(t, y) dx dy \\ &+ \frac{1}{m_g m_p} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{r_p+r_g}(|x-y|) \rho_\ell(t, x) \rho_\ell(t, y) dx dy, \end{aligned} \quad (4.2.12)$$

where potential function β_r for Enskog collision integral is defined by

$$\beta_r(s) := \int_s^\infty \delta(s-r)ds = H(r-s)$$

Proposition 4.2.2. *Let f and F be classical solution of (4.2.1). Assume that $(x, v) \mapsto F(t, x, v)$ and $(x, w) \mapsto f(t, x, w)$ rapidly decaying at infinity, while $(x, w) \mapsto \ln f(t, x, w)$ and $(x, v) \mapsto \ln F(t, x, v)$ have at most polynomial growth at infinity. Then, for the Boltzmann-Enskog collision integrals ($Y^{(1,1)} = Y^{(0,2)} = Y^{(2,0)} \equiv 1$), we have*

$$\frac{d}{dt} S_{EE} = -\Lambda \leq 0, \quad (4.2.13)$$

where Λ is defined by

$$\begin{aligned} \Lambda := & \frac{1}{2m_g^2} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} f(t, x, w) f(t, x + 2r_g n, w_1) \lambda \left(\frac{f(t, x, w^o) f(t, x + 2r_g n, w_1^o)}{f(t, x, w) f(t, x + 2r_g n, w_1)} \right) \\ & \times (w - w_1) \cdot n H((w - w_1) \cdot n) dx dn dw dw_1 \\ & + \frac{1}{2m_p^2} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} F(t, x, v) F(t, x + 2r_p n, v_1) \lambda \left(\frac{F(t, x, v^o) F(t, x + 2r_p n, v_1^o)}{F(t, x, v) F(t, x + 2r_p n, v_1)} \right) \\ & \times (v - v_1) \cdot n H((v - v_1) \cdot n) dx dn dv dv_1 \\ & + \frac{1}{m_g m_p} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} f(t, x + (r_g + r_p)n, w) F(t, x, v) \lambda \left(\frac{f(t, x + (r_g + r_p)n, w') F(t, x, v')}{f(t, x + (r_g + r_p)n, w) F(t, x, v)} \right) \\ & \times (v - w) \cdot n H((v - w) \cdot n) dx dn dv dw, \end{aligned}$$

where $v', w', v_*^o, v^o, w^o, w_*^o$ are given by (4.1.3) and (4.1.3), respectively.

Proof. Similarly, we directly compute the time derivative of S_{EE} . We decompose it into 3 parts:

$$\frac{d}{dt} S_{EE} = \Gamma_1 + \Gamma_2 + \Gamma_3,$$

where

$$\begin{aligned} \Gamma_1 := & \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{E}_0[f] \ln f(t, x, w) dx dw + \frac{d}{dt} \left(\frac{1}{2m_g^2} \int_{\mathbb{R}^3} \beta_{2r_g}(|\cdot|) \star \rho_g \rho_g(t, x) dx \right) \\ \Gamma_2 := & \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{E}_3[F] \ln F(t, x, v) dx dv + \frac{d}{dt} \left(\frac{1}{2m_p^2} \int_{\mathbb{R}^3} \beta_{2r_p}(|\cdot|) \star \rho_\ell \rho_\ell(t, x) dx \right) \\ \Gamma_3 := & \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{E}_1[f, F] \ln f dx dw + \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{E}_2[F, f] \ln F dx dv \\ & + \frac{1}{m_g m_p} \frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{r_g+r_p}(|x-y|) \rho_\ell(x) \rho_g(y) dx dy \end{aligned}$$

We begin with considering Γ_3

$$m_p \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{E}_1[f, F] \ln f dx dw + m_g \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathcal{E}_2[F, f] \ln F dx dv$$

$$= (r_g + r_p)^2 \int_{(v-w) \cdot n > 0} (v-w) \cdot n f(x + (r_g + r_p)n, w) F(x, v) \ln \frac{f(x + (r_g + r_p)n, w') F(x, v')}{f(x + (r_g + r_p)n, w) F(x, v)} dx dv dw dn.$$

Thanks to (4.1.22), the quantity above is no larger than

$$\begin{aligned} & (r_g + r_p)^2 \int_{(v-w) \cdot n > 0} (v-w) \cdot n [f(x + (r_g + r_p)n, w') F(x, v') - f(x + (r_g + r_p)n, w) F(x, v)] dx dv dw dn \\ &= - (r_g + r_p)^2 \int_{\mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{S}^2} (v-w) \cdot n f(x + (r_g + r_p)n, w) F(x, v) dx dv dw dn \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} (v-w) \cdot \frac{x-y}{|x-y|} f(y, w) F(x, v) \delta(|x-y| - (r_g + r_p)) dx dy \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_\ell(x) \rho_g(y) \frac{x-y}{|x-y|} \cdot [u_\ell(x) - u_g(y)] \delta(|x-y| - (r_g + r_p)) dx dy \end{aligned}$$

On the other hand, the equations (4.2.9) and integration by parts yield that

$$\begin{aligned} & \frac{d}{dt} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{r_g+r_p}(|x-y|) \rho_\ell(x) \rho_g(y) dx dy \\ &= - \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{r_g+r_p}(|x-y|) \operatorname{div}_x(\rho_\ell(x) u_\ell(x)) \rho_g(y) dx dy - \int_{\mathbb{R}^3 \times \mathbb{R}^3} \beta_{r_g+r_p}(|x-y|) \rho_\ell(x) \operatorname{div}_y(\rho_g(y) u_g(y)) dx dy \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_\ell(x) \rho_g(y) \{ \nabla_x [\beta_{r_g+r_p}(|x-y|)] \cdot u_\ell(x) + \nabla_y [\beta_{r_g+r_p}(|x-y|)] \cdot u_g(y) \} dx dy \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \rho_\ell(x) \rho_g(y) \frac{x-y}{|x-y|} \cdot [u_\ell(x) - u_g(y)] \beta'_{r_g+r_p}(|x-y|) dx dy. \end{aligned}$$

Recall that $\beta'_s(r) = -\delta(r-s)$. Therefore, we could rewrite Γ_3 term as

$$\begin{aligned} \Gamma_3 &= \frac{1}{m_g m_p} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} f(t, x + (r_g + r_p)n, w) F(t, x, v) \lambda \left(\frac{f(t, x + (r_g + r_p)n, w') F(t, x, v')}{f(t, x + (r_g + r_p)n, w) F(t, x, v)} \right) \\ &\quad (v-w) \cdot n H((v-w) \cdot n) dx dn dv dw \geq 0. \end{aligned} \quad (4.2.14)$$

Due to the same reason, or by the Theorem 3.4 in [CCG24], we have the following estimates

$$\begin{aligned} \Gamma_1 &= \frac{1}{2m_g^2} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} f(t, x, w) f(t, x + 2r_g n, w_1) \lambda \left(\frac{f(t, x, w^o) f(t, x + 2r_g n, w_1^o)}{f(t, x, w) f(t, x + 2r_g n, w_1)} \right) \\ &\quad (w - w_1) \cdot n H((w - w_1) \cdot n) dx dn dw dw_1 \geq 0, \end{aligned} \quad (4.2.15)$$

and

$$\begin{aligned} \Gamma_2 &= \frac{1}{2m_p^2} \int_{(\mathbb{R}^3)^3 \times \mathbb{S}^2} F(t, x, v) F(t, x + 2r_p n, v_1) \lambda \left(\frac{F(t, x, v^o) F(t, x + 2r_p n, v_1^o)}{F(t, x, v) F(t, x + 2r_p n, v_1)} \right) \\ &\quad (v - v_1) \cdot n H((v - v_1) \cdot n) dx dn dv dv_1 \geq 0, \end{aligned} \quad (4.2.16)$$

Finally, we conclude the result by combining (4.2.15), (4.2.16), and (4.2.14). $\square$

This result bases on the Theorem 3.4 in [CCG24], which treats the entropy inequality

for single-species Boltzmann-Enskog equation. The detailed proof is provided in Section ?? . From this proposition, we observe that the entropy of the Enskog-Enskog system is not merely the sum of the individual entropies of each species, as in the case of the coupled Boltzmann equations, but also includes additional cross-interaction terms.

4.3 Formal derivation of kinetic equation with delocalized collision integral

In this section, we aim to derive the coupled Enskog equations (4.2.1). The technique bases on Grad's approach. One can refer to, for instance, Chapter 2 in [Cer94], also Appendix A in [Son07] for formal derivation. Rigorously, for short time, the proof can be found in [Lan75]. We begin with Newtonian mechanics. The system consists of N_p "heavy" particles and N_g "light" gas molecules, with positions $X_i \equiv X_i(t), Y_k \equiv Y_k(t) \in \mathbb{R}^3$ and velocities $V_i \equiv V_i(t), W_k \equiv W_k(t) \in \mathbb{R}^3$, for $1 \leq i \leq N_p, 1 \leq k \leq N_g$. Let r_p and r_g denote the radii of the particles and gas molecules, respectively. For the N -particle system consisting of two species, we denote the full state vector by

$$Z(t) := (X_1, \dots, X_{N_p}, Y_1, \dots, Y_{N_g}, V_1, \dots, V_{N_p}, W_1, \dots, W_{N_g}) \in \mathbb{R}^{6(N_p+N_g)}.$$

The evolution of the system is governed by Hamilton's equations:

$$\begin{cases} \frac{dX_i}{dt} = \frac{\partial \mathcal{H}}{\partial V_i}, & \frac{dY_k}{dt} = \frac{\partial \mathcal{H}}{\partial W_k}, \\ \frac{dV_i}{dt} = -\frac{\partial \mathcal{H}}{\partial X_i}, & \frac{dW_k}{dt} = -\frac{\partial \mathcal{H}}{\partial Y_k}, \end{cases} \quad \text{for } 1 \leq i \leq N_p, 1 \leq k \leq N_g, Z \in \Omega \quad (4.3.1)$$

where the Hamiltonian $\mathcal{H}$ is given by

$$\mathcal{H}(t, Z(t)) = \sum_{i=1}^{N_p} \frac{|V_i(t)|^2}{2} + \sum_{k=1}^{N_g} \frac{|W_k(t)|^2}{2}.$$

and the admissible phase space domain Ω is defined as

$$\Omega := \{Z \in \mathbb{R}^{6(N_p+N_g)} : |X_i - X_j| \geq 2r_p, |X_i - Y_k| \geq r_p + r_g, |Y_k - Y_l| \geq 2r_g\}.$$

We then define the flow map S_t associated with the Hamiltonian dynamics as

$$S_t(X, Y, V, W) := Z(t)$$

where $Z(t)$ given by (4.3.1), and $X, V \in \mathbb{R}^{3N_p}, Y, W \in \mathbb{R}^{3N_g}$. Let $P = P(t, Z(t))$ denote the joint distribution function. By the Liouville's theorem, the flow S_t preserves volume in phase space, meaning the Jacobian determinant of S_t is equal to 1 for all t . Consequently, the distribution function satisfies the identity

$$P(t, S_t(X, Y, V, W)) = P(0, X, Y, V, W).$$

Applying the chain rule to the total time derivative, we obtain

$$0 = \frac{d}{dt}P(t, Z(t)) = \frac{\partial}{\partial t}P(t, Z(t)) + \frac{dX(t)}{dt} \cdot \frac{\partial}{\partial X}P(t, Z(t)) + \frac{dY(t)}{dt} \cdot \frac{\partial}{\partial Y}P(t, Z(t)) \\ + \frac{dV(t)}{dt} \cdot \frac{\partial}{\partial V}P(t, Z(t)) + \frac{dW(t)}{dt} \cdot \frac{\partial}{\partial W}P(t, Z(t)).$$

Combining with the Hamilton equations (4.3.1), we arrive at the Liouville equation:

$$\partial_t P(t, Z(t)) + V \cdot \nabla_X P(t, Z(t)) + W \cdot \nabla_Y P(t, Z(t)) = 0, \quad \text{for } Z \in \Omega$$

which governs the evolution of the joint distribution function under the deterministic particle dynamics.

We now consider the boundary conditions imposed by elastic collisions between particles and gas molecules. Suppose the i -th particle collides with k -th gas molecule. On the collision surface $|X_i - Y_k| = r_g + r_p$, the post-collision velocities are V_i and W_k , while the pre-collision velocities V'_i and W'_k must satisfy the conservation of momentum and kinetic energy

$$\begin{cases} m_g W'_k + m_p V'_i = m_g W_k + m_p V_i, \\ m_g |W'_k|^2 + m_p |V'_i|^2 = m_g |W_k|^2 + m_p |V_i|^2. \end{cases} \quad (4.3.2)$$

Additionally, since the collision is specular, the change in relative velocity is orthogonal to the contact normal:

$$(W_k + V_i - W'_k - V'_i) \cdot \frac{X_i - Y_k}{|X_i - Y_k|} = 0.$$

These constraints uniquely determine the pre-collision velocities, yielding the collision transformation:

$$\begin{cases} V'_i \equiv V'_i(V_i, W_k, \frac{X_i - Y_k}{|X_i - Y_k|}, \eta) = V_i - \frac{2\eta}{1+\eta}(V_i - W_k) \cdot \frac{X_i - Y_k}{|X_i - Y_k|} \frac{X_i - Y_k}{|X_i - Y_k|} \delta(|X_i - Y_k| - r_g - r_p), \\ W'_k \equiv W'_k(V_i, W_k, \frac{X_i - Y_k}{|X_i - Y_k|}, \eta) = W_k + \frac{2}{1+\eta}(V_i - W_k) \cdot \frac{X_i - Y_k}{|X_i - Y_k|} \frac{X_i - Y_k}{|X_i - Y_k|} \delta(|X_i - Y_k| - r_g - r_p), \end{cases} \quad (4.3.3)$$

where $\eta := \frac{m_g}{m_p} \ll 1$ is the mass ratio. Similarly, for collisions between two particles of the same species, say particles i and j , the pre-collision velocities V_i^o and V_j^o are given by

$$\begin{cases} V_i^o \equiv V_i^o(V_i, V_j, \frac{X_i - X_j}{|X_i - X_j|}) = V_i - (V_i - V_j) \cdot \frac{X_i - X_j}{|X_i - X_j|} \frac{X_i - X_j}{|X_i - X_j|} \delta(|X_i - X_j| - 2r_p), \\ V_j^o \equiv V_j^o(V_i, V_j, \frac{X_i - X_j}{|X_i - X_j|}) = V_j + (V_i - V_j) \cdot \frac{X_i - X_j}{|X_i - X_j|} \frac{X_i - X_j}{|X_i - X_j|} \delta(|X_i - X_j| - 2r_p), \end{cases} \quad (4.3.4)$$

Let $X_{(N_p)} = (x_1, \dots, x_{N_p}) \in \mathbb{R}^{3N_p}$ and $V_{(N_p)} = (v_1, \dots, v_{N_p}) \in \mathbb{R}^{3N_p}$ denote the position and velocity vectors of the particles. Similarly, let $Y_{(N_g)}$ and $W_{(N_g)}$ represent the positions and velocities of the gas molecules.

The joint velocity distribution function is defined as

$$\tilde{P}^{(N_p, N_g)} \equiv \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}), \quad \text{in } \mathbb{R}_+ \times \Omega^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g)},$$

where the admissible domain $\Omega^{(N_p, N_g)}$ excludes overlap between any two spheres, defined as

$$\Omega^{(N_p, N_g)} := \{(X_{(N_p)}, Y_{(N_g)}) : |x_i - x_j| \geq 2r_p, |x_i - y_k| \geq r_p + r_g, |y_k - y_l| \geq 2r_g \\ \forall i, j, k, l, \text{ such that } 1 \leq i < j \leq N_p, 1 \leq k < l \leq N_g\}.$$

The distribution function $\tilde{P}^{(N_p, N_g)}$ evolves according to the Liouville equation:

$$\partial_t \tilde{P}^{(N_p, N_g)} + \sum_{i=1}^{N_p} v_i \cdot \nabla_{x_i} \tilde{P}^{(N_p, N_g)} + \sum_{j=1}^{N_g} w_j \cdot \nabla_{y_j} \tilde{P}^{(N_p, N_g)} = 0 \\ \text{in } \Omega^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g)} \quad (4.3.5)$$

with the boundary conditions

$$\left\{ \begin{array}{l} \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) = \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, R_{ij}V_{(N_p)}, W_{(N_g)}), \\ \quad \text{on } \{(X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) : (x_i - x_j) \cdot (v_i - v_j) > 0, |x_i - x_j| = 2r_p\} ; \\ \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) = \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, C_{ij}(V_{(N_p)}, W_{(N_g)})), \\ \quad \text{on } \{(X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) : (x_i - y_j) \cdot (v_i - w_j) > 0, |x_i - y_j| = r_p + r_g\} ; \\ \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) = \tilde{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, R_{ij}W_{(N_g)}), \\ \quad \text{on } \{(X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) : (y_i - y_j) \cdot (w_i - w_j) > 0, |y_i - y_j| = 2r_g\} . \end{array} \right. \quad (4.3.6)$$

where the reflection operators R_{ij} and C_{ij} are defined as

$$\left\{ \begin{array}{l} R_{ij}(V_{(N_p)}) := \left(v_1, \dots, v_{i-1}, v_i^o \left(v_i, v_j, \frac{x_i - x_j}{|x_i - x_j|} \right), v_{i+1}, \dots, v_{j-1}, \right. \\ \quad \left. v_j^o \left(v_i, v_j, \frac{x_i - x_j}{|x_i - x_j|} \right), v_{j+1}, \dots, v_{N_p} \right), \quad 1 \leq i < j \leq N_p, \\ C_{ij}(V_{(N_p)}, W_{(N_g)}) := \left(v_1, \dots, v_i' \left(v_i, w_j, \frac{x_i - y_j}{|x_i - y_j|}, \eta \right), \dots, v_{N_p}, w_1, \dots, \right. \\ \quad \left. w_j' \left(v_i, w_j, \frac{x_i - y_j}{|x_i - y_j|}, \eta \right), \dots, w_{N_g} \right), \quad 1 \leq i \leq N_p, 1 \leq j \leq N_g, \\ R_{ij}(W_{(N_g)}) := \left(w_1, \dots, w_{i-1}, w_i^o \left(w_i, w_j, \frac{y_i - y_j}{|y_i - y_j|} \right), w_{i+1}, \dots, w_{j-1}, \right. \\ \quad \left. w_j^o \left(w_i, w_j, \frac{y_i - y_j}{|y_i - y_j|} \right), w_{j+1}, \dots, w_{N_g} \right), \quad 1 \leq i < j \leq N_g, \end{array} \right.$$

where the pre-collision velocities are given by (4.3.3) and (4.3.4).

