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On the Numerical Simulation of a Class of Reactive Boltzmann Type Equation

by Dorin Marinescu [1]

Contents

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1. Introduction

It is known that the classical Boltzmann equation describes the evolution of the simple gas. The Boltzmann equation represents the connecting bridge between the microscopic and macroscopic description of the simple fluid evolution. The kinetics of the simple gas is essentially governed by elastic binary collisions between structureless particles belonging to a unique species, the multiple collisions being very improbable Ref. [1]. However, this equation is not able to describe the evolution of the real gas with chemical reactions and/or ionization processes. Then inelastic collisions must be considered by the kinetic models. Boltzmann himself was aware of the importance of the inelastic collisions in the real fluid evolution Ref. [9].

The classical Boltzmann equation is almost unanimously considered as appropriate for the kinetics of the rarefied simple gas. A kinetic theory for the reactive (real) gas is a more difficult task Ref. [30, 21]. As compared to the classical Boltzmann equation for the simple gas, kinetic reactive models exhibit new mathematical difficulties due the contribution of the particle internal states to the gas evolution (in particular the presence or reaction thresholds) and the existence of collision channels with multiple reaction participants Ref. [8, 25, 24, 29]. In the case of the reacting gas mixtures the mass balance does not hold for a given species. Then, the mass conservation for a specie must be replaced by the total mass balance. In the reactive models is present a transfer between the kinetic energy and the internal molecular energy. Consequently, the kinetic energy balance must be replaced by the total energy balance (i.e. kinetic energy + internal molecular energy). Then, the transport properties of the reacting gas mixtures differ from the properties of the simple gas.

Various models have been introduced to describe the kinetics of the real (reactive) gas. An important role is played by the Boltzmann-like semi-quantum equations. A known example is the Wang-Chang-Uhlenbeck-de Boer system of kinetic equations [32] for the real gas with binary collisions. This model refers to a gas of particles with classical translational motion, but with quantum internal structure. Essentially, the difference from the Boltzmann model Ref. [11] for the simple gas is to associate to each internal state a distribution function, and to relate each transition from one quantum internal state (of some chemical species) to another with a cross-section matrix.

A more general model introduced by Ludwig and Heil [25] extends Wang-Chang-Uhlenbeck-de Boer model. This model describes reactions in a diatomic gas without emission or absorption of radiation. It includes processes

of recombinations by triple collisions, as well as three post-collisional products like dissociation and ionization induced by collisions Ref. [8, 25, 24].

In some Wang-Chang-Uhlenbeck-de Boer or Ludwig and Heil model the number of equations depends on the number of distribution functions, i.e. on the number of different quantum internal states owned by the gas particles during the gas evolution. It is known that, there exists only at most a countable set of internal states. However, only a finite number of internal states will significantly contribute to the gas kinetics. Consequently, the Wang-Chang-Uhlenbeck-de Boer and Ludwig and Heil models are described by a finite number of equations.

For analytical purposes, in Ref. [16, 17, 18], the Wang-Chang-Uhlenbeck-de Boer and Ludwig and Heil equations corresponding to the model with finite number of internal states have been transcribed in abstract form, revealing the mathematical structure of the equations. In Ref. [17] was proved the existence and uniqueness of the solutions for the Cauchy problem. It was shown that the solutions verify the conservation of the total mass, momentum and energy respectively. Moreover, it was proved the existence of equilibrium solutions. H-theorem and a generalized law of the mass action have been rigorously proved under extended balance conditions.

The interest for reactive kinetics is not only intrinsic, but also of practical nature, in plasma physics, nuclear physics, physical chemistry of the high atmosphere, combustion theory, modeling of missiles flight.

Accurate numerical modeling of nonlinear processes in dilute, flows is critical for solving transport problems both in fundamental and applied science. In this respect Babovsky and Illner [4, 5] have proposed an efficient numerical scheme consistent with the classical Boltzmann equation. Using Nambu's ideas [26], by time discretization and local space-homogenization, Babovsky and Illner have obtained a convenient approximate form of the equation. At this point, the nonlinear character of the collision operators involve a power-like growth of the numerical complexity. To provide an algorithm, with small numerical effort, they have introduced an additonal stochastic approximation. Finally, they have proved the convergence almost sure, in some sense, of the approximation scheme. The techniques developed by Nambu [26], Babovsky and Illner of [4, 5] were also applied Ref. [6] to Pullin's equation [27] with Larsen-Borgnakke [10] scattering cross section for the one-component diatomic gas with classical internal degrees of freedom.

For the abstract model Ref. [16, 17, 18] describing the real reacting gas, in Ref. [19] was introduced a rigorous and efficient approximation scheme. This method represents a nontrivial extension of the techniques of Ref. [4, 5] for

solving space-homogeneous Boltzmann-like models of reacting gas mixtures Ref. [32, 8, 25, 24, 16, 17].

The methods of this chapter have been tested Ref. [14, 13] on the Krook-Wu [22] two-component Boltzmann equation as well as on the reactive Boltzmann models with three and four components Ref. [12, 20].

This review presents the theoretical approximation method for the solutions of the Boltzmann model introduced in Ref. [17] following the line of Ref. [19] and adding some improvements sketched in Ref. [12].

The present chapter is organized as follows.

In the next section one first recalls the main features of the Boltzmann-like equations introduced in Ref. [17]. Then, one formulates the approximation problem. In Section 3 one investigates the initial value problem for the space-homogeneous kinetic equations of Section 2, formulated in a suitable space of functions. In Section 4 one obtains a convergent, time-discretized version of the aforementioned Boltzmann-like equations. Section 5 is devoted to the generalizations of certain probabilistic selection results of Ref. [4, 5]. This is possible due to some clarifications with respect to the nature of the convergence introduced by Babovsky and Illner. More precisely, the probabilistic part of the convergence proof of Ref. [4, 5] is based on the central limit theorem for row-wise i.i.d. random variables and the Borel-Cantelli Lemma. Our argument follows from a simple version of the strong law of large numbers for arrays of (not necessarily identically distributed) row-wise independent, random variables. (Which results from the Chebyshev inequality and the Borel-Cantelli Lemma.) In Section 6, the results of Section 5 are applied to the discretized scheme obtained in Section 4. Consequently, one obtains the numerical algorithm for the original Cauchy problem. This represents our main result, namely the convergence of the numerical scheme. Finally, we discuss the limitations and possible generalizations of the model.

2. The Kinetic Model and the Approximation Procedure

Here, we briefly recall the features of the model presented in Ref. [17, 18] (see also Ref. [16]).

The leading idea behind the model is that, unequal internal states of a gas particle with internal structure can be considered as describing structure-less particles belonging to distinct chemical species. Then, a real gas mixture

of particles with internal structure can be thought as a mixture of several chemical species of mass points with unique internal states.

Specifically, the model refers to a gas consisting of N distinct species of point masses, with one-state internal energy, evolving without external forces. The following assumptions are general: (i) gas particles have free classical motion in space, between (in)elastic, instant, local collisions, without emission or absorption of photons; (ii) collision (reactions) may change momenta, as well as the chemical nature (in particular mass and internal energy) of the gas particles; any collision occurs with conservation of total mass, momentum and (kinetic+internal) energy, according to the laws of classical mechanics. (iii) in each collision (reaction) channel, the number of identical partners cannot exceed some number, say $M \geq 2$ and any collision (reaction) channel contains, at least, two particles.

Denote by $\mathcal{M}$ the folowing multi-index set

$$\mathcal{M} := \{\boldsymbol{\gamma} = (\gamma_k)_{k=1,\ldots,N} | \gamma_k \in \{0, 1, \ldots, M\}\}. \tag{2.1}$$

A gas collision (reaction) process is specified by a couple $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$. Here, the multi-index $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_N)$ represents the pre-collision (in) channel, with $\alpha_n \in \{0, 1, \ldots, M\}$ identical participants of the $n-th$ species. The multi-index $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_N)$ represents the post-collision (out) channel, with $\beta_n \in \{0, 1, \ldots, M\}$ identical participants of the $n-th$ species.

The pair of multi-indexes $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ corresponds to a reaction of the following type

$$\alpha_1 X_1 +, \ldots, +\alpha_N X_N \to \beta_1 X_1 +, \ldots, +\beta_N X_N, \tag{2.2}$$

between the species X_1,...,X_N, with stoichiometric coefficients $\alpha_1, \ldots, \alpha_N$, $\beta_1, .., \beta_N$. Note that if $\alpha = \beta$, the collision is elastic and if $\alpha \neq \beta$, the collision is inelastic.

For each channel $\boldsymbol{\gamma} \in \mathcal{M}$ the family $\mathcal{N}(\boldsymbol{\gamma}) := \{k \mid \gamma_k > 0 \text{ for } k = 1, \ldots, N\}$ represents the species existing in that channel. Obviously, if $k \notin \mathcal{N}(\boldsymbol{\gamma})$ the species k is not present inside the channel $\boldsymbol{\gamma}$. If $k \in \mathcal{N}(\boldsymbol{\gamma})$, then there are γ_k identical particles of the species k in the channel $\boldsymbol{\gamma}$. We denote the total number of particles in the channel $\boldsymbol{\gamma}$ by

$$|\boldsymbol{\gamma}| := \sum_{k=1}^{N} \gamma_k. \tag{2.3}$$

Their velocities are denoted by $\mathbf{w}_{k,1}, \ldots, \mathbf{w}_{k,\gamma_k} \in \mathbb{R}^3$. Also set $\mathbf{w} := ((\mathbf{w}_{k,i})_{i=1,\ldots,\gamma_k})_{k \in \mathcal{N}(\boldsymbol{\gamma})}$, understanding that $\mathbf{w} \in \mathbb{R}^{3|\boldsymbol{\gamma}|}$. We denote by

$m_k > 0$ and $E_k \in \mathbb{R}$, the mass and the internal energy, respectively of a mass-point of the species $k = 1, \ldots, N$.

Let

$$V_{\boldsymbol{\gamma}}(\mathbf{w}) := (\sum_{k=1}^{N} \gamma_k m_k)^{-1} \sum_{k \in \mathcal{N}(\boldsymbol{\gamma})} \sum_{i=1}^{\gamma_k} m_k \mathbf{w}_{k,i}, \tag{2.4}$$

and

$$W_{\boldsymbol{\gamma}}(\mathbf{w}) := \sum_{k \in \mathcal{N}(\boldsymbol{\gamma})} \sum_{i=1}^{\gamma_k} (2^{-1} m_k \mathbf{w}_{k,i}^2 + E_k). \tag{2.5}$$

be the classical mass center velocity and the total energy, respectively, for the particles in the channel $\boldsymbol{\gamma}$. According to the conservation assumptions, in the description of the gas kinetics, for each couple $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$ we consider only the collisions satisfying the relations

$$\sum_{k=1}^{N} m_k(\alpha_k - \beta_k) = 0, \tag{2.6}$$

$$V_{\boldsymbol{\alpha}}(\mathbf{w}) = V_{\boldsymbol{\beta}}(\mathbf{u}), \quad W_{\boldsymbol{\alpha}}(\mathbf{w}) = W_{\boldsymbol{\beta}}(\mathbf{u}), \tag{2.7}$$

In (2.7) $\mathbf{w} = ((\mathbf{w}_{k,i})_{i=1,\ldots,\gamma_k})_{k \in \mathcal{N}(\boldsymbol{\alpha})}$ and $\mathbf{u} = ((\mathbf{u}_{k,i})_{i=1,\ldots,\beta_k})_{k \in \mathcal{N}(\boldsymbol{\beta})}$ are the velocities of the particles in the channels $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$, respectively.

Note that reactions with at most one particle in some collision channel are excluded by (2.6) and (2.7), because in the absence of radiative processes, the conservation laws (2.6) and (2.7) cannot be simultaneously fulfilled. Therefore, $|\boldsymbol{\gamma}| \geq 2$. This inequality explains the restriction $M \geq 2$ in the definition (2.1) of $\mathcal{M}$. Remark that, the conservation of the total energy stated in (2.7) implies the existence of reaction thresholds and shows what happens with the internal energies of the particles participating in reactions. For instance in the case of endothermic collisions $(\boldsymbol{\alpha}, \boldsymbol{\beta})$, i.e.

$$\sum_{k \in \mathcal{N}(\boldsymbol{\alpha})} \alpha_k E_k < \sum_{k \in \mathcal{N}(\boldsymbol{\beta})} \beta_k E_k, \tag{2.8}$$

the kinetic energy of the resulting products is lost as binding energy. In such a case the collision can be forbidden if the kinetic energy in the channel $\boldsymbol{\alpha}$ is bellow the reaction threshold. Note that, the model accepts also reaction thresholds for exothermic collisions $(\boldsymbol{\alpha}, \boldsymbol{\beta})$

$$\sum_{k \in \mathcal{N}(\boldsymbol{\alpha})} \alpha_k E_k > \sum_{k \in \mathcal{N}(\boldsymbol{\beta})} \beta_k E_k. \tag{2.9}$$

Following the standard Boltzmann procedure (based on the molecular chaos assumption) we introduce the system of kinetic equations

$$\partial_t f_k + \mathbf{v} \cdot \nabla_x f_k = P_k(\mathbf{f}) - S_k(\mathbf{f}), \text{ for } k = 1, \dots, N, \tag{2.10}$$

as an abstract transcription of the Wang-Chang-Uhlenbeck-de Boer and Ludwig and Heil equations. Here $f_k : \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}_+$ are the unknowns for $k = 1, \dots, N$, (with $\mathbb{R}_+ := [0, \infty)$) and $\mathbf{f} := (f_1, \dots, f_N)$. Each $f_k = f_k(t, \mathbf{v}, \mathbf{x})$ (t-time, $\mathbf{v}$ -velocity, $\mathbf{x}$ -position) is the one-particle distribution function for species $k = 1, \dots, N$ of particles. In (2.10) the gain operators P_k and the loss operators $S_k(\mathbf{f})$ describe the collision processes.

