

## Chapter 2

# A Brief Introduction to the Mathematical Kinetic Theory of Classical Particles

### 2.1 Plan of the Chapter

The contents of this chapter are motivated by the second key question posed in Section 1.3, namely by the search of mathematical tools suitable to model living systems (specifically, we deal with systems composed of many interacting entities). The strategy to pursue this challenging objective consists in designing a general mathematical framework suitable to capture, by a differential system, the ten key complexity features presented in Section 1.4. This topic will be exhaustively treated in the next chapter. However, the classical kinetic theory represents an important reference background. Therefore, this present section provides a brief introduction to this topic.

Bearing this in mind, let us report about the methods of the kinetic theory of diluted gases and, specifically, of the celebrated Boltzmann equation. A common feature shared by the classical and the new approach is that the state of the overall system is described by a probability distribution over the state at the microscopic scale of the interacting entities, namely classical particles in the first case and active particles in the second case, where the microscopic state includes, as we shall see, an additional variable suitable to model the living features of each specific system.

The time and space dynamics of the said distribution is obtained, in both cases, by a balance of particles in the elementary volume of the space of the microscopic states. However, substantial conceptual differences can be put in evidence. In the classical kinetic theory, interactions are reversible, binary, and ruled by laws of classical mechanics, while in the kinetic theory of active particles, they are not reversible, may involve multiple entities, and do not follow, as already mentioned, rules from a field theory.

Understanding the important conceptual differences between these two approaches can contribute to a deeper insight over the new approach. Therefore, a brief introduction to the Boltzmann equation will be presented also with the aim of enlightening the said differences.

Details of the contents of this chapter can now be given:

- Section 2.2 provides a brief introduction to the derivation of the Boltzmann equation and to its properties. This section also presents an overview of mathematical problems generated by the application of the models to the study of real flows, namely the initial value problem in unbounded domains within the framework of non-equilibrium thermodynamics and initial-boundary problems for internal or external flows.
- Section 2.3 rapidly introduces some generalizations of the Boltzmann equations, namely the so-called discrete velocity Boltzmann Equation (in short BE) to obtain a mathematical model apparently simpler than the original model, the Enskog equation, where the dimension of the particles is not neglected with the aims of modeling some dense gas effects, and Vlasov-type equation, where interactions with self-consistent force fields are accounted for.
- Section 2.4 provides a brief introduction to numerical methods which can be used to solve kinetic equations. The presentation remains at a technical level, namely for practical use, while the reader is addressed to the pertinent literature for a deeper insight into theoretical topics. Later in the book, this approach will be adapted to the specific case studies proposed in the next chapters.
- Section 2.5 proposes a critical analysis focused on the substantial differences of the physical framework, which leads to the classical kinetic theory and that of complex living systems.

It is worth stressing that the contents of this chapter is presented at a very introductory level. The reader who already possesses a basic knowledge of the mathematical kinetic theory can rapidly skip over this chapter and simply look at the last critical section. On the other hand, the reader who might think that it is exhaustive is invited to forget about this idea and go to the book by Cercignani, Illner, and Pulvirenti [82], which is the main reference for the contents of this present chapter.

## 2.2 Phenomenological Derivation of the Boltzmann Equation

Let us consider a system composed by spherically symmetrical classical particles modeled as point masses, where their microscopic state is given by position  $\mathbf{x} \in \mathbb{R}^3$  and velocity  $\mathbf{v} \in \mathbb{R}^3$ , and suppose that the mean free path is large enough that only binary collisions are important; namely, the probability of multiple collisions is not significant.

The system is supposed to be set in an unbounded domain with periodic boundary conditions or with decaying density and velocity of particles at infinity.

Molecular physical theories allow to define an interaction potential of the forces exchanged by pair of particles, and hence, the exchanged positional forces can be formally written as follows:

$$\varphi_{ij} = \varphi(\mathbf{x}_i, \mathbf{x}_j), \quad \mathbf{x}_i, \mathbf{x}_j \in \mathbb{R}^3, \quad i \neq j, \quad (2.1)$$

under the assumption that binary interactions are not influenced by the other particles.

When physical conditions make plausible all above assumptions, the dynamics of the particles is described by a large system of ordinary differential equations as follows:

$$\begin{cases} \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \\ m \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^N \varphi(\mathbf{x}_i, \mathbf{x}_j) + \mathbf{F}_i(\mathbf{x}_i), \end{cases} \quad (2.2)$$

where  $i = 1, \dots, N$  for a system of  $N$  equal particles subject to an external positional field  $\mathbf{F}_i(\mathbf{x})$ . The exchanged force  $\varphi_{ij}$  is repulsive for very short distances and attractive for large ones depending on the specific physical features of the interacting pairs. Further developments can take into account also a velocity dependence.

Disparate gas mixtures can be treated by the same approach, by including interactions of particles with different mass and adding new terms related to interactions of all components of the mixture.

Macroscopic quantities such as mass, linear momentum, and kinetic energy can be computed by local averages in small finite volumes. Fluctuations cannot be avoided by this technical averaging process.

An alternative to this approach consists in representing the overall system by a probability distribution and by looking for an equation suitable to describe the dynamics in time and space of the said distribution. Bearing this in mind, let us introduce the  $N$ -particles distribution function

$$f_N = f_N(t, \mathbf{x}_1, \dots, \mathbf{x}_N, \mathbf{v}_1, \dots, \mathbf{v}_N), \quad (2.3)$$

such that  $f_N d\mathbf{x}_1 \dots d\mathbf{x}_N d\mathbf{v}_1 \dots d\mathbf{v}_N$  represents the probability of finding, at time  $t$ , and a particle in the elementary volume of the  $N$ -particles in the phase space and the microscopic state at time  $t$  is the vector variable defined in the elementary volume of said space of all positions and velocities.