Let us clarify this more precisely. Consider a collision between particle i and gas molecule k . The pre-collision configuration corresponds to the particles approaching each other, which is characterized by the condition:

$$(x_i - y_k) \cdot (v_i' - w_k') < 0.$$

Conversely, after the collision, the relative velocity should be directed outward, indicating

that the particles are moving apart:

$$(x_i - y_k) \cdot (v_i - w_k) > 0.$$

Assuming sufficient regularity of the distribution function, it is reasonable to impose the boundary condition on the interaction sphere $\{|x_i - y_k| = r_p + r_g\}$ in the following form:

$$\begin{aligned} P(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) & H(- (x_i - y_k) \cdot (v'_i - w'_k)) \delta(|x_i - y_k| - r_p - r_g) \\ &= P(t, X_{(N_p)}, Y_{(N_g)}, C_{ik}(V_{(N_p)}, W_{(N_g)})) H((x_i - y_k) \cdot (v_i - w_k)) \delta(|x_i - y_k| - r_p - r_g), \end{aligned}$$

Thanks to the collision property (5.3.12), this boundary condition is naturally imposed on the outgoing hemisphere:

$$\{|x_i - y_k| = r_p + r_g, \quad (x_i - y_k) \cdot (v_i - w_k) > 0\},$$

See the following Figure 4.1 for illustration:

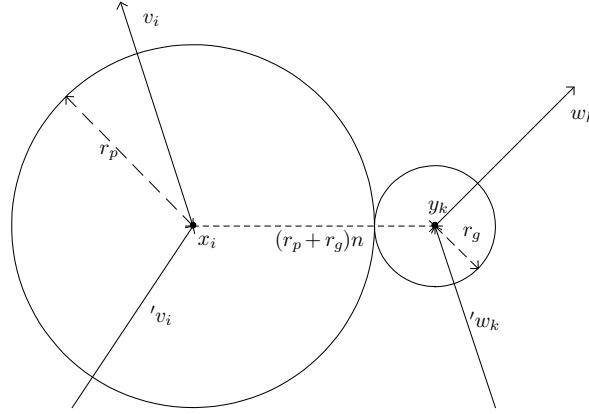


Figure 4.1: Collision Between Two Dissimilar Particles

We symmetrize distribution function $\tilde{P}^{(N_p, N_g)}$ by

$$\begin{aligned} \bar{P}^{(N_p, N_g)} &:= \frac{1}{N_p! N_g!} \sum_{\sigma, \tau} \tilde{P}^{(N_p, N_g)}(t, x_{\sigma(1)}, \dots, x_{\sigma(N_p)}, y_{\tau(1)}, \dots, y_{\tau(N_g)}, \\ &\quad v_{\sigma(1)}, \dots, v_{\sigma(N_p)}, w_{\tau(1)}, \dots, w_{\tau(N_g)}), \end{aligned} \quad (4.3.7)$$

where σ and τ are permutations in S_{N_p} and S_{N_g} , respectively. Hence, function $\bar{P}^{(N_p, N_g)}$ is permutation invariant, i.e.,

$$\begin{aligned} \bar{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}, V_{(N_p)}, W_{(N_g)}) &= \bar{P}^{(N_p, N_g)}(t, x_{\sigma(1)}, \dots, x_{\sigma(N_p)}, \\ &\quad y_{\tau(1)}, \dots, y_{\tau(N_g)}, v_{\sigma(1)}, \dots, v_{\sigma(N_p)}, w_{\tau(1)}, \dots, w_{\tau(N_g)}), \end{aligned} \quad (4.3.8)$$

ensuring indistinguishability of molecules within the same species. Next, we extend $\bar{P}^{(N_p, N_g)}$

in $\mathbb{R}_+ \times \mathbb{R}^{6(N_p+N_g)}$ by

$$\begin{aligned} P^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}) &:= \bar{P}^{(N_p, N_g)}(t, X_{(N_p)}, Y_{(N_g)}) \mathbf{1}_{\Omega^{(N_p, N_g)}}(X_{(N_p)}, Y_{(N_g)}) \\ &= \begin{cases} \bar{P}^{(N_p, N_g)}, & \text{if } (X_{(N_p)}, Y_{(N_g)}) \in \Omega^{(N_p, N_g)} \\ 0, & \text{if } (X_{(N_p)}, Y_{(N_g)}) \notin \Omega^{(N_p, N_g)} \end{cases}, \quad (4.3.9) \end{aligned}$$

We denote the variables by $X_{(s)} = (x_1, \dots, x_s) \in \mathbb{R}^{3s}$, $Y_{(l)} = (y_1, \dots, y_l) \in \mathbb{R}^{3l}$, $V_{(s)} = (v_1, \dots, v_s) \in \mathbb{R}^{3s}$, and $W_{(l)} = (w_1, \dots, w_l) \in \mathbb{R}^{3l}$. Similarly, the complementary variables are defined as $X_{(N_p)}^{(s)} := (x_{s+1}, \dots, x_{N_p}) \in \mathbb{R}^{3(N_p-s)}$, $Y_{(N_g)}^{(l)} := (y_{l+1}, \dots, y_{N_g}) \in \mathbb{R}^{3(N_g-l)}$, $V_{(N_p)}^{(s)} := (v_{s+1}, \dots, v_{N_p}) \in \mathbb{R}^{3(N_p-s)}$, and $W_{(N_g)}^{(l)} := (w_{l+1}, \dots, w_{N_g}) \in \mathbb{R}^{3(N_g-l)}$. Then we introduce the marginals of $P^{(N_p, N_g)}$

$$P^{(s, l)}(t, X_{(s)}, Y_{(l)}, V_{(s)}, W_{(l)}) := \int_{\mathbb{R}^{6(N_p+N_g-s-l)}} P^{(N_p, N_g)} dX_{(N_p)}^{(s)} dY_{(N_g)}^{(l)} dV_{(N_p)}^{(s)} dW_{(N_g)}^{(l)} \quad (4.3.10)$$

To study the dynamics of first marginal for both species, we integrate (4.3.5) in the admissible domain for single molecule:

$$\begin{aligned} \Omega_{(1,0)}^{(N_p, N_g)} &:= \{(x_2, \dots, x_{N_p}, Y_{(N_g)}) \in \mathbb{R}^{3(N_p+N_g-1)} : |x_i - x_1| \geq 2r_p, |x_1 - y_j| \geq r_p + r_g, \\ &\quad |x_i - x_j| \geq 2r_p, |y_j - y_l| \geq 2r_g, |x_i - y_j| \geq r_g + r_p \\ &\quad \forall 2 \leq i \neq j \leq N_p, 1 \leq k \neq l \leq N_g\} \\ \Omega_{(0,1)}^{(N_p, N_g)} &:= \{(X_{(N_p)}, y_2, \dots, y_{N_g}) \in \mathbb{R}^{3(N_p+N_g-1)} : |x_i - x_k| \geq 2r_p, |x_i - y_1| \geq r_p + r_g, \\ &\quad |x_i - x_j| \geq 2r_p, |y_j - y_l| \geq 2r_g, |x_i - y_j| \geq r_g + r_p \\ &\quad \forall 2 \leq i \neq j \leq N_p, 1 \leq k \neq l \leq N_g\}. \end{aligned}$$

The equation for particles (4.3.5) follows

$$\begin{aligned} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p+N_g-1)}} \partial_t P^{(N_p, N_g)} + \sum_{i=1}^{N_p} v_i \cdot \nabla_{x_i} P^{(N_p, N_g)} \\ + \sum_{j=1}^{N_g} w_j \cdot \nabla_{y_j} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} = 0. \quad (4.3.11) \end{aligned}$$

If we assume $\partial_t P^{(N_p, N_g)} \in L^1(\mathbb{R}_+ \times \mathbb{R}^{6(N_p+N_g)})$, the definition of marginals (4.3.10) shows

$$\int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{2(N_p+N_g-1)}} \partial_t P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} = \partial_t P^{(1,0)}. \quad (4.3.12)$$

If $v_1 \cdot \nabla_{x_1} P^{(N_p, N_g)} \in L^1(\mathbb{R}_+ \times \mathbb{R}^{6(N_p+N_g)})$, we change the order of integration. Due to the existence of boundary, it reads

$$\int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p+N_g-1)}} v_1 \cdot \nabla_{x_1} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} = v_1 \cdot \nabla_{x_1} P^{(1,0)}$$

$$\begin{aligned}
& - \sum_{j=2}^{N_p} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_1 \cdot \frac{x_1 - x_j}{|x_1 - x_j|} \delta(|x_1 - x_j| - 2r_p) P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
& - \sum_{k=1}^{N_g} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_1 \cdot \frac{x_1 - y_k}{|x_1 - y_k|} \delta(|x_1 - y_k| - r_g - r_p) P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}.
\end{aligned}$$

Therefore, the symmetry property (4.3.8) allows us to simplify the integral by replacing all indices $2 \leq j \leq N_p$ with 2, and $1 \leq k \leq N_g$ with 1, due to the assumed symmetry within each species.

$$\begin{aligned}
& \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_1 \cdot \nabla_{x_1} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
& = v_1 \cdot \nabla_{x_1} P^{(1,0)} - (N_p - 1) \int_{\mathbb{R}^6} v_1 \cdot \frac{x_1 - x_2}{|x_1 - x_2|} \delta(|x_1 - x_2| - 2r_p) P^{(2,0)} dx_2 dv_2 \\
& \quad - N_g \int_{\mathbb{R}^6} v_1 \cdot \frac{x_1 - y_1}{|x_1 - y_1|} \delta(|x_1 - y_1| - r_g - r_p) P^{(1,1)} dy_1 dw_1. \quad (4.3.13)
\end{aligned}$$

For $2 \leq i \leq N_p$, we apply the Gauss theorem on the boundary consists of three parts:

- Sphere centered at unintegrated variable x_1 : $\{(X_{(N_p)}, Y_{(N_p)}) : |x_i - x_1| = 2r_p\}$;
- Sphere centered at integrated variables x_j for $2 \leq j \neq i \leq N_p$: $\{(X_{(N_p)}, Y_{(N_p)}) : |x_i - x_1| = 2r_p\}$;
- Sphere centered at another species y_k for $1 \leq k \leq N_g$: $\{(X_{(N_p)}, Y_{(N_p)}) : |x_i - y_k| = r_g + r_p\}$.

$$\begin{aligned}
& \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_i \cdot \nabla_{x_i} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
& = \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_i \cdot \frac{x_i - x_1}{|x_i - x_1|} P^{(N_p, N_g)} \delta(|x_i - x_1| - 2r_g) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
& + \sum_{1 \leq j \neq i \leq N_p} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_i \cdot \frac{x_i - x_j}{|x_i - x_j|} P^{(N_p, N_g)} \delta(|x_i - x_j| - 2r_g) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
& + \sum_{1 \leq k \leq N_g} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_i \cdot \frac{x_i - y_k}{|x_i - y_k|} P^{(N_p, N_g)} \delta(|x_i - y_k| - r_g - r_p) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}
\end{aligned}$$

Thanks to the symmetry of the distribution function (4.3.8), we can, without loss of generality, relabel the indices in the integrals and summations: replace i by 2 in the first integral, replace each pair (i, j) with $(2, 3)$ for $2 \leq i \neq j \leq N_p$ in the first summation, and replace each pair (i, k) with $(2, 1)$ in the second summation. This leads to the following simplified expression:

$$\int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_i \cdot \nabla_{x_i} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}$$

$$\begin{aligned}
&= \int_{\mathbb{R}^6} v_2 \cdot \frac{x_2 - x_1}{|x_2 - x_1|} P^{(2,0)}(t, x_1, x_2, v_1, v_2) dx_2 dv_2 \\
&+ (N_p - 1) \int_{\mathbb{R}^{12}} v_2 \cdot \frac{x_2 - x_3}{|x_2 - x_3|} P^{(3,0)}(t, x_1, x_2, x_3, v_1, v_2, v_3) \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&+ N_g \int_{\mathbb{R}^{12}} v_2 \cdot \frac{x_2 - y_1}{|x_2 - y_1|} P^{(2,1)}(t, x_1, x_2, y_1, v_1, v_2, w_1) \delta(|x_2 - y_1| - r_g - r_p) dy_1 dx_2 dw_1 dv_2.
\end{aligned}$$

We then sum the above formula over all $2 \leq i \leq N_p$, which yields

$$\begin{aligned}
&\sum_{i=2}^{N_p} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} v_i \cdot \nabla_{x_i} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
&= (N_p - 1) \int_{\mathbb{R}^6} v_2 \cdot \frac{x_2 - x_1}{|x_2 - x_1|} P^{(2,0)} dx_2 dv_2 \\
&+ (N_p - 1)(N_p - 2) \int_{\mathbb{R}^{12}} v_2 \cdot \frac{x_2 - x_1}{|x_2 - x_1|} P^{(3,0)} \delta(|x_2 - x_1| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&+ (N_p - 1)N_g \int_{\mathbb{R}^{12}} v_2 \cdot \frac{x_2 - y_1}{|x_2 - y_1|} P^{(2,1)} \delta(|x_2 - y_1| - r_g - r_p) dy_1 dx_2 dw_1 dv_2. \quad (4.3.14)
\end{aligned}$$

For $1 \leq k \leq N_g$, we compute the following integral using the Gauss theorem on the boundary $\{y_k \in \mathbb{R}^3 : |y_k - x_i| = r_g + r_p, |y_k - y_l| = 2r_g, \forall 1 \leq i \leq N_p, 1 \leq l \neq k \leq N_g\}$:

$$\begin{aligned}
&\int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} w_k \cdot \nabla_{y_k} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
&= \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} w_k \cdot \frac{y_k - x_1}{|y_k - x_1|} P^{(N_p, N_g)} \delta(|y_k - x_1| - r_g - r_p) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
&+ \sum_{2 \leq i \leq N_p} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} w_k \cdot \frac{y_k - x_i}{|y_k - x_i|} P^{(N_p, N_g)} \delta(|y_k - x_i| - r_g - r_p) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
&+ \sum_{1 \leq l \neq k \leq N_g} \int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} w_k \cdot \frac{y_k - y_l}{|y_k - y_l|} P^{(N_p, N_g)} \delta(|y_k - y_l| - 2r_g) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}.
\end{aligned}$$

The symmetry of g and definition of marginals shows:

$$\begin{aligned}
&\int_{\Omega_{(1,0)}^{(N_p, N_g)} \times \mathbb{R}^{3(N_p + N_g - 1)}} w_k \cdot \nabla_{y_k} P^{(N_p, N_g)} dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\
&= \int_{\mathbb{R}^6} w_1 \cdot \frac{y_1 - x_1}{|y_1 - x_1|} P^{(1,1)} \delta(|y_1 - x_1| - r_g - r_p) dy_1 dw_1 \\
&+ (N_p - 1) \int_{\mathbb{R}^{12}} w_1 \cdot \frac{y_1 - x_2}{|y_1 - x_2|} P^{(2,1)} \delta(|y_1 - x_2| - r_g - r_p) dy_1 dx_2 dw_1 dv_2 \\
&+ (N_g - 1) \int_{\mathbb{R}^{12}} w_1 \cdot \frac{y_1 - y_2}{|y_1 - y_2|} P^{(1,2)} \delta(|y_1 - y_2| - 2r_g) dy_1 dy_2 dw_1 dw_2. \quad (4.3.15)
\end{aligned}$$

Substituting (4.3.12), (4.3.13), (4.3.14), and (4.3.15) into (4.3.11), it follows,

$$\begin{aligned}
& \partial_t P^{(1,0)} + v_1 \cdot \nabla_{x_1} P^{(1,0)} \\
&= -(N_p - 1)(N_p - 2) \int_{\mathbb{R}^{12}} v_2 \cdot \frac{x_2 - x_3}{|x_2 - x_3|} P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&\quad - N_g(N_g - 1) \int_{\mathbb{R}^{12}} w_1 \cdot \frac{y_1 - y_2}{|y_1 - y_2|} P^{(1,2)} \delta(|y_1 - y_2| - 2r_g) dy_1 dy_2 dw_1 dw_2 \\
&\quad + (N_p - 1)N_g \int_{\mathbb{R}^{12}} (v_2 - w_1) \cdot \frac{y_1 - x_2}{|y_1 - x_2|} P^{(2,1)} \delta(|y_1 - x_2| - r_g - r_p) dy_1 dx_2 dw_1 dv_2 \\
&\quad + (N_p - 1) \int_{\mathbb{R}^6} (v_1 - v_2) \cdot \frac{x_1 - x_2}{|x_1 - x_2|} \delta(|x_1 - x_2| - 2r_p) P^{(2,0)} dx_2 dv_2 \\
&\quad + N_g \int_{\mathbb{R}^6} (v_1 - w_1) \cdot \frac{x_1 - y_1}{|x_1 - y_1|} \delta(|x_1 - y_1| - r_g - r_p) P^{(1,1)} dy_1 dw_1. \quad (4.3.16)
\end{aligned}$$

Next, we simplify the expression term by term. We will show that the interaction involving three molecules ultimately contributes zero. Meanwhile, the pairwise collisions between two molecules can be reformulated as collision integrals—specifically, as either Boltzmann or Enskog collision integrals. Let's take the first integral in (4.3.16) as an example. By the symmetry of g , we can exchange the indices 2 and 3, hence we obtain:

$$\begin{aligned}
& \int_{\mathbb{R}^{12}} v_2 \cdot \frac{x_2 - x_3}{|x_2 - x_3|} P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&= \int_{\mathbb{R}^{12}} v_3 \cdot \frac{x_3 - x_2}{|x_2 - x_3|} P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&= \frac{1}{2} \int_{\mathbb{R}^{12}} (v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3.
\end{aligned}$$

Next, we decompose $(v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|}$ into its positive and negative parts, that is,

$$\begin{aligned}
(v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} &= \left| (v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} \right| H[(v_2 - v_3) \cdot (x_2 - x_3)] \\
&\quad - \left| (v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} \right| H[-(v_2 - v_3) \cdot (x_2 - x_3)].
\end{aligned}$$

For the negative part, we perform the change of variables $V_{(N_p)} \mapsto R_{23}(V_{(N_p)})$ with Jacobian given by (5.3.11). The boundary condition (4.3.6) guarantees the invariance of $P^{(3,0)}$ under the transformation. Hence, we obtain,

$$\begin{aligned}
& \int_{\mathbb{R}^{12}} (v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&= \int_{\mathbb{R}^{12}} \left| (v_2 - v_3) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} \right| H[(v_2 - v_3) \cdot (x_2 - x_3)] P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3 \\
&\quad - \int_{\mathbb{R}^{12}} \left| (v_2^o - v_3^o) \cdot \frac{x_2 - x_3}{|x_2 - x_3|} \right| H[-(v_2^o - v_3^o) \cdot (x_2 - x_3)] P^{(3,0)} \delta(|x_2 - x_3| - 2r_p) dx_2 dx_3 dv_2 dv_3.
\end{aligned}$$

Thanks to (5.3.12), we know the positive and the negative parts cancel each other out. Due

to the same reason, we have

$$\begin{aligned} \int_{\mathbb{R}^{12}} w_1 \cdot \frac{y_1 - y_2}{|y_1 - y_2|} P^{(1,2)} \delta(|y_1 - y_2| - 2r_g) dy_1 dy_2 dw_1 dw_2 \\ = \frac{1}{2} \int_{\mathbb{R}^{12}} (w_1 - w_2) \cdot \frac{y_1 - y_2}{|y_1 - y_2|} P^{(1,2)} \delta(|y_1 - y_2| - 2r_g) dy_1 dy_2 dw_1 dw_2 = 0, \end{aligned}$$

and

$$\int_{\mathbb{R}^{12}} (v_2 - w_1) \cdot \frac{y_1 - x_2}{|y_1 - x_2|} P^{(2,1)} \delta(|y_1 - x_2| - r_g - r_p) dy_1 dx_2 dw_1 dv_2 = 0$$

We decompose the remaining two integrals in (4.3.16) into positive part and negative part called gain terms and loss terms, respectively, as done previously,

$$\begin{aligned} \partial_t P^{(1,0)} + v_1 \cdot \nabla_{x_1} P^{(1,0)} \\ = (N_p - 1) \int_{\mathbb{R}^6} \left| (v_1 - v_2) \cdot \frac{x_1 - x_2}{|x_1 - x_2|} \right| \delta(|x_1 - x_2| - 2r_p) \left[P^{(2,0)}(x_1, x_2, v_1, v_2) \right. \\ \times H((v_1 - v_2) \cdot (x_1 - x_2)) - P^{(2,0)}(x_1, x_2, v_1, v_2) H(-(v_1 - v_2) \cdot (x_1 - x_2)) \Big] dx_2 dv_2 \\ + N_g \int_{\mathbb{R}^6} (v_1 - w_1) \cdot \frac{x_1 - y_1}{|x_1 - y_1|} \delta(|x_1 - y_1| - r_g - r_p) \left[P^{(1,1)}(x_1, y_1, v_1, w_1) \right. \\ \times H((x_1 - y_1) \cdot (v_1 - w_1)) - P^{(1,1)}(x_1, y_1, v_1, w_1) H(-(x_1 - y_1) \cdot (v_1 - w_1)) \Big] dy_1 dw_1. \end{aligned}$$

We then apply the boundary condition (4.3.6) on the out-going hemisphere,

$$\begin{aligned} \partial_t P^{(1,0)} + v_1 \cdot \nabla_{x_1} P^{(1,0)} \\ = (N_p - 1) \int_{\mathbb{R}^6} \left| (v_1 - v_2) \cdot \frac{x_1 - x_2}{|x_1 - x_2|} \right| \delta(|x_1 - x_2| - 2r_p) \left[P^{(2,0)}(x_1, x_2, v_1^o, v_2^o) \right. \\ \times H((v_1 - v_2) \cdot (x_1 - x_2)) - P^{(2,0)}(x_1, x_2, v_1, v_2) H(-(v_1 - v_2) \cdot (x_1 - x_2)) \Big] dx_2 dv_2 \\ + N_g \int_{\mathbb{R}^6} \left| (v_1 - w_1) \cdot \frac{x_1 - y_1}{|x_1 - y_1|} \right| \delta(|x_1 - y_1| - r_g - r_p) \left[P^{(1,1)}(x_1, y_1, v_1', w_1') \right. \\ \times H((x_1 - y_1) \cdot (v_1 - w_1)) - P^{(1,1)}(x_1, y_1, v_1, w_1) H(-(x_1 - y_1) \cdot (v_1 - w_1)) \Big] dy_1 dw_1. \end{aligned}$$

We then change the coordinate from $x_2, y_1 \in \mathbb{R}^3$ to surface element on the unit sphere $n \in \mathbb{S}^2$ by $x_2 = x_1 - 2r_p n$ and $y_1 = x_1 - (r_g + r_p)n$, respectively. Noting that $\delta(|x_1 - x_2| - 2r_p) dx_2 = (2r_p)^2 dn$, and $\delta(|x_1 - y_1| - r_g - r_p) dy_1 = (r_g + r_p)^2 dn$. After that, we change $n \mapsto -n$ on the in-going hemisphere:

$$\begin{aligned} \partial_t P^{(1,0)} + v_1 \cdot \nabla_{x_1} P^{(1,0)} &= (N_p - 1)(2r_p)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} |(v_1 - v_2) \cdot n| H((v_1 - v_2) \cdot n) \\ &\times \left[P^{(2,0)}(x_1, x_1 - 2r_p n, v_1^o, v_2^o) - P^{(2,0)}(x_1, x_1 + 2r_p n, v_1, v_2) \right] dn dv_2 \\ &+ N_g (r_g + r_p)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} |(v_1 - w_1) \cdot n| H((v_1 - w_1) \cdot n) \left[P^{(1,1)}(x_1, x_1 - (r_g + r_p)n, v_1', w_1') \right. \end{aligned}$$

$$- P^{(1,1)}(x_1, x_1 + (r_g + r_p)n, v_1, w_1) \Big] dn dw_1.$$

In fact, $P^{(s,l)}$ represent the $(s+l)$ th marginal of distribution function. We plan to establish their connections to density distribution function for particle and gas molecule. The mass density distribution function for particles $g^{(1,0)}$ is defined as

$$g^{(1,0)}(t, x, v) := m_p \sum_{i=1}^{N_p} \int_{\mathbb{R}^{6(N_g+N_p-1)}} \tilde{P}^{(N_p, N_g)}(t, x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_{N_p}, Y_{(N_g)}, \\ v_1, \dots, v_{i-1}, v, v_{i+1}, \dots, v_{N_p}, W_{(N_g)}) \\ dX_{(i-1)} dX_{(N_p)}^{(i+1)} dY_{(N_g)} dV_{(i-1)} dV_{(N_p)}^{(i+1)} dW_{(N_g)}.$$