For $\mathbf{g} = (g_1, \dots, g_N)$ (with $g_1, \dots, g_N : \mathbb{R}^3 \to \mathbb{R}$) define,

$$\mathbf{g}_{\boldsymbol{\gamma}}(\mathbf{w}) := \prod_{k \in \mathcal{N}(\boldsymbol{\gamma})} \prod_{i=1}^{\gamma_k} g_k(\mathbf{w}_{k,i}), \quad \boldsymbol{\gamma} \in \mathcal{M}. \tag{2.11}$$

Formally the gain and the loss operators are defined by

$$P_k(\mathbf{g})(\mathbf{v}) = \sum_{\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M}} \alpha_k \int_{\mathbb{R}^{3|\boldsymbol{\beta}|} \times \mathbb{R}^{3|\boldsymbol{\alpha}|}} \sigma_{\boldsymbol{\beta}, \boldsymbol{\alpha}, k}(\mathbf{u}, \mathbf{w}, \mathbf{v}) \mathbf{g}_{\boldsymbol{\beta}}(\mathbf{u}) \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{w}, \tag{2.12}$$

and

$$S_k(\mathbf{g})(\mathbf{v}) = \sum_{\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M}} \alpha_k \int_{\mathbb{R}^{3|\boldsymbol{\beta}|} \times \mathbb{R}^{3|\boldsymbol{\alpha}|}} \sigma_{\boldsymbol{\alpha}, \boldsymbol{\beta}, k}(\mathbf{w}, \mathbf{u}, \mathbf{v}) \mathbf{g}_{\boldsymbol{\alpha}}(\mathbf{w}) \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{w}. \tag{2.13}$$

Here, for each $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$ and $k = 1, \dots, N$,

$$\begin{aligned} &\sigma_{\boldsymbol{\alpha}, \boldsymbol{\beta}, k}(\mathbf{w}, \mathbf{u}, \mathbf{v}) := K_{\boldsymbol{\alpha}, \boldsymbol{\beta}}(\mathbf{w}, \mathbf{u}) \cdot \\ &\delta(\mathbf{w}_{k, \alpha_k} - \mathbf{v}) \cdot \delta(V_{\boldsymbol{\beta}}(\mathbf{u}) - V_{\boldsymbol{\alpha}}(\mathbf{w})) \cdot \delta(W_{\boldsymbol{\beta}}(\mathbf{u}) - W_{\boldsymbol{\alpha}}(\mathbf{w})), \end{aligned} \tag{2.14}$$

where $K_{\boldsymbol{\alpha}, \boldsymbol{\beta}} : \mathbb{R}^{3|\boldsymbol{\alpha}|} \times \mathbb{R}^{3|\boldsymbol{\beta}|} \to \mathbb{R}_+$ are given functions related to the probability of the reaction $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$. The following general properties are assumed:

1^o $K_{\boldsymbol{\alpha}, \boldsymbol{\beta}} \equiv 0$ if $|\boldsymbol{\alpha}| < 0$, or $|\boldsymbol{\beta}| < 0$.

2^o $K_{\boldsymbol{\alpha}, \boldsymbol{\beta}} \equiv 0$ when the probability of the collision $(\boldsymbol{\alpha}, \boldsymbol{\beta})$ is zero.

3^o $K_{\boldsymbol{\alpha}, \boldsymbol{\beta}} \equiv 0$ if for some $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$, the condition (2.6) does not hold.

4^o $K_{\boldsymbol{\alpha}, \boldsymbol{\beta}}(\mathbf{w}, \mathbf{u})$ is invariant at the permutation of the components $\mathbf{w}_{n,1}, \dots, \mathbf{w}_{n, \alpha_n}$ of $\mathbf{w}$ for each fixed $\mathbf{u} \in \mathbb{R}^{3|\boldsymbol{\alpha}|}$, $\mathbf{w} \in \mathbb{R}^{3|\boldsymbol{\beta}|}$ and $n \in \mathcal{N}(\boldsymbol{\alpha})$; a similar

statement holds for the components of $\mathbf{u}$. (This condition expresses the "indistinguishability" of identical collision partners.)

5^o For all $\mathbf{a} \in \mathbb{R}^3$ $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$,

$$K_{\alpha,\beta}(T(\mathbf{a})\mathbf{w}, T(\mathbf{a})\mathbf{u}) \equiv K_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{w}, \mathbf{u}), \tag{2.15}$$

where $T(\mathbf{a})\mathbf{w}$ is defined on components by $(T(\mathbf{a})\mathbf{w})_{k,i} = \mathbf{w}_{k,i} + \mathbf{a}$ for $k \in \mathcal{N}(\boldsymbol{\alpha})$ and $i = 1, \ldots, \alpha_k$.

6^o There exist some given constants $C_1, \ldots, C_N > 0$, such that

$$C^{\boldsymbol{\beta}} K_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{w}, \mathbf{u}) \equiv C^{\boldsymbol{\alpha}} K_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{u}, \mathbf{w}). \tag{2.16}$$

are verified for all $(\mathbf{w}, \mathbf{u}) \in \mathbb{R}^{3|\boldsymbol{\alpha}|} \times \mathbb{R}^{3|\boldsymbol{\beta}|}$ and $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{M} \times \mathcal{M}$, where

$$C^{\boldsymbol{\gamma}} := C_1^{\gamma_1} \cdot \ldots \cdot C_N^{\gamma_N}, \tag{2.17}$$

for all $\boldsymbol{\gamma} \in \mathcal{M}$.

Note that assumption 1^o excludes the "spontaneous dissociation" as well as the "total fussion". The condition 3^o refers to the microscopic conservation of the mass. The form of $\sigma_{\boldsymbol{\alpha},\boldsymbol{\beta},k}$ in (2.14) takes into account the microscopic conservation laws of the total energy and momentum. The explicit use of only one variable, $\mathbf{w}_{k,\alpha_k}$ in $\delta(\mathbf{w}_{k,\alpha_k} - \mathbf{v})$, is possible due to "indistinguishability" of identical collision partners (condition 4^o). Assumption 5^o expresses the absence of the external fields. The generalization of the classical collision reversibility is given by the condition 6^o.

As announced before, we refer only to the space-homogeneous version of (2.10), i.e.

$$\partial_t f_k = P_k(\mathbf{f}) - S_k(\mathbf{f}), \qquad k = 1, \ldots, N. \tag{2.18}$$

Several properties (also valid in the space-inhomogeneous case [17, 18]) can be formally established as for the Ludwig and Heil equations [25], and rigorously proved by giving a meaning to (2.18) and finding classes of solutions with convenient regularity properties. Thus, formally,

$$\sum_{k=1}^{N} \int_{\mathbb{R}^3} \Phi_k^i(\mathbf{v}) \left[P_k(\mathbf{f})(\mathbf{v}) - S_k(\mathbf{f})(\mathbf{v})\right] \mathrm{d}\mathbf{v} = 0, \quad i = 0, \ldots, 4, \tag{2.19}$$

provided that all integrals involved are convergent, where $\Phi_n^0(\mathbf{v}) := m_n$, $\Phi_n^i(\mathbf{v}) = m_n v_i$, for the component v_i, $i = 1, 2, 3$, of $\mathbf{v}$, and $\Phi_n^4(\mathbf{v}) := m_n \mathbf{v}^2/2 + E_n$. By (2.19) the solutions of (2.18) are formally compatible

with the conservation of the mass ($i = 0$), bulk momentum ($i = 1, 2, 3$) and energy ($i = 4$), respectively.

One can define the H-function

$$H(\mathbf{f})(t) = \sum_{k=1}^{N} \int_{\mathbb{R}^3} \left[\log C_k f_k(t, \mathbf{v}) - 1\right] f_k(t, \mathbf{v}) \mathrm{d}\mathbf{v}, \tag{2.20}$$

for those solutions $\mathbf{f}(t, \mathbf{v})$ of (2.18), with positive components, provided that the integrals exist. In (2.20) the constants C_k are the same to the constants from the assumption 6^o. Formally, by a few algebraic manipulations, one obtains

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} H(\mathbf{f})(t) &= \sum_{k=1}^{N} \int_{\mathbb{R}^3} \left[P_k(\mathbf{f})(t, \mathbf{v}) - S_k(\mathbf{f})(t, \mathbf{v})\right] \log C_k f_k(t, \mathbf{v}) \mathrm{d}\mathbf{v} = \\ &= \sum_{\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M}} \int_{\mathbb{R}^{3|\boldsymbol{\beta}|} \times \mathbb{R}^{3|\boldsymbol{\alpha}|}} K_{\boldsymbol{\beta}, \boldsymbol{\alpha}}(\mathbf{u}, \mathbf{w}) \mathbf{f}_{\boldsymbol{\beta}}(t, \mathbf{u}) F\left[\frac{C^{\boldsymbol{\alpha}} \mathbf{f}_{\boldsymbol{\alpha}}(t, \mathbf{w})}{C^{\boldsymbol{\beta}} \mathbf{f}_{\boldsymbol{\beta}}(t, \mathbf{u})}\right] \mathrm{d}\mathbf{u}\mathrm{d}\mathbf{w} \leq 0, \end{aligned} \tag{2.21}$$

where $F(x) := \frac{1}{2}(1 - x) \log x \leq 0$ for $x \geq 0$.

The equilibrium solutions of (2.18) are Maxwellian (Gaussian) functions with determining constants (concentration, bulk velocity and temperature) related to the internal energies E_n and the constants C_n of (2.16), by the law of the mass action (for more details see e.g. Ref. [25, 17]).

We distinguish the following particular cases:

1. If $M = 3$ in (2.10-2.13), and the conditions of (2.16) are verified, then (2.10) essentially reduces to the Ludwig and Heil system of equations with discrete internal energies.

2. If $M = 2$ and the conditions of (2.16) are fulfilled with $C_1 = C_2 = 1$, then we obtain the Wang-Chang-Uhlenbeck-de Boer system of equations.

3. If $M = 2$, $N = 1$, the condition (2.16) are fulfilled and the transition functions depend only on the relative velocities of the encounters in each collision channel, then one gets the classical Boltzmann equation.

In order to introduce the numerical scheme associated to the equations (2.18), in the next section we solve a Cauchy problem for (2.18) formulated in a product of $\mathbb{L}^1$ spaces. Besides the uniqueness and global existence of the

solution, we also need the positivity of the solution and the macroscopic mass conservation. Note that, other conservation properties, as well as the existence of a H-theorem play no role in this numerical scheme. In particular, property (2.16) is not needed. However, we will state without proof a general result concerning the conservation relations and a H-theorem (only for the sake of completeness).

Roughly speaking, we would like to approximate the measures $d\mu_k^t(\mathbf{v}) := f_k(t,\mathbf{v})d\mathbf{v}$ induced by the solutions $f_k(t,\mathbf{v})$ of (2.18), $k = 1,\dots,N$, by convenient homogeneous sums of point measures, defined as follows.

Let μ be a finite positive measure on $\mathbb{R}^m$. For $a_n > 0$, where $n \in \mathbb{N}^* := \{1,2,\dots\}$, let

$$\sigma_n = \frac{a_n}{n}\sum_{i=1}^{n}\delta_{x_{i,n}}, \quad n \in \mathbb{N}^*. \tag{2.22}$$

Here $\delta_{x_{i,n}}$ is the Dirac measure on $\mathbb{R}^m$ concentrated at point $x_{i,n}$ for $i = 1,\dots,n$. The sequence of measures $(\sigma_n)_{n\in\mathbb{N}^*}$ is called a *homogeneous sum of point measures* (HSPM) approximating the measure μ, if it converges weakly to μ (in the weak sens of the measures) i.e. $\sigma_n \rightharpoonup \mu$ as $n \to \infty$.

We call a sequence $(\sigma_n)_{n\in\mathbb{N}^*}$ of the form

$$\sigma_n = \sum_{i=1}^{n}\frac{a_{i,n}}{n}\delta_{x_{i,n}}, \quad n \in \mathbb{N}^*, \tag{2.23}$$

(where $a_{i,n} > 0$ for $i \in \{1,\dots,n\}$ and $n \in \mathbb{N}^*$) a *weighted sum of point measures* (WSPM) approximating the measure μ, if it converges weakly to μ, i.e. $\sigma_n \rightharpoonup \mu$ as $n \to \infty$. Obviously, if $a_{i,n} = a_{j,n}$ for $i,j \in \{1,\dots,n\}$ and $n \in \mathbb{N}^*$, the WSPM approximation becomes a HSPM approximation.

The HSPM approximation is convenient for numerical solving of equations where the solutions are finite (probability) measures on $\mathbb{R}^m$, and where one also wishes to approximate moments of some (random) variables with respect to solutions. In this case, the control of the approximation can be made by means of the Koksma-Hlavka inequality Ref. [23], in terms of discrepancy.