If the number of particles is constant in time and if the dynamics follows Newton rules, a continuity equation in the phase space is satisfied. Formal calculations, related to conservation of particles, yield

$$\partial_t f_N + \sum_{i=1}^N \mathbf{v}_i \cdot \nabla_{\mathbf{x}} f_N + \frac{1}{m} \sum_{i=1}^N \nabla_{\mathbf{x}} (\mathbf{F}_i \cdot f_N) = 0, \quad (2.4)$$

where  $m$  is the mass of the particle and  $\mathbf{F}_i = \mathbf{F}_i(t, \mathbf{x})$  is the force applied to each particle by the overall system as shown by Eq. (2.2).

This equation, which is known as “Liouville equation”, is not practical as it involves a too large number of variables. The “great” idea by Ludwig Boltzmann has been the description of the overall state by a continuous probability distribution

over the microscopic state of the particles, namely position and velocity of the *test particle* representative of the whole. Therefore, he introduced the one-particle distribution function as follows:

$$f = f(t, \mathbf{x}, \mathbf{v}) : [0, T] \times \mathbf{R}^3 \times \mathbf{R}^3 \rightarrow \mathbf{R}_+, \quad (2.5)$$

such that under suitable integrability conditions  $f(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}$  defines the number of particles that at time  $t$  are in the elementary volume  $[\mathbf{x}, \mathbf{x} + d\mathbf{x}] \times [\mathbf{v}, \mathbf{v} + d\mathbf{v}]$  space, called phase space, of the microscopic states.

Suppose now that

$$\mathbf{v}^r f(t, \mathbf{x}, \mathbf{v}) \in L_1(\mathbf{R}^3), \quad \text{for } r = 0, 1, 2, \dots,$$

then macroscale quantities are obtained by weighted moments as follows:

$$M_r = M_r[f](t, \mathbf{x}) = \int_{\mathbf{R}^3} m \mathbf{v}^r f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}, \quad (2.6)$$

where  $m$  is the mass of the particles,  $r = 0$  corresponds to the local density  $\rho(t, \mathbf{x})$  and  $r = 1$  to the linear momentum  $\mathbf{Q}(t, \mathbf{x})$ , while  $r = 2$  to the mechanical energy. Therefore, the local density and mean velocity are computed as follows:

$$\rho(t, \mathbf{x}) = m \int_{\mathbf{R}^3} f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}, \quad (2.7)$$

$$\mathbf{U} = \mathbf{U}(t, \mathbf{x}) = \frac{1}{\rho(t, \mathbf{x})} \int_{\mathbf{R}^3} m \mathbf{v} f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}, \quad (2.8)$$

while the kinetic translational energy is given by the second-order moment

$$\mathcal{E} = \mathcal{E}(t, \mathbf{x}) = \frac{1}{2\rho(t, \mathbf{x})} \int_{\mathbf{R}^3} m (\mathbf{v} - \mathbf{U})^2 f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}, \quad (2.9)$$

which, at equilibrium conditions, can be related to the local temperature based on the principle of repartition of energy, which is however valid only in equilibrium conditions.

Suppose now that a mathematical model can be derived to describe the time and space dynamics of  $f$ , formally as follows:

$$\mathcal{L} f = \mathcal{N} f, \quad (2.10)$$

where  $\mathcal{L}$  and  $\mathcal{N}$  are a linear and nonlinear operators, still to be defined explicitly. Then, solving Eq. (2.10) and using Eq. (2.6) yield the desired macroscale information.

Boltzmann's contribution was the derivation of Eq. (2.10) based on some fundamental concepts of non-equilibrium statistical mechanics mixed with some heuristic simplification of physical reality. This celebrated result has generated a huge

bibliography not only in the field of physics, but also in that of mathematics due to the challenging hints that this equation induced to applied mathematicians.

The aforementioned mathematical literature tackles a variety of topics including rigorous derivation, qualitative analysis of initial and initial-boundary value problems, and asymptotic limits to derive macroscale equations from the underlying description at the microscopic scale.

However, since dealing with this topic is not the most important aim of this book, we will focus only on those aspects that are relevant to the objective of developing mathematical tools for the derivation of models for living systems. The reader who likes the mathematical kinetic theory also knows that the literature includes some criticism to this model, some of which made difficult the life of the great Boltzmann.

Only the hallmarks followed for the derivation of the Boltzmann equation will be given. As already mentioned, the interested reader is addressed to the book [82] which is, according to the author's bias, the most appropriate for the aforesaid purpose. The reader who is more interested in fluid dynamics applications is addressed to the classical book by Kogan [164], not yet obsolete although appeared more than fifty years ago. The said hallmarks and related technical calculations for the derivation of the model are as follows:

1. Development of detailed calculations of the interaction dynamics of perfectly elastic pair of spherically shaped particles;
2. Computation of the net flow of particles entering into the elementary volume  $[\mathbf{x} + d\mathbf{x}] \times [\mathbf{v} + d\mathbf{v}]$  of the phase space and leaving it due to the interaction (collision) dynamics;
3. Modeling the time and space dynamics, in the said elementary volume, for the one-particle distribution function, Eq. (2.5), by equating the local evolution of the distribution function to the net flow of particles due to collisions.

Detailed calculations are reported in the next two subsections.