We shift the indices $1, 2, \dots, i-1$ back by one position in the sequence. Specifically, we relabel $(x_1, x_2, \dots, x_{i-1}, v_1, v_2, \dots, v_{i-1})$ as $(x_2, x_3, \dots, x_i, v_2, v_3, \dots, v_i)$, and then substitute (x, v) with (x_1, v_1) .

$$g^{(1,0)}(t, x_1, v_1) = m_p \sum_{i=1}^{N_p} \int_{\mathbb{R}^{6(N_g+N_p-1)}} \tilde{P}^{(N_p, N_g)}(t, x_2, \dots, x_i, x_1, x_{i+1}, \dots, x_{N_p}, Y_{(N_g)} \\ , v_2, \dots, v_i, v_1, v_{i+1}, \dots, v_{N_p}, W_{(N_g)}) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}.$$

For any the permutation $\tilde{\sigma}_i \in S_{N_p-1} : \{2, \dots, N_p\} \rightarrow \{2, \dots, N_p\}$ with $1 \leq i \leq N_p$, we identify

$$\int_{\mathbb{R}^{6(N_g+N_p-1)}} \tilde{P}^{(N_p, N_g)}(t, x_2, \dots, x_i, x_1, x_{i+1}, \dots, x_{N_p}, Y_{(N_g)} \\ , v_2, \dots, v_i, v_1, v_{i+1}, \dots, v_{N_p}, W_{(N_g)}) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)} \\ = \int_{\mathbb{R}^{6(N_g+N_p-1)}} \tilde{P}^{(N_p, N_g)}(t, x_{\tilde{\sigma}_i(2)}, \dots, x_{\tilde{\sigma}_i(i)}, x_1, x_{\tilde{\sigma}_i(i+1)}, \dots, x_{\tilde{\sigma}_i(N_p)}, Y_{(N_g)} \\ , v_{\tilde{\sigma}_i(2)}, \dots, v_{\tilde{\sigma}_i(i)}, v_1, v_{\tilde{\sigma}_i(i+1)}, \dots, v_{\tilde{\sigma}_i(N_p)}, W_{(N_g)}) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}.$$

Summing over $\tilde{\sigma}_i \in S_{N_p-1}$, we rewrite $g^{(1,0)}(t, x_1, v_1)$ as

$$g^{(1,0)}(t, x_1, v_1) = m_p \sum_{i=1}^{N_p} \frac{1}{(N_p-1)!} \sum_{\tilde{\sigma}_i \in S_{N_p-1}} \int_{\mathbb{R}^{6(N_g+N_p-1)}} \tilde{P}^{(N_p, N_g)} \left(t, x_{\tilde{\sigma}_i(2)}, \dots \right. \\ \left. , x_{\tilde{\sigma}_i(i)}, x_1, x_{\tilde{\sigma}_i(i+1)}, \dots, x_{\tilde{\sigma}_i(N_p)}, Y_{(N_g)}, v_{\tilde{\sigma}_i(2)}, \dots, v_{\tilde{\sigma}_i(i)}, v_1, v_{\tilde{\sigma}_i(i+1)}, \dots, v_{\tilde{\sigma}_i(N_p)}, W_{(N_g)} \right) \\ dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}.$$

By defining permutation $\sigma_i : \{1, \dots, N_p\} \rightarrow \{1, \dots, N_p\}$ maps i to 1:

$$\sigma_i(k) := \begin{cases} \tilde{\sigma}_i(k+1), & 1 \leq k \leq i-1; \\ 1, & k = i; \\ \tilde{\sigma}_i(k), & i+1 \leq k \leq N_p, \end{cases}$$

we can combine the two summations

$$g^{(1,0)}(t, x_1, v_1) = m_p N_p \frac{1}{N_p!} \sum_{\sigma \in S_{N_p}} \int_{\mathbb{R}^{6(N_g+N_p-1)}} \tilde{P}^{(N_p, N_g)} \left(t, x_{\sigma(1)}, \dots, x_{\sigma(N_p)}, Y_{(N_g)}, v_{\sigma(1)}, \dots, v_{\sigma(N_p)}, W_{(N_g)} \right) dX_{(N_p)}^{(2)} dY_{(N_g)} dV_{(N_p)}^{(2)} dW_{(N_g)}.$$

The definition of averaged particles distribution function (4.3.7) and definition of marginal (4.3.10) shows that

$$g^{(1,0)}(t, x, v) = m_p N_p P^{(1,0)}(t, x, v). \quad (4.3.17)$$

Due to the same reason, we have

$$g^{(0,1)}(t, x, w) = m_g N_g P^{(0,1)}(t, x, w). \quad (4.3.18)$$

Similarly, we can establish the connection between the second marginal $P^{(1,1)}$ and the two-particle distribution function $g^{(2,0)}$ using the same idea. The definition of $g^{(2,0)}$ is given by

$$\begin{aligned} g^{(2,0)}(t, \xi_1, \xi_2, \nu_1, \nu_2) \\ := m_p^2 \sum_{1 \leq i < j \leq N_p} \int_{\mathbb{R}^{6(N_g+N_p-2)}} \tilde{P}^{(N_p, N_g)}(t, x_1, \dots, x_{i-1}, \xi_1, x_{i+1}, \dots, x_{j-1}, \xi_2, x_{j+1}, \dots, x_{N_p}, \\ Y_{(N_g)}, v_1, \dots, v_{i-1}, \nu_1, v_{i+1}, \dots, v_{j-1}, \nu_2, v_{j+1}, \dots, v_{N_p}, W_{(N_g)}) \\ dX_{(i-1)} dX_{(j-1)}^{(i+1)} dX_{(N_p)}^{(j+1)} dY_{(N_g)} dV_{(i-1)} dV_{(j-1)}^{(i+1)} dV_{(N_p)}^{(j+1)} dW_{(N_g)}. \end{aligned}$$

Thanks of the change of variables, we can symmetrize it as follows

$$\begin{aligned} g^{(2,0)}(t, \xi_1, \xi_2, \nu_1, \nu_2) \\ := m_p^2 \sum_{1 \leq i < j \leq N_p} \frac{1}{(N_p - 2)!} \sum_{\tilde{\sigma}_{ij} \in S_{N_p-2}} \int_{\mathbb{R}^{6(N_g+N_p-2)}} \tilde{P}^{(N_p, N_g)} \left(t, x_{\tilde{\sigma}_{ij}(3)}, \dots, \right. \\ \left. x_{\tilde{\sigma}_{ij}(i+1)}, \xi_1, x_{\tilde{\sigma}_{ij}(i+2)}, \dots, x_{\tilde{\sigma}_{ij}(j)}, \xi_2, x_{\tilde{\sigma}_{ij}(j+1)}, \dots, x_{\tilde{\sigma}_{ij}(N_p)}, Y_{(N_g)} \right. \\ \left. v_{\tilde{\sigma}_{ij}(3)}, \dots, v_{\tilde{\sigma}_{ij}(i+1)}, \nu_1, v_{\tilde{\sigma}_{ij}(i+2)}, \dots, v_{\tilde{\sigma}_{ij}(j)}, \nu_2, v_{\tilde{\sigma}_{ij}(j+1)}, \dots, v_{\tilde{\sigma}_{ij}(N_p)} \right) \\ dX_{(i-1)} dX_{(j-1)}^{(i+1)} dX_{(N_p)}^{(j+1)} dY_{(N_g)} dV_{(i-1)} dV_{(j-1)}^{(i+1)} dV_{(N_p)}^{(j+1)} dW_{(N_g)}. \end{aligned}$$

Extend $\tilde{\sigma}_{ij} \in S_{N_p-2}$ to $\sigma_{ij} \in S_{N_p}$ by defining

$$\sigma_{ij}(k) := \begin{cases} \tilde{\sigma}_{ij}(k+2), & 1 \leq k \leq i-1; \\ 1, & k = i; \\ \tilde{\sigma}_{ij}(k+1), & i+1 \leq k \leq j-1; \\ 2, & k = j; \\ \tilde{\sigma}_{ij}(k), & i+1 \leq k \leq N_p. \end{cases}$$

Hence,

$$g^{(2,0)}(t, x_1, x_2, v_1, v_2) = m_p^2 N_p (N_p - 1) P^{(2,0)}(t, x_1, x_2, v_1, v_2).$$

A similar computation yields

$$\begin{aligned} g^{(1,1)}(t, x_1, y_1, v_1, w_1) &= m_p m_g N_p N_g P^{(1,1)}(t, x_1, y_1, v_1, w_1), \\ g^{(0,2)}(t, y_1, y_2, w_1, w_2) &= m_g^2 N_g (N_g - 1) P^{(0,2)}(t, y_1, y_2, w_1, w_2). \end{aligned}$$

Therefore, We can write the equation for density distribution function of particles by replacing $P^{(i,j)}$ by $g^{(i,j)}$

$$\begin{aligned} \partial_t g^{(1,0)} + v_1 \cdot \nabla_{x_1} g^{(1,0)} &= \frac{(2r_p)^2}{m_p} \int_{\mathbb{R}^3 \times \mathbb{S}^2} |(v_1 - v_2) \cdot n| H((v_1 - v_2) \cdot n) \\ &\quad \times \left[g^{(2,0)}(x_1, x_1 - 2r_p n, v_1^o, v_2^o) - g^{(2,0)}(x_1, x_1 + 2r_p n, v_1, v_2) \right] dndv_2 \\ &+ \frac{(r_g + r_p)^2}{m_g} \int_{\mathbb{R}^3 \times \mathbb{S}^2} |(v_1 - w_1) \cdot n| H((v_1 - w_1) \cdot n) \left[g^{(1,1)}(x_1, x_1 - (r_g + r_p)n, v_1', w_1') \right. \\ &\quad \left. - g^{(1,1)}(x_1, x_1 + (r_g + r_p)n, v_1, w_1) \right] dndw_1. \end{aligned}$$

It is clear that the equation remains unclosed, even when combined with the equation for the gas molecules $g^{(0,1)}$. To achieve closure, we invoke the propagation of chaos assumption, stated as follows:

$$g^{(0,2)} = Y^{(0,2)}[f, f] f \otimes f, \quad g^{(2,0)} = Y^{(2,0)}[F, F] F \otimes F, \quad g^{(1,1)} = Y^{(1,1)}[F, f] F \otimes f, \quad (4.3.19)$$

where $F \equiv F(t, x, v) := g^{(1,0)}(t, x, v)$ and $f \equiv f(t, x, w) := g^{(0,1)}(t, x, w)$, for notational simplicity, and $Y^{(i,j)}[\varphi, \phi] \equiv Y^{(i,j)}[\varphi, \phi](t, x)$, with $i, j \in \{0, 1, 2\}$, that account for the correction to collision probabilities due to volume exclusion effects arising from finite particle size. Furthermore, $Y^{(1,1)}[F, f]$ is a symmetric functional with respect to f and F ; that is,

$$Y^{(1,1)}[F, f] = Y^{(1,1)}[f, F].$$

We obtain the equation (4.2.1) with collision integrals (4.2.2)(4.2.3)(4.2.4)(4.2.5) using a similar argument for the equation of gas molecules by integrating (4.3.5) with respect to $dX_{(N_p)} dV_{(N_p)} dY_{(N_g)}^{(2)} dW_{(N_g)}^{(2)}$.

4.4 Conclusion

We have verified the coupled Enskog equations from the underlying particle system. Two essential features emerge that are absent in the single-species Boltzmann case:

- the delocalization effects between different species;
- the precise coefficients appearing in front of each collision integral

The directions of these delocalization effects is important in understanding their impacts on macroscopic quantities such as pressure, density, and bulk velocity. Meanwhile, the coefficients in front of the collision integrals play a role when we nondimensionalize the coupled Enskog equations.

A natural question arises: can one have the general collision kernel instead of hard sphere case for the coupled Enskog equations? The answer is yes, but the generalization becomes meaningless in a physical sense. For general interaction potentials, the molecular radius is irrelevant; what matters is the range of the force. Thus, the system is better viewed as a short-range potential model. For dilute gases, this has already been studied in [PSS14]. For dense gases, however, substantial difficulties appear: the collision frequency may fail to remain finite, recollisions may no longer be negligible, and key estimates (such as estimate (5.5) in [PSS14]) break down, since $\varepsilon^2(N - j)$ is no longer less than 1.

The rigorous derivation of such models is certainly of great interest. Yet even the rigorous derivation of the Boltzmann equation itself for long times remains an open problem at the time of this writing.

Chapter 5

A Formal Derivation of the Thick Spray Model from the Enskog-Boltzmann System

This chapter is based on the preprint [Che25a], which has been submitted to a journal for publication.

Introduction

An aerosol, or spray, is a binary mixture composed of a dispersed phase— typically liquid droplets, or solid particles—suspended in a gaseous medium known as the propellant. There are various types of equations to describe such a system; see, for instance [Des10]. A significant class of models describing the dynamics of aerosol or spray flows couples

- (a) a kinetic equation governing the dispersed phase, with
- (b) a fluid equation describing the evolution of the propellant.

These fluid-kinetic equations, also known as Eulerian-Lagrangian or gas-particles model, are coupled through the drag force.

According to the proportions of the dispersed phase, sprays regimes can be classified into three categories (see, for instance, Chapter 1 in [ORo81]): the very thin sprays, where the volume fraction of the dispersed phase's proportion is much less than 10^{-3} ; the thin sprays, where the proportion is much less than 10^{-1} ; and thick sprays, where the dispersed phase occupies up to approximately 10^{-1} of the total volume. From a microscopic point of view, let N_p denotes the total number of particles and r_p the radius of each particle, these regimes correspond to different scaling behaviors: very dilute scale $r_p N_p = O(1)$; the Boltzmann-Grad scale $r_p^2 N_p = O(1)$; dense gas scale $r_p^3 N_p = O(1)$. Any dense scaling, such as, $N_p r_p^4 = O(1)$, would imply that the total volume of the dispersed phase, $N_p r_p^3$, diverges as $r_p \rightarrow 0$, which is physically inconsistent.

Intuitively speaking, as the concentration of the dispersed phase (dusts or droplets) increases, the interaction between two species becomes stronger.

In the case of a *very thin spray*, we only take into account interactions of order $O(r_p)$. This, for instance, gives rise to the Brinkman force; see [All90; DGR08]. However, in the Euler regime, the friction force appears only at order $O(r_p^2)$. As a result, the gas phase dynamics can be computed independently of the influence of the droplets.

When the spray becomes *thin*, the proportion of the dispersed phase grows, and its feedback on the gas phase become non-negligible—although its volume remains small. In this intermediate regime, the dispersed phase influences the exchange rates of momentum and energy with gas. The viscous force emerges at this stage and is intuitively proportional to the surface area of the spherical particles, i.e. $O(r_p^2)$. At this level of approximation, the volume of the dispersed phase, which scales as $O(r_p^3)$, is still neglected. [Ber+17; Ber+18] provided the formal derivation from coupled Boltzmann equations to Vlasov-Navier-Stokes, and Vlasov-Stokes respectively. [DGR19] provided the formal derivation from the same system to Vlasov-Euler equations.

In the *thick sprays* regime, the volume of particles become significant. Consequently, the drag force between two species becomes more complex—it includes not only the viscous effects but also the modification of the pressure due to the volume occupation. This leads to the the notion of “boundary” between dispersed phase and the propellant. On such boundaries, pressure imbalance may arise in non-equilibrium state. To address this, [THa76] introduced the concept of the volume fraction (or void) function, which behaves like $1 - O(r_p^3)$. This modifies the drag force to include not only viscous effects but also corrections associated with volume exclusion.

A key contribution of this work is the derivation of higher-order perturbations (of order $O(r_p^3)$) in the viscous force from a mesoscopic perspective—corrections that were missed in previous models such as those proposed in [ORo81; Duk80]. Moreover, we provide a justification for the plausibility of these extended models from the kinetic-kinetic framework.

The outline of this paper is as follows: we introduce the equation of Boltzmann and its variant—the Enskog equation—are presented in Section 5.1.1 and 5.1.2, respectively. The Section 5.2 introduce the target equations which we aim to derive. In Section 5.3, we formulate the initial coupled kinetic system. In section 5.4, we state the main result of this paper. Section 5.5 demonstrates how to derive the Vlasov equation from the Enskog-Boltzmann equation. In section 5.6, we establish the conservation laws for the gas phase using the moment method. Finally, we conclude the result with some remarks in Section 5.7.

5.1 The Boltzmann equation and Enskog-Boltzmann equation

Let $f \equiv f(t, x, w) \geq 0$ and $F \equiv F(t, x, v) \geq 0$ denote the number distribution functions of gas molecules and particles, respectively, depending on time $t \in \mathbb{R}_+$, position $x \in \mathbb{R}$, and velocities $w, v \in \mathbb{R}$.

Calligraphic letters such as $\mathcal{B}$ and $\mathcal{E}$ are used to denote the collision integrals. In the notation used throughout this paper, square brackets $[]$ indicate functional dependence, while parentheses $()$ indicate dependence on variables.

5.1.1 The Boltzmann equation

The Boltzmann equation is the classical collisional kinetic model describing the dynamics of a dilute gas, and it takes the following form:

$$\partial_t f(t, x, w) + w \cdot \nabla_x f(t, x, w) = \mathcal{B}[f, f](t, x, w), \quad (5.1.1)$$

where the Boltzmann collision integral is

$$\mathcal{B}[f, f](w) = \iint_{\mathbb{R}^3 \times \mathbb{S}^2} \left(f({}^o w) f({}^o w_1) - f(w) f(w_1) \right) b(w - w_1, \mathbf{n}) dw_1 d\mathbf{n}. \quad (5.1.2)$$

Here ${}^o w$ and ${}^o w_1$ denote the velocities just before the collision, while w and w_1 are the velocities immediately after the collision. The positive term $f({}^o w) f({}^o w_1)$ in the collision integral above accounts for the “gain” of gas molecules with velocity w , while the negative term $-f(w) f(w_1)$ represents the “lose” of such molecules with velocity w . For elastic collision between gas molecules, it's natural to require conservation of momentum and energy:

$${}^o w + {}^o w_1 = w + w_1; \quad |{}^o w|^2 + |{}^o w_1|^2 = |w|^2 + |w_1|^2.$$

The system involves 6 unknowns (3 component for each pre-collision velocity), and 4 constraints, leaving 2-degree of freedom. To parametrize ${}^o w$ and ${}^o w_1$, we introduce additional variable $\mathbf{n} \in \mathbb{S}^2$, and it's easy to verify the following representation satisfy the conservation of momentum and energy:

$$\begin{aligned} {}^o w &\equiv {}^o w(w, w_1, \mathbf{n}) = w - (w - w_1) \cdot \mathbf{n} \mathbf{n}, \\ {}^o w_1 &\equiv {}^o w_1(w, w_1, \mathbf{n}) = w_1 + (w - w_1) \cdot \mathbf{n} \mathbf{n}, \end{aligned}$$

where $\mathbf{n}$ varies over the unit sphere $\mathbb{S}^2 \subset \mathbb{R}^3$. Note that here the pre-collision velocities are parametrized by the unit vector $\mathbf{n}$. However, this is not the standard σ -representation commonly used in the Boltzmann collision integral. The representation of the pre-collision velocities ${}^o w$ and ${}^o w_1$ are not unique. The relationship between these vectors can be visualized in Figure 5.1.

The collision kernel $b(z, \omega)$ is of the form

$$b(z, \omega) = |z| \Sigma(|z|, \cos(\widehat{z, \omega})) \quad \text{with } \Sigma > 0.$$

One can (formally) derive the Boltzmann equation from Hamilton's equation for an N -particle system in the case of hard sphere—rigorously established for the short time by Lanford [Lan75]—under the Boltzmann-Grad scaling: $N(2r)^2 \sim 1$. In this case, collision kernel takes of the form $b(z, \omega) = (2r)^2 |\cos(\widehat{z, \omega})|$. Moreover, the excluded volume $N(2r)^3 = O(r)$ becomes negligible in the N -particle limit (namely, $N \rightarrow \infty$ and $r \rightarrow 0$). This indicates that the gas described by the Boltzmann equation must be sufficiently “dilute”.