We recall that, by definition Ref. [5, 15, 23], the discrepancy between the nonnegative measures μ and ν on $\mathbb{R}^m$ is given by the following formula,

$$D(\mu,\nu) := \sup_{\mathbf{a}\in\mathbb{R}^m}\left|\mu(\Lambda(\mathbf{a})) - \nu(\Lambda(\mathbf{a}))\right|, \tag{2.24}$$

where $\Lambda(\mathbf{a}) := \{\mathbf{x} \in \mathbb{R}^m \,|\, x_l \le a_l,\ l = 1,\dots,m\}$.

We also recall, Ref. [5], that a sequence of measures μ_n is said to converge to μ with respect to discrepancy if, $D(\mu_n, \mu) \to 0$ as $n \to \infty$.

It is known, Ref. [5], that if μ is a measure absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^m$, then the convergence of μ_n to μ with respect to discrepancy is equivalent to the weak convergence in the sense of measures.

Starting with HSPM approximation for each μ_k^0 induced by the initial data in (2.18), with $k = 1, \ldots, N$, our purpose is to provide a convergent algorithm generating HSPM approximations for the measures μ_k^t, where $k = 1, \ldots, N$, at any $t > 0$.

In this respect, one chooses some fixed timestep $\Delta t < T$. Let

$$T_\Delta := \left[\left[\frac{T}{\Delta t}\right]\right], \tag{2.25}$$

where $[[x]]$ denotes the integer part of $x \in \mathbb{R}$. One associates a time-discretized version of equations to (2.18). Starting with an initial data, $f_k^0 = f_k^0(\mathbf{v})$, $k = 1, \ldots, N$, one obtains a family of functions $f_k^j(\mathbf{v})$, $j = 1, \ldots, T_\Delta$ verifying the discretized form of (2.18). The discretized version of (2.18) can be formulated in the weak form for the measures $d\bar{\mu}_k^j(\mathbf{v}) := f_k^j(\mathbf{v})d\mathbf{v}$, where $k = 1, \ldots, N$. We shall prove that if, each $\bar{\mu}_k^0$ is close, to μ_k^0, in some sense, then (for Δt sufficiently small), $\bar{\mu}_k^j$ is close to μ_k^t on the interval $((j-1)\Delta t, j\Delta t]$, with an error of order Δt, for all $j = 1, \ldots, T_\Delta$ and $k = 1, \ldots, N$.

The scheme is initialized for $k = 1, \ldots, N$ by approximating for the measures $\bar{\mu}_k^0$ by a HSPM approximation of the form:

$$\mu_{k,n}^0 := \frac{a_{k,n}}{n} \sum_{i=1}^{n} \delta_{\mathbf{v}_{k,n}} \rightharpoonup \bar{\mu}_k^0, \quad \text{as } n \to \infty. \tag{2.26}$$

The above approximation provides for all $j = 1, \ldots, T_\Delta$ and $k = 1, \ldots, N$ approximations by discrete measures $\mu_{k,n}^j \rightharpoonup \bar{\mu}_k^j$ as $n \to \infty$.

Because of the nonlinearity of the initial problem, each step of the iteration produces a power-like growing number of terms in the sums of point measures expressing $\mu_{k,n}^j$. In computations, the numerical effort would also be power-like increasing, so that the algorithm could not be effective at this level.

To approximate $\bar{\mu}_k^j$ by sums of Dirac measures with a non-increasing number of terms, for technical reasons, it is necessary to have a HSPM approximation. However, in general, $\mu_{k,n}^j$ appears as a WSPM of the form (2.23). For this reason we introduce a *homogenization procedure* of approximation to obtain measures of the form (2.22). At this level, one can reduce the numerical

effort by using probabilistic techniques of selection. Then, the convergence of the numerical scheme is proved in probabilistic terms.

3. The Existence of the Solution

Define the space $\mathbb{X} := \underbrace{\mathbb{L}^1(\mathbb{R}^3) \times \ldots \times \mathbb{L}^1(\mathbb{R}^3)}_{N \text{ times}}$ — *real*, equipped with the norm

$$\|\mathbf{g}\|_{\mathbb{X}} := \sum_{k=1}^{N} m_k \|g_k\|_{\mathbb{L}^1}, \tag{3.1}$$

where $\mathbf{g} = (g_1, \ldots, g_N)$ and $g_k \in \mathbb{L}^1(\mathbb{R}^3)$, $k = 1, \ldots, N$. We recall that $m_k > 0$ denotes the mass of a particle of species k for each $k = 1, \ldots, N$.

Note that if $\mathbf{g} \geq 0$ (i.e. $g_k \geq 0$ a.e. for all $k = 1, \ldots, N$) then the norm $\|g\|_{\mathbb{X}}$ is equal to the mass of the gas in the state described by the distribution functions given by the components of $\mathbf{g}$.

For approximation purposes, we suppose that the functions of the family $\{K_{\boldsymbol{\alpha},\boldsymbol{\beta}}\}_{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}}$ are *continuous*. We formulate the Cauchy problem for (2.18) in the space $\mathbb{X}$.

Before, we must give a meaning to the collision operators P_k and S_k as operators acting in the space $\mathbb{X}$. This can be performed, using regularization as in Ref. [16, 17] to define $\sigma_{\boldsymbol{\alpha},\boldsymbol{\beta},k}$ as distributions for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M} \times \mathcal{M}$ and $k = 1, \ldots, N$.

For $m \in \mathbb{N}^*$ denote by $C_b(\mathbb{R}^m)$ the space of the bounded functions of $C(\mathbb{R}^m; \mathbb{R})$, endowed with the usual sup norm. Let $C_c(\mathbb{R}^m)$ be the subset of the functions of $C_b(\mathbb{R}^m)$ with compact support.

Let $J \in C_c(\mathbb{R})$ be positive and even function, such that $\text{supp}(J) = [-1, 1]$ and $\|J\|_{\mathbb{L}^1} = 1$. For $\varepsilon > 0$ denote by $\delta_\varepsilon(t) =: \varepsilon^{-1} J(\varepsilon^{-1} \cdot t)$ and $\delta_\varepsilon^3(y) := \delta_\varepsilon(y_1) \cdot \delta_\varepsilon(y_2) \cdot \delta_\varepsilon(y_3)$, where $y = (y_1, y_2, y_3) \in \mathbb{R}^3$. Define

$$\sigma^{\varepsilon,\eta}_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{u}, \mathbf{w}) := K_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{w}, \mathbf{u}) \delta_\varepsilon^3(V_{\boldsymbol{\beta}}(\mathbf{u}) - V_{\boldsymbol{\alpha}}(\mathbf{w})) \delta_\eta(W_{\boldsymbol{\beta}}(\mathbf{u})) - W_{\boldsymbol{\alpha}}(\mathbf{w})), \tag{3.2}$$

$$P_{k\varepsilon\eta}(\mathbf{g})(\mathbf{v}) := \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}} \boldsymbol{\alpha}_k \left[\int_{\mathbb{R}^{3|\boldsymbol{\beta}|} \times \mathbb{R}^{3|\boldsymbol{\alpha}|-3}} \sigma^{\varepsilon,\eta}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{u}, \mathbf{w}) \mathbf{g}_{\boldsymbol{\beta}}(\mathbf{u}) \mathrm{d}\mathbf{u} \mathrm{d}\tilde{\mathbf{w}}_k \right]_{\mathbf{w}_{k,\alpha_k} = \mathbf{v}} \tag{3.3}$$

and

$$S_{k\varepsilon\eta}(\mathbf{g})(\mathbf{v}) := \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}} \alpha_k \left[\int_{\mathbb{R}^{3|\boldsymbol{\beta}|}\times\mathbb{R}^{3|\boldsymbol{\alpha}|-3}} \sigma^{\varepsilon,\eta}_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{w},\mathbf{u})\mathbf{g}_{\boldsymbol{\alpha}}(\mathbf{w})\mathrm{d}\mathbf{u}\mathrm{d}\tilde{\mathbf{w}}_k\right]_{\mathbf{w}_{k,\alpha_k}=\mathbf{v}}, \tag{3.4}$$

with $\mathbf{g}_{\boldsymbol{\alpha}}$ and $\mathbf{g}_{\boldsymbol{\beta}}$ as in (2.11), for all $\mathbf{g}\in C_c(\mathbb{R}^3)^N := \underbrace{C_c(\mathbb{R}^3)\times\ldots\times C_c(\mathbb{R}^3)}_{N \text{ times}}$; $\mathbf{v}\in\mathbb{R}^3$, $k\in 1,\ldots,N$. In (3.3) and (3.4), the terms with $\alpha_k = 0$, vanish, by definition, and $d\tilde{\mathbf{w}}_k$ is the Euclidean element of area on the manifold $\left\{\mathbf{w}\in\mathbb{R}^{3|\boldsymbol{\alpha}|} | \mathbf{w}_{k,\alpha_k} = \mathbf{v}\right\}$.

Let $\boldsymbol{\Omega}_{\boldsymbol{\gamma}}$ be the unit sphere in $\mathbb{R}^{3|\boldsymbol{\gamma}|-3}$, where $\boldsymbol{\gamma}\in\mathcal{M}$. The operators P_k and S_k can be defined by means of the following result.

LEMMA **3.1** *For each $\mathbf{g}\in C_c^N(\mathbb{R}^3)$, there exist the limits*

$$\dot{P}_k(\mathbf{g})(\mathbf{v}) := \lim_{\eta\to 0}\lim_{\varepsilon\to 0} P_{k\varepsilon\eta}(\mathbf{g})(\mathbf{v}), \qquad \dot{S}_k(\mathbf{g})(\mathbf{v}) := \lim_{\eta\to 0}\lim_{\varepsilon\to 0} S_{k\varepsilon\eta}(\mathbf{g})(\mathbf{v}). \tag{3.5}$$

There are the families of functions $\{r_{\boldsymbol{\beta},\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}}$, $\{p_{\boldsymbol{\beta},\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}} \subset C(\mathbb{R}^{3|\boldsymbol{\alpha}|}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}};\mathbb{R}_+)$ and $\{\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}} \subset C(\mathbb{R}^{3|\boldsymbol{\alpha}|}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}};\mathbb{R}^{3|\boldsymbol{\beta}|})$ such that

$$\dot{P}_k(\mathbf{g})(\mathbf{v}) = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}} \alpha_k \left[\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|-3}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}}} p_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})\mathbf{g}_{\boldsymbol{\beta}}(\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}))\mathrm{d}\tilde{\mathbf{w}}_k\mathrm{d}\mathbf{n}\right]_{\mathbf{w}_{k,\alpha_k}=\mathbf{v}}, \tag{3.6}$$

$$\dot{S}_k(\mathbf{g})(\mathbf{v}) = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}} \alpha_k \left[\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|-3}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}}} r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})\mathbf{g}_{\boldsymbol{\alpha}}(\mathbf{w})\mathrm{d}\tilde{\mathbf{w}}_k\mathrm{d}\mathbf{n}\right]_{\mathbf{w}_{k,\alpha_k}=\mathbf{v}}, \tag{3.7}$$

for all $\mathbf{g}\in C_c^N(\mathbb{R}^3)$, and the following properties are verified:

i) *there are some constants $c,d>0$ such that $|\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})| \geq c|\mathbf{w}|$ for all $|\mathbf{w}|\geq d$ and $\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}$.*

ii) *if $W_{\boldsymbol{\alpha}}(\mathbf{w}) - 2^{-1}(\sum_{n=1}^N \alpha_n m_n)V_{\boldsymbol{\alpha}}(\mathbf{w})^2 - \sum_{n=1}^N \beta_n E_n \leq 0$ for some $\mathbf{w}\in\mathbb{R}^{3|\boldsymbol{\alpha}|}$, then*

$$r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}) = p_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}) = 0, \quad \text{for all } \mathbf{n}\in\boldsymbol{\Omega}_{\boldsymbol{\beta}} \text{ and } \boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}. \tag{3.8}$$

iii) *for each $\varphi\in C(\mathbb{R}^{3|\boldsymbol{\alpha}|})$ and $f\in C_c(\mathbb{R}^{3|\boldsymbol{\beta}|})$ and $\forall\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}$*

$$\begin{aligned}&\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}}} \varphi(\mathbf{w})\cdot p_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})\cdot\mathbf{f}(\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}))\mathrm{d}\mathbf{w}\mathrm{d}\mathbf{n} = \\ &= \int_{\mathbb{R}^{3|\boldsymbol{\beta}|}\times\boldsymbol{\Omega}_{\boldsymbol{\alpha}}} \varphi(\mathbf{u}_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{u},\mathbf{n}))\cdot r_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{u},\mathbf{n})\cdot\mathbf{f}(\mathbf{u})\mathrm{d}\mathbf{u}\mathrm{d}\mathbf{n}.\end{aligned} \tag{3.9}$$

The results of the above Lemma were obtained in Ref. [17]. However, for the sake of completeness, the proof is outlined in Appendix[2].

Property (3.8) follows by the presence of reaction thresholds (in the frame of the conservation relations (2.6) and (2.7)). Moreover, (3.6) and (3.7) are well defined, because of property i) in Lemma 3.1.