### 2.2.1 Interaction dynamics

Let us consider binary interactions (collisions) preserving mass, linear momentum, and energy between two particles with equal mass. Moreover, let us denote by  $\mathbf{v}$  and  $\mathbf{v}_*$  their velocities before interaction (collision) and by  $\mathbf{v}'$  and  $\mathbf{v}'_*$  those after interaction (collision). The said conservation of mechanical quantities implies:

$$\begin{cases} \mathbf{v} + \mathbf{v}_* = \mathbf{v}' + \mathbf{v}'_* \\ v^2 + v_*^2 = v'^2 + v_*'^2 \end{cases} \quad (2.11)$$

The system of four scalar equations is not sufficient to compute the six component of the post-collision velocities. Usually, see [82], the post-collision velocities are related to the precollision ones as follows:

$$\begin{cases} \mathbf{v}' = \mathbf{v} + \mathbf{k}(\mathbf{k} \cdot \mathbf{q}), \\ \mathbf{v}'_* = \mathbf{v} - \mathbf{k}(\mathbf{k} \cdot \mathbf{q}). \end{cases} \quad (2.12)$$

where  $q = \mathbf{v}_* - \mathbf{v}$  is the relative velocity.

The integration domain of  $\mathbf{n}$  is

$$\mathcal{S} = \{\mathbf{k} \in \mathbf{R}^2 : \|\mathbf{k}\| = 1, \mathbf{k} \cdot \mathbf{q} \geq 0\}.$$

### 2.2.2 The Boltzmann equation

The Boltzmann equation can be derived by a balance of particles in the elementary volume of the phase space  $[\mathbf{x}, \mathbf{x} + d\mathbf{x}] \times [\mathbf{v}, \mathbf{v} + d\mathbf{v}]$ . Such a balance can be formally obtained by equating the flow due to transport

$$\mathcal{L}f = (\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} + \mathbf{F}(t, \mathbf{x}) \cdot \nabla_{\mathbf{v}}) f(t, \mathbf{x}, \mathbf{v}), \quad (2.13)$$

to the net flow due to collisions

$$\mathcal{L}f = \mathcal{N}f = G[f, f](t, \mathbf{x}, \mathbf{v}) - L[f, f](t, \mathbf{x}, \mathbf{v}), \quad (2.14)$$

where  $\mathbf{F}$  is an external force field, while  $G$  and  $L$  denote the so-called *gain* and *loss* terms amounting to the inlet and outlet of particles due to collisions.

The calculation of these quantities needs some heuristic assumptions:

1. The probability of collisions involving more than two particles is much smaller than the one of binary encounters;
2. The effect of external forces on the molecules during the mean collision time is negligible in comparison to the interacting molecular forces;
3. Both asymptotic pre-collision and post-collision velocities are not correlated. This hypothesis is referred to as *molecular chaos* and implies that the joint-particle distribution function of the two interacting particles can be factorized, namely is given by the product  $f(t, \mathbf{x}, \mathbf{v})f(t, \mathbf{x}, \mathbf{v}_*)$ ;
4. The distribution function does not significantly change over a time interval which is larger than the mean collision time but smaller than the mean free time. Likewise, the distribution function does not change very much over a distance of the order of the range of the intermolecular forces.

These assumptions have an impact on the validity of the BE and on the qualitative analysis of the mathematical problems related to its fluid dynamics applications. Many studies have been devoted to these topics and part of them can be regarded as fundamental contributions to applied mathematics. However, these issues are not deeply dealt with in this book, where the BE is simply presented as a conceptual parallel to the mathematical approach hereinafter developed. Additional

bibliographic references will be given in the following, in addition to the already cited book [82].

Bearing all above in mind, the terms  $G$  and  $L$  can be computed explicitly according to the aforementioned assumptions.

Let us consider two gas molecules whose asymptotic pre-collision velocities are denoted by  $\mathbf{v}$  and  $\mathbf{v}_*$ . In Fig. 2.1, the molecule which has velocity  $\mathbf{v}$  is at the point  $O$ , while the other molecule is approaching with relative velocity  $\mathbf{q} = \mathbf{v}_* - \mathbf{v}$  and with impact parameter  $b$  in the reference plane forming the azimuthal angle  $\varepsilon$  with respect to the reference plane.

During a small the time interval  $\Delta t$  all molecules with velocities within the range  $\mathbf{v}_*$  and  $\mathbf{v}_* + d\mathbf{v}_*$ , and that are inside the cylinder of volume  $q \Delta t b db d\varepsilon$  will collide with the molecules located in a volume element  $d\mathbf{x}$  around the point  $O$  and whose velocities are within the range  $\mathbf{v}$  and  $\mathbf{v} + d\mathbf{v}$ . The number of the former is given by  $f(t, \mathbf{x}, \mathbf{v}_*) q \Delta t b db d\varepsilon$  while the number of the latter is  $f(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}$ . Therefore, the total number of particles which are expected to loose the velocity  $\mathbf{v}$  per unit of time in the phase volume element  $d\mathbf{x} d\mathbf{v}$  is given by

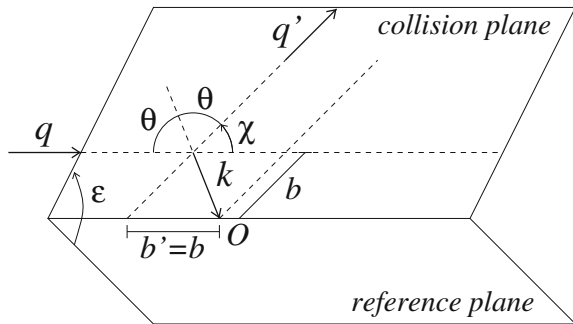
$$L(f, f)(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v} \Delta t = d\mathbf{x} d\mathbf{v} \Delta t \int f(t, \mathbf{x}, \mathbf{v}) f(t, \mathbf{x}, \mathbf{v}_*) q b db d\varepsilon d\mathbf{v}_*, \quad (2.15)$$

where integration is over the domain of the variables under the integral sign.