It's well-known that for all $f \in L^1(\mathbb{R}, (1 + |w|^2)^3 dw)$, the collision integral conserves mass, momentum, energy locally (see, for instance, section 3.1 and section 3.3 in [Cer94]), meaning

$$\int_{\mathbb{R}^3} \mathcal{B}[f, f](w) \begin{pmatrix} 1 \\ w \\ |w|^2 \end{pmatrix} dw = 0. \quad (5.1.3)$$

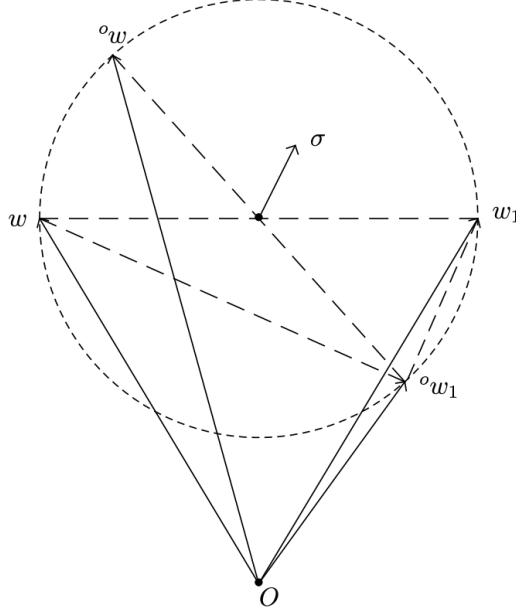


Figure 5.1: Illustration of a geometric configuration relevant to Boltzmann collisions

This property implies that the Boltzmann collision integral does not contribute to the macroscopic equation *directly*, but only in an indirect way. In other words, we multiply equation (5.1.1) by 1, w , or $|w|^2/2$ and integrate it with respect to w . If $f, \partial_t f$ and $\nabla_x f \in L^1(\mathbb{R}, (1 + |w|^2)^3 dw)$ we can write

$$\begin{cases} \partial_t \int_{\mathbb{R}^3} f(t, x, w) dw + \operatorname{div}_x \int_{\mathbb{R}^3} w f(t, x, w) dw = 0, \\ \partial_t \int_{\mathbb{R}^3} w f(t, x, w) dw + \operatorname{div}_x \int_{\mathbb{R}^3} w^{\otimes 2} f(t, x, w) dw = 0, \\ \partial_t \int_{\mathbb{R}^3} \frac{|w|^2}{2} f(t, x, w) dw + \operatorname{div}_x \int_{\mathbb{R}^3} w \frac{|w|^2}{2} f(t, x, w) dw = 0, \end{cases}$$

where the divergence of a 2-tensor $A \equiv (A_{ij})$ with respect to variable x is defined componentwise by $(\operatorname{div}_x A)_i = (\partial_{x_j} A_{ij})$.

Under the following definitions, we can establish the connection between kinetic de-

scription of gas and the framework of continuum mechanics. Let's introduce:

$$\begin{aligned}
 R(t, x) &:= \int_{\mathbb{R}^3} f(t, x, w) dw, && \text{Local number density} \\
 U(t, x) &:= \frac{H(R(t, x))}{R(t, x)} \int_{\mathbb{R}^3} w f(t, x, w) dw, && \text{Bulk velocity} \\
 P(t, x) &:= \int_{\mathbb{R}^3} (w - U(t, x))^{\otimes 2} f(t, x, w) dw, && \text{Stress tensor} \\
 E_{\text{int}}(t, x) &:= \frac{H(R(t, x))}{2R(t, x)} \int_{\mathbb{R}^3} |w - U(t, x)|^2 f(t, x, w) dw, && \text{Internal energy} \\
 \Lambda(t, x) &:= \frac{1}{2} \int_{\mathbb{R}^3} (w - U(t, x)) |w - U(t, x)|^2 f(t, x, w) dw, && \text{Energy flux}
 \end{aligned}$$

where $H : \mathbb{R} \rightarrow \{0, 1\}$ denotes the Heaviside step function is defined by

$$H(r) = \begin{cases} 1 & \text{for } r > 0 \\ 0 & \text{for } r \leq 0. \end{cases}$$

These definitions leads to the following fluid equations:

$$\begin{cases} \partial_t R + \operatorname{div}_x (RU) = 0, \\ \partial_t (RU_i) + \sum_{j=1}^3 \partial_{x_j} (RU_i U_j + P_{ij}) = 0, & i = 1, 2, 3 \\ \partial_t (R (\frac{1}{2}|U|^2 + E_{\text{int}})) + \operatorname{div}_x (RU (\frac{1}{2}|U|^2 + E_{\text{int}})) + \sum_{i=1}^3 \partial_{x_i} \left[\sum_{j=1}^3 U_j P_{ij} + \Lambda_i \right] = 0, \end{cases}$$

These equations represent, respectively, the conservation of mass, momentum, and energy in the fluid regime derived from kinetic theory. Obviously, the system of macroscopic equation is not closed, as it involves 16 unknowns subject to only 5 constrains. To close the system, we consider the high-collision regime, which ensures that f take the form of a local Maxwellian distribution (see, for instance, Section 3.2 in [Cer94]). Under this assumption, it's straightforward to verify the following relations:

$$P(t, x) = \frac{2}{3} R(t, x) E_{\text{int}}(t, x) \operatorname{Id}; \quad \Lambda(t, x) = 0.$$

These constitute the classical equation of state for dilute (or ideal) gas.

This illustrates how the Boltzmann collision integral contributes to the fluid equations, in contrast to the free transport equation $\partial_t f + w \cdot \nabla_x f = 0$, where no such closure naturally arises—yet the stress tensor still appears in the macroscopic description.

For the binary mixture, we can consider the following coupled Boltzmann equations:

$$\begin{cases} (\partial_t + w \cdot \nabla_x) f(t, x, w) &= \mathcal{R}[f, F](t, x, w) + \mathcal{C}[f, f](t, x, w), \\ (\partial_t + v \cdot \nabla_x) F(t, x, v) &= \mathcal{D}[F, f](t, x, v) + \mathcal{Q}[F, F](t, x, v). \end{cases} \quad (5.1.4)$$

Here, the collision integrals $\mathcal{R}, \mathcal{D}$ describe the interactions between two different species,

while collision integrals $\mathcal{Q}, \mathcal{C}$ represent the self-collision within each species. Previous works are largely based on specific choices and modifications on the Boltzmann collision integral. For example, [Ber+17] and [Ber+18] use the Boltzmann collision integrals with different scalings for velocities and mass ratio. [CD09] considers the size of particles in the modeling. [CD25] and [CMS25] modified the Boltzmann collision integral. In this work, we adopt the Enskog collision integral, which will be introduced in the next subsection, as a refinement of the Boltzmann operator to more accurately capture the finite-volume effects in moderately to densely packed regimes.

5.1.2 The Enskog equation

When the radius of molecules cannot be ignored, precisely, the Boltzmann-Grad assumption fails, we should seek for another model to describe such a system (dense gas). Later on, Enskog [Ens22] proposed the so-called (standard) Enskog equation which shares the same structure with the Boltzmann equation, while the collision integral is different:

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \mathcal{E}[f, f](t, x, v), \quad (5.1.5)$$

where collision integral $\mathcal{E}$ is given by

$$\begin{aligned} \mathcal{E}[f, g](t, x, v) := & \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left[\chi[f, g](t, x, y) f(t, x, {}^o v) g(t, y, {}^o v_1) - \chi[f, g](t, x, y) f(t, x, v) g(t, y, v_1) \right] \\ & (v - v_1) \cdot \frac{y - x}{|y - x|} H \left((v - v_1) \cdot \frac{y - x}{|y - x|} \right) \delta(|x - y| - 2r_p) dy dv_1. \end{aligned} \quad (5.1.6)$$

Here, $r_p > 0$ denotes the diameter of the particle, and $\chi \equiv \chi[f, g](t, x, y)$ is the correlation function, which captures the effects of volume exclusion—such as shielding influence. Further details can be found in Chapter 16 of [CC90]. In other words, the presence of finite-size particles reduces the statistical independence of two-particle configurations compared to the dilute gas case. If we assume the propagation of chaos holds—that is, the two-particle distribution function $f^{(2)}(t, x_1, x_2, w_1, w_2)$ can be approximated by the product of two single-particle distribution functions $f(t, x_1, w_1) f(t, x_2, w_2)$ —then we may set $\chi \equiv 1$ in the Enskog collision integral. Under this assumption, we refer to equation (5.1.5) with such a simplified collision integral as the *Enskog-Boltzmann equation*. For the remainder of this work, we consider only this case, i.e. we always assume $\chi \equiv 1$. As we will see, this assumption is sufficient to capture the necessary modification of the pressure in the macroscopic fluid equations.

Unlike in the Boltzmann case, the pre-collision velocities in the Enskog setting are determined uniquely by conservation momentum, conservation of energy, and the positions of the colliding particles

$$\begin{cases} {}^o v \equiv {}^o v(x, v_1, x - y) = v - (v - v_1) \cdot \frac{y - x}{|y - x|} \frac{y - x}{|y - x|}, \\ {}^o v_1 \equiv {}^o v_1(x, v_1, x - y) = v_1 + (v - v_1) \cdot \frac{y - x}{|y - x|} \frac{y - x}{|y - x|}. \end{cases}$$

This determinism arises because, unlike in the Boltzmann model where particles are treated as point masses, the Enskog model accounts for the finite size of particles. Thus, it dis-

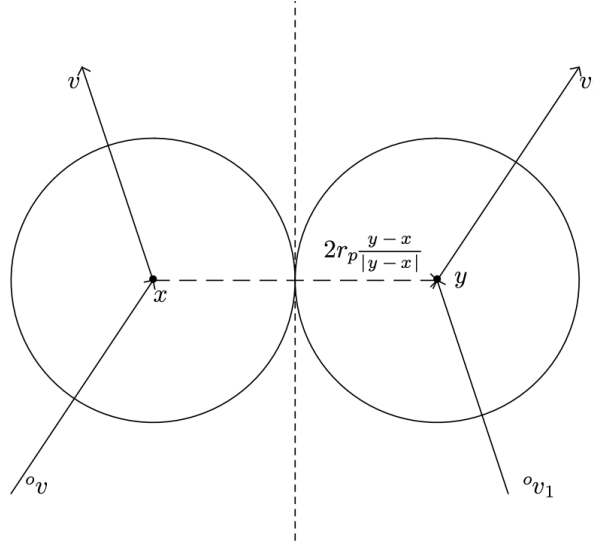


Figure 5.2: Diagram illustrating particle positions and velocities during a collision.

tinguishes between the collision point and the center of mass of each particles. See the illustrative diagram 5.2. More details about Enskog equation can be found in Chapter 16 of [CC90]. In the following, we adopt the $\mathbf{n}$ -representation of the Enskog-Boltzmann collision integral, which corresponds to the change of variables $y = x \pm 2r_p \mathbf{n}$ in the gain (positive) and loss (negative) terms, respectively. Under this transformation, the collision integral (5.1.6) can be rewritten as:

$$\mathcal{E}[f, g](t, x, v) := \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left[f(t, x, {}^o v) g(t, x - 2r_p \mathbf{n}, {}^o v_1) - f(t, x, v) g(t, x + 2r_p \mathbf{n}, v_1) \right] (v - v_1) \cdot \mathbf{n} H((v - v_1) \cdot \mathbf{n}) (2r_p)^2 d\mathbf{n} dv_1.$$

Parallel to the result for the Boltzmann collision, integral, one may ask whether the Enskog collision integral locally conserves mass, momentum, and energy? The answer is *no*. However, it does conserve these quantities globally. As shown in [CCG24], the Enskog-Boltzmann collision integral admits the following conservative form (in the sense of distributions):

$$\mathcal{E}[f, f](w) \begin{pmatrix} 1 \\ w_1 \\ w_2 \\ w_3 \\ |w|^2 \end{pmatrix} = \begin{pmatrix} \operatorname{div}_v \mathbb{J}_0 \\ \operatorname{div}_x \mathbb{I}_1 + \operatorname{div}_v \mathbb{J}_1 \\ \operatorname{div}_x \mathbb{I}_2 + \operatorname{div}_v \mathbb{J}_2 \\ \operatorname{div}_x \mathbb{I}_3 + \operatorname{div}_v \mathbb{J}_3 \\ \operatorname{div}_x \mathbb{I}_4 + \operatorname{div}_v \mathbb{J}_4 \end{pmatrix},$$

for some specific vectors $\mathbb{I}_1, \dots, \mathbb{I}_4, \mathbb{J}_0, \dots, \mathbb{J}_4$. This indicates that, unlike the Boltzmann case, the Enskog collision integral contribute *directly* to the macroscopic equations due to the presence of the term $\mathbb{I}$. More specifically, using the same notations as before, we obtain the following macroscopic equations by multiplying equation (5.1.5) by 1, w , or $|w|^2/2$, and

integrate it with respect to w

$$\begin{cases} \partial_t R + \operatorname{div}_x(RU) = 0, \\ \partial_t(RU_i) + \sum_{j=1}^3 \partial_{x_j}(RU_i U_j + P_{ij}) - \operatorname{div}_x \mathbb{I}_i = 0, & i = 1, 2, 3 \\ \partial_t \left(R \left(\frac{1}{2} |U|^2 + E_{\text{int}} \right) \right) + \operatorname{div}_x \left(RU \left(\frac{1}{2} |U|^2 + E_{\text{int}} \right) \right) + \sum_{i=1}^3 \partial_{x_i} \left[\sum_{j=1}^3 U_j P_{ij} + \Lambda_i \right] - \operatorname{div}_x \mathbb{I}_4 = 0, \end{cases}$$

Another approach to derive the corresponding hydrodynamics equations for Enskog gas—Enskog-Euler system—is through the Hilbert expansion, as in [Lac98]. However, unlike the system derived above, this approach yields an asymptotic result. As a byproduct, the influence of particle volume on the equation for the Enskog gases becomes apparent. The pressure is modified as follows

$$p_E = \frac{2}{3} R E_{\text{int}} \left(1 + \frac{4}{3} \pi r_p R \right), \quad (5.1.7)$$

highlighting a correction to the ideal gas law due to finite-size effects. At this point, we have strong motivation to introduce the Enskog collision integral to capture the effect of volume fraction on stress tensor in the macroscopic equation for thick sprays.

5.2 The kinetic-fluid description: Vlasov-Euler system

Beyond the kinetic description of collisions, an alternative framework involves coupling a fluid equation—such as the Navier-Stokes, Stokes, or Euler equations—with a kinetic equation, typically of Vlasov type. When the volume fraction of the dispersed phase is sufficiently small, the system is described by the so-called thin sprays model:

$$\begin{cases} \partial_t \rho + \operatorname{div}_x(\rho u) = 0, \\ \partial_t(\rho u) + \operatorname{div}_x(\rho u \otimes u) + \nabla_x p = m_g \int_{\mathbb{R}^3} F(v) D(v - u) dv, \\ \partial_t(\rho E) + \operatorname{div}_x(\rho u E) + \operatorname{div}_x(p u) = m_g \int_{\mathbb{R}^3} v \cdot D(v - u) F(v) dv, \\ \partial_t F + v \cdot \nabla_x F + \operatorname{div}_v[F(v) D(v - u)] = 0, \\ p = n\theta, E = \frac{|u|^2}{2} + \frac{3\theta}{2m_g}, n = \frac{\rho}{m_g} \end{cases} \quad (5.2.1)$$

where ρ, u, θ, p, E represent the local density, velocity, temperature, pressure, and internal energy of gas respectively, $F = F(t, x, v)$ denotes the distribution of particles bedding in the gas, $D \equiv D(v - u)$ is a given function describing the friction between the two species, typically defined by the linear case $D(\xi) = \xi$, or the quadratic case $D(\xi) = \xi|\xi|$. However, it may depending on gas density and internal energy. A formal derivation of this model has been presented in [DGR19].

To account for the volume contribution in the pressure, we introduce the volume fraction

function by

$$\check{\alpha}(t, x) := 1 - \frac{4\pi}{3} r_p^3 \int_{\mathbb{R}^3} F(t, x, v) dv,$$

where r_p represent the radius of spherical suspension, and $F(t, x, v)$ is the density function of suspensions. Thus, $\int_{\mathbb{R}^3} F(t, x, v) dv$ represents the total number of suspensions. Here, we give an intuitive explanation of how the volume fraction contributes when it cannot be neglected. From a macroscopic perspective, one can understand why volume occupation contributes to the pressure; see [THa76] for reference. The buoyancy force on a spherical droplet can be expressed as $(F_{\text{buoy}})_i = -\int_{\partial B_i} p(t, x) n(x) dS(x)$, where dS is surface element, $\mathbf{n}$ denotes the outer normal vector to i -th ball $B_i = B(X_i, r_p)$. By the Gauss theorem, we obtain $(F_{\text{buoy}})_i = -\int_{B_i} \nabla_x p(t, x) dV(x)$. If the density of the droplet does not vary significantly on its surface, or if the droplet is sufficiently small, the buoyancy can be approximated by $(F_{\text{buoy}})_i \sim -\frac{4\pi}{3} r_p^3 \nabla_x p$. Repeating this argument for N_p particles, we obtain

$$F_{\text{buoy}} \sim -\frac{4\pi}{3} r_p^3 N_p \nabla_x p.$$

From the mesoscopic point of view, the number of particles is replaced by the particle distribution function F , leading to the approximation

$$F_{\text{buoy}} \sim -\frac{4\pi}{3} r_p^3 \int_{\mathbb{R}^3} F(t, x, v) dv \nabla_x p.$$

This explains, in an extremely formal way, why the volume fraction function appears outside the pressure gradient in the following system. We will revisit and discuss this reasoning from a mesoscopic point of view in Section 5.7. Therefore, we can formally write the following Vlasov-Euler equations for thick sprays which is widely accepted:

$$\left\{ \begin{array}{l} \partial_t(\check{\alpha}\rho) + \text{div}_x(\check{\alpha}\rho u) = 0, \\ \partial_t(\check{\alpha}\rho u) + \text{div}_x(\check{\alpha}\rho u^{\otimes 2}) + \nabla_x p = m_g \int_{\mathbb{R}^3} F(v) \Gamma(v - u) dv, \\ \partial_t(\check{\alpha}\rho E) + \text{div}_x(\check{\alpha}\rho u E) + \text{div}_x(\check{\alpha} u p) + p \partial_t \check{\alpha} = m_g \int_{\mathbb{R}^3} D(v - u) \cdot v F(v) dv, \\ \partial_t F + v \cdot \nabla_x F + \text{div}_v(F \Gamma) = 0, \\ \Gamma(v - u) = \frac{4\pi}{3} r_p^3 \nabla_x p + D(v - u), \\ p = n\theta, \quad E = \frac{|u|^2}{2} + \frac{3\theta}{2m_g}, \quad \rho = m_g n, \\ \check{\alpha} = 1 - \frac{4\pi}{3} r_p^3 \int_{\mathbb{R}^3} F(v) dv, \end{array} \right. \quad (5.2.2)$$

where Γ represents the drag force between gas and particle. Here the drag force includes not only the friction term D , as in the case of thin sprays, but also an additional contribution accounting for pressure modification. If we set $\check{\alpha} = 1$ in equations (5.2.2), we recover the Vlasov-Euler system for thin sprays (5.2.1).

A substantial body of work has focused on modeling and analysis of gas-particle systems, particularly thick sprays. The foundational model of many particles suspended in

a gas was considered in [THa76]. A more systematic and comprehensive model for thick sprays—including collisions, cooling process, energy exchange, and more— was developed in [ORo81]. This model has served as the basis for many subsequent studies and computational developments, especially in the content of the Kiva code; see, for instance [AOB89]. [BDM03] conducted a numerical study of this model, and demonstrated the global conservation of total energy. [Ben+12] provided a one-dimensional simulation of a thick sprays system within a pipe.

From a theoretical perspective, [FBD24] established the well-posedness for the modified thick sprays model by averaging the pressure term and volume fraction. [EH23] shows the well-posedness of this system under initial data satisfying a Penrose-type stability, which is shown to be necessary for the long-time stability. [FBD24; Fou24] studied the linearized thick sprays model, they showed that the system have similar behavior as Landau damping, in both numerical and theoretical ways. More recently, [Bia+25] shows the thick sprays model can exhibit linear ill-posedness, even locally in time.

Beyond this system, [DM10] formally derive the Eulerian-Eulerian description for the thick sprays.

Compared to general gas-particle models without finite-volume effect, the setting we consider involves the following simplifications: the radius of particles is fixed; there isn't energy exchanged, and collision between particles are elastic; all the collisions are elastic. The case with variable radii is addressed in [CD09]. A model incorporating inelastic collisions can be found in [CDS12] with numerical scheme. Models that include energy exchange between different species have been studied in more recent works, such as [CD25; CMS25].