From (3.7), we can write

$$\dot{S}_k(\mathbf{g})(\mathbf{v}) = \dot{R}_k(\mathbf{g})(\mathbf{v})g_k(\mathbf{v}), \tag{3.10}$$

where

$$\begin{aligned} &\dot{R}_k(\mathbf{g})(\mathbf{v}) := \\ &:= \sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}} \boldsymbol{\alpha}_k \left[\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|-3}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}}} r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})\mathbf{g}_{\boldsymbol{\gamma};k}(\mathbf{w}_{s,i})\mathrm{d}\tilde{\mathbf{w}}_k\mathrm{d}\mathbf{n} \right]_{\mathbf{w}_{k,\alpha_k}=\mathbf{v}} . \end{aligned} \tag{3.11}$$

In (3.11), for $\boldsymbol{\gamma}\in\mathcal{N}(\boldsymbol{\gamma})$ we assumed the convention

$$\mathbf{g}_{\boldsymbol{\gamma};k}(\mathbf{w}) := \mathbf{g}_{\boldsymbol{\gamma}}(\mathbf{w})/g_k(\mathbf{w}_{k,\alpha_k}), \tag{3.12}$$

where the r.h.s. makes sense and $\mathbf{g}_{\boldsymbol{\gamma};k}(\mathbf{w}) := 0$ otherwise.

Our results are based on the following

Assumption

There is a constant $K > 0$, such that

$$\int_{\boldsymbol{\Omega}_{\boldsymbol{\beta}}} r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})\mathrm{d}\mathbf{n} < K, \tag{3.13}$$

for all $\mathbf{w}\in\mathbb{R}^{3|\boldsymbol{\alpha}|}$ and $\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}$.

From (3.13), it is immediate that the maps

$$\begin{aligned} &\mathbb{X}\supset C_c(\mathbb{R}^3)^N \ni \mathbf{g}\to \dot{S}_k(\mathbf{g})\in\mathbb{L}^1(\mathbb{R}^3), \\ &\mathbb{X}\supset C_c(\mathbb{R}^3)^N \ni \mathbf{g}\to \dot{R}_k(\mathbf{g})\in C_b(\mathbb{R}^3) \end{aligned} \tag{3.14}$$

are continuous for each $k = 1,\ldots,N$. Moreover, using property (3.9) (with $\varphi = 1$, $f = \mathbf{g}_{\boldsymbol{\beta}}$) combined with Fubini's theorem, it also follows that the map

$$\mathbb{X}\supset C_c(\mathbb{R}^3)^N \ni \mathbf{g}\to \dot{P}_k(\mathbf{g})\in\mathbb{L}^1(\mathbb{R}^3) \tag{3.15}$$

[2]Note that the functions $r_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ and $p_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ appear in explicit form in the proof of Lemma 3.1 (see the Appendix).

is continuous for each $k = 1, \ldots, N$.

Since $C_c(\mathbb{R}^3)^N$ is dense in $\mathbb{X}$, the maps given by (3.14-3.15) have continuous extensions to $\mathbb{X}$. These extensions will be also denoted S_k, R_k and P_k, respectively.

Note that (3.10) can be extended to all $\mathbf{g} \in \mathbb{X}$, in the sense that a.e.,

$$S_k(\mathbf{g})(\mathbf{v}) = R_k(\mathbf{g})(\mathbf{v}) g_k(\mathbf{v}), \tag{3.16}$$

for all $k = 1, \ldots, N$.

Define $\mathbf{P}, \mathbf{S} : \mathbb{X} \to \mathbb{X}$ by

$$\begin{aligned} \mathbf{P}(\mathbf{g}) &= (P_1(\mathbf{g}), \ldots, P_N(\mathbf{g})), \\ \mathbf{S}(\mathbf{g}) &= (S_1(\mathbf{g}), \ldots, S_N(\mathbf{g})), \end{aligned} \tag{3.17}$$

for all $\mathbf{g} \in \mathbb{X}$.

We consider the Cauchy problem for equation (2.18) in $\mathbb{X}$.

$$d_t f(\mathbf{f}) = \mathbf{P}(\mathbf{f}(t)) - \mathbf{S}(\mathbf{f}(t)), \quad \mathbf{f}(0) = \mathbf{f}_0. \tag{3.18}$$

THEOREM **3.1** *Let $\mathbf{f}_0 > 0$. For each $T > 0$, equation (3.18) has a unique solution $\mathbf{f}(t)$ in $\mathbb{X}$ on $[0, T]$. Moreover, for all $t \in [0, T]$ one has $\mathbf{f}(t) > 0$ and*

$$\sum_{k=1}^{N} m_k \int_{\mathbb{R}^3} f_k(t, \mathbf{v}) \mathrm{d}\mathbf{v} = \sum_{k=1}^{N} m_k \int_{\mathbb{R}^3} f_{0,k}(\mathbf{v}) \mathrm{d}\mathbf{v}. \tag{3.19}$$

Proof. One applies the Banach fixed point theorem to (3.18) written in convenient form.

Consider the cone $C_T^+ := \{\mathbf{f} \in C(0, T; \mathbb{X}) | \mathbf{f}(t) \geq 0, \text{for all } t \in [0, T]\}$ with the norm

$$\|\mathbf{f}\| := \sup_{t \in [0,T]} \|\mathbf{f}(t)\|_{\mathbb{X}}. \tag{3.20}$$

Observe that for all $k = 1, \ldots, N$, if $\mathbf{f} \in C_T^+$ then $R_k(\mathbf{f}), P_k(\mathbf{f}) \geq 0$ (since $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}$, $p_{\boldsymbol{\beta},\boldsymbol{\alpha}} \geq 0$, for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M}$). Moreover, if $\mathbf{f} \in C_T^+$, then $R_k(\mathbf{f}) \in C(0, T; C_b(\mathbb{R}^3))$. Consequently the Riemann integral $\int_s^t R_k(\mathbf{f}(\tau)) \mathrm{d}\tau$ is well defined in $C_b(\mathbb{R}^3)$ for all $s, t \in [0, T]$ and $k \in \{1, \ldots, N\}$.

Let $\mathbf{f} \in C_T^+$. We define the map $[0, T] \ni t \to \mathbf{I}(\mathbf{f})(t) \in \mathbb{X}$ by the components of $\mathbf{I}(\mathbf{f})(t)$, as:

$$I_k(\mathbf{f})(t) = \exp\left[-\int_0^t R_k(\mathbf{f}(\tau))\mathrm{d}\tau\right]\cdot \mathbf{f}_{0,k}+ \\ +\int_0^t \exp\left[-\int_s^t R_k(\mathbf{f}(\tau))\mathrm{d}\tau\right]\cdot P_k(\mathbf{f}(s))\mathrm{d}s, \tag{3.21}$$

where $t\in[0,T]$. Here, the integration with respect to ds is in the sense of Riemann in $\mathbb{L}^1(\mathbb{R}^3)$.

Obviously $I_k(\mathbf{f})(t)\geq 0$ for all $t\in[0,T]$, $k=1,\ldots,N$.

The problem (3.18) can be rewritten in C_T^+, as it follows.

$$\mathbf{f}=\mathbf{I}(\mathbf{f}) \tag{3.22}$$

Let $R>\|\mathbf{f}_0\|_{\mathbb{X}}$. Define

$$\mathcal{B}(R):=\left\{\mathbf{f}\in C_T^+ \,|\, \|\mathbf{f}\|\leq R, \quad \mathbf{f}\,(0)=\mathbf{f}_0\right\}. \tag{3.23}$$

Using (3.11), (3.6) and (3.13), one can find some positive numbers $k_1(R)$ and $k_2(R)$, such that

$$\|\mathbf{I}(\mathbf{f})\|\leq \|\mathbf{f}_0\|_{\mathbb{X}}+T\cdot k_1(R), \tag{3.24}$$

and

$$\|\mathbf{I}(\mathbf{f})-\mathbf{I}(\mathbf{h})\|\leq T\cdot k_2(R)\cdot\|\mathbf{f}-\mathbf{h}\|, \tag{3.25}$$

for all $\mathbf{f},\mathbf{h}\in\mathcal{B}(R)$. Obviously, from (3.24) and (3.25), for T small enough, the map $\mathbf{I}$ becomes a strict contraction on $\mathcal{B}(R)$. Consequently $\mathbf{I}:\mathcal{B}(R)\to\mathcal{B}(R)$ and has a unique fixed point. This proves that (3.18) has a unique positive solution on $[0,T]$.

The positivity of f_k, implies that

$$\|\mathbf{f}(t)\|_{\mathbb{X}}=\sum_{k=1}^N m_k\int_{\mathbb{R}^3} f_k(t,\mathbf{v})\mathrm{d}\mathbf{v}, 0\leq t\leq T. \tag{3.26}$$

By (3.18) and using (2.6), (3.11), (3.6) and (3.9) (applied to $\varphi\equiv 1$) one obtains

$$d_t\|\mathbf{f}(t)\|_{\mathbb{X}}=\sum_{k=1}^N m_k\int_{\mathbb{R}^3}\left[P_k(\mathbf{f})-S_k(\mathbf{f})\right]\mathrm{d}\mathbf{v}=0, \tag{3.27}$$

which proves (3.19). Moreover,

$$\|\mathbf{f}\|=\sup_{0\leq t\leq T}\|\mathbf{f}(t)\|_{\mathbb{X}}=\|\mathbf{f}_0\|_{\mathbb{X}}. \tag{3.28}$$

By continuation, and uniqueness, the local solution $\mathbf{f}(t)$ can be made time-global. This ends the proof. □

For the sake of completeness we state the following result.

Let Φ_n^i be as in (2.19) for $i = 1, \ldots, 4$. With the remark that the mass conservation (3.19) has been already proved, the solution of (3.18) has the following properties.

PROPOSITION **3.1** *Let* $\mathbf{f}(t)$ *be the solution of* (3.18) *given by Theorem* 3.1.

a) *If*

$$f_{0,k},\ (1+\mathbf{v}^2)f_{0,k} \in \mathbb{L}^1(\mathbb{R}^3) \tag{3.29}$$

for each $k = 1, \ldots, N$, *then*

$$(1+\mathbf{v}^2)f_k(t) \in \mathbb{L}^1(\mathbb{R}^3) \tag{3.30}$$

and

$$\sum_{n=1}^{N} \int_{\mathbb{R}^3} \Phi_n^i(\mathbf{v}) f_n(t,\mathbf{v}) \mathrm{d}\mathbf{v} = \sum_{n=1}^{N} \int_{\mathbb{R}^3} \Phi_n^i(\mathbf{v}) f_{0,n}(\mathbf{v}) d\mathbf{v} = 0, \tag{3.31}$$

for each $k = 1, \ldots, N$ *and* $i = 1, \ldots, 4$ *and all* $t \geq 0$.

b) *In addition to the conditions (3.29), suppose that there are some constants* $C_1, \ldots, C_N > 0$ *such that conditions (2.16) hold. If*

$$f_{0,k} \log f_{0,k} \in \mathbb{L}^1(\mathbb{R}^3) \tag{3.32}$$

for each $k = 1, \ldots, N$, *then*

$$f_k(t) \log f_k(t) \in \mathbb{L}^1(\mathbb{R}^3; \mathrm{d}\mathbf{v}) \tag{3.33}$$

and

$$H(\mathbf{f})(t) := \sum_{n=1}^{N} \int_{\mathbb{R}^3} \left[\log C_n f_n(t,\mathbf{v}) - 1\right] f_n(t,\mathbf{v}) \mathrm{d}\mathbf{v} \tag{3.34}$$

is non-increasing as a function of t, *for each* $k = 1, \ldots, N$ *and all* $t \geq 0$.

The proof of this proposition is beyond the present purposes. Though, we mention that the proof uses Lemma 3.1 and the ideas introduced by of Arkeryd [2, 3] to prove results of the same nature in the case of the classical space-homogeneous Boltzmann equation.

4. Time Discretization

Let $\Delta t \in (0,T)$ be a fixed timestep. We consider the following discretized version of (3.18).

$$\begin{aligned} &\mathbf{f}^j = \mathbf{f}^{j-1} + \Delta t \cdot \left[\mathbf{P}(\mathbf{f}^{j-1}) - \mathbf{S}(\mathbf{f}^{j-1})\right], \\ &\mathbf{f}^0 = \mathbf{f}_0 \geq 0, \ a.e., \quad j = 1, \ldots, T_\Delta, \end{aligned} \tag{4.1}$$

where $\mathbf{f}^j = (f_1^j, \ldots, f_N^j)$ and $f_k^j = f_k^j(\mathbf{v})$.

The discretized scheme (4.1) may destroy the positivity of the functions $\mathbf{f}^j$ for $j \geq 1$. However, one can prove that for Δt small enough, $\mathbf{f}^j$ is positive and close, in some sense, to the solution $\mathbf{f}$ provided by Theorem 3.1.

PROPOSITION **4.1**

a) *If Δt is sufficiently small, then $\mathbf{f}^j \geq 0$ for all $j = 1, \ldots, T_\Delta$. Moreover,*

$$\left\|\mathbf{f}^j\right\| = \left\|\mathbf{f}_0\right\|, \tag{4.2}$$

for all $j = 1, \ldots, T_\Delta$.

b) *There exists some number $C = C(\|\mathbf{f}_0\|_{\mathbb{X}}) > 0$, depending only on $\|\mathbf{f}_0\|_{\mathbb{X}}$, such that*

$$\left\|\mathbf{f}(t) - \mathbf{f}^j\right\|_{\mathbb{X}} \leq C \cdot \Delta t, \tag{4.3}$$

for all $j = 1, \ldots, T_\Delta$ and $t \in ((j-1)\Delta t, j\Delta t]$.