However, collisions are reversible and, in the reversed interactions, particles can also assume a velocity between  $\mathbf{v}$  and  $\mathbf{v} + d\mathbf{v}$  as a result of collisions with the following characteristics:

- (i) Asymptotic pre-collision velocities  $\mathbf{v}'$  and  $\mathbf{v}'_*$ ;
- (ii) Asymptotic post-collision velocities  $\mathbf{v}$  and  $\mathbf{v}_*$ ;
- (iii) Apsidal vector  $\mathbf{k}' = \mathbf{k}$ ,
- (iv) Impact parameter  $b' = b$ ;
- (v) Azimuthal angle  $\varepsilon' = \pi + \varepsilon$ .

**Fig. 2.1** Interaction dynamics.  $\mathbf{q}$  and  $\mathbf{q}'$  are the pre-collision and post-collision relative velocities,  $b$  is the impact parameter, and  $\chi$  is the scattering angle



These collisions can be referred to as inverse collisions to distinguish them from the former which are called direct collisions. The geometry of direct and inverse collisions is represented in Fig. 2.2.

In analogy with the treatment of the direct collisions, it is not difficult to conclude that the total number of particles which are expected to gain the velocity  $\mathbf{v}$  per unit of time in the phase volume element  $d\mathbf{x}d\mathbf{v}$  is given by

$$G(f, f)(t, \mathbf{x}, \mathbf{v})d\mathbf{x}d\mathbf{v}\Delta t = d\mathbf{x}d\mathbf{v}\Delta t \int f(t, \mathbf{x}, \mathbf{v}')f(t, \mathbf{x}, \mathbf{v}_*)q b db d\varepsilon d\mathbf{v}_*, \quad (2.16)$$

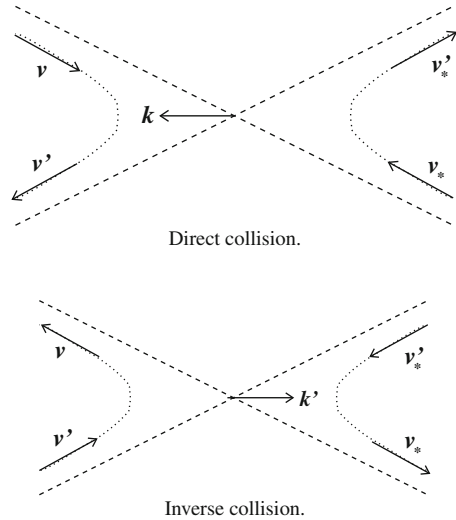
where it has been used the fact that the modulus of the Jacobian for the equations that relate the post- and pre-collision asymptotic velocities is equal to one, i.e.,  $d\mathbf{v}'d\mathbf{v}_* = d\mathbf{v}d\mathbf{v}_*$ , and, due to the energy conservation law, the modulus of the pre- and post-collision relative velocities are equal to each other, i.e.,  $q' = q$ .

By using Eqs. (2.16) and (2.15), the Boltzmann equation can be thus written:

$$\begin{aligned} & (\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} + \mathbf{F}(t, \mathbf{x}) \cdot \nabla_{\mathbf{v}}) f(t, \mathbf{x}, \mathbf{v}) \\ &= \int [f(t, \mathbf{x}, \mathbf{v}')f(t, \mathbf{x}, \mathbf{v}_*) - f(t, \mathbf{x}, \mathbf{v})f(t, \mathbf{x}, \mathbf{v}_*)] q b db d\varepsilon d\mathbf{v}_*. \end{aligned} \quad (2.17)$$

Various modifications of this kinetic equation are known in the literature. Some of them are analyzed in the next section still looking at the development of mathematical tools for living systems.

**Fig. 2.2** Direct and inverse collisions



### 2.2.3 Properties of the Boltzmann equation

Although the Boltzmann equation is derived under various approximations of physical reality, it still retains some important features of the physics of system composed of many interacting classical particles. Let us first observe that the local density and mean velocity are computed by Eqs. (2.7) and (2.8), while the local temperature can be related to the kinetic energy by assuming that the principle of repartition of the energy for a perfect gas can be applied.

Bearing this in mind, some important properties can be recalled referring to the classical literature:

1. The collision operator  $\mathcal{N}[f, f]$  admits collision invariants corresponding to mass, momentum, and energy, namely

$$\langle \phi_r, \mathcal{N}[f, f] \rangle = 0, \quad \text{for } r = 0, 1, 2, \quad \text{with } \phi_r = \mathbf{v}^r, \quad (2.18)$$

where the notation  $\langle, \rangle$  is used for product under the integral sign. Equation (2.18) states conservation of mass, linear momentum, and energy.

2. A unique solution  $f_e$  to the equilibrium equation  $\mathcal{N}[f] = 0$  exists and is the Maxwellian distribution:

$$f_e(t, \mathbf{x}, \mathbf{v}) = \frac{\rho(t, \mathbf{x})}{[2\pi(k/m)\Theta(t, \mathbf{x})]^{3/2}} \exp \left\{ -\frac{|\mathbf{v} - \mathbf{U}(t, \mathbf{x})|^2}{2(k/m)\Theta(t, \mathbf{x})} \right\}, \quad (2.19)$$

where  $k$  is the Boltzmann constant, and  $\Theta$  is the temperature given, for a monatomic gas, by the approximation of a perfect gas, namely

$$\mathcal{E} = \frac{3}{2} \frac{k}{m} \Theta,$$

where  $\mathcal{E}$  is the already defined kinetic energy.