5.3 Building on the dimensionless kinetic equations

As motivated in the last subsection, to model the thick sprays, we introduce the Enskog-Boltzmann collision integral into the system (5.1.2) with the following (elastic) collision laws:

$$m_p v' + m_g w' = m_p v + m_g w \quad (5.3.1)$$

$$m_p |v'|^2 + m_g |w'|^2 = m_p |v|^2 + m_g |w|^2, \quad (5.3.2)$$

Where m_p and m_g denote the mass of particle and gas molecule, respectively. These velocity distribution functions should satisfy the coupled Enskog-Boltzmann equations:

$$\begin{cases} (\partial_t + w \cdot \nabla_x) f(t, x, w) &= \mathcal{E}_1[f, F](t, x, w) + \mathcal{E}_0[f, f](t, x, w) \\ (\partial_t + v \cdot \nabla_x) F(t, x, v) &= \mathcal{E}_2[F, f](t, x, v) + \mathcal{E}_3[F, F](t, x, v) \end{cases} \quad (5.3.3)$$

where the Enskog-Boltzmann collision integrals are given by

$$\mathcal{E}_0[f, f](x, w) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} [f(x, {}^o w) f(x - 2r_g \mathbf{n}, {}^o w_1) - f(x, w) f(x + 2r_g \mathbf{n}, w_1)] b_g(w - w_1, \mathbf{n}) d\mathbf{n} dw_1,$$

$$\mathcal{E}_1[f, F](x, w) = (r_g + r_p)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} [F(x + (r_g + r_p) \mathbf{n}, {}' v) f(x, {}' w) - F(x - (r_g + r_p) \mathbf{n}, v) f(x, w)] (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dv$$

$$\mathcal{E}_2[F, f](x, v) = (r_g + r_p)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} [f(x - (r_g + r_p)\mathbf{n}, 'w)F(x, 'v) - f(x + (r_g + r_p)\mathbf{n}, w)F(x, v)] \\ (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw$$

$$\mathcal{E}_3[F, F](x, v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} [F(x, {}^o v)F(x - 2r_p\mathbf{n}, {}^o v_1) - F(x, v)F(x + 2r_p\mathbf{n}, v_1)] b_p(v - v_1, \mathbf{n}) d\mathbf{n} dv_1,$$

where the collision kernel b_β is of the form $b_\beta(\xi, \sigma) = |\xi| \Sigma_\beta(|\xi|, \sigma)$. For the case of hard sphere, $\Sigma_\beta(\xi, \sigma)$ is given by $\frac{2r_\beta^2}{m_\beta} |\cos(\widehat{\xi, \sigma})|$. Here r_β denotes the radius of molecule. Specifically, $\beta = g$ and p correspond to the collision kernel b_g and b_p respectively, and pre-collision velocities between same species are given by

$$\begin{cases} {}^o v = {}^o v(v, v_1, \mathbf{n}) = v - (v - v_1) \cdot \mathbf{n} \mathbf{n} \\ {}^o v_1 = {}^o v_1(v, v_1, \mathbf{n}) = v_1 - (v_1 - v) \cdot \mathbf{n} \mathbf{n}, \end{cases}$$

and the pre-collision velocities between different species are given by

$$\begin{cases} 'v = 'v(v, w, \mathbf{n}, \eta) = v - \frac{2\eta}{1+\eta} (v - w) \cdot \mathbf{n} \mathbf{n} \\ 'w = 'w(v, w, \mathbf{n}, \eta) = w - \frac{2}{1+\eta} (w - v) \cdot \mathbf{n} \mathbf{n}, \end{cases}$$

where $\eta = \frac{m_g}{m_p}$ denotes the mass ratio, supposing to be sufficient small.

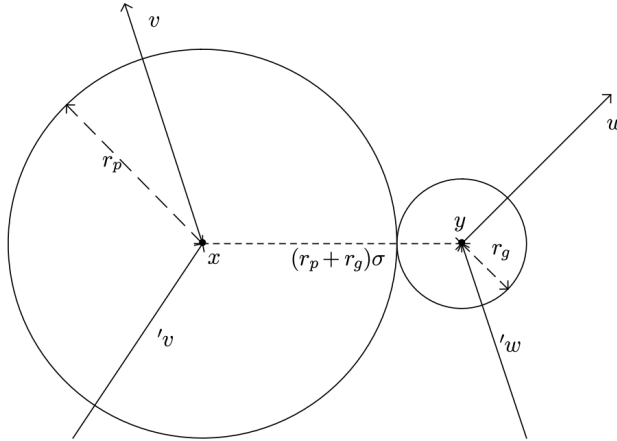


Figure 5.3: Schematic diagram of collision between different species

We then introduce the following table of physical parameters (Table 5.1). Throughout, subscript g, p refer to gas molecules and particles, respectively. The table of parameters is the same as in [Ber+17; Ber+18; DGR19]. We begin with equation (5.3.3). The dimensionless quantities are given by

$$\hat{x} = \frac{x}{L}, \quad \hat{t} = \frac{t}{T}, \quad \hat{v} = \frac{v}{V_p}, \quad \hat{w} = \frac{w}{V_g}$$

Parameter	Meaning
L	size of the container (periodic box)
T	time scale
N_p	number of particles/ L^3
N_g	number of gas molecules / L^3
V_p	thermal speed of particles
V_g	thermal speed of gas molecules
S_p	the average collision cross section between particles
S_g	the average collision cross section between gas molecules
r_p	the radius of particles
r_g	the radius of gas molecules
m_p	the mass of each particle
m_g	the mass of each gas molecule
$\eta := m_g/m_p$	mass ratio (≤ 1)
$\epsilon := V_p/V_g$	thermal speed ratio (≤ 1)

Table 5.1: Physical parameters

and the dimensionless distribution functions are

$$\hat{F}(\hat{t}, \hat{x}, \hat{v}) = \frac{F(t, x, v)}{N_p/V_p^3}; \quad \hat{f}(\hat{t}, \hat{x}, \hat{w}) = \frac{f(t, x, w)}{N_g/V_g^3}$$

The collision kernels in the Boltzmann collision integrals are rescaled by

$$\hat{b}_g(\hat{z}, \omega) = \frac{b_g(z, \omega)}{S_g V_g}, \quad \hat{b}_p(\hat{z}, \omega) = \frac{b_p(z, \omega)}{S_p V_p}.$$

The scaling comes from the dimension of the collision integral should match with the left hand side of the Boltzmann equation, see formula 2.2 in [LP81].

Summarizing these definitions, we can express the dimensionless collision integrals as follows:

$$\begin{aligned} \mathcal{E}_0[f, f] &= \frac{N_g^2}{V_g^6} S_g V_g^4 \hat{\mathcal{E}}_0[\hat{f}, \hat{f}], \\ \mathcal{E}_1[f, F] &= L^2 \frac{N_p}{V_p^3} \frac{N_g}{V_g^3} V_g V_p^3 \hat{\mathcal{E}}_1[\hat{f}, \hat{F}], \\ \mathcal{E}_2[F, f] &= L^2 \frac{N_p}{V_p^3} \frac{N_g}{V_g^3} V_g^4 \hat{\mathcal{E}}_2[\hat{F}, \hat{f}], \\ \mathcal{E}_3[F, F] &= \frac{N_p^2}{V_p^6} S_p V_p^4 \hat{\mathcal{E}}_3[\hat{F}, \hat{F}], \end{aligned}$$

where dimensionless collision integrals are given by

$$\hat{\mathcal{E}}_0[\hat{f}, \hat{f}](\hat{t}, \hat{x}, \hat{w}) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} [\hat{f}(\hat{x}, \hat{w}^\circ) \hat{f}(\hat{x} - \frac{2r_g}{L}, \hat{w}_1^\circ) - \hat{f}(\hat{x}, \hat{w}) \hat{f}(\hat{x} + \frac{2r_g}{L}, \hat{w}_1)] \hat{b}_g(\hat{w} - \hat{w}_1, \mathbf{n}) d\mathbf{n} d\hat{w}_1,$$

$$\begin{aligned}\hat{\mathcal{E}}_1[\hat{f}, \hat{F}](\hat{t}, \hat{x}, \hat{w}) &= S_g \left(\frac{r_g + r_p}{L} \right)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} [\hat{F}(\hat{x} + \frac{r_g + r_p}{L} \mathbf{n}, \hat{v}') \hat{f}(\hat{x}, \hat{w}') - \hat{F}(\hat{x} - \frac{r_g + r_p}{L} \mathbf{n}, \hat{v}) \hat{f}(\hat{x}, \hat{w})] \\ &\quad \times (\epsilon \hat{v} - \hat{w}) \cdot \mathbf{n} H((\epsilon \hat{v} - \hat{w}) \cdot \mathbf{n}) d\mathbf{n} d\hat{v}\end{aligned}$$

$$\begin{aligned}\hat{\mathcal{E}}_2[\hat{F}, \hat{f}](\hat{t}, \hat{x}, \hat{v}) &= \left(\frac{r_g + r_p}{L} \right)^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} [\hat{f}(\hat{x} - \frac{r_g + r_p}{L} \mathbf{n}, \hat{w}') \hat{F}(\hat{x}, \hat{v}') - \hat{f}(\hat{x} + \frac{r_g + r_p}{L} \mathbf{n}, \hat{w}) \hat{F}(\hat{x}, \hat{v})] \\ &\quad \times (\epsilon \hat{v} - \hat{w}) \cdot \mathbf{n} H((\epsilon \hat{v} - \hat{w}) \cdot \mathbf{n}) d\mathbf{n} d\hat{w}\end{aligned}$$

$$\hat{\mathcal{E}}_3[\hat{F}, \hat{F}](\hat{t}, \hat{x}, \hat{v}) = S_p \int_{\mathbb{R}^3 \times \mathbb{S}^2} [\hat{F}(\hat{x}, \hat{v}^o) \hat{F}(\hat{x} - \frac{2r_p}{L} \mathbf{n}, \hat{v}_1^o) - \hat{F}(\hat{x}, \hat{v}) \hat{F}(\hat{x} + \frac{2r_p}{L} \mathbf{n}, \hat{v}_1)] \hat{b}_p(\hat{v} - \hat{v}_1, \mathbf{n}) d\mathbf{n} d\hat{v}_1,$$

and the rescaled pre-collision velocities between same species are given by

$$\begin{cases} \hat{w}^o(\hat{w}, \hat{w}_1, \mathbf{n}) := \widehat{o\hat{w}} = \hat{w} - (\hat{w} - \hat{w}_1) \cdot \mathbf{n} \mathbf{n}, \\ \hat{w}_1^o(\hat{w}, \hat{w}_1, \mathbf{n}) := \widehat{o\hat{w}_1} = \hat{w}_1 - (\hat{w}_1 - \hat{w}) \cdot \mathbf{n} \mathbf{n}. \end{cases}$$

The rescaled pre-collision velocities between different species are given by

$$\begin{cases} \hat{v}'(\hat{v}, \hat{w}, \mathbf{n}) = \widehat{v'} = \hat{v} - \frac{2\eta}{1+\eta} (\hat{v} - \frac{1}{\epsilon} \hat{w}) \cdot \mathbf{n} \mathbf{n}, \\ \hat{w}'(\hat{v}, \hat{w}, \mathbf{n}) = \widehat{w'} = \hat{w} - \frac{2}{1+\eta} (\hat{w} - \epsilon \hat{v}) \cdot \mathbf{n} \mathbf{n}, \end{cases}$$

where we recall that $\epsilon := V_p/V_g$ is the thermal speed ratio, and $\mathbf{n}$ denotes the unit vector along the line connecting the centers of the colliding particles. The dimensionless form of the left-hand side equations should be

$$\begin{cases} (\partial_t + w \cdot \nabla_x) f(t, x, w) = \frac{N_g}{V_g^3} \left(\frac{1}{T} \partial_t + \frac{V_g}{L} \hat{w} \cdot \nabla_{\hat{x}} \right) \hat{f}(\hat{t}, \hat{x}, \hat{w}), \\ (\partial_t + v \cdot \nabla_x) F(t, x, v) = \frac{N_p}{V_p^3} \left(\frac{1}{T} \partial_t + \frac{V_p}{L} \hat{v} \cdot \nabla_{\hat{x}} \right) \hat{F}(\hat{t}, \hat{x}, \hat{v}). \end{cases}$$

Combining these two parts and dropping the hats on each variable and function, we can write the dimensionless kinetic equations as follows

$$\begin{cases} \partial_t f + \frac{V_g T}{L} w \cdot \nabla_x f = L^2 N_p V_g T \mathcal{E}_1[f, F] + N_g S_g T V_g \mathcal{E}_0[f, f] \\ \partial_t F + \frac{V_p T}{L} v \cdot \nabla_x F = L^2 N_g V_g T \mathcal{E}_2[F, f] + N_p S_p T V_p \mathcal{E}_3[F, F], \end{cases}$$

To simplify the equations, we assume the following conditions

(A1) The velocity scale of gas molecules is the same as that of the particles: $\epsilon = 1$.

(A2) We choose the time scale as: $T = L/V_g$.

(A3) The length scale satisfies: $L^3 N_p = 1$.

- (A4) The mass ratio is equal to the number ratio, and they are sufficient small: $\frac{N_p}{N_g} = \eta \ll 1$.
- (A5) We assume the averaged gas molecule cross section S_g such that: $1/\delta := N_g L S_g \gg 1^1$.
- (A6) The collisions between particles can be ignored: $N_p L S_p \ll 1$. We will neglect this term in the following discussion.
- (A7) The radius of gas molecules is sufficient small compared to the length scale: $r_g/L \ll 1$. This assumption degenerates Enskog-Boltzmann collision integral $\mathcal{E}_0$ into a classical Boltzmann collision integral $\mathcal{B}$.

In fact, these assumptions are nearly identical to those in [DGR19], which are specified for the case of a hard-sphere collision kernel between two species.

Therefore, we arrive at the rescaled kinetic equations:

$$\begin{cases} \partial_t f + w \cdot \nabla_x f = \mathcal{E}_1^\eta[f, F] + \frac{1}{\delta} \mathcal{B}[f, f] \\ \partial_t F + v \cdot \nabla_x F = \frac{1}{\eta} \mathcal{E}_2^\eta[F, f], \end{cases} \quad (5.3.4)$$

where the rescaled Enskog-Boltzmann collision integrals are given by

$$\mathcal{B}[f, f](x, w) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} [f(x, w^o) f(x, w_1^o) - f(x, w) f(x, w_1)] (w - w_1) \cdot \mathbf{n} H((w - w_1) \cdot \mathbf{n}) d\mathbf{n} dw_1, \quad (5.3.5)$$

$$\mathcal{E}_1^\eta[f, F](x, w) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} a^2 [f(x, w') F(x + a\mathbf{n}, v') - f(x, w) F(x - a\mathbf{n}, v)] (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dv, \quad (5.3.6)$$

$$\mathcal{E}_2^\eta[F, f](x, v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} a^2 [f(x - a\mathbf{n}, w') F(x, v') - f(x + a\mathbf{n}, w) F(x, v)] (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw, \quad (5.3.7)$$

where the dimensionless radius is defined as

$$a := \frac{r_p}{L},$$

and the pre-collision velocities between different species with mass ratio and velocity scaling are given by

$$\begin{cases} v' \equiv v'(v, w, \mathbf{n}, \eta) = v - \frac{2\eta}{1+\eta} (v - w) \cdot \mathbf{n} \mathbf{n}, \\ w' \equiv w'(v, w, \mathbf{n}, \eta) = w - \frac{2}{1+\eta} (w - v) \cdot \mathbf{n} \mathbf{n}, \end{cases} \quad (5.3.8)$$

and the pre-collision velocities between molecules of the same species with velocity scaling given by

$$\begin{cases} v^o \equiv v^o(v, v_1, \mathbf{n}) = v - (v - v_1) \cdot \mathbf{n} \mathbf{n} \\ v_1^o \equiv v_1^o(v, v_1, \mathbf{n}) = v_1 - (v_1 - v) \cdot \mathbf{n} \mathbf{n}. \end{cases}$$

It's easy to check the following collision properties.

¹Here $\delta > 0$ is a parameter, not Dirac mass.

- Pre-collision velocities are even function with respect to $\mathbf{n}$

$$v'(v, w, \mathbf{n}, \eta) = v'(v, w, -\mathbf{n}, \eta); w'(v, w, \mathbf{n}, \eta) = w'(v, w, -\mathbf{n}, \eta). \quad (5.3.9)$$

- The collision process is reversible: Let $\Phi^\eta(v, w) := (v'(v, w, \mathbf{n}, \eta), w'(v, w, \mathbf{n}, \eta))$, then

$$\Phi^\eta \circ \Phi^\eta(v, w) = (v, w). \quad (5.3.10)$$

- The result above gives the absolute value the determinant of the Jacobian of the change of variable is 1

$$\left| \det \frac{\partial \Phi^\eta(v, w)}{\partial (v, w)} \right| = 1. \quad (5.3.11)$$

- The collision is specular reflection with respect to norm vector $\mathbf{n}$

$$(v'(v, w, \mathbf{n}, \eta) - w'(v, w, \mathbf{n}, \eta)) \cdot \mathbf{n} = -(v - w) \cdot \mathbf{n}. \quad (5.3.12)$$

By simply taking $\eta = 1$, we obtain the same properties for the pre-collision velocities (v^o, v_1^o) and (w^o, w_1^o) .

At the end of this subsection, we remark that if we adopt a different scaling, for example, if we introduce distinct thermal velocities V_g and V_p — it becomes possible to derive the Vlasov-Stokes, or Vlasov-Navier-Stokes system; see [Ber+17; Ber+18].

5.4 Main result: Derivation of the Euler-Vlasov system for thick sprays

Each term in the macroscopic equation can be interpreted from a mesoscopic point of view. By retaining leading-order contributions and carefully estimating higher-order terms, the derived macroscopic equation provides a consistent approximation of the underlying kinetic model while revealing the original of each term from kinetic level.

In the following sections, we aim to prove the following theorem, which derive the experimental kinetic-fluid equations (5.2.2) from the more fundamental equations—namely, the coupled Enskog-Boltzmann equations, at a formal asymptotic level:

Theorem 5.4.1. *Let $f^{\eta, \delta} = f^{\eta, \delta}(t, x, w)$, and $F^{\eta, \delta} = F^{\eta, \delta}(t, x, v)$ solve the following coupled Enskog-Boltzmann equations*

$$\begin{cases} \partial_t f^{\eta, \delta} + w \cdot \nabla_x f^{\eta, \delta} = \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] + \frac{1}{\delta} \mathcal{B}[f^{\eta, \delta}, f^{\eta, \delta}], \\ \partial_t F^{\eta, \delta} + v \cdot \nabla_x F^{\eta, \delta} = \frac{1}{\eta} \mathcal{E}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}]. \end{cases} \quad (5.4.1)$$

Assume that, for each (η, δ) , $f^{\eta, \delta}(w)$, $f^{\eta, \delta}(w)w$, $f^{\eta, \delta}(w)|w|^2 \in L^1(\mathbb{R}_w)$, and $F^{\eta, \delta} \in W^{2, \infty}(\mathbb{R}_x) \cap W^{1, 1}(\mathbb{R}_v)$. Moreover, suppose $\partial_t f^{\eta, \delta}$, $w \cdot \nabla_x f^{\eta, \delta}$, and $\mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}]$ has uniform bound with respect to δ and η . Assume further that there exists $\alpha, n, u, \theta \in C^1(\mathbb{R}_+ \times \mathbb{R})$, $F \in C^1(\mathbb{R}_+, W^{2, \infty}(\mathbb{R}_x, W^{1, 1}(\mathbb{R}_v)))$, $f^{\eta, \delta} \rightarrow \mu \equiv \mu[\alpha(t, x)n(t, x), u(t, x), \theta(t, x)/m_g](w)$, $F^{\eta, \delta} \rightarrow F(t, x, v)$, and $\nabla_x F^{\eta, \delta} \rightarrow \nabla_x F(t, x, v)$ almost everywhere as $\delta, \eta \rightarrow 0$ where μ is Maxwellian

distribution

$$\mu[\alpha n, u, \theta/m_g](t, x, w) := \frac{\alpha(t, x)n(t, x)}{(2\pi\theta(t, x)/m_g)^{3/2}} \exp\left(-\frac{m_g|w - u(t, x)|^2}{2\theta(t, x)}\right). \quad (5.4.2)$$

Then $(\alpha, n, u, \theta, F)$ solve the following equations in the weak sense

$$\partial_t(\alpha\rho) + \operatorname{div}_x(\alpha\rho u) = 0, \quad (5.4.3)$$

$$\partial_t(\alpha\rho u) + \operatorname{div}_x(\alpha\rho u^{\otimes 2}) + \alpha\nabla_x p = m_g \int_{\mathbb{R}^3} F(v)D(v-u)dv - \operatorname{div}_x\left(\alpha\rho \int_{\mathbb{R}^3} F(v)Q(v-u)dv\right) + \mathcal{R}, \quad (5.4.4)$$

$$\partial_t(\alpha\rho E) + \operatorname{div}_x(\alpha\rho uE) + \operatorname{div}_x(\alpha\rho u) + p\partial_t\alpha \quad (5.4.5)$$

$$= m_g \int_{\mathbb{R}^3} F(v)D(v-u)v dv - \operatorname{div}_x\left(\alpha\rho \int_{\mathbb{R}^3} F(v)Q(v-u)v dv\right) + \mathcal{P},$$

$$\partial_t F + v \cdot \nabla_x F + \operatorname{div}_v \left[F \left(D(v-u) + \frac{4\pi}{3} a^3 \nabla_x p \right) \right] = \mathcal{Q}, \quad (5.4.6)$$

$$p = n\theta, \quad E = \frac{|u|^2}{2} + \frac{3\theta}{2m_g}, \quad \rho = m_g n \quad (5.4.7)$$

$$\alpha = 1 - \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} F(v)dv. \quad (5.4.8)$$

The friction force $D(v-u) \equiv D[\alpha n, u, \theta](v-u)$ is given by

$$D[\alpha n, u, \theta](v-u) := \pi a^2 \alpha n \frac{\theta}{m_g} q\left(\frac{v-u}{\sqrt{\theta/m_g}}\right) + \operatorname{div}_x[\alpha n Q(v-u)], \quad (5.4.9)$$

where $q \in \mathbb{R}$ is defined as

$$q(\xi) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} (\xi - y) |\xi - y| e^{-|y|^2/2} dy, \quad (5.4.10)$$

Q is a 2-tensor defined as

$$Q(\xi) := \frac{4\pi}{15} a^3 [2\xi^{\otimes 2} + |\xi|^2 \operatorname{Id}]. \quad (5.4.11)$$

And the remainder terms $\mathcal{P}, \mathcal{Q} \in \mathbb{R}$ and $\mathcal{R} \in \mathbb{R}$ are of order $o(a^3)$, explicitly given by

$$\begin{aligned}
\mathcal{P}(t, x) &:= 2a^2 m_g \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} \mu[\alpha n, u, \theta](x, w) [F(x, v) - F(x - a\mathbf{n}, v) + a\mathbf{n} \cdot \nabla_x F(x, v)] ((v - w) \cdot \mathbf{n})^2 v \cdot \mathbf{n} \\
&\quad H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw - ((1 - \alpha)n\theta \partial_t \alpha)(t, x) \\
\mathcal{Q}(t, x) &:= a^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} F(x, v) \left[\mu[\alpha n, u, \theta](x - a\mathbf{n}, w + 2(v - w) \cdot \mathbf{n}\mathbf{n}) - \mu[\alpha n, u, \theta](x, w + 2(v - w) \cdot \mathbf{n}\mathbf{n}) \right. \\
&\quad + a\mathbf{n} \cdot \nabla_x \mu[\alpha n, u, \theta](x, w + 2(v - w) \cdot \mathbf{n}\mathbf{n}) - \mu[\alpha n, u, \theta](x + a\mathbf{n}, w) + \mu[\alpha n, u, \theta](x, w) \\
&\quad \left. + a\mathbf{n} \cdot \nabla_x \mu[\alpha n, u, \theta](x, w) \right] (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} \\
&\quad + \frac{4\pi}{3m_g} a^3 n \theta \nabla_v F(x, v) \cdot \nabla_x \alpha(t, x) - \frac{4\pi}{3m_g} a^3 (1 - \alpha) \nabla_v F(x, v) \cdot (\nabla_x (n\theta))(t, x) \\
\mathcal{R}(t, x) &:= 2a^2 m_g \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} \mu[\alpha n, u, \theta](x, w) [F(x - a\mathbf{n}, v) - F(x, v) + a\mathbf{n} \cdot \nabla_x F(x, v)] [(v - w) \cdot \mathbf{n}]^2 \mathbf{n} \\
&\quad H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw + ((1 - \alpha)n\theta \nabla_x \alpha)(t, x),
\end{aligned} \tag{5.4.12}$$

The theorem is primarily based on the following two propositions, which are proved in Section 5.5 and Section 5.6, respectively. Proposition 5.4.1 aims to derive the Vlasov-type equation (5.4.6) from (5.3.4).