Proof. a) First we write (4.1) more conveniently.

Let

$$\mathcal{U} := \{\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_N) \,|\gamma_k \in \{0, 1, \ldots, NM\}, |\boldsymbol{\gamma}| \geq 2\}. \tag{4.4}$$

For any $\boldsymbol{\xi} = (\xi_1, ..., \xi_N) \in \mathbb{R}^N$ for $k = 1, ..., N$ and $\boldsymbol{\alpha} \in \mathcal{M}$, denote

$$\boldsymbol{\xi}_{\boldsymbol{\alpha},k} := \begin{cases} \dfrac{1}{\xi_k} \displaystyle\prod_{n \in \mathcal{N}(\boldsymbol{\alpha})} \xi_n^{\alpha_n} & \text{if } \alpha_k \geq 1 \text{ and } \xi_k \neq 0, \\ \\ 0 & \text{if } \alpha_k = 0 \text{ or } \quad \xi_k = 0. \end{cases} \tag{4.5}$$

For $k = 1, \ldots, N$ and $\boldsymbol{\alpha} \in \mathcal{M}$, using the multinomial formula, we get

$$\sum_{p=2}^{NM} (\xi_1 + \ldots + \xi_N)^{p-1} = \sum_{p=2}^{NM} p^{-1} \partial_{\xi_k} (\xi_1 + \ldots + \xi_N)^p = \sum_{\boldsymbol{\alpha} \in \mathcal{U}} c^{\boldsymbol{\alpha}} \alpha_k \boldsymbol{\xi}_{\boldsymbol{\alpha},k}, \tag{4.6}$$

where

$$c^{\boldsymbol{\alpha}} := (|\boldsymbol{\alpha}| - 1)! \left(\prod_{k=1}^{N} \alpha_k! \right)^{-1}. \tag{4.7}$$

If

$$\xi_1 + \ldots + \xi_N = 1, \tag{4.8}$$

then, by (4.6) we get

$$MN - 1 = \left[\frac{1}{(M+1)^N - N - 1} \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}} \alpha_k c_{\boldsymbol{\alpha}} \boldsymbol{\xi}_{\boldsymbol{\alpha},k} + \sum_{\boldsymbol{\alpha} \in \mathcal{U} \setminus \mathcal{M}} \alpha_k c_{\boldsymbol{\alpha}} \boldsymbol{\xi}_{\boldsymbol{\alpha},k} \right]. \tag{4.9}$$

For each $k = 1, \ldots, N$, put

$$\xi_k = \mu_k \mathfrak{I}_k, \tag{4.10}$$

where

$$\mu_k = m_k \left(\sum_{n=1}^{N} m_n \int_{\mathbb{R}^3} f_{0,n}(\mathbf{v}) \mathrm{d}\mathbf{v} \right)^{-1} \tag{4.11}$$

and

$$\mathfrak{I}_k = \int_{\mathbb{R}^3} f_k^j(\mathbf{v}) \mathrm{d}\mathbf{v}. \tag{4.12}$$

It follows that (4.8) is satisfied, due to (4.19). Consequently, by (4.9),

$$1 = \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}} \alpha_k \cdot \Gamma^{\boldsymbol{\alpha},k} \cdot \mathbf{I}_{\boldsymbol{\alpha},k} + \sum_{\boldsymbol{\alpha} \in \mathcal{U} \setminus \mathcal{M}} \Lambda^{\boldsymbol{\alpha},k} \cdot \mathbf{I}_{\boldsymbol{\alpha},k}, \tag{4.13}$$

where the notation $\mathbf{I}_{\boldsymbol{\alpha},k}$ is given by (4.5) for $\mathbf{I} = (\mathfrak{I}_1, \ldots, \mathfrak{I}_N)$. In (4.13),

$$\Lambda^{\boldsymbol{\alpha},k} := \frac{\alpha_k c^{\boldsymbol{\alpha}} \mu_1^{\alpha_1} \cdot \ldots \mu_{k-1}^{\alpha_{k-1}} \cdot \mu_k^{\alpha_k - 1} \cdot \mu_{k+1}^{\alpha_{k+1}} \cdot \ldots \cdot \mu_N^{\alpha_N}}{MN - 1} \tag{4.14}$$

and

$$\Gamma^{\boldsymbol{\alpha},k} := \frac{c^{\boldsymbol{\alpha}} \mu_1^{\alpha_1} \cdot \ldots \mu_{k-1}^{\alpha_{k-1}} \cdot \mu_k^{\alpha_k - 1} \cdot \mu_{k+1}^{\alpha_{k+1}} \cdot \ldots \cdot \mu_N^{\alpha_N}}{(MN - 1)\left[(M+1)^N - N - 1\right]}. \tag{4.15}$$

Multiplying on components ($k = 1, \ldots, N$), the first term of the right side of (4.1) by (4.13) and using (3.11), equation (4.1) becomes

$$f_k^j = Q_k(\mathbf{f}^{j-1}) + L_k(\mathbf{f}^{j-1}) + \Delta t \cdot P_k(\mathbf{f}^{j-1}), \tag{4.16}$$

for $k=1,\dots,N$. Here

$$Q_k(\mathbf{f}^j)(\mathbf{v}):=$$

$$=\sum_{\boldsymbol{\alpha},\boldsymbol{\beta}\in\mathcal{M}}\alpha_k\left[\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|-3}}\left(\Gamma^{\boldsymbol{\alpha},k}-\Delta t\int_{\boldsymbol{\Omega}_{\boldsymbol{\beta}}}r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})\mathrm{d}\mathbf{n}\right)\mathbf{f}^j_{\boldsymbol{\alpha}}(\mathbf{w})\mathrm{d}\mathbf{w}_{(k)}\right]_{\mathbf{w}_{\boldsymbol{\alpha},k}=\mathbf{v}},\tag{4.17}$$

$$L_k(\mathbf{f}^j)(\mathbf{v}):=\sum_{\boldsymbol{\alpha}\in\mathcal{U}\setminus\mathcal{M}}\Lambda^{\boldsymbol{\alpha},k}\left[\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|-3}}\mathrm{d}\mathbf{w}_{(k)}\mathbf{f}^j_{\boldsymbol{\alpha}}(\mathbf{w})\right]_{\mathbf{w}_{\boldsymbol{\alpha},k}=\mathbf{v}}.\tag{4.18}$$

If K is the constant introduced in (3.13), we can choose Δt such that $\Delta t\cdot K\leq\inf_{\boldsymbol{\alpha},k}\Gamma^{\boldsymbol{\alpha},k}$.

Then, the positivity of $\mathbf{f}^j$, for all $j=1,\dots,T_\Delta$, follows by induction, using Assumption (3.13). As $\mathbf{f}^j\geq 0$ for all $j=1,\dots,T_\Delta$, then the mass conservation is always fulfilled. Indeed, by induction and using the same argument as in (3.27) we have

$$\sum_{k=1}^N m_k\int_{\mathbb{R}^3}f_k^j(\mathbf{v})\mathrm{d}\mathbf{v}=\sum_{k=1}^N m_k\int_{\mathbb{R}^3}f_{k,0}(\mathbf{v})\mathrm{d}\mathbf{v}\tag{4.19}$$

for all $j=1,\dots,T_\Delta$.

b) Combining (3.18) and (4.1), for all $j=1,\dots,T_\Delta$ we can write

$$\begin{aligned}\left\|\mathbf{f}(j\cdot\Delta t)-\mathbf{f}^j\right\|_{\mathbb{X}}&\leq\left\|\mathbf{f}(j-1)\cdot\Delta t)-\mathbf{f}^{j-1}\right\|_{\mathbb{X}}+\\&+\int_{(j-1)\cdot\Delta t}^{j\cdot\Delta t}\left\|P(\mathbf{f}(s))-P(\mathbf{f}^{j-1})\right\|_{\mathbb{X}}\mathrm{d}s+\\&+\int_{(j-1)\cdot\Delta t}^{j\cdot\Delta t}\left\|S(\mathbf{f}(s))-S(\mathbf{f}^{j-1})\right\|_{\mathbb{X}}\mathrm{d}s.\end{aligned}\tag{4.20}$$

Denote by $\mathcal{O}_j:=\left\|\mathbf{f}(j\Delta t)-\mathbf{f}^j\right\|_{\mathbb{X}}$. Using the explicit forms of $\mathbf{P}$ and $\mathbf{S}$, taking account of the conservation relations (3.19) and (4.19), we find that there is some number $c_0>0$, depending on $\|\mathbf{f}_0\|_{\mathbb{X}}$ such that $\mathcal{O}_j<\mathcal{O}_{j-1}(1+c_0\Delta t)$ for all $j=2,\dots,T_\Delta$ and $\mathcal{O}_1\leq c_0\Delta t$. Then

$$\mathcal{O}_j\leq\mathcal{O}_1(1+c_0\Delta t)^{T_\Delta}\leq c_1\cdot\Delta t,\tag{4.21}$$

with $c_1>0$ depending only on $\|\mathbf{f}_0\|_{\mathbb{X}}$. Suppose that $t\in((j-1)\Delta t,j\Delta t]$.

The explicit forms of $\mathbf{P}$ and $\mathbf{S}$ together with (3.18) and (3.19) lead to

$$\begin{aligned} &\|\mathbf{f}(t) - \mathbf{f}((j-1)\Delta t)\|_{\mathbb{X}} \leq \\ &\leq \int_{(j-1)\Delta t}^{j\Delta t} (\|\mathbf{P}(\mathbf{f}(s))\|_{\mathbb{X}} + \|\mathbf{S}(\mathbf{f}(s))\|_{\mathbb{X}}) \mathrm{d}s \leq c_2 \cdot \Delta t, \end{aligned} \tag{4.22}$$

where c_2 depends only on $\|f_0\|_{\mathbb{X}}$. Now estimation (4.3) is an immediate consequence of (4.21) and (4.22). □

For numerical purposes, one has to write the equation (4.1) in the weak form for measures. In this respect, we associate the the following measures to the solutions $\mathbf{f}(t)$ and $\mathbf{f}^j$ appearing in Proposition 4.1. For $k = 1, \ldots, N$ define

$$\mathrm{d}\mu_k^t(\mathbf{v}) := f_k(t, \mathbf{v})\mathrm{d}\mathbf{v}, \tag{4.23}$$

where $t \geq 0$, and

$$\mathrm{d}\bar{\mu}_k^j(\mathbf{v}) := f_k^j(\mathbf{v})\mathrm{d}\mathbf{v}, \tag{4.24}$$

for $j = 1, \ldots, T_\Delta$.

Proposition 4.1 has the following consequence expressed in terms of the discrepancy defined by (2.24).

COROLLARY **4.1** *If the conditions of Proposition* 4.1 *are fulfilled, then*

$$\max_{k=1,\ldots,N} \max_{j=1,\ldots,T_\Delta} D(\mu_k^{j\Delta t}, \bar{\mu}_k^j) \to 0 \quad \textit{as } \Delta t \to 0. \tag{4.25}$$

5. The Probabilistic Frame

The central result of this section extends, in some sense, the probabilistic methods of selection used by Babovsky and Illner [4, 5] (see e.g. Lemma 2 of Ref. [4]).

We start with a simple generalization (to row-wise independent random variables) of the strong law of large numbers for independent random variables with bounded fourth momentum (see, e.g., Theorem IV.§3-1 in Ref. [28], p.363).

Let (Ω, β, P) be a probability space. For some real random variable X, by $\langle X \rangle$ we denote its mean with respect to P.

Let $\mathbb{N}^* \ni n \to q_n \in \mathbb{N}^*$. We call the family $((X_{n,i})_{i \in \{1,\ldots,q_n\}})_{n \in \mathbb{N}^*}$ of real valued random variables on Ω an *array of row-wise independent random variables*, if for each fixed $n \in \mathbb{N}^*$ the random variables $(X_{n,i})_{i \in \{1,\ldots,q_n\}}$ are independent.

PROPOSITION **5.1** *Let $((X_{n,i})_{i\in\{1,\dots,q_n\}})_{n\in\mathbb{N}^*}$ be an array of row-wise independent random variables with zero mean. Denote $A_n := \sup\limits_{i\in\{1,\dots,q_n\}} \langle X_{n,i}^4\rangle$.*

If

$$\sum_{n=1}^{\infty} \frac{A_n}{q_n^2} < \infty, \tag{5.1}$$

then, with probability one,

$$\frac{1}{q_n}\sum_{i=1}^{q_n} X_{n,i} \to 0, \ \ as\ n\to\infty. \tag{5.2}$$

Proof. According to a version of the Borel-Cantelli Lemma, it is sufficient to show that for each $\varepsilon > 0$,

$$\sum_{n=1}^{\infty} P\left(\left|\frac{1}{q_n}\sum_{i=1}^{q_n} X_{n,i}\right| > \varepsilon\right) < \infty. \tag{5.3}$$

To this end, by Chebyshev's inequality, we obtain

$$P\left(\left|\sum_{i=1}^{q_n} X_{n,i}\right| > \varepsilon\cdot q_n\right) \le \frac{1}{\varepsilon^4 q_n^4}\left\langle\left|\sum_{i=1}^{q_n} X_{n,i}\right|^4\right\rangle. \tag{5.4}$$

Expanding the fourth power, we invoke the independence of $X_{n,i}$ and use the fact that $\langle X_{n,i}\rangle = 0$. Then a simple computation shows that for all $\varepsilon > 0$,

$$0 \le \sum_{n=1}^{\infty} P\left(\frac{1}{q_n}\left|\sum_{i=1}^{q_n} X_{n,i}\right| > \varepsilon\right) \le \frac{3}{\varepsilon^4}\sum_{n=1}^{\infty}\frac{A_n}{q_n^2} < \infty. \tag{5.5}$$

This concludes the proof. □

Consider $\mathbb{N}^* \ni n \to m_n \in \mathbb{N}^*$ a sequence, such that $m_n \to \infty$ as $n\to\infty$.