The first item states conservation of mass

$$\int f(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v} = \int f_0(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v},$$

linear momentum

$$\int \mathbf{v} f(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v} = \int \mathbf{v} f_0(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v},$$

and energy

$$\int v^2 f(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v} = \int v^2 f_0(\mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v},$$

where  $f_0(\mathbf{x}, \mathbf{v}) = f(t = 0, \mathbf{x}, \mathbf{v})$ .

Trend to equilibrium is assured by the *kinetic entropy*, namely the  $H$ -Boltzmann functional:

$$H[f](t) = \int_{\mathbf{R}^3 \times \mathbf{R}^3} (f \log f)(t, \mathbf{x}, \mathbf{v}) d\mathbf{x} d\mathbf{v}, \quad (2.20)$$

which, in the spatially homogeneous case, is monotonically decreasing along the solutions and is equal to zero at  $f = f_e$ . Therefore, the Maxwellian distribution with parameters  $\rho$ ,  $\mathbf{U}$ , and  $\Theta$  minimizes  $H$  (this is the celebrated  $H$ -Theorem).

Mathematical problems for the Boltzmann equation can be classified as the initial value (Cauchy) problem in unbounded domains and the initial-boundary value problem in bounded domains or external flows. Applications refer generally to non-equilibrium thermodynamics or fluid dynamics applications for molecular flows. The *Cauchy problem* can be stated in more detail, in the absence of an external force, as follows:

$$\begin{cases} \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = J(f, f), \\ f(t = 0, \mathbf{x}, \mathbf{v}) = f_0(\mathbf{x}, \mathbf{v}), \end{cases} \quad (2.21)$$

where the initial datum can either be assumed to decay at infinity in the phase space or be periodic in space and decaying with velocity.

The literature on this challenging problem is documented in various books, for instance [13, 49, 131], which report about the solution of Cauchy problem for initial data given as perturbation of vacuum, spatially homogeneous case, and Maxwellian equilibrium. In particular, the book by Glassey [131] reports also about the Cauchy problem for the mean field models, namely the Vlasov equation.

Particularly important is the celebrated global existence result by Di Perna and Lions [99, 100], who succeeded to prove existence in the sense of distributions for a large class of initial data for a gas with bounded mass momentum and energy. This result gave, as it is known, a great hint to research activity as all previous results were limited to small perturbation although the existence theorem [53] also included the case of an infinite mass of the gas.

The statement of the initial-boundary value problem requires the modeling of gas-surface interaction dynamics. Two specific problems, among various ones, can be stated:

- The *interior domain problem*, which corresponds to a gas contained in a volume bounded by a solid surface;
- The *exterior domain problem*, which corresponds to a gas in the whole space  $\mathbf{R}^3$  which contains an obstacle.

The surface of the solid wall is defined in both cases by  $\Sigma_w$ , and the normal to the surface directed toward the gas is  $\nu$ . Moreover, in order to define the boundary conditions on a solid wall, we need to define the partial incoming and outgoing traces  $f^+$  and  $f^-$  on the boundary  $\Sigma_w$ , which, for continuous  $f$ , can be defined as follows:

$$f^+(\mathbf{x}, \mathbf{v}) = f(\mathbf{x} \in \Sigma_w, \mathbf{v} | \mathbf{v} \cdot \nu(\mathbf{x}) > 0), \quad (2.22)$$

and

$$f^-(\mathbf{x}, \mathbf{v}) = f(\mathbf{x} \in \Sigma_w, \mathbf{v} | \mathbf{v} \cdot \nu(\mathbf{x}) < 0). \quad (2.23)$$

The boundary conditions can be formally defined by the operator map:

$$f^+(t, \mathbf{x}, \mathbf{v}) = \mathcal{R} f^-(t, \mathbf{x}, \mathbf{v}), \quad (2.24)$$

where the operator  $\mathcal{R}$ , which maps the distribution function of the particles which arrive to the surface into the one of particles leaving the surface, is featured by the following properties:

1.  $\mathcal{R}$  is linear, of local type with respect to  $\mathbf{x}$ , and is positive:

$$f^- \geq 0 \Rightarrow \mathcal{R} f^- \geq 0. \quad (2.25)$$

2.  $\mathcal{R}$  preserves mass, i.e., the flux of the incoming particles equals the one of the particles which leaves the surface.
3.  $\mathcal{R}$  preserves local equilibrium at the boundary:  $\omega_w^+ = \mathcal{R} \omega_w^-$ , where  $\omega_w$  is the Maxwellian distribution at the wall temperature.
4.  $\mathcal{R}$  is dissipative, i.e., satisfies the inequality at the wall:

$$\int_{\mathbf{R}^3} \langle \mathbf{v} \cdot \nu \rangle (f^- + \mathcal{R} f^-) (\log f + |\mathbf{v}|^2/T) d\mathbf{v} \leq 0. \quad (2.26)$$

The formulation of the initial-boundary value problem, in the case of the *interior domain problem*, consists in linking the BE to the initial and boundary conditions. In the case of the *exterior domain problems*, in addition to the boundary conditions on the wall, suitable Maxwellian equilibrium conditions need to be assumed at infinity. The already cited book [82] reports some specific examples of the operator  $\mathcal{R}$ .

## 2.3 Some Generalized Models

The mathematical developments of the kinetic theory have generated a variety of models somehow related to the original Boltzmann equation. Most of them are motivated by the need of reducing the analytic and computational complexity of the equation, while others aim at taking into account physical effects that are not included in the original model. This section focuses on three different classes of models, selected among various ones, which present features of interest for a comparison with the approach addressed to living systems that will be presented in the next chapter.

Specifically, we consider the so-called BGK model, where the complexity of the right-hand-side term modeling collisions is strongly simplified by replacing the original term by an algebraic structure modeling, a trend toward equilibrium. The

second class of models corresponds to the so-called Discrete Boltzmann equation, where particles are supposed to attain only a finite number of velocities. Finally, the Enskog equation is rapidly introduced as a model, which attempts to include some dense gas effects. The next three paragraphs present these models waiting for the critical analysis proposed in the last section.