Proposition 5.4.1. *For any test function $\varphi(v) \in C^\infty(\mathbb{R})$, and Enskog-Boltzmann collision integral $\mathcal{E}_2^\eta[F, f]$ defined in (5.3.7), $f^{\eta, \delta}, F^{\eta, \delta}$ satisfy the assumptions shown in Theorem 5.4.1, then we have the following weak formulation:*

$$\lim_{\eta, \delta \rightarrow 0} \frac{1}{\eta} \int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}] \varphi(v) dv = \int_{\mathbb{R}^3} \left[F(v) \left(D(v - u) + \frac{4\pi}{3} a^3 \nabla_x p \right) \right] \cdot \nabla_v \varphi(v) dv + \int_{\mathbb{R}^3} \mathcal{Q} \varphi(v) dv \tag{5.4.13}$$

where the drag force Γ is defined in (5.4.9), and remain term $\mathcal{Q}$ is defined in (5.4.12).

With the help of this proposition, we multiply the test function $\varphi(v)$ on both sides of Enskog-Boltzmann equation for particles in (5.3.4), and integrate it with respect to $v \in \mathbb{R}$. As $\eta \rightarrow 0$, the distribution function F should satisfies

$$\begin{aligned}
\int_{\mathbb{R}^3} \partial_t \varphi(v) F(v) dv + \int_{\mathbb{R}^3} \nabla_x \varphi(v) \cdot v F(v) dv + \int_{\mathbb{R}^3} \nabla_v \varphi(v) \cdot \left[F(v) \left(D(v - u) + \frac{4\pi}{3} a^3 \nabla_x p \right) \right] dv \\
= - \int_{\mathbb{R}^3} \mathcal{Q} \varphi(v) dv,
\end{aligned}$$

which corresponds to a Vlasov-type equation in the weak sense. Proposition 5.4.2 aims to obtain the gas phase equations (5.4.3), (5.4.4), and (5.4.5)—Euler-like equations—from coupled Enskog-Boltzmann equations (5.3.4).

Proposition 5.4.2. *Let $f^{\eta, \delta}, F^{\eta, \delta}$ satisfy the assumptions shown in Theorem 5.4.1, then the parameter functions α, n, u, θ of $\mu[\alpha n, u, \theta/m_g]$, the limit function of $f^{\eta, \delta}$, obeys the*

following equations:

$$\begin{cases} \partial_t(\alpha\rho) + \operatorname{div}_x(\alpha\rho u) = 0 \\ \partial_t(\alpha\rho u) + \nabla_x(\alpha\rho u^{\otimes 2}) + \alpha\nabla_x(n\theta) = m_g \int_{\mathbb{R}^3} D(v-u)F(v)dv - \operatorname{div}_x \left(\alpha\rho \int_{\mathbb{R}^3} Q(v-u)F(v)dv \right) + \mathcal{R}, \\ \partial_t \left(\alpha \left(\frac{\rho|u|^2}{2} + \frac{3n\theta}{2} \right) \right) + \operatorname{div}_x \left(\alpha u \left(\frac{\rho|u|^2}{2} + \frac{3n\theta}{2} \right) \right) + \operatorname{div}_x(\alpha n\theta u) + n\theta\partial_t\alpha \\ = m_g \int_{\mathbb{R}^3} F(v)D(v-u) \cdot v dv - \operatorname{div}_x \left(\alpha\rho \int_{\mathbb{R}^3} Q(v-u)vF(v)dv \right) + \mathcal{P}, \end{cases} \quad (5.4.14)$$

where the friction force $D(v-u)$ is defined in (5.4.9), and $Q(v-u)$ is defined in (5.4.11). ρ is local mass density of gas defined by $\rho(t, x) = m_g n(t, x)$.

This theorem explains why the volume fraction α appears outside the pressure gradient term $\nabla_x p$: the microscopic drag force inherently contains a pressure contribution. When this term interacts with density distribution of the particles, it yields an additional volume fraction function, specifically, $\frac{4\pi}{3}a^3 \int_{\mathbb{R}^3} F(v)dv \nabla_x p$. If we separate this volume effect and friction force, and combine it with the pressure gradient $\nabla_x(\alpha p)$ that arises from the free transport (i.e., the gas phase's self-interaction), we are naturally led to a term of the form $\alpha \nabla_x(\alpha p)$. In fact, under the assumption that α is close to 1, it can be approximated by $\alpha \nabla_x p + o(a^3)$, which justifies writing the effective pressure gradient as $\alpha \nabla_x p$ at leading order. This formal argument reveals the microscopic origin of the pressure modification observed in thick sprays models.

The appearance of the coefficient $\frac{4}{3}\pi a^3$ is not coincidental. In fact, if this problem is treated in dimension d , the corresponding coefficient would precisely be the volume of a d -dimensional ball. See Appendix C.

The leading-order term q of the friction force D can be expressed as

$$q \left(\frac{v-u}{\sqrt{\theta/m_g}} \right) = \bar{q} \left(\frac{|v-u|}{\sqrt{\theta/m_g}} \right) (v-u),$$

where the explicit formula for $\bar{q}$ can be found in Lemma 3.3 of [DGR19]. However, the delocalization effect introduce not only a modification to the pressure term but also an additional friction term $\operatorname{div}_x(\alpha\rho Q(v-u))$. If we write friction force D in terms of a viscous tensor $\bar{D}(v-u)$ acting on the relative velocity $v-u$, that is,

$$D[\alpha n, u, \theta] = \bar{D}[\alpha n, u, \theta](v-u),$$

we observe that the viscous tensor is no longer a scalar. Instead, the resulting friction force may deviate toward the direction of $\nabla_x(\alpha n)$, and its structure also depends on the compressibility of the gas phase. The explicit expression for viscous tensor $\bar{D}(v-u)$ can be found in Appendix D. Nonetheless, since this deviation $\operatorname{div}_x(\alpha\rho Q(v-u))$ is arises at higher order $O(a^3)$ compared to the leading-order friction term q , it may be regraded as a small perturbation.

Another way to derive the gas phase equation is combining the following proposition with proposition 5.4.1.

Proposition 5.4.3. *For Enskog-Boltzmann collision integrals defined in (5.3.6),(5.3.7) obeys the collision laws (5.3.8). For any test function $\varphi(x, v) \in C^\infty(\mathbb{R} \times \mathbb{R})$, we have the following identity*

$$\begin{aligned} & \eta \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f, F](w) \varphi(x, w) dw + \int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F, f](v) \varphi(x, v) dv + \eta \operatorname{div}_x I[f, F; \varphi] \\ &= \int_{\mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} a^2 f(x, w) F(x - a\mathbf{n}, v) (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) \left[\varphi(x - a\mathbf{n}, w') + \varphi(x, v') \right. \\ & \quad \left. - \varphi(x - a\mathbf{n}, w) - \varphi(x, v) \right] d\mathbf{n} dv dw, \quad (5.4.15) \end{aligned}$$

where

$$\begin{aligned} I[f, F; \varphi] &:= \int_{\mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} \int_0^a a^2 \mathbf{n} (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) (\varphi(x + s\mathbf{n}, w') - \varphi(x + s\mathbf{n}, w)) \\ & \quad f(x + s\mathbf{n}, w) F(x - (a - s)\mathbf{n}, v) d\mathbf{n} dv dw ds. \end{aligned}$$

The proof of the Proposition 5.4.3 can be found in Appendix A. In fact, the terms $\alpha \rho \int_{\mathbb{R}^3} F Q dv$ and $\alpha \rho \int_{\mathbb{R}^3} F Q v dv$ correspond precisely to the leading-order contributions (of order $O(a^3)$) of $I[f, F; \varphi]$ for $\varphi(x, \xi) = \xi$ and $\varphi(x, \xi) = \frac{|\xi|^2}{2}$ respectively.

The results for general delocalized collision integral in the single-species case can be found in [CCG24], and the corresponding result for the Boltzmann collision integral for binary mixture can be found in [Ber+17; Ber+18; DGR19].

This proposition illustrates more clearly the origin of the pressure imbalance, and explain that the pressure imbalance is inevitable when we introduce “delocalized collision” models. Although, these pressures do not balance locally, their integral over $x \in \mathbb{R}$ causes the “extra pressure” to vanishes. Moreover, in non-equilibrium gas-particle systems, this phenomena occurs, see, for example [GHS04; DM10]. It’s referred to as interfacial pressure.

5.5 Proof of Proposition 5.4.1

In this section, we start from equation (5.3.4), with the goal of deriving equation (5.4.6) which incorporates the drag force (5.4.9) and the volume fraction (5.4.8). We first derive the Maxwellian distribution from the Enskog-Boltzmann equation for gas phase. Next, we obtain the leading order drag force in the following subsection. In the final subsection, we derive the higher-order correction to drag force, which includes contribution from the volume fraction and pressure.

5.5.1 The leading order gives the Maxwellian distribution

We assume that $(f^{\eta, \delta}, F^{\eta, \delta})$ solves the equation (5.3.4). Hence

$$\mathcal{B}[f^{\eta, \delta}, f^{\eta, \delta}] = \delta(\partial_t f^{\eta, \delta} + w \cdot \nabla_x f^{\eta, \delta} - \mathcal{E}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}]).$$

Since right-hand side is uniformly bounded in δ , as $\eta, \delta \rightarrow 0$, the limit function f should satisfy

$$\mathcal{B}[f, f](t, x, w) = 0. \quad (5.5.1)$$

It implies that f is a Maxwellian distribution; see for instance, Chapter 3 of [Cer94]. Moreover, we introduce the following macroscopic quantities

$$\rho(t, x) = m_g n(t, x) = \frac{H(\alpha(t, x))}{\alpha(t, x)} \int_{\mathbb{R}^3} m_g f(t, x, w) dw, \quad \text{the local mass density of gas} \quad (5.5.2)$$

$$u(t, x) = \frac{H(\alpha(t, x)n(t, x))}{\alpha(t, x)n(t, x)} \int_{\mathbb{R}^3} w f(t, x, w) dw, \quad \text{the bulk velocity of gas} \quad (5.5.3)$$

$$\theta(t, x) = \frac{H(\alpha(t, x)n(t, x))}{\alpha(t, x)n(t, x)} \int_{\mathbb{R}^3} m_g \frac{|w - u(t, x)|^2}{3} f(t, x, w) dw, \quad \text{the internal energy of gas} \quad (5.5.4)$$

then $f^\eta(t, x, w)$ should be of the form of Maxwellian distribution $\mu[\alpha n, u, \theta/m_g](w)$ in (5.4.2), where the volume fraction function $\alpha = \alpha(t, x)$ is defined by

$$\alpha(t, x) := 1 - \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} F(t, x, v) dv, \quad (5.5.5)$$

to describe the volume occupation of gas which is close to 1 but not negligible. These quantities are well-defined thanks to the strict positivity of volume fraction α . This can be established in the simplified case (with linear viscous force). We refer the reader to the Proposition 2.1 in [BDD23].

5.5.2 Drag force from Boltzmann collision integral

As in [DGR19], we can construct the term $q(v - u)F$ from $\frac{1}{\eta} E_2[F, f]$. This motivates us to remove the delocalization effect on f by using the approximation

$$f^{\eta, \delta}(x \pm a\mathbf{n}, w) = f^{\eta, \delta}(x, w) \pm a\mathbf{n} \cdot \nabla_x f^{\eta, \delta}(x, w) + o(a).$$

Asymptotically, the Enskog-Boltzmann collision integral can be rewritten as

$$\mathcal{E}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}] = \mathcal{R}_1^\eta[F^{\eta, \delta}, f^{\eta, \delta}] - \mathcal{R}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}] + o(a^3), \quad (5.5.6)$$

where $\mathcal{R}_1^\eta[F^{\eta, \delta}, f^{\eta, \delta}]$ and $\mathcal{R}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}]$ are defined by

$$\mathcal{R}_1^\eta[F^{\eta, \delta}, f^{\eta, \delta}](t, x) := a^2 \int_{\mathbb{R}^3 \times \mathbb{S}^2} [f^{\eta, \delta}(x, w') F^{\eta, \delta}(x, v') - f^{\eta, \delta}(x, w) F^{\eta, \delta}(x, v)] (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw, \quad (5.5.7)$$

$$\begin{aligned} \mathcal{R}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}](t, x) := & a^3 \int_{\mathbb{R}^3 \times \mathbb{S}^2} \mathbf{n} \cdot [\nabla_x f^{\eta, \delta}(x, w') F^{\eta, \delta}(x, v') + \nabla_x f^{\eta, \delta}(x, w) F^{\eta, \delta}(x, v)] (v - w) \cdot \mathbf{n} \\ & \times H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw. \end{aligned}$$

Hence, we define

$$\mathcal{Q}_1^{\eta,\delta} := \mathcal{E}_2^\eta[F^{\eta,\delta}, f^{\eta,\delta}] - \mathcal{R}_1^\eta[F^{\eta,\delta}, f^{\eta,\delta}] + \mathcal{R}_2^\eta[F^{\eta,\delta}, f^{\eta,\delta}], \quad (5.5.8)$$

and $\mathcal{Q}_1 := \lim_{\eta,\delta \rightarrow 0} \mathcal{Q}_1^{\eta,\delta}$. The computation of leading term follows the same approach as in [CDS12]. We summarize only the main idea here; for the inelastic case, one may refer to [CDS12], also in [DGR19]. For a test function $\varphi(v) \in C^2(\mathbb{R}^3)$, with $\nabla\varphi, \nabla^2\varphi \in L^\infty(\mathbb{R})$, we apply the change of variables $(v, w, \mathbf{n}) \mapsto (v', w', -\mathbf{n})$ in the gain term of $\mathcal{R}_1^\eta$. Properties (5.3.10), (5.3.11), and (5.3.12) guarantee that

$$\begin{aligned} & \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} [f^{\eta,\delta}(w')F^{\eta,\delta}(v') - f^{\eta,\delta}(w)F^{\eta,\delta}(v)](v-w) \cdot \mathbf{n} H((v-w) \cdot \mathbf{n}) \varphi(v) dv d\mathbf{n} dw \\ &= \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta,\delta}(w)F^{\eta,\delta}(v)[\varphi(v') - \varphi(v)](v-w) \cdot \mathbf{n} H((v-w) \cdot \mathbf{n}) dv d\mathbf{n} dw. \end{aligned}$$

The fundamental theorem of calculus, and (5.3.8) show that

$$\varphi(v') - \varphi(v) = (v' - v) \cdot \nabla_v \varphi(v) + o(v' - v) = -\frac{2\eta}{1+\eta} (v-w) \cdot \mathbf{nn} \cdot \nabla_v \varphi(v) + o(\eta), \quad (5.5.9)$$

hence

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{R}_1^\eta[F^{\eta,\delta}, f^{\eta,\delta}](x, v) \varphi(v) dv \\ &= -\frac{2a^2\eta}{1+\eta} \int_{\mathbb{R}^3} \left(F^{\eta,\delta}(x, v) \int_{\mathbb{S}^2} f^{\eta,\delta}(w) ((v-w) \cdot \mathbf{n})^2 H((v-w) \cdot \mathbf{n}) d\mathbf{n} dw \right) \cdot \nabla_v \varphi(v) dv + o(\eta), \end{aligned} \quad (5.5.10)$$

which is the weak formulation for Boltzmann collision integral $\mathcal{R}_1^\eta$. After integrating in $\mathbf{n}$ (see, for instance, section 16.8 of [CC70], or in the Appendix ??), we obtain

$$\int_{\mathbb{S}^2} \mathbf{n} ((v-w) \cdot \mathbf{n})^2 H((v-w) \cdot \mathbf{n}) f^{\eta,\delta}(w) d\mathbf{n} = \frac{\pi}{2} \int (v-w) |v-w| f^{\eta,\delta}(w) dw. \quad (5.5.11)$$

Since $f^{\eta,\delta} \rightarrow f^\eta$ takes the form of a Maxwellian $\mu[\alpha n, u, \theta/m_g]$,

$$\int_{\mathbb{R}^3} (v-w) |v-w| \mathcal{M}[\alpha n, u, \theta/m_g](w) dw = \alpha n \frac{\theta}{m_g} q \left(\frac{v-u}{\sqrt{\theta/m_g}} \right) \quad (5.5.12)$$

where q is defined in (5.4.10). The explicit formulas for q can be found in Lemma 3.3 of [DGR19], and their asymptotic behavior is discussed in [CMS25]. As a result, we obtain the leading-order friction force as

$$\lim_{\delta, \eta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{R}_1^\eta[F^{\eta,\delta}, f^{\eta,\delta}](x, v) \varphi(v) dv = -\pi a^2 \alpha n \frac{\theta}{m_g} \int_{\mathbb{R}^3} F(v) q \left(\frac{v-u}{\sqrt{\theta/m_g}} \right) \cdot \nabla_v \varphi(v) dv, \quad (5.5.13)$$

5.5.3 Volume fraction from delocalization effect

We repeat the same procedure as in the previous subsection to derive the weak formulation of $\mathcal{R}_2^\eta$. For any test function $\varphi \in C^2(\mathbb{R}^3)$ with $\nabla\varphi, \nabla^2\varphi \in L^\infty(\mathbb{R}^3)$, we perform the change of variables $(v, w, n) \mapsto (v'(v, w, n, \eta), w'(v, w, n, \eta), -n)$ in the gain term (first half part) of $\mathcal{R}_2^\eta$. Consequently, we obtain:

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{R}_2^\eta[F^{\eta,\delta}, f^{\eta,\delta}](x, v) \varphi(v) dv \\ &= a^3 \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} \mathbf{n} \cdot \nabla_x f^{\eta,\delta}(w) F^{\eta,\delta}(v) [-\varphi(v') + \varphi(v)] (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw. \end{aligned}$$

Then, the approximation (5.5.9) shows

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{R}_2^\eta[F^{\eta,\delta}, f^{\eta,\delta}](x, v) \varphi(v) dv \\ &= \frac{2a^3\eta}{1+\eta} \int_{\mathbb{R}^3} \left(F^{\eta,\delta}(x, v) \int_{\mathbb{S}^2} \mathbf{n} \cdot \nabla_x f^{\eta,\delta}(w) ((v - w) \cdot \mathbf{n})^2 H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw \right) \cdot \nabla_v \varphi(v) dv + o(\eta). \end{aligned} \quad (5.5.14)$$