For each $n\in\mathbb{N}^*$, let $\mathcal{I}_n := \{1,2,\dots,m_n\}$ be an index set and let $\mathcal{I}_n^p := \underbrace{\mathcal{I}_n\times\ldots\times\mathcal{I}_n}_{p \text{ times}}$ for a fixed $p\in\mathbb{N}^*$.

Consider some given set $\mathbf{X}\subset\mathbb{R}^m$ and a given sequence $(F_n)_{n\in\mathbb{N}^*}$ of functions $F_n : \mathbf{X}\times\mathcal{I}_n^p \to \mathbb{R}$. Define $S_n : \mathbf{X}\to\mathbb{R}$ by

$$S_n(x) := \begin{cases} \dfrac{1}{m_n^p}\displaystyle\sum_{\mathbf{j}\in\mathcal{I}_n} F_n(x,\mathbf{j}) & \text{if} \quad p\ge 2, \\ \\ \displaystyle\sum_{j=1}^{m_n} a_{n,j}F_n(x,j) & \text{if} \quad p=1, \end{cases} \tag{5.6}$$

where $((a_{n,l})_{l\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ is a family of nonnegative numbers, such that

$$\begin{aligned}&\sup_{n\in\mathbb{N}^*}\sum_{l=1}^{m_n}a_{n,j}<\infty,\\&\sum_{l=1}^{m_n}a_{n,l}>0,\ \text{for all } n\in\mathbb{N}^*.\end{aligned}\tag{5.7}$$

Suppose that there is some function $F:\mathbf{X}\to\mathbb{R}$ such that, for each $x\in\mathbf{X}$,

$$F(x)=\lim_{n\to\infty}S_n(x).\tag{5.8}$$

In general, for a given n, the sum S_n contains m_n^p terms. Roughly speaking, our problem is to conveniently diminish the numbers of terms in S_n, by random selection of the terms in (5.6) and "renormalize" the resulting sum such that the convergence to $F(x)$ be kept, in some sense. In this respect, we define some special families of random variables.

Let (Ω,β,P) be a probability space, where $\Omega:=[0,1)^\infty$ (in the countable sense) is endowed with the usual product Borel $\sigma-$algebra β and P the usual product probability induced on Ω by the uniform distribution of $[0,1)$.

For each $n\in\mathbb{N}^*$ and $j\in\mathcal{I}_n$, define the weights

$$p_{n,j}:=\frac{a_{n,j}}{\sum\limits_{l=1}^{m_n}a_{n,l}},\tag{5.9}$$

where $((a_{n,l})_{l\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ is the family with properties (5.7). For each $n\in\mathbb{N}^*$, let

$$q_{n,s}:=\begin{cases}0 & \text{if}\quad s=0,\\ \displaystyle\sum_{j=1}^{s}p_{n,j} & \text{if}\quad s\in\mathcal{I}_n.\end{cases}\tag{5.10}$$

For each $n\in\mathbb{N}^*$ and $l\in\mathcal{I}_n$ we consider the random variables $c_{n,l}\,,\tilde{c}_{n,l}:\Omega\to\mathcal{I}_n$ given by

$$c_{n,l}(\boldsymbol{\omega}):=[[\omega_l\cdot m_n]]+1,\tag{5.11}$$

and

$$\tilde{c}_{n,l}(\boldsymbol{\omega}):=s\ \text{ if }\omega_l\in[q_{n,s-1},q_{n,s})\,,\tag{5.12}$$

where ω_l is the l^{th} component of $\boldsymbol{\omega} = (\omega_1, \omega_2, \ldots) \in \Omega$. In (5.12) we make the convention that $[x, x) := \phi$ (the void set) for any $x \in \mathbb{R}$. Obviously, for each $j \in \mathcal{I}_n$

$$P\left(c_{n,l}(\boldsymbol{\omega}) = j\right) = \frac{1}{m_n}, \tag{5.13}$$

and

$$P\left(\tilde{c}_{n,l}(\boldsymbol{\omega}) = j\right) = p_{n,j}. \tag{5.14}$$

Consequently, $((c_{n,l})_{l\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ and $((\tilde{c}_{n,l})_{l\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$, are arrays of row-wise independent random variables.

Remark that the random variables $c_{n,l}$ are particular forms of $\tilde{c}_{n,l}$, with $p_{n,j} = m_n^{-1}$ in (5.9).

Let $p \geq 2$. For $n \in \mathbb{N}^*$ and $l \in \mathcal{I}_n$, define the random variables $\mathbf{J}_{n,l} : \Omega \to \mathcal{I}_n^p$ by

$$\mathbf{J}_{n,l}(\boldsymbol{\omega}) := (i, c_{n,(l-1)p+1}(\boldsymbol{\omega}), c_{n,(l-1)p+2}(\boldsymbol{\omega}), \ldots, c_{n,lp-1}(\boldsymbol{\omega})), \tag{5.15}$$

where $\boldsymbol{\omega} = (\omega_1, \omega_2, \ldots) \in \Omega$.

Observe that $ip + j = i'p + j'$ if and only if $i = i'$ and $j = j'$, for all $i, i' \in N^*$ and $j, j' \in \{1, 2, \ldots, p\}$. Then, using the row-wise independence of $((c_{n,l})_{l\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$, we conclude the row-wise independence of $((\mathbf{J}_{n,l})_{l\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$.

Suppose that one of the following conditions is fulfilled:

1. $\mathbf{X}$ is at most countable.

2. $\mathbf{X}$ is the whole $\mathbb{R}^m$, the function F is continuous and each $F_n(\cdot, \mathbf{j})$ is increasing with respect to the order of $\mathbb{R}^m$ for each fixed $n \in \mathbb{N}^*$ and $\mathbf{j} \in \mathcal{I}_n^p$. Define for each $n \in \mathbb{N}^*$ and $x \in \mathbf{X}$ by

$$a_n(x) := \max_{\mathbf{j}\in\mathcal{I}_n^p} \left|F_n(x, \mathbf{j})\right|. \tag{5.16}$$

PROPOSITION **5.2** 1. *Let $p \geq 2$. If*

$$\sum_{n=1}^{\infty} \frac{a_n(x)^4}{m_n^2} < \infty \tag{5.17}$$

for all $x \in \mathbf{X}$, then for each $x \in \mathbf{X}$, with probability one,

$$\lim_{n\to\infty} \frac{1}{m_n} \sum_{i=1}^{m_n} F_n(x, \cdot) \circ \mathbf{J}_{n,i} = F(x). \tag{5.18}$$

2. *Let $p = 1$. Consider $\mathbb{N}^* \ni n \to k_n \in \mathbb{N}^*$ a sequence such that, $k_n \to \infty$ as $n \to \infty$. If $k_n \leq m_n$ for all $n \in \mathbb{N}^*$, and*

$$\sum_{n=1}^{\infty} \frac{a_n(x)^4}{k_n^2} < \infty, \tag{5.19}$$

for all $x \in \mathbf{X}$, then for all $x \in \mathbf{X}$, with probability one,

$$\lim_{n\to\infty} \left(\sum_{j-1}^{m_n} a_{n,j} \right) \frac{1}{k_n} \sum_{i=1}^{k_n} F_n(x, \cdot) \circ \tilde{c}_{n,i} = F(x). \tag{5.20}$$

Proof. Remark that it is sufficient to consider the case in which all functions F_n are positive.

Case $\mathbf{X}$ *countable*

1. Let $x \in \mathbf{X}$ be fixed. For each $n \in \mathbb{N}^*$ and $i \in \mathcal{I}_n$, define

$$Y_{n,i} := F_n(x, \cdot) \circ \mathbf{J}_{n,i}. \tag{5.21}$$

The row-wise independence of $((\mathbf{J}_{n,i})_{i\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ implies that $((Y_{n,i})_{i\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ is an array of row-wise independent random variables. Let $\mathbf{j} = (j_1, \ldots, j_p) \in \mathcal{I}_n^p$. Using (5.13) and the definition (5.15) of $\mathbf{J}_{n,i}$, we get

$$P(\{\mathbf{J}_{n,i}(\boldsymbol{\omega}) = \mathbf{j}\}) = \begin{cases} m_n^{1-p} & \text{if} \quad i = j_1, \\ \\ 0 & \text{if} \quad i \neq j_1, \end{cases} \tag{5.22}$$

for all $n \in \mathbb{N}^*$ and $\mathbf{j} \in \mathcal{I}_n$. Consequently,

$$\langle Y_{n,i} \rangle = \frac{1}{m_n^{p-1}} \sum_{j_2,\ldots,j_p=1}^{m_n} F_n(x, (i, j_2, \ldots, j_p)), \tag{5.23}$$

so that

$$\frac{1}{m_n} \sum_{i=1}^{m_n} \langle Y_{n,i} \rangle = \frac{1}{m_n^p} \sum_{\mathbf{j}\in\mathcal{I}_n^p} F_n(x, \mathbf{j}) = S_n(x). \tag{5.24}$$

Put $X_{n,i} := Y_{n,i} - \langle Y_{n,i} \rangle$. Then, the family $((X_{n,i})_{i\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ satisfies the conditions of Proposition 5.1, with $A_n \leq (2a_n(x))^4$. Therefore, for each fixed x, by (5.24) and (5.6) one obtains (5.18). For each $x \in \mathbf{X}$, let Ω_x be the subset of Ω where the limit (5.18) holds. Define $\Omega_{\mathbf{X}} := \bigcap_{x\in\mathbf{X}} \Omega_x$. Since $\mathbf{X}$ is countable, we have $P(\Omega_{\mathbf{X}}) = 1$, so that the argument is complete.

2. Let $x \in \mathbf{X}$ be fixed. For each $n \in \mathbb{N}^*$ and $i \in \mathcal{I}_n$ define

$$Y_{n,i} := \left(\sum_{l=1}^{m_n} a_{n,l} \right) F_n(x, \cdot) \circ \tilde{c}_{n,i}. \tag{5.25}$$

The row-wise independence of $((\tilde{c}_{n,i})_{i \in \mathcal{I}_n})_{n \in \mathbb{N}^*}$ ensures that $((Y_{n,i})_{i \in \mathcal{I}_n})_{n \in \mathbb{N}^*}$ is an array row-wise independent family of random variables. From (5.14), we get

$$\langle Y_{n,i} \rangle = \sum_{l=1}^{m_n} a_{n,l} F_n(x, l), \tag{5.26}$$

for all $i \in \mathcal{I}_n$ and $n \in \mathbb{N}^*$. Consequently,

$$\frac{1}{k_n} \sum_{i=1}^{k_n} \langle Y_{n,i} \rangle = S_n(x). \tag{5.27}$$

Define $X_{n,i} := Y_{n,i} - \langle Y_{n,i} \rangle$. From here the argument works similarly as in 1.

Case $\mathbf{X} = \mathbb{R}^m$

1. Observe that the argument with **X** *countable* is valid on the countable set $\mathbb{Q}^m$ of the vectors of $\mathbb{R}^m$ with rational components. Further, remark that for any $x \in \mathbb{R}^m \setminus \mathbb{Q}^m$ and $\varepsilon > 0$, by the continuity of F and the monotonicity of F_n, we can find two elements $x^-, x^+ \in \mathbb{Q}^m$, with $x^- \leq x \leq x^+$ such that

$$\begin{aligned} &F(x^+) - \frac{1}{m_n} \sum_{i=1}^{m_n} F_n(x^+, \cdot) \circ \mathbf{J}_{n,i}(\boldsymbol{\omega}) - \varepsilon \leq \\ &\leq F(x) - \frac{1}{m_n} \sum_{i=1}^{m_n} F_n(x, \cdot) \circ \mathbf{J}_{n,i}(\boldsymbol{\omega}) \leq \\ &\leq F(x^-) - \frac{1}{m_n} \sum_{i=1}^{m_n} F_n(x^-, \cdot) \circ \mathbf{J}_{n,i}(\boldsymbol{\omega}) + \varepsilon, \end{aligned} \tag{5.28}$$

for all $\boldsymbol{\omega} \in \Omega$. Now we approximate x by two sequences $\left\{x_p^+\right\}_{p \in \mathbb{N}}, \left\{x_p^-\right\}_{p \in \mathbb{N}} \subset \mathbb{Q}^m$, with $x_p^- \leq x \leq x_p^+$. Then, to conclude the proof in the *case* $\mathbf{X} = \mathbb{R}^m$, we refer to the result in the *case* **X** *countable*.