### 2.3.1 The BGK model

This model was proposed, as already mentioned, to reduce the analytic and computational complexity of the Boltzmann equation. The hallmarks that guided the design of this model can be listed as follows:

- If the distribution function  $f$  is known, then the local Maxwellian can be computed by the first three moments. Formally:  $f_e = f_e[f] =: f_e(\rho, \mathbf{U}, \Theta)$ .
- A molecular fluid is featured by a natural trend to local equilibrium as described by the H-function.
- Models can be derived simply by replacing the collision right-hand-side integral operator by a decay term modeling trend to equilibrium.

Consequently, in the absence of an external force field, the model is written as follows:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = c[f](f_e[f] - f), \quad (2.27)$$

where  $c$  gives the decay rate. The latter can be assumed to be a function of the local density  $\rho$ , i.e.,  $c = c(\rho)$ . Otherwise, the simplest approximation suggests to take a constant value  $c = c_0$ .

Model (2.27) definitely requires less sophisticated tools toward computing than the original Boltzmann equation. However, one has necessarily to put in discussion the validity of the decay assumptions in conditions largely far from equilibrium.

In addition, let us stress that the BGK model is nonlinear even in the case of  $c = c_0$ . In fact,  $f_e$  nonlinearly depends on  $f$ . It becomes a simple linear model only by linearization or by assuming that  $f_e = f_{e0}$ , which is rather unrealistic hypothesis.

The substantial conceptual difference with respect to the Boltzmann equation is that in the original model, the Maxwellian distribution is an emerging behavior that is induced by the dynamics at the microscopic scale, while it is artificially imposed in the BGK model.

### 2.3.2 The discrete Boltzmann equation

Discrete velocity models of the Boltzmann equation can be obtained, assuming that particles allowed to move with a finite number of velocities. The model is an evolution equation for the number densities  $N_i$  linked to the admissible velocities  $\mathbf{v}_i$ , for

$i = 1, \dots, n$  with  $i \in L = \{1, \dots, n\}$ . The set  $\{N_i(t, \mathbf{x})\}_{i=1}^n$  corresponds, for certain aspects, to the one-particle distribution function of the continuous Boltzmann equation.

The mathematical theory of the discrete kinetic theory is exhaustively treated in the Lecture Notes by Gatignol [125], which provides a detailed analysis of the relevant aspects of the discrete kinetic theory: modeling, analysis of thermodynamic equilibrium, and application to fluid-dynamic problems. The contents mainly refer to a simple monatomic gas and to the related thermodynamic aspects.

After such a fundamental contribution, several developments have been proposed in order to deal with more general physical systems: gas mixtures, chemically reacting gases, particles undergoing multiple collisions, and so on. Analytic topics, such as the qualitative analysis of the initial value and of the initial-boundary value problem, have been object of continuous interest of applied mathematicians as reported in the survey [45]. Additional sources of information are the review paper by Platkowski and Illner [201] and the edited book [42], where various applications and developments of the model are reported.

The formal expression of the evolution equation corresponds, as for the full Boltzmann equation, to the balance of particles in the elementary volume of the space of the microscopic states:

$$(\partial_t + \mathbf{v}_i \cdot \nabla_{\mathbf{x}}) N_i = J_i[N] = \frac{1}{2} \sum_{j,h,k=1}^n A_{ij}^{hk} (N_h N_k - N_i N_j), \quad (2.28)$$

which is a system of partial differential equations, where the dependent variables are the number of densities linked to the discrete velocities:

$$N_i = N_i(t, \mathbf{x}) : (t, \mathbf{x}) \in [0, T] \times \mathbf{R}^v \rightarrow \mathbf{R}_+, \quad i = 1, \dots, n, \quad v = 1, 2, 3.$$

Collisions  $(\mathbf{v}_i, \mathbf{v}_j) \longleftrightarrow (\mathbf{v}_h, \mathbf{v}_k)$  are binary and reversible, and preserve mass momentum and energy. Their modeling is left to the so-called *transition rates*  $A_{ij}^{hk}$ , which are positive constants and, according to the reversibility properties, satisfy the following relations:  $A_{ji}^{hk} = A_{ij}^{kh} = A_{ji}^{kh}$ .

Analogously to the Boltzmann equation, it is possible to define the space of collision invariants and of the Maxwellian state [125]. In more detail, the following definitions can be used:

**Collision Invariant:** A vector  $\phi = \{\phi_i\}_{i \in L} \in \mathbf{R}^n$  is defined *collision invariant* if:

$$\langle \phi, J[N] \rangle = 0, \quad J[N] = \{J_i[N] \in \mathbf{R}^n\},$$

where the inner product is defined in  $\mathbf{R}^n$ .

**Space of the collision invariants:** The set of the totality of collision invariants is called *space of the collision invariants* and is a linear subspace of  $\mathbf{R}^n$ . Such a space will be denoted, in what follows, by  $\mathcal{M}$ .

**Maxwellian:** Let  $N_i > 0$  for any  $i \in L$ , then the vector  $N$  is defined *Maxwellian* if  $J[N] = 0$ . In particular, let  $N \in \mathbf{R}^n$ , then the following conditions are equivalent:

- (i)  $N$  is a Maxwellian;
- (ii)  $\{\log N_i\}_{i \in L} \in \mathcal{M}$ ;
- (iii)  $J[N] = 0$ .