Note the following identity (see, for instance, section 16.8 of [CC70], or in the Appendix B)

$$2a^3 \int_{|\mathbf{n}|=1, \mathbf{n} \cdot \xi > 0} (\mathbf{n} \cdot \xi)^2 \mathbf{n}^{\otimes 2} d\mathbf{n} = \frac{4\pi}{15} a^3 (2\xi^{\otimes 2} + |\xi|^2 \text{Id}) =: Q(\xi). \quad (5.5.15)$$

It follows

$$\begin{aligned} & \int_{\mathbb{R}^3 \times \mathbb{S}^2} \mathbf{n} \cdot \nabla_x f^{\eta,\delta}(w) ((v - w) \cdot \mathbf{n})^2 H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw \\ &= \frac{2\pi}{15} \left(\text{div}_x \int 2(v - w)^{\otimes 2} f^{\eta,\delta}(w) dw + \nabla_x \int |v - w|^2 f^{\eta,\delta}(w) dw \right). \end{aligned} \quad (5.5.16)$$

We decompose $v - w$ as $(v - u) + (u - w)$. The component depending on $v - u$ contributes to the pressure term, while the component depending on $u - w$ gives rise to a higher order friction force. In other words,

$$\begin{aligned} & \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} (v - w)^{\otimes 2} f^{\eta,\delta}(w) dw = (v - u)^{\otimes 2} \int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) dw + \int_{\mathbb{R}^3} (u - w)^{\otimes 2} \mu[\alpha n, u, \theta/m_g](w) dw \\ &+ (v - u) \otimes \int_{\mathbb{R}^3} (u - w) \mu[\alpha n, u, \theta/m_g](w) dw + \int_{\mathbb{R}^3} (u - w) \mu[\alpha n, u, \theta/m_g](w) dw \otimes (v - u). \end{aligned}$$

Since, $\mu[\alpha n, u, \theta/m_g](w)$ is a radial function centered at $w = u$, we have

$$\int_{\mathbb{R}^3} (w - u) \mu[\alpha n, u, \theta/m_g](w) dw = 0.$$

Therefore,

$$\lim_{\delta, \eta \rightarrow 0} \int_{\mathbb{R}^3} (v - w)^{\otimes 2} f^{\eta, \delta}(w) dw = \alpha n (v - u)^{\otimes 2} + \alpha n \frac{\theta}{m_g} \text{Id}. \quad (5.5.17)$$

Take the trace of the identity (5.5.17) for both sides, we obtain

$$\lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} |v - w|^2 f^{\eta, \delta}(w) dw = \alpha n |v - u|^2 + 3\alpha n \frac{\theta}{m_g}. \quad (5.5.18)$$

Substituting (5.5.17) and (5.5.18) into (5.5.16), we deduce that

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3 \times \mathbb{S}^2} \mathbf{n} \cdot \nabla_x f^{\eta, \delta}(w) ((v - w) \cdot \mathbf{n})^2 H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw d\mathbf{n} \\ = \frac{2\pi}{3m_g} \nabla_x (\alpha n \theta) + \frac{2\pi}{15m_g} [\text{div}_x (2\alpha n (v - u)^{\otimes 2}) + \nabla_x (\alpha n |v - u|^2)]. \end{aligned}$$

Next, we aim to eliminate the double appearance of α by discarding terms of order $O(a^3)$. In other words, we will show that the leading-order approximation of $\alpha \nabla_x (\alpha n \theta)$ is $\alpha \nabla_x (n \theta)$. Since $1 - \alpha = O(a^3)$ and $\nabla_x \alpha = O(a^3)$, we define

$$\mathcal{Q}_2 := \frac{1}{m_g} \frac{4\pi}{3} a^3 [n \theta \nabla_v F \cdot \nabla_x \alpha - (1 - \alpha) \nabla_v F \cdot \nabla_x (n \theta)] = o(a^3).$$

Therefore, by applying the production rule repeatedly, we have

$$\begin{aligned} & \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} F(v) \nabla_x (n \theta) \cdot \nabla_v \varphi(v) dv - \int_{\mathbb{R}^3} \mathcal{Q}_2(v) \varphi(v) dv \\ &= -\frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \nabla_v F(v) \cdot \nabla_x (n \theta) \varphi(v) dv - \int_{\mathbb{R}^3} \mathcal{Q}_2(v) \varphi(v) dv \\ &= \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \nabla_v F(v) \cdot [-\nabla_x (n \theta) - n \theta \nabla_x \alpha + (1 - \alpha) \nabla_x (n \theta)] \varphi(v) dv \\ &= -\frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \nabla_v F(v) \cdot \nabla_x (\alpha n \theta) \varphi(v) dv \\ &= \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} F(v) \nabla_x (\alpha n \theta) \cdot \nabla_v \varphi(v) dv. \end{aligned}$$

Then the weak formulation of $\mathcal{R}_2[F, f]$ can be reacted as

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \frac{1}{\eta} \int_{\mathbb{R}^3} \mathcal{R}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}](v) \varphi(v) dv &= \int_{\mathbb{R}^3} F(v) \left(\frac{1}{m_g} \frac{4\pi}{3} a^3 \nabla_x (n \theta) + \text{div}_x [\alpha n Q(v - u)] \right) \cdot \nabla_v \varphi(v) dv \\ &\quad - \int_{\mathbb{R}^3} \mathcal{Q}_2 \varphi(v) dv. \quad (5.5.19) \end{aligned}$$

Finally, we conclude the results by combining (5.5.8), (5.5.13) and (5.5.19):

$$\lim_{\eta, \delta \rightarrow 0} \frac{1}{\eta} \int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F^{\eta, \delta}, f^{\eta, \delta}] \varphi(v) dv = - \int_{\mathbb{R}^3} \left[F(v) \left(D(v - u) + \frac{1}{m_g} \frac{4\pi}{3} a^3 \nabla_x (n \theta) \right) \right] \cdot \nabla_v \varphi(v) dv$$

$$+ \int_{\mathbb{R}^3} \mathcal{Q}\varphi(v)dv,$$

where the remainder term $\mathcal{Q}$ is defined by $\mathcal{Q} := \mathcal{Q}_1 + \mathcal{Q}_2$.

5.6 Proof of proposition 5.4.2

In this section, we use the moment method to derive the equations of gas phase by taking moments of kinetic equation of gas in (5.3.4) with respect to the functions $m_g, m_g w$, and $\frac{m_g |w|^2}{2}$.

5.6.1 Gas phase mass equation

Once we integrate the gas phase equation in (5.3.4) with respect to w , we obtain

$$m_g \partial_t \int_{\mathbb{R}^3} f^{\eta, \delta} dw + m_g \operatorname{div}_x \int_{\mathbb{R}^3} w f^{\eta, \delta} dw = m_g \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] dw + m_g \int_{\mathbb{R}^3} \mathcal{B}^\eta[f^{\eta, \delta}, f^{\eta, \delta}] dw = 0.$$

Let $\eta, \delta \rightarrow 0$, we obtain

$$m_g \partial_t \int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) dw + m_g \operatorname{div}_x \int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) w dw = 0.$$

The definitions (5.5.2), (5.5.3) and assumption (5.4.2) yield

$$\partial_t(\alpha \rho) + \operatorname{div}_x(\alpha \rho u) = 0. \quad (5.6.1)$$

The last identity holds because the Enskog-Boltzmann collision integral for two species preserves mass for suitable functions f and F . The general form of this property can be found in [CCG24].

5.6.2 Gas phase momentum equations

Similarly, we multiply gas the phase equation in (5.3.4) by $m_g w$, and then integrate it with respect to w , then the left-hand side should be

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} m_g \int_{\mathbb{R}^3} w \partial_t f^{\eta, \delta}(w) dw + m_g \int_{\mathbb{R}^3} w^{\otimes 2} : \nabla_x f^{\eta, \delta}(w) dw \\ = \partial_t \int_{\mathbb{R}^3} m_g \mu[\alpha n, u, \theta/m_g](w) w dw + \operatorname{div}_x \int_{\mathbb{R}^3} m_g \mu[\alpha n, u, \theta/m_g](w) w^{\otimes 2} dw. \end{aligned} \quad (5.6.2)$$

We split $w^{\otimes 2}$ into $w - u$ and u . Noting that $\mu[\alpha n, u, \theta/m_g](w)(w - u)$ is an odd function with respect to $w - u$,

$$\int_{\mathbb{R}^3} m_g \mu[\alpha n, u, \theta/m_g](w) w^{\otimes 2} dw = u^{\otimes 2} \int_{\mathbb{R}^3} m_g \mu[\alpha n, u, \theta/m_g](w) dw + \int_{\mathbb{R}^3} m_g \mu[\alpha n, u, \theta/m_g](w) (w - u)^{\otimes 2} dw,$$

The limit becomes

$$\lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} m_g w \partial_t f^{\eta, \delta}(w) dw + \int_{\mathbb{R}^3} m_g w^{\otimes 2} : \operatorname{div}_x f^{\eta, \delta}(w) dw = \partial_t(\alpha \rho u) + \nabla_x(\alpha \rho u^{\otimes 2}) + \nabla_x(\alpha n \theta) \quad (5.6.3)$$

We proceed with a similar computation shown in Section 5.5. The property (5.3.10) allows us combining the gain term and lose term in collision integral $\mathcal{E}_1[f, F]$:

$$\begin{aligned} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] w dw &= \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} a^2 f^{\eta, \delta}(x, w) F^{\eta, \delta}(x - a\mathbf{n}, v) (w' - w)(v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw \\ &= \frac{2a^2}{1 + \eta} \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta, \delta}(x, w) F^{\eta, \delta}(x - a\mathbf{n}, v) ((v - w) \cdot \mathbf{n})^2 \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw. \end{aligned}$$

By approximating $F^{\eta, \delta}(x - a\mathbf{n}, \xi)$ as $F^{\eta, \delta}(x, \xi) - a\mathbf{n} \cdot \nabla_x F^{\eta, \delta}(x, \xi) + o(a)$ in $\int_{\mathbb{R}^3} \mathcal{E}_1[f^{\eta, \delta}, F^{\eta, \delta}] w dw$, one has

$$\begin{aligned} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] w dw &= \frac{2a^2}{1 + \eta} \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta, \delta}(w) F^{\eta, \delta}(v) ((v - w) \cdot \mathbf{n})^2 \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw \\ &\quad - \frac{2a^3}{1 + \eta} \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta, \delta}(w) ((v - w) \cdot \mathbf{n})^2 \mathbf{n}^{\otimes 2} \nabla_x F^{\eta, \delta}(v) H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw + \mathcal{R}_1^{\eta, \delta}, \end{aligned}$$

where $\mathcal{R}_1^{\eta, \delta} = o(a^3)$ is given by

$$\begin{aligned} \mathcal{R}_1^{\eta, \delta} &:= \frac{2a^2}{1 + \eta} \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta, \delta}(x, w) [F^{\eta, \delta}(x - a\mathbf{n}, v) - F^{\eta, \delta}(x, v) + a\mathbf{n} \cdot \nabla_x F^{\eta, \delta}(x, v)] ((v - w) \cdot \mathbf{n})^2 \mathbf{n} \\ &\quad H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw. \end{aligned}$$

Then, integrating with respect to $\mathbf{n} \in \mathbb{S}^2$, and using identities (5.5.11), and (5.5.15), we obtain

$$\begin{aligned} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] w dw &= \frac{\pi a^2}{1 + \eta} \int_{\mathbb{R} \times \mathbb{R}^3} F^{\eta, \delta}(v) f^{\eta, \delta}(w) |v - w| (v - w) dv dw \\ &\quad - \frac{4\pi a^3}{15(1 + \eta)} \int_{\mathbb{R} \times \mathbb{R}^3} [2(v - w)^{\otimes 2} + |v - w|^2 \operatorname{Id}] \nabla_x F^{\eta, \delta}(v) f^{\eta, \delta}(w) dv dw + \mathcal{R}_1^{\eta, \delta}. \end{aligned}$$

After that, after taking $\eta, \delta \rightarrow 0$, identities (5.5.13), (5.5.17), and (5.5.18) yield

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] m_g w dw &= \pi a^2 \alpha n \theta \int_{\mathbb{R}^3} F(v) q \left(\frac{v - u}{\sqrt{\theta/m_g}} \right) dv \\ &\quad - \int_{\mathbb{R}^3} \left\{ \frac{4\pi}{3} a^3 \alpha n \theta \operatorname{Id} + \alpha \rho Q(v - u) \right\} \nabla_x F(v) dv + \mathcal{R}_1, \end{aligned}$$

where $\mathcal{R}_1$ is defined by

$$\mathcal{R}_1(t, x) := 2a^2 m_g \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} \mu[\alpha n, u, \theta/m_g](x, w) [F(x - a\mathbf{n}, v) - F(x, v) + a\mathbf{n} \cdot \nabla_x F(x, v)] [(v - w) \cdot \mathbf{n}]^2 \mathbf{n}$$

$$H((v-w) \cdot \mathbf{n}) dv dw d\mathbf{n}. \quad (5.6.4)$$

Note that $\mathcal{R}_1$ is of order $o(a^3)$. We take the gradient of the volume fraction function α defined in (5.5.5),

$$\nabla_x \alpha = -\frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \nabla_x F(v) dv.$$

Hence, we have

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}](w) m_g w dw &= \pi a^2 \alpha n \theta \int_{\mathbb{R}^3} F(v) q \left(\frac{v-u}{\sqrt{\theta/m_g}} \right) dv \\ &+ \alpha n \theta \nabla_x \alpha - \alpha \rho \int_{\mathbb{R}^3} Q(v-u) \nabla_x F(v) dv + \mathcal{R}_1, \end{aligned} \quad (5.6.5)$$

where Q is defined in (5.4.11). By the product rule, we have

$$\alpha \rho \int_{\mathbb{R}^3} Q(v-u) \nabla_x F(v) dv = \operatorname{div}_x \left(\alpha \rho \int_{\mathbb{R}^3} Q(v-u) F(v) dv \right) - \int_{\mathbb{R}^3} \operatorname{div}_x [\alpha \rho Q(v-u)] F(v) dv. \quad (5.6.6)$$

Note that the volume fraction function remains close to 1, since the gas remains the dominant component even in the thick sprays regime. Consequently, the product $\alpha \nabla_x \alpha$ behaves similarly to $\nabla_x \alpha$ up to higher-order terms. More precisely, we expand the volume function α by definition (5.5.5):

$$\begin{aligned} \alpha \nabla_x \alpha &= \left(1 - \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} F(v) dv \right) \left(-\frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \nabla_x F(v) dv \right) = -\frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \nabla_x F(v) dv + o(a^3) \\ &= \nabla_x \alpha + o(a^3). \end{aligned} \quad (5.6.7)$$

And the difference is defined to be $\mathcal{R}_2$:

$$\mathcal{R}_2 := (1 - \alpha) n \theta \nabla_x \alpha = o(a^3) \quad (5.6.8)$$

Then, we substitute (5.6.6) and (5.6.8) into (5.6.5). It shows

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}](w) m_g w dw &= \pi a^2 \alpha n \theta \int_{\mathbb{R}^3} F(v) q \left(\frac{v-u}{\sqrt{\theta/m_g}} \right) dv + n \theta \nabla_x \alpha \\ &- \operatorname{div}_x \left(\alpha \rho \int_{\mathbb{R}^3} Q(v-u) F(v) dv \right) + \int_{\mathbb{R}^3} \operatorname{div}_x [\alpha \rho Q(v-u)] F(v) dv + \mathcal{R}, \end{aligned} \quad (5.6.9)$$

where $\mathcal{R} := \mathcal{R}_1 + \mathcal{R}_2$. Combining (5.6.3) and (5.6.9), we obtain the momentum equation for the gas phase

$$\partial_t(\alpha \rho u) + \nabla_x(\alpha \rho u^{\otimes 2}) + \alpha \nabla_x(n \theta) = m_g \int_{\mathbb{R}^3} D(v-u) F(v) dv - \operatorname{div}_x \left(\alpha \rho \int_{\mathbb{R}^3} Q(v-u) F(v) dv \right) + \mathcal{R}(t, x), \quad (5.6.10)$$

where the microscopic friction force $D \equiv D[\alpha\rho, u, \theta](t, x, v)$ is defined by

$$D[\alpha\rho, u, \theta](v) := \pi a^2 \alpha n \frac{\theta}{m_g} q \left(\frac{v - u}{\sqrt{\theta/m_g}} \right) + \operatorname{div}_x(\alpha n Q(v - u)).$$

5.6.3 Gas phase energy equation

Again, we multiply gas the phase equation in (5.3.4) by $\frac{m_g |w|^2}{2}$, and then integrate it with respect to w , note the following identity

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \frac{|w|^2}{2} \partial_t f^{\eta, \delta} dw + \int_{\mathbb{R}^3} \frac{|w|^2}{2} \nabla_x f^{\eta, \delta} dw \\ = \partial_t \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) \frac{|w|^2}{2} dw \right) + \operatorname{div}_x \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) \frac{|w|^2}{2} w dw \right). \end{aligned}$$

We process the same steps: we split w into $w - u$ and u , and the terms including odd orders of $w - u$ vanishes. Therefore,

$$\begin{aligned} \partial_t \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) \frac{|w|^2}{2} dw \right) + \operatorname{div}_x \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) \frac{|w|^2}{2} w dw \right) \\ = \partial_t \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) \frac{|w - u|^2}{2} dw + \frac{|u|^2}{2} \int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) dw \right) \\ + \operatorname{div}_x \left[\left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) \frac{|w - u|^2}{2} dw \right) u + \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) (w - u)^{\otimes 2} dw \right) u \right. \\ \left. + \left(\int_{\mathbb{R}^3} \mu[\alpha n, u, \theta/m_g](w) dw \right) \frac{|u|^2}{2} u \right]. \end{aligned}$$

It follows,

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \frac{m_g |w|^2}{2} \partial_t f^{\eta, \delta} dw + \int_{\mathbb{R}^3} \frac{m_g |w|^2}{2} \nabla_x f^{\eta, \delta} dw = \partial_t \left(\alpha \rho \left(\frac{|u|^2}{2} + \frac{3\theta}{2m_g} \right) \right) \\ + \operatorname{div}_x \left(\alpha \rho u \left(\frac{|u|^2}{2} + \frac{5\theta}{2m_g} \right) \right). \quad (5.6.11) \end{aligned}$$

We repeat the same approach as shown in the momentum equation,

$$\begin{aligned} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}] \frac{|w|^2}{2} dw \\ = \frac{2a^2}{(1 + \eta)^2} \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta, \delta}(w) F^{\eta, \delta}(v) ((v - w) \cdot \mathbf{n})^2 (v + \eta w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw \\ - \frac{2a^3}{(1 + \eta)^2} \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta, \delta}(w) ((v - w) \cdot \mathbf{n})^2 (v + \eta w) \cdot \mathbf{n} \nabla_x F^{\eta, \delta}(v) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw + \mathcal{P}_1^{\eta, \delta}, \end{aligned}$$

where $\mathcal{P}_1^{\eta, \delta}$ is given by

$$\begin{aligned} \mathcal{P}_1^{\eta,\delta} := & 2a^2 \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} f^{\eta,\delta}(x, w) [F^{\eta,\delta}(x, v) - F^{\eta,\delta}(x - a\mathbf{n}, v) + a\mathbf{n} \cdot \nabla_x F^{\eta,\delta}(x, v)] \\ & ((v - w) \cdot \mathbf{n})^2 (v + \eta w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw \end{aligned}$$

As $\eta, \delta \rightarrow 0$, we integrate over $\mathbf{n} \in \mathbb{S}^2$. For the same reason,

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta,\delta}, F^{\eta,\delta}] \frac{m_g |w|^2}{2} dw &= \pi a^2 \alpha n \theta \int_{\mathbb{R}^3} F(v) q \left(\frac{v - u}{\sqrt{\theta/m_g}} \right) \cdot v dv \\ &\quad - \frac{4\pi}{3} a^3 \alpha n \theta \int_{\mathbb{R}^3} v \cdot \nabla_x F(v) dv - \alpha \rho \int_{\mathbb{R}^3} Q(v - u) : v \otimes \nabla_x F(v) dv + \mathcal{P}_1, \end{aligned}$$

where $\mathcal{P}_1$ is defined as

$$\begin{aligned} \mathcal{P}_1 := & 2a^2 m_g \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} \mu[\alpha n, u, \theta/m_g](w) [F(x, v) - F(x - a\mathbf{n}, v) + a\mathbf{n} \cdot \nabla_x F(x, v)] ((v - w) \cdot \mathbf{n})^2 v \cdot \mathbf{n} \\ & H((v - w) \cdot \mathbf{n}) dv d\mathbf{n} dw \quad (5.6.12) \end{aligned}$$

Thanks to the mass conservation of the particles, and the definition of the volume fraction,

$$-\partial_t \alpha + \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} v \cdot \nabla_x F dv = \frac{4\pi}{3} a^3 \left(\int_{\mathbb{R}^3} \partial_t F dv + \int_{\mathbb{R}^3} v \cdot \nabla_x F dv \right) = \frac{4\pi}{3} a^3 \int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F, f] dv = 0,$$

the energy exchange becomes

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta,\delta}, F^{\eta,\delta}] \frac{m_g |w|^2}{2} dw &= \pi a^2 \alpha n \theta \int_{\mathbb{R}^3} F(v) q \left(\frac{v - u}{\sqrt{\theta/m_g}} \right) \cdot v dv \\ &\quad - \alpha \rho \int_{\mathbb{R}^3} Q(v - u) : v \otimes \nabla_x F(v) dv - \alpha n \theta \partial_t \alpha + \mathcal{P}_1. \quad (5.6.13) \end{aligned}$$