2. Replacing only (5.28) with

$$F(x^+) - \frac{1}{k_n}\sum_{i=1}^{k_n} F_n(x^+,\cdot)\circ\tilde{c}_{n,i}(\boldsymbol{\omega}) - \varepsilon \leq$$

$$\leq F(x) - \frac{1}{k_n}\sum_{i=1}^{k_n} F_n(x,\cdot)\circ\tilde{c}_{n,i}(\boldsymbol{\omega}) \leq \tag{5.29}$$

$$\leq F(x^-) - \frac{1}{k_n}\sum_{i=1}^{k_n} F_n(x^-,\cdot)\circ\tilde{c}_{n,i}(\boldsymbol{\omega}) + \varepsilon,$$

one repeats step by step the arguments of the part 1 to conclude the proof of the part 2. □

The index set $\mathcal{I}_n^p$ being defined as before, let $((\mu_{n,\mathbf{j}})_{\mathbf{j}\in\mathcal{I}_n^p})_{n\in\mathbb{N}^*}$ be a bounded family of positive measures on $\mathbb{R}^m$, i.e. there exists some constant $a>0$, such that $|\mu_{n,\mathbf{j}}| \leq a$ for all $\mathbf{j}\in\mathcal{I}_n^p$ and $n\in\mathbb{N}^*$ (we recall the notation $|\mu| := \mu(\mathbb{R}^m)$ for some finite measure μ on $\mathbb{R}^m$).

Let (Ω,β,P) be the probability space be as in Proposition 5.2 and the arrays of row-wise random variables $((\mathbf{J}_{n,i})_{i\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ and $((\tilde{c}_{n,i})_{i\in\mathcal{I}_n})_{n\in\mathbb{N}^*}$ defined by (5.15) and (5.12) respectively.

THEOREM **5.1** 1. *Let $p\geq 2$. Suppose that there is a positive measure μ on $\mathbb{R}^m$, absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^m$, such that*

$$\frac{1}{m_n^p}\sum_{\mathbf{j}\in\mathcal{I}_n^p}\mu_{n,\mathbf{j}} \rightharpoonup \mu, \ \text{as } n\to\infty. \tag{5.30}$$

Define $\mu_{n,i}(\boldsymbol{\omega}) := \mu_{n,\mathbf{j}}|_{\mathbf{j}=\mathbf{J}_{n,i}(\boldsymbol{\omega})}$ for all $\boldsymbol{\omega}\in\Omega$, all $i\in\mathcal{I}_n$ and $n\in\mathbb{N}^*$. If

$$\sum_{n=1}^{\infty}\frac{1}{m_n^2} < \infty, \tag{5.31}$$

then for $P-$almost all $\boldsymbol{\omega}$,

$$\sigma_{1,n}(\boldsymbol{\omega}) := \frac{1}{m_n}\sum_{i=1}^{m_n}\mu_{n,i}(\boldsymbol{\omega}) \rightharpoonup \mu \ \text{as } n\to\infty. \tag{5.32}$$

2. *Let $p=1$. Suppose that there is a positive measure μ on $\mathbb{R}^m$, absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^m$, such that*

$$\sum_{l=1}^{m_n} a_{n,l}\cdot\mu_{n,l} \rightharpoonup \mu, \ \text{as } n\to\infty. \tag{5.33}$$

Define $\mu_{n,i}(\boldsymbol{\omega}) := \mu_{n,l}|_{l=\tilde{c}_{n,i}(\boldsymbol{\omega})}$ *for all* $\boldsymbol{\omega} \in \Omega$, *all* $i \in \mathcal{I}_n$ *and* $n \in \mathbb{N}^*$. *Let* $\mathbb{N}^* \ni n \to k_n \in \mathbb{N}^*$ *be a sequence such that* $k_n \leq m_n$, *for all* $n \in \mathbb{N}^*$ *and*

$$\sum_{n=1}^{\infty} \frac{1}{k_n^2} < \infty. \tag{5.34}$$

Then, for $P-$*almost all* $\boldsymbol{\omega}$,

$$\sigma_{2,n}(\boldsymbol{\omega}) := \frac{1}{k_n} \sum_{i=1}^{k_n} \mu_{n,i}(\boldsymbol{\omega}) \rightharpoonup \mu \text{ as } n \to \infty. \tag{5.35}$$

Proof. Define for each $x \in \mathbb{R}^m$

$$F_n(x, \mathbf{j}) := \int_{y \leq x} \mathrm{d}\mu_{n,\mathbf{j}}(y), \tag{5.36}$$

and

$$F(x) := \int_{y \leq x} \mathrm{d}\mu(y). \tag{5.37}$$

Then it is sufficient to observe that F and $F_n(x, \mathbf{j})$ satisfy the conditions of Proposition 5.2, (with $a_n(x) = a$) and the family $\{y \in \mathbb{R}^m \,|y \leq x\}_{x \in \mathbb{R}^m}$ is determining, Ref. [28], for the weak convergence of the measures $\mu_{n,\mathbf{j}}$. □

REMARK **5.1** *It can be easily seen that Babovsky Lemma (see Lemma* 2 *of Ref.* [4]*) is a particular case of Theorem* 5.1.1 *with* $m_n = n^2$, *for all* $n \in \mathbb{N}^*$ *and with* $\mu_{n,\mathbf{j}}$ *given by a product of two point measures.*

REMARK **5.2** *As we have mentioned in Section 1, our purpose is to approximate the solutions of* (2.18) *by sums of Dirac measures of the form* (2.22).

Due to the nonlinear character of the collision operators $\mathbf{P}$ *and* $\mathbf{S}$, *at each timestep, the numerical complexity increases dramatically (power-like). Although, we are able to reduce the computational effort using repeatedly the Theorem* 5.1.1.

However, except the case of (2.18) *modelling the one component gas with purely elastic collisions, a certain step of the numerical scheme destroys the homogeneity of the sums of Dirac measures, i.e. instead of HSPM approximations one obtains WSPM approximations. This difficulty will be surmounted by using Theorem* 5.1.2, *which converts the WSPM approximations into HSPM approximations.*

Theorem 5.1 will be the basic point of the probabilistic part of our numerical scheme for the solutions of (2.18) in the next section.

6. The Main Result

For our numerical scheme, we need a weak form of (4.16), where the functions f_k^j are replaced by the measures $\bar{\mu}_k^j$ given by (4.24). Denote

$$(\varphi, h) := \int_{\mathbb{R}^3} \varphi(\mathbf{v}) h(\mathbf{v}) \mathrm{d}\mathbf{v}, \tag{6.1}$$

for $\varphi \in C_b(\mathbb{R}^3)$ and $h \in \mathbb{L}^1(\mathbb{R}^3)$. From (4.16) using (6.1) we get

$$\left(\varphi, f_k^j\right) = (\varphi, Q_k(\mathbf{f}^{j-1})) + (\varphi, L_k(\mathbf{f}^{j-1})) + \Delta t \cdot (\varphi, P_k(\mathbf{f}^{j-1})) \tag{6.2}$$

for all $\varphi \in C_b(\mathbb{R}^3)$, all $j = 1, \ldots, T_\Delta$ and $k = 1, \ldots, N$. Denoting by

$$V(\mathbf{\Omega}_{\boldsymbol{\beta}}) := \int_{\mathbf{\Omega}_{\boldsymbol{\beta}}} \mathrm{d}\mathbf{n}, \tag{6.3}$$

in (6.2),

$$\begin{aligned} (\varphi, Q_k(\mathbf{f}^j)) := \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}} \alpha_k \int_{\mathbb{R}^{3|\boldsymbol{\alpha}|} \times \mathbf{\Omega}_{\boldsymbol{\beta}}} (\varphi \circ i_{k,\boldsymbol{\alpha}})(\mathbf{w}) \times \\ \times \left(\frac{\Gamma^{\boldsymbol{\alpha},k}}{V(\mathbf{\Omega}_{\boldsymbol{\beta}})} - \Delta t \cdot r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n}) \right) \mathbf{f}_{\boldsymbol{\alpha}}^j(\mathbf{w}) \mathrm{d}\mathbf{w} \mathrm{d}\mathbf{n}, \end{aligned} \tag{6.4}$$

and

$$(\varphi, L_k(\mathbf{f}^j)(\mathbf{v})) := \sum_{\boldsymbol{\alpha} \in \mathcal{U} \setminus \mathcal{M}} \Lambda^{\boldsymbol{\alpha},k} \int_{\mathbb{R}^{3|\boldsymbol{\alpha}|}} (\varphi \circ i_{k,\boldsymbol{\alpha}})(\mathbf{w}) \mathbf{f}_{\boldsymbol{\alpha}}^j(\mathbf{w}) \mathrm{d}\mathbf{w}. \tag{6.5}$$

In the formulas (6.4) and (6.5), the projection application $i_{k,\boldsymbol{\gamma}} : \mathbb{R}^{3|\boldsymbol{\gamma}|} \to \mathbb{R}^3$ is defined by $i_{k,\boldsymbol{\gamma}}(\mathbf{w}) = \mathbf{w}_{k,\gamma_k}$, for $\boldsymbol{\gamma} \in \mathcal{M}$ and $k = 1, \ldots, N$. Using (3.6) and (3.9) we get

$$\begin{aligned} &(\varphi, P_k(\mathbf{f}^j)) = \\ &= \sum_{\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}} \beta_k \int_{\mathbb{R}^{3|\boldsymbol{\alpha}|} \times \mathbf{\Omega}_{\boldsymbol{\beta}}} \varphi \circ i_{k,\boldsymbol{\beta}}(\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n})) r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n}) \mathbf{f}_{\boldsymbol{\alpha}}^j(\mathbf{w}) \mathrm{d}\mathbf{w} \mathrm{d}\mathbf{n}, \end{aligned} \tag{6.6}$$

for all $\varphi \in C_b(\mathbb{R}^3)$, all $j = 0, 1, \ldots, T_\Delta$ and $k = 1, \ldots, N$.

Now, we are able to formulate (6.2) as an equation for measures. For some $\boldsymbol{\gamma} \in \mathcal{M}$ and $j = 0, 1, \ldots, T_\Delta$, define the measure $\bar{\mu}_{\boldsymbol{\gamma}}^j$ on $\mathbb{R}^{3|\boldsymbol{\gamma}|}$ by

$$\mathrm{d}\bar{\mu}_{\boldsymbol{\gamma}}^j(\mathbf{w}) = \bigotimes_{k \in \mathcal{N}_\gamma} \bigotimes_{i=1}^{\gamma_k} \mathrm{d}\bar{\mu}_k^j(\mathbf{w}_{k,i}). \tag{6.7}$$

From (6.2-6.6), using spherical coordinates

$$[0,\pi)^{3|\boldsymbol{\beta}|-5}\times[0,2\pi)\ni(\theta,\varphi)\to\mathbf{n}(\theta,\varphi)\in\boldsymbol{\Omega}_{\boldsymbol{\beta}}, \tag{6.8}$$

to integrate on each unit sphere $\boldsymbol{\Omega}_{\boldsymbol{\beta}}$, it follows that there are some sets $\mathcal{A}\subset\mathcal{U}$, $\mathcal{B}\subset\mathcal{M}$, the functions $q_{\boldsymbol{\alpha},\boldsymbol{\beta},k}\in C(\mathbb{R}^{3|\boldsymbol{\alpha}|}\times[0,\pi)^{3|\boldsymbol{\beta}|-5}\times[0,2\pi)\,;\mathbb{R}_+)$ and $H_{\boldsymbol{\alpha},\boldsymbol{\beta},k}\in C(\mathbb{R}^{3|\boldsymbol{\alpha}|}\times[0,\pi)^{3|\boldsymbol{\beta}|-5}\times[0,2\pi)\,;\mathbb{R}^3)$ such that we can write (6.2) in the compressed form

$$\begin{aligned}\int_{\mathbb{R}^3}\varphi(\mathbf{v})\mathrm{d}\bar{\mu}_k^j(\mathbf{v})=&\sum_{\boldsymbol{\alpha}\in\mathcal{A},\boldsymbol{\beta}\in\mathcal{B}}\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|}}\mathrm{d}\bar{\mu}_{\boldsymbol{\alpha}}^{j-1}(\mathbf{w})\times\\ &\times\int_{[0,\pi)^{3|\boldsymbol{\beta}|-5}}\mathrm{d}\theta\int_0^{2\pi}(\varphi\circ H_{\boldsymbol{\alpha},\boldsymbol{\beta},k})(\mathbf{w},\theta,\phi)q_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,\phi)\mathrm{d}\phi,\end{aligned} \tag{6.9}$$

for $\varphi\in C_b(\mathbb{R}^3)$ and $k\in 1,\dots,N$.

First, we consider $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}$ verifying the properties of Lemma 3.1 and we construct the algorithm starting from (6.9). Then, we show how the numerical scheme can be improved, if one introduces additional conditions on $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}$.