Applied mathematicians have attempted in the last decade to design models with arbitrarily large number of velocities and hence to analyze convergence of discretized models toward the full Boltzmann equation. However, various technical difficulties have to be tackled, such as:

1. Discretization schemes for each couple of incoming velocities do not assure a pair of outgoing velocities such that conservation of mass and momentum is preserved;
2. Specific models may have a number of spurious collision invariants in addition to the classical ones corresponding to conservation of mass, linear momentum, and energy;
3. Convergence of the solutions of discretized equation to those of the full Boltzmann equation, when the number of discretization points tends to infinity, under suitable hypotheses which have to be properly defined.

A technical difficulty in dealing with the above convergence proof consists in obtaining an existence theorem for the Boltzmann equation in a function space which can be properly exploited for the development of the computational scheme.

These difficulties generated the so-called *semi-continuous Boltzmann equation*, where particles are allowed to attain all directions in space, but only a finite number of velocity modules. This approach allows to overcome the difficulty in integration of the whole velocity space, namely  $\mathbf{R}^3$ . Particularly important is the result of paper [171], where it is shown that a particular choice of the sequence of velocity modules maximizes the number of collisions consistent with conservation of momentum and energy; hence, the model appears closer to physical reality.

### 2.3.3 Vlasov and Enskog equations

Further models have been developed to take into account some alternative ways of modeling interactions. For instance, the Boltzmann equation is such that the distribution function is modified only by external actions and short range interactions and, on the other hand, various physical systems are such that also long-range interactions may be significant as in the mean field approaches which lead to the Vlasov equation. Moreover, one can consider localized interactions, but at a fixed distance imposed by the finite dimension of the particles.

Both types of interactions can occur in the case of living systems although in a technically different way. Therefore, it is worth providing a brief introduction to the said alternative derivation methods.

Focusing on the mean field approach, let us consider the vector action  $\mathcal{P} = \mathcal{P}(\mathbf{x}, \mathbf{v}, \mathbf{x}_*, \mathbf{v}_*)$  on the subject with microscopic state  $\mathbf{x}, \mathbf{v}$  (test particle) due to the subject with microscopic state  $\mathbf{x}_*, \mathbf{v}_*$  (field particle). The resultant action is:

$$\mathcal{F}[f](t, \mathbf{x}, \mathbf{v}) = \int_{\mathbf{R}^3 \times \mathcal{D}_\Omega} \mathcal{P}(\mathbf{x}, \mathbf{v}, \mathbf{x}_*, \mathbf{v}_*) f(t, \mathbf{x}_*, \mathbf{v}_*) d\mathbf{x}_* d\mathbf{v}_*, \quad (2.29)$$

where  $\mathcal{D}_\Omega$  is the domain around the test particle, where the action of the field particle is effectively felt; namely, the action  $\mathcal{P}$  decays with the distance between test and field particles and is equal to zero on the boundary of  $\mathcal{D}_\Omega$ .

Based on the aforesaid assumptions, the mean field equation writes:

$$\partial_t f + (\mathbf{v} \cdot \nabla_{\mathbf{x}})f + \mathbf{F} \cdot \nabla_{\mathbf{v}} f + \nabla_{\mathbf{v}} \cdot (\mathcal{F}[f] f) = 0, \quad (2.30)$$

where  $\mathbf{F}$  is the positional macroscopic force acting on the system.

Another model to be considered is the so-called *Enskog equation*, which introduces some effects of the finite dimensions of the particles. This specific feature is introduced in the model by two ways:

1. The distribution functions of the interacting pairs (indeed, only binary collisions are considered) are computed in the centers of the two spheres, namely not in a common point for both distributions;
2. The collision frequency is reduced by the dimension of the interacting spheres, which reduces the probability of further interactions by shielding the free volume available for further interactions. This amounts to introducing a functional local density which correlates with the distribution functions of the interacting pairs and increases with the increasing local density.

This model has been interpreted for a long time as the first step toward the derivation of kinetic models for dense fluid. On the other hand, the limitation to binary mixtures technically prevents such interesting generalization. In fact, multiple interactions appear to be necessary to describe the physics of transition from rarefied to dense fluid.

However, as it is, the model offers to applied mathematicians a variety of challenging problems such as existence and uniqueness of solutions to mathematical problems and asymptotic limits either to hydrodynamics when the intermolecular distances tends to zero, or to the Boltzmann equation when the dimension of the particles is allowed to tend to zero. The book [48] was devoted to this model and mainly to the analytic problems generated by its applications. The bibliography reported in it also includes useful indications in the field of physics.

## 2.4 Computational Methods

Kinetic equations have the form of nonlinear integro-differential equations in which the unknown function depends on seven variables. The mathematical difficulties connected with them are such that only numerical solutions can be obtained in cases of practical interest. The common strategy consists in decoupling the transport and the collision terms by time-splitting the evolution operator into a *drift step*, in which collisions are neglected, and a *collision step*, in which spatial motion is frozen.

Numerical methods can be roughly divided into three groups depending on how drift and collision steps are dealt with, namely regular, semi-regular, and particle. Valuable references are provided by standard books [10, 64, 197, 208] as well as recent review papers [106].

Regular and semi-regular methods adopt similar strategies in discretizing the distribution function on a grid in the phase space [10]. The drift step requires to solve a system of hyperbolic conservation laws coupled at the boundaries. Their discretization can be performed in a variety of ways, including finite-difference, finite-volume, finite-element, or spectral methods [170]. The collision step consists of solving a spatially homogeneous relaxation equation. This is the more computationally demanding part since it involves the computation of a high-dimensional integral defining the collision operator. Regular and semi-regular methods differ in the way the collision term is evaluated.