Since α is close to 1, we can approximate $\alpha \partial_t \alpha = (1 + O(a^3)) \partial_t \alpha = \partial_t \alpha + O(a^6)$. We define the remainder term $\mathcal{P}_2$ as

$$\mathcal{P}_2 := -(1 - \alpha) n \theta \partial_t \alpha. \quad (5.6.14)$$

Substituting (5.6.14) into (5.6.13), we obtain

$$\begin{aligned} \lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta,\delta}, F^{\eta,\delta}](w) \frac{m_g |w|^2}{2} dw &= \pi a^2 \alpha n \theta \int_{\mathbb{R}^3} F(v) q \left(\frac{v - u}{\sqrt{\theta/m_g}} \right) \cdot v dv \\ &\quad - \alpha \rho \int_{\mathbb{R}^3} Q(v - u) : v \otimes \nabla_x F(v) dv - n \theta \partial_t \alpha + \mathcal{P}, \end{aligned}$$

where $\mathcal{P} = \mathcal{P}_1 + \mathcal{P}_2$. Next, we move the gradient outside the integral,

$$\alpha \rho \int_{\mathbb{R}^3} Q(v - u) : v \otimes \nabla_x F(v) dv = \operatorname{div}_x \left(\alpha \rho \int_{\mathbb{R}^3} F(v) Q(v - u) v dv \right) - \int_{\mathbb{R}^3} F(v) \operatorname{div}_x (\alpha \rho Q(v - u)) \cdot v dv.$$

Recall the definition of friction force D , we obtain

$$\lim_{\eta, \delta \rightarrow 0} \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f^{\eta, \delta}, F^{\eta, \delta}](w) \frac{m_g |w|^2}{2} dw = m_g \int_{\mathbb{R}^3} F(v) D(v-u) \cdot v dv - \operatorname{div}_x \left(\alpha \rho \int_{\mathbb{R}^3} F(v) Q(v-u) v dv \right) - n \theta \partial_t \alpha + \mathcal{P}. \quad (5.6.15)$$

Combining (5.6.11) and (5.6.15), we obtain the energy equation for the gas phase

$$\begin{aligned} \partial_t \left(\alpha \rho \left(\frac{|u|^2}{2} + \frac{3\theta}{2m_g} \right) \right) + \operatorname{div}_x \left(\alpha \rho u \left(\frac{|u|^2}{2} + \frac{3\theta}{2m_g} \right) \right) + \operatorname{div}_x (\alpha n \theta u) + n \theta \partial_t \alpha \\ = m_g \int_{\mathbb{R}^3} F(v) D(v-u) \cdot v dv - \operatorname{div}_x \left(\alpha \rho \int_{\mathbb{R}^3} F(v) Q(v-u) v dv \right) + \mathcal{P}. \end{aligned} \quad (5.6.16)$$

5.7 Conclusion

To obtain the commonly used model, we combine equations (5.6.1), (5.6.10), and (5.6.16), and make the following conventions:

- The gas phase is ideal gas: $p(t, x) = n(t, x) \theta(t, x)$,
- Total energy per unit mass is: $E(t, x) = \frac{|u(t, x)|^2}{2} + \frac{3\theta(t, x)}{2m_g}$.

Readers may wonder whether it's reasonable to assume that the gas governed by Enskog equation is still behaves as an ideal gas. This is justified by the fact that we use the Enskog collision integral specifically to describe the collisions *between particle and gas*, while the collision among gas molecules themselves are still governed by Boltzmann collision integral $\mathcal{B}[f, f]$.

A natural question arises: can we generalize the cross-section $b_{pg}(z, \omega)$ within the Enskog–Boltzmann collision integral to account for more complex particle interactions beyond hard-sphere collisions? If we adopt such a generalized cross-section, the familiar coefficient $\frac{4\pi}{3} a^3$ (corresponds to the volume of sphere with radius a), which arises in the standard Enskog theory for hard spheres of radius a , is no longer exact. In the generalized setting, the coefficient in front of the pressure gradient term $\nabla_x p$ instead depends on the angular integrals

$$\int_{\mathbb{S}^2} b_{pg}(z, \omega) d\omega \quad \text{and} \quad \int_{\mathbb{S}^2} b_{pg}(z, \omega) (z \cdot \omega)^2 d\omega,$$

which capture how the effective collision geometry and scattering vary with orientation ω and relative position z . These integrals account for more general interaction mechanisms, including anisotropic or soft potentials, rather than assuming a fixed collision diameter. Consequently, the parameter a , previously interpreted as the hard-sphere radius, should be replaced with an effective interaction range. This interaction range reflects the spatial extent over which particles influence each other and aligns conceptually with the van der Waals correction to real gas behavior, where the microscopic structure of intermolecular forces alters the macroscopic thermodynamic quantities. Thus, in models employing a generalized cross-section, the geometric interpretation of a must be reconsidered in terms of the physical nature of the particle interactions. See, for instance, §74 in [LL80].

Finally, we must emphasize that this result is still far from a rigorous derivation. Although the well-posedness for suitable initial datum is obtained in [EH23] recently, as of the time of this writing, very little is known about the existence, uniqueness, or qualitative behavior of solutions to the coupled Enskog-Boltzmann equations. The well-posedness of coupled kinetic equation remains largely open at the time of writing. Moreover, the reminder terms $\mathcal{P}$, $\mathcal{Q}$ and $\mathcal{R}$ are highly intricate, involving not only the expansions on distribution functions, but also the density product between two species.

Appendix A. Proof of Proposition 5.4.3

Proof. We do the change of variables $(v, w, \mathbf{n}) \mapsto (v', w', -\mathbf{n})$ for the gain terms of $\int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f, F]\varphi(x, w)dw$ and $\int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F, f]\varphi(x, v)dv$, the properties (5.3.9)-(5.3.12) show

$$\int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f, F]\varphi(x, w)dw = \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} a^2(\varphi(x, w') - \varphi(x, w))f(x, w)F(x - a\mathbf{n}, v)(v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dv dw,$$

and

$$\int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F, f]\varphi(x, v)dv = \int_{\mathbb{R} \times \mathbb{R}^3 \times \mathbb{S}^2} a^2(\varphi(x, v') - \varphi(x, v))f(x + a\mathbf{n}, w)F(x, v)(v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dv dw.$$

Therefore, we have

$$\begin{aligned} & \eta \int_{\mathbb{R}^3} \mathcal{E}_1^\eta[f, F]\varphi(x, w)dw + \int_{\mathbb{R}^3} \mathcal{E}_2^\eta[F, f]\varphi(x, v)dv \\ &= \int_{\mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} a^2 f(x + a\mathbf{n}, w)F(x, v)(v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) \left[\varphi(x, w') + \varphi(x + a\mathbf{n}, v') \right. \\ & \quad \left. - \eta \varphi(x, w) - \eta \varphi(x + a\mathbf{n}, v) \right] d\mathbf{n} dv dw \\ &+ \eta \int_{\mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} a^2 (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) \left[(\varphi(x, w') - \varphi(x, w))f(x, w)F(x - a\mathbf{n}, v) \right. \\ & \quad \left. - (\varphi(x + a\mathbf{n}, w') - \varphi(x + a\mathbf{n}, w))f(x + a\mathbf{n}, w)F(x, v) \right] d\mathbf{n} dv dw. \end{aligned}$$

The fundamental theorem of calculus shows

$$\Phi(x + a\mathbf{n}) - \Phi(x) = \int_0^a \frac{d}{ds} \Phi(x + s\mathbf{n}) ds = \int_0^a \mathbf{n} \cdot \nabla_x \Phi(x + s\mathbf{n}) ds.$$

Since φ is smooth, and furthermore if $f(\cdot, w)F(\cdot, w)$ is smooth, then the last line of the right-hand side can be rewritten as

$$\begin{aligned} & -\eta \operatorname{div}_x \int_{\mathbb{R}^3 \times \mathbb{S}^2 \times \mathbb{R}^3} \int_0^a a^2 \mathbf{n} (v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) (\varphi(x + s\mathbf{n}, w') - \varphi(x + s\mathbf{n}, w)) \\ & \quad f(x + s\mathbf{n}, w)F(x - (a - s)\mathbf{n}, v) d\mathbf{n} dv dw ds. \end{aligned}$$

□

Appendix B. Two integrals

Let $\xi \in \mathbb{R}^3 \setminus \{0\}$ be a fixed vector. We compute these two integrals

$$K(\xi) := \int_{\mathbb{S}^2} (\omega \cdot \xi)^2 \omega H(\omega \cdot \xi) d\omega \quad \text{and} \quad K_d(\xi) := \int_{\mathbb{S}^{d-1}} \omega^{\otimes 2} (\omega \cdot \xi)^2 H(\omega \cdot \xi) d\omega.$$

In the following, we adopt the Einstein summation convention for tensor calculation. δ_{ij} is the Kronecker delta. The colon symbol $:$ denotes a double contraction. For 2-tensors $A \equiv (A_{ij})$ and $B \equiv (B_{ij})$, We define $A : B = A_{ij} B_{ij}$.

Compute $K(\xi)$:

Because of the rotational symmetry of the sphere, we can assume without loss of generality that $\frac{\xi}{|\xi|} = e_3 = (0, 0, 1)$, and express the unit vector in spherical coordinates as:

$$\omega = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$$

with $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$, and the surface element:

$$d\omega = \sin \theta d\theta d\phi.$$

The function $H(\omega \cdot \xi)$ becomes $H(\cos \theta)$, which restricts the integral to the northern hemisphere $\theta \in [0, \pi/2]$.

$$K(\xi) = |\xi|^2 \int_0^{2\pi} \int_0^{\pi/2} \omega \cos^2 \theta \sin \theta d\theta d\phi.$$

Noting that ϕ goes through $[0, 2\pi]$, the entry containing $\sin \phi$ or $\cos \phi$ vanishes. Thus

$$K(\xi) = 2\pi |\xi|^2 \int_0^{\pi/2} e_3 \cos^3 \theta \sin \theta d\theta d\phi = \frac{\pi}{2} |\xi| \xi.$$

Compute $K_d(\xi)$: We identify $K_d(\xi)$ as the contraction of a 4-tensor with a 2-tensor:

$$\left(\int_{\mathbb{S}^{d-1}} \omega^{\otimes 4} H(\omega \cdot \xi) d\omega \right) : \xi^{\otimes 2}.$$

By substituting $\omega \rightarrow -\omega$ in $\int_{\mathbb{S}^2} \omega^{\otimes 4} H(\omega \cdot \xi) d\omega$, we observe that

$$\int_{\mathbb{S}^{d-1}} \omega^{\otimes 4} H(\omega \cdot \xi) d\omega = \frac{1}{2} \int_{\mathbb{S}^{d-1}} \omega^{\otimes 4} d\omega.$$

This is a rank-4 isotropic and symmetric tensor, whose general form is given by:

$$\int_{\mathbb{S}^{d-1}} \omega_i \omega_j \omega_k \omega_l d\omega = C_d (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}).$$

To determine the constant C_d , we contract both sides by $\delta_{ij} \delta_{kl}$:

$$\delta_{ij} \delta_{kl} \int_{\mathbb{S}^{d-1}} \omega_i \omega_j \omega_k \omega_l d\omega = C_d \delta_{ij} \delta_{kl} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}).$$

It follows

$$\int_{\mathbb{S}^{d-1}} (\omega_i \omega_i)(\omega_k \omega_k) d\omega = C_d[(\delta_{ii})(\delta_{kk}) + 2\delta_{ik}\delta_{ik}].$$

In the three dimensions, we obtain $4\pi = \int_{\mathbb{S}^2} 1 d\omega = 15C_3$, namely, $C_3 = \frac{4\pi}{15}$. Substituting back into $K_d(\xi)$, its entries are

$$(K_3(\xi))_{ij} = \frac{2\pi}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\xi_k\xi_l = \frac{2\pi}{15}(\delta_{ij}(\xi_k\xi_k) + \xi_i\xi_j + x_i x_j \xi_i).$$

It can be also written as

$$K_3(\xi) = \frac{2\pi}{15}(|\xi|^2 \text{Id} + 2\xi^{\otimes 2}).$$

Appendix C.Generalization to Dimension d

After taking limit, the coefficient in front of the pressure modification appears solely in

$$a^d \int_{\mathbb{R}^d \times \mathbb{S}^{d-1}} \mathbf{n} \cdot [\nabla_x \mu(x, w') F^{\eta, \delta}(x, v') + \nabla_x \mu(x, w) F(x, v)](v - w) \cdot \mathbf{n} H((v - w) \cdot \mathbf{n}) d\mathbf{n} dw$$

It's not difficult to verify that, in d -dimensional space, it can be reacted as

$$2a^d F(v) \text{div}_x \int_{\mathbb{R}^d} K_d(v - w) \mu(w) dw.$$

To determinate K_d which we've defined in Appendix ??, we note the identity

$$|\mathbb{S}^{d-1}| = \int_{\mathbb{S}^{d-1}} 1 d\omega = C_d(d^2 + 2d).$$

Therefore,

$$\mathcal{R}_2[F, \mu] = a^d F(v) \frac{|\mathbb{S}^{d-1}|}{d(d+2)} \text{div}_x \int_{\mathbb{R}^d} [2(v - w)^{\otimes 2} + |v - w|^2 \text{Id}] \mu dw.$$

Then we decompose $v - w = (v - u) + (u - w)$, while the terms involving $v - u$ don't contribute to pressure correction. Using the identity:

$$\int_{\mathbb{R}^d} (w - U)^{\otimes 2} \mu[R, U, T] dw = RT \text{Id},$$

we obtain, in dimension d ,

$$a^d \frac{|\mathbb{S}^{d-1}|}{d(d+2)} F(v) \text{div}_x (2\alpha n \theta \text{Id} + d\alpha n \theta \text{Id}) = a^d \frac{|\mathbb{S}^{d-1}|}{d} F(v) \nabla_x (\alpha n \theta).$$

Since $d|B_d| = |\mathbb{S}^{d-1}|$, where B_d denotes the unit ball in $\mathbb{R}^d$, we conclude that the coefficient in front of the pressure modification is exactly the volume of a ball of radius a in d -dimensional space.

Appendix D. More on the friction force

As shown in [DGR19], the leading-order friction force $q \left(\frac{v-u}{\sqrt{\theta/m_g}} \right)$ can be expressed as

$$q(\xi) = \bar{q}(|\xi|)\xi \quad (.0.1)$$

Furthermore, we represent

$$\operatorname{div}_x(\alpha\rho Q(v-u)) = \frac{4\pi}{15}a^3\operatorname{div}_x[2\alpha\rho(v-u)^{\otimes 2} + \alpha\rho|v-u|^2\operatorname{Id}]$$

as a viscous tensor acting on relative velocity $v-u$ by using indices to represent the tensors to express the tensor component

$$\begin{aligned} (\operatorname{div}_x(\alpha\rho(v-u)^{\otimes 2}))_j &= \partial_{x_i}(\alpha\rho(v_i-u_i)(v_j-u_j)) \\ &= \partial_{x_i}(\alpha\rho)(v_i-u_i)(v_j-u_j) - \alpha\rho\partial_{x_i}u_i(v_j-u_j) - \alpha\rho(v_i-u_i)\partial_{x_i}u_j \end{aligned}$$

hence

$$\operatorname{div}_x(\alpha\rho(v-u)^{\otimes 2}) = [\nabla_x(\alpha\rho) \cdot (v-u)\operatorname{Id} - \alpha\rho(\operatorname{div}_xu)\operatorname{Id} - \alpha\rho\nabla_xu](v-u). \quad (.0.2)$$

Similarly,

$$(\nabla_x(\alpha\rho|v-u|^2))_j = \partial_{x_j}(\alpha\rho(v_i-u_i)(v_i-u_i)) = \partial_{x_j}(\alpha\rho)(v_i-u_i)(v_i-u_i) - 2\alpha\rho\partial_{x_j}u_i(v_i-u_i),$$

so that

$$\nabla_x(\alpha\rho|v-u|^2) = [\nabla_x(\alpha\rho) \otimes (v-u) - 2\alpha\rho(\nabla_xu)^T](v-u). \quad (.0.3)$$

By substituting (.0.2) and (.0.3) into $\operatorname{div}_x(\alpha\rho Q(v-u))$, and combining with (.0.1), we can the friction force in the form of viscous tensor applying on relative velocity

$$D[\alpha n, u, \theta] = \bar{D}[\alpha n, v-u, \theta, u](v-u), \quad (.0.4)$$

where

$$\begin{aligned} \bar{D}[\alpha n, v-u, \theta, u] &:= \pi a^2 \alpha n \sqrt{\frac{m_g}{\theta}} \bar{q} \left(\frac{|v-u|}{\sqrt{\theta/m_g}} \right) \operatorname{Id} \\ &+ \frac{2\pi}{15} a^3 [2(\nabla_x(\alpha\rho) \cdot (v-u))\operatorname{Id} + \nabla_x(\alpha\rho) \otimes (v-u)] - \frac{4\pi}{15} a^3 \alpha \rho [\operatorname{div}_xu\operatorname{Id} + \nabla_xu + (\nabla_xu)^T]. \end{aligned} \quad (.0.5)$$

Note that both $\pi a^2 \alpha n \sqrt{\frac{m_g}{\theta}} \bar{q} \left(\frac{|v-u|}{\sqrt{\theta/m_g}} \right) \operatorname{Id}$ and $\frac{4\pi a^3}{15} (\nabla_x(\alpha\rho) \cdot (v-u))\operatorname{Id}$ are scalar multiples of the identity matrix and thus do not alter the direction of the force. In contrast, the term $[\nabla_x(\alpha\rho) \otimes (v-u)](v-u) = |v-u|^2 \nabla_x(\alpha\rho)$ introduces a directional deflection aligned with $\nabla_x(\alpha\rho)$. The expression $\operatorname{div}_xu\operatorname{Id} + \nabla_xu + (\nabla_xu)^T$ forms a symmetric tensor depending solely on the bulk velocity field of the gas phase.

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Study of Nonlocal Collisional Kinetic Models and Their Applications to Thick Sprays

Étude de modèles cinétiques à collisions délocalisées et applications aux sprays épais

Abstract

This thesis is devoted to the study of delocalized collision models and to the establishment of links between particle systems, delocalized kinetic models, and fluid–kinetic models for thick sprays.

Chapters 2 and 3 investigate the properties of several delocalized collision models. In Chapter 2, we present a unified framework for the revised Enskog model, Cercignani’s soft sphere model, and a modified Povzner model. Local conservative representations are established, from which the corresponding conservation laws are derived using the moment method, together with associated entropy inequalities. Chapter 3 applies the same method to the standard Enskog model and the original Povzner model, where conservative forms are obtained but the resulting entropy inequalities are weaker and of limited interest.

The second part of the thesis focuses on the formal derivation of the coupled Enskog and Vlasov–Euler equations for thick sprays. Chapter 4 derives the coupled Enskog equations from the underlying particle system, establishes conservation of mass, momentum, and energy, and proves an H-theorem. Chapter 5 studies the Eulerian–Lagrangian model as a hydrodynamic limit of the coupled Boltzmann–Enskog equations.

Keywords: kinetic models, fluid dynamics, aerosols, nonlocal collisions, Enskog model, conservation laws, entropy inequalities, moment method, particle systems, hydrodynamic limit, fluid–kinetic coupling, thick sprays

Résumé

Cette thèse est consacrée à l’étude de modèles cinétiques avec collisions délocalisées et à l’établissement de liens entre des systèmes de particules, des modèles cinétiques délocalisés et des modèles fluide-cinétiques pour les sprays épais.

La première partie étudie les propriétés de plusieurs modèles de collisions délocalisées. Le chapitre 2 analyse le modèle d’Enskog révisé, le modèle de sphères molles de Cercignani et un modèle modifié de Povzner, et montre qu’ils peuvent être unifiés dans un cadre commun. Des représentations conservatives locales sont établies, permettant de dériver les lois de conservation macroscopiques correspondantes par la méthode des moments, ainsi que les inégalités d’entropie associées. Le chapitre 3 applique la même approche méthodologique au modèle standard d’Enskog et au modèle original de Povzner ; bien que des formes conservatives soient obtenues, les inégalités d’entropie qui en résultent sont plus faibles et d’intérêt limité.

La seconde partie est consacrée à la dérivation formelle des équations couplées d’Enskog et d’un système de type Vlasov–Euler pour les sprays épais. Le chapitre 4 dérive les équations d’Enskog couplées à partir du système de particules, établit la conservation de la masse, de la quantité de mouvement et de l’énergie, et démontre un théorème H pour le système. Enfin, le chapitre 5 étudie le couplage fluide-cinétique comme limite hydrodynamique des équations couplées de Boltzmann–Enskog.

Mots clés : modèles cinétiques, mécanique des fluides, aérosols, collisions délocalisées, modèle d’Enskog, lois de conservation, inégalités d’entropie, méthode des moments, systèmes de particules, limite hydrodynamique, couplage fluide-cinétique, sprays épais

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