Most of the regular methods adopt a Galerkin discretization of the velocity space [106]. These methods consist of expanding the velocity dependence of the distribution function in a set of trial functions with expansion coefficients that depend on position and time. The Galerkin ansatz is substituted in the space homogeneous relaxation equation which is subsequently multiplied by test functions and integrated into the velocity space. According to the Galerkin approach, test and trial functions are assumed to be the same. The above procedure yields a coupled system of ordinary differential equations for the expansion coefficients. Galerkin discretization can be further distinguished depending on the basis functions which they employ.

In Fourier–Galerkin approach, the distribution function is expanded in trigonometric polynomials and the fast Fourier transform is used to accelerate the computation of the collision integral in the velocity space [114, 122, 178, 196], while discontinuous Galerkin methods adopt discontinuous piecewise polynomials as test and trial functions [9, 126].

Hybrid approaches have been also developed where the distribution function is expanded in Laguerre polynomials with respect to the velocity components parallel to solid surfaces, whereas quadratic finite-element functions have been used for the normal velocity component [190, 225].

In semi-regular methods, the collision integral is computed by Monte Carlo or quasi-Monte Carlo quadrature. These schemes originate from the work by Nordsieck and Hicks [185] and have been further developed over the years by a number of authors [11, 116].

Particle methods originate from the Direct Simulation Monte Carlo (DSMC) scheme [64] which, introduced firstly based on physical reasoning [65], has been later proved to converge, in a suitable limit, to the solution of the Boltzmann equation [238]. The distribution function is represented by a number of particles which move in the computational domain and collide according to stochastic rules derived from the kinetic equations.

The space domain to be simulated is covered by a mesh of cells. These cells are used to collect together particles that may collide and also for the sampling of macroscopic field such as density and mean velocity. Macroscopic flow properties are obtained by time averaging particle properties. Variants of the DSMC have been proposed over the years which differ in the way the collision step is performed.

These methods include the majoring Frequency scheme [158], the null Collision scheme [165], the Nanbu scheme [182] and its modified version [17], the Ballot Box scheme [249], the Simplified Bernoulli trials scheme [227].

Particle schemes and particle methods are by far the most popular and widely used simulation methods in rarefied gas dynamics. Indeed, they permit to easily handle complex geometries while keeping the computing effort requirements at a reasonable level. Furthermore, they permit to easily insert new physics.

Particle methods are not well suited to simulate unsteady gas flows. Indeed, in this case, the possibility of time averaging is lost or reduced. Acceptable accuracy can only be achieved by increasing the number of simulation particles or superposing several flow snapshots obtained from statistically independent simulations of the same flow but, in both cases, the computing effort is considerably increased. Weighted particles can also be used to increase the result accuracy without additional computational cost [208].

Although the adoption of such a grid limits the applicability of regular and semi-regular schemes to problems where particular symmetries reduce the number of spatial and velocity variables, these are a feasible alternative to particle methods in studying unsteady flows since the possibility of a direct steady-state formulation.

Moreover, unlike particle-based methods, their implementation on massively parallel computers with Single Instruction Multiple Data (SIMD) architecture, such as multicores and Graphic Processing Units (GPUs), can easily realize the full potential of these processors [119, 120]. These aspects also prompted the development of deterministic methods of solution.

## 2.5 Critical Analysis

Let us now elaborate a critical overview of the contents of our book referring it to the complexity features presented in Chapter 1. Criticisms should not be addressed to the mathematical kinetic theory as it is. Indeed, it remains a fundamental research field of applied mathematics in interaction with physics and, as far as some applications are concerned, with technological sciences. On the other hand, we wish to understand the drawbacks of kinetic theory methods when referred to the modeling of living systems.

The aim is also to avoid an uncritical use of classical methods and to understand how the classical methods should be modified to tackle the challenging task of capturing the aforesaid complexity features.

Bearing all above in mind, it can be rapidly understood that the mathematical structures of the kinetic theory do not retain the main features of complex systems, where the causality principles which rule the dynamics of classical particles are lost. On the other hand, it can be argued that the representation by a probability distribution over the microscopic state can provide a useful description of the whole system. In fact, it retains some stochastic features of living systems and can rapidly provide, simply by weighted moments, the information on macroscale properties, which are often needed by applications.

An example can be rapidly selected to understand the conceptual differences between classical and living particles. Then, let us consider the statement of the boundary conditions as in Eq. (2.25). Classical particles collide with the wall where they sharply modify their trajectory. Living particles feel (see) the wall and gradually modify their trajectory before reaching it.

Furthermore, the microscopic state cannot be limited to mechanical variables as it should capture, in an appropriate way, the ability that interacting entities have to express their strategy.

In addition, the use of a distribution function can be made technically consistent with the presence of a birth and death dynamics, which is a typical feature of living systems including features not precisely related to classical mechanics. For instance, birth processes can even generate mutations and selection within a Darwinian-type framework [57].

According to all above reasonings, it can be argued that the idea of representing the system by some modified (generalized) distribution function can be accepted as a useful step toward modeling. Moreover, the balance of particles in the elementary volume of the space of the microscopic states can still be used to compute the time and space dynamics of the aforesaid distribution function. However, interactions cannot be described by the deterministic causality principles of classical mechanics, starting from the fact that interactions are not reversible. Therefore, new ideas need to be developed.

The rationale that guides the approach of this book is that theoretical tools of game theory need to be properly developed to model interactions. Of course, one cannot naively follow a straightforward application of the classical game theory, but has to look for developments suitable to include multiple interactions and learning ability, which has a progressive influence on the rules of interactions that evolve in time [186, 187]. Furthermore, modeling interactions should necessarily taken into account stochastic aspects, which are somehow related to the heterogeneous behavior of living entities, and space nonlocality, as when interactions can occur in networks [162, 163, 184].

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Bellomo, N.; Bellouquid, A.; Gibelli, L.; Outada, N.

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