Now, we write (6.9) in a more convenient form. Note that, we can find some $L\in\mathbb{N}^*$ and

1. a family $\{\boldsymbol{\alpha}(l)\}_{l=1,\dots,L}\subset\mathcal{U}$ of multi-indexes,
2. a family $\{q(l)\}_{l=1,\dots,L}\subset\mathbb{N}^*$,
3. a family $\{\pi_l\}_{l=1,\dots,L}$ of measures absolute continuous with respect to the Lebesgue measure on $\mathbb{R}^{q(l)}$,
4. a family $\{R_{k,l}\}_{k=1,\dots,N;l=1,\dots,L}\subset C(\mathbb{R}^{3|\boldsymbol{\alpha}(l)|+q(l)};\mathbb{R}_+)$ of functions,
5. a family $\{h_{k,l}\}_{k=1,\dots,N;l=1,\dots,L}\subset C(\mathbb{R}^{3|\boldsymbol{\alpha}(l)|+q(l)};\mathbb{R}^3)$ of functions,

such that (6.9) can be written

$$\int_{\mathbb{R}^3}\varphi(\mathbf{v})\mathrm{d}\bar{\mu}_k^j(\mathbf{v})=\sum_{l=1}^L\int_{\mathbb{R}^{3|\boldsymbol{\alpha}(l)|+q(l)}}R_{k,l}(\mathbf{z})(\varphi\circ h_{k,l})(\mathbf{z})\mathrm{d}(\bar{\mu}_{\boldsymbol{\alpha}(l)}^{j-1}\otimes\pi_l)(\mathbf{z}). \tag{6.10}$$

Let (Ω,β,P) be as in Theorem 5.1.

a) For each $l = 1, \ldots, L$, we approximate π_l by a convenient HSPM of the form (2.22), containing n-terms, $\pi_{l,n} \rightharpoonup \pi_l$ as $n \to \infty$ (this can be done, e.g. by means of low discrepancy, well distributed sequences Ref. [6, 27]).

b) The initialization of the scheme is done by giving n-terms HSPM approximations $\nu^0_{k,n}$ of the initial data $\bar{\mu}^0_k$, where $k = 1, \ldots, N$.

c) The n-terms HSPM approximations $\nu^1_{k,n}$ of $\bar{\mu}^1_k$, with $k = 1, \ldots, N$, resulting from the scheme, can be obtained as follows:

Step 1 *(first selection).* For each $l = 1, \ldots, L$ and $k = 1, \ldots, N$ we replace $\bar{\mu}^0_k$ by $\nu^0_{k,n}$ in (6.7) (for $\boldsymbol{\gamma} = \boldsymbol{\alpha}(l)$, $j = 0$). Then for each $l = 1, \ldots, L$, we obtain a sequence of finite measures $\nu^0_{\boldsymbol{\alpha}(l),n} \rightharpoonup \bar{\mu}^0_{\boldsymbol{\alpha}(l)}$ as $n \to \infty$, implying $\nu^0_{\boldsymbol{\alpha}(l),n} \otimes \pi_{l,n} \rightharpoonup \bar{\mu}^0_{\boldsymbol{\alpha}(l)} \otimes \pi_l$ as $n \to \infty$. Obviously, each $\nu^0_{\boldsymbol{\alpha}(l),n} \otimes \pi_{l,n}$ is a sum of the form (5.30), containing $n^{|\boldsymbol{\alpha}(l)|+1}$ terms. We apply the selection algorithm cf. Theorem 5.1.1 (with $m_n = n$ and $p = |\boldsymbol{\alpha}(l)|+1$) to construct n - -terms HSPM approximations for all $\nu^0_{\boldsymbol{\alpha}(l),n} \otimes \pi_{l,n}$. Thus, by Theorem 5.1.1, for each $l = 1, \ldots, L$, there exists some set $\Omega_l \subset \Omega$, with $P(\Omega_l) = 1$, such that from $\nu^0_{\boldsymbol{\alpha}(l),n} \otimes \pi_{l,n}$, one can extract a n-terms HSPM approximation (of the form (5.32)) $\sigma_{1,l,n}(\boldsymbol{\omega}^l) \rightharpoonup \bar{\mu}^0_{\boldsymbol{\alpha}(l)} \otimes \pi_l$ as $n \to \infty$, for almost all $\boldsymbol{\omega}^l \in \Omega_l$.

Step 2 *(second selection).* In the right side of (6.10), written for $j = 1$, replace each $\bar{\mu}^0_{\boldsymbol{\alpha}(l)} \otimes \pi_l$ by the corresponding $\sigma_{1,l,n}$. Then the right side of (6.10) defines the measures $M_{k,n}$ on $\mathbb{R}^3$, for $k = 1, \ldots, N$ and $n \in \mathbb{N}^*$,

$$M_{k,n} = \frac{1}{n} \sum_{l=1}^{L} \sum_{i=1}^{n} a_l R_{k,l}(\mathbf{z}_{l,i,n}(\boldsymbol{\omega}^l)) \delta_{h_{k,l}(\mathbf{z}_{l,i,n}(\boldsymbol{\omega}^l))}, \tag{6.11}$$

concentrated at the points $h_{k,l}(\mathbf{z}_{l,i,n}(\boldsymbol{\omega}^l))$, where $\mathbf{z}_{l,i,n}(\boldsymbol{\omega}^l) \in \mathbb{R}^{3|\boldsymbol{\alpha}(l)|+q(l)}$ and $a_l \geq 0$ are some constants (for $l = 1, \ldots, L$ and $i = 1, \ldots, n$). By Step 1, it follows that

$$M_{k,n} \rightharpoonup \bar{\mu}^1_k \text{ as } n \to \infty, \tag{6.12}$$

for all $\boldsymbol{\omega}^1 \in \Omega_1$, $\boldsymbol{\omega}^2 \in \Omega_2$, ..., $\boldsymbol{\omega}^L \in \Omega_L$ and for $k = 1, \ldots, N$. Now, it can be easily seen that (6.11) can be written as WSPM, containing, at most $L \cdot n$ terms.

As we mentioned before, we want to obtain HSPM approximations at the end of each step of time. We fix, for the moment, some $\boldsymbol{\omega}^1 \in \Omega_1, \ldots, \boldsymbol{\omega}^L \in \Omega_L$, so that (6.12) holds. We apply the selection algorithm formulated Theorem 5.1.2

for each fixed $k = 1, \ldots, N$, as follows. For $l = 1, \ldots, L \cdot n$ defining

$$\iota(l) := \left[\left[\frac{l-1}{L}\right]\right] + 1,$$
$$\lambda(l) := \left[\left[\frac{l-1}{n}\right]\right] + 1, \tag{6.13}$$

put

$$a_{n,l} = \frac{1}{n} a_{\lambda(l)} R_{k,\lambda(l)}(\mathbf{z}_{\lambda(l),\iota(l),n}(\boldsymbol{\omega}^{\lambda(l)})). \tag{6.14}$$

We choose $m_n = L \cdot n$ and $k_n = n$. Then, for each $k = 1, \ldots, N$, there exists some $\Omega_{L+k} \subset \Omega$, with $P(\Omega_{L+k}) = 1$, such that from $M_{k,n}$, we obtain a n-terms HSPM approximation (of the form (5.35)) $\sigma_{2,k,n}(\boldsymbol{\omega}^{L+k}; \boldsymbol{\omega}^1, \ldots, \boldsymbol{\omega}^L) \rightharpoonup \bar{\mu}_k^1$ as $n \to \infty$, for all $\boldsymbol{\omega}^{L+k} \in \Omega_{L+k}$. Set $\bar{\nu}_{k,n}^1(\boldsymbol{\omega}^1, \ldots, \boldsymbol{\omega}^{L+k}) := \sigma_{2,k,n}(\boldsymbol{\omega}^{L+k}; \boldsymbol{\omega}^1, \ldots, \boldsymbol{\omega}^L)$. Therefore for each $\bar{\mu}_k^1$ in (6.10), we obtain a corresponding n-terms HSPM approximation $\bar{\nu}_{k,n}^1 \rightharpoonup \bar{\mu}_k^1$ as $n \to \infty$, for all $\boldsymbol{\omega}^1 \in \Omega_1, \ldots, \boldsymbol{\omega}^{L+k} \in \Omega_{L+k}$ and for all $k = 1, \ldots, N$.

e) The procedure can be repeated, with the entering data $\bar{\nu}_{k,n}^1$, to obtain HSPM approximations $\bar{\nu}_{k,n}^2(\boldsymbol{\omega}^1, \ldots, \boldsymbol{\omega}^{2L+N+k})$ of $\bar{\mu}_k^2$ for $k = 1, \ldots, N$.

f) Repeating this procedure over and over, after j timesteps, we provide the n-terms HSPM approximations $\bar{\nu}_{k,n}^j(\boldsymbol{\omega}^1, \ldots, \boldsymbol{\omega}^{jL+(j-1)N+k}) \rightharpoonup \bar{\mu}_k^j$ for all $\boldsymbol{\omega}^1 \in \Omega_1$, $\boldsymbol{\omega}^2 \in \Omega_2, \ldots, \boldsymbol{\omega}^{jL+(j-1)N+k} \in \Omega_{jL+(j-1)N+k}$, all $j = 1, \ldots, T_\Delta$ and all $k = 1, \ldots, N$, where $\Omega_l \subset \Omega$ with $P(\Omega_l) = 1$, for $l = 1, \ldots, T_\Delta(L+N)$.

Now, observe that we can find a family $\{Q_l\}_{l \in \mathbb{N}^*}$ of measurable maps $Q_l : \Omega \to \Omega$, with $P(Q_l^{-1}(A)) = 1$, for all $A \subset \Omega$ with $P(A) = 1$. For instance, we can consider $U, V : \Omega \to \Omega$, given by

$$U(\boldsymbol{\omega}) = U(\omega_1, \omega_2, \ldots, \omega_{2n-1}, \omega_{2n}, \ldots) := (\omega_1, \omega_3, \ldots \omega_{2n-1}, \omega_{2n+1}, \ldots), \tag{6.15}$$

$$V(\boldsymbol{\omega}) = V(\omega_1, \omega_2, \ldots, \omega_{2n-1}, \omega_{2n}, \ldots) := (\omega_2, \omega_4, \ldots, \omega_{2n}, \omega_{2n+2}, \ldots), \tag{6.16}$$

respectively, for all $\boldsymbol{\omega} = (\omega_1, \omega_2, \ldots, \omega_{2n-1}, \omega_{2n}, \ldots) \in \Omega$. Then it is sufficient to put $Q_1 = U$ and $Q_l := U \circ V^{l-1}$, $l = 2, 3, \ldots$ Let

$$\Omega_{\Delta t} := \bigcap_{l=1}^{T_\Delta(L+N)} Q_l^{-1}(\Omega_l). \tag{6.17}$$

Since $P(Q_l^{-1}(\Omega_l)) = 1$ for all $l = 1, \ldots, T_\Delta(L+N)$, clearly $P(\Omega_{\Delta t}) = 1$. Defining $\nu_{k,n}^j(\boldsymbol{\omega}) := \bar{\nu}_{k,n}^j(Q_1(\boldsymbol{\omega}), \ldots, Q_{jL+(j-1)N+k}(\boldsymbol{\omega}))$ for all $\boldsymbol{\omega} \in \Omega$, $j =$

$1, \ldots, T_\Delta$, $k = 1, \ldots, N$, it follows that $\nu_{k,n}^j(\boldsymbol{\omega}) \rightharpoonup \bar{\mu}_k^j$ as $n \to \infty$, for all $\boldsymbol{\omega} \in \Omega_{\Delta t}$, $j = 1, \ldots, T_\Delta$, $k = 1, \ldots, N$.

In particular, if $D(\cdot, \cdot)$ is the discrepancy introduced in Section 2., then

$$\lim_{n\to\infty} \max_{k=1,\ldots,N} \max_{j=1,\ldots,T_\Delta} D\left(\nu_{k,n}^j(\boldsymbol{\omega}), \bar{\mu}_k^j\right) = 0, \tag{6.18}$$

for almost all $\boldsymbol{\omega} \in \Omega$.

All these and Corollary 4.1 lead to our main result.

Let $\mathbf{f}(t)$ be the solution of equation (3.18), provided by Theorem 3.1 and let μ_k^t be given by $\mathrm{d}\mu_k^t(\mathbf{v}) := f_k(t, \mathbf{v})\mathrm{d}\mathbf{v}$, for all $t \geq 0$ and $k = 1, \ldots, N$. Consider some family $\{\Delta t_p\}_{p\in\mathbb{N}}$ of discretization timesteps as in Section 4.. For each Δt_p and for the initial data $\bar{\mu}_k^0$, consider the solutions $\bar{\mu}_{k,p}^j$ of (6.10), with $j = 1, \ldots, T_\Delta$ and $k = 1, \ldots, N$. For each $\bar{\mu}_{k,p}^j$, denote by $\nu_{k,p,n}^j$ the corresponding n-terms HSPM approximation obtained by the above scheme.

Similar to (2.25), we introduce the following notation $T_{\Delta p} := [[T/\Delta t_p]]$, for all $p \in \mathbb{N}$.

THEOREM **6.1** *For each sequence of timesteps $\Delta t_p \to 0$ as $p \to \infty$, there is a sequence of positive integers $n(p) \to \infty$ as $p \to \infty$, such that*

$$\lim_{p\to\infty} \max_{k=1,\ldots,N} \max_{j=1,\ldots,T_{\Delta p}} D\left(\nu_{k,p,n(p)}^j(\boldsymbol{\omega}), \mu_k^{j\cdot\Delta t_p}\right) = 0, \tag{6.19}$$

for almost all $\boldsymbol{\omega} \in \Omega$.

Proof. Let

$$d_{p,n}(\boldsymbol{\omega}) := \max_{k=1,\ldots,N} \max_{j=1,\ldots,T_{\Delta p}} D\left(\nu_{k,p,n}^j(\boldsymbol{\omega}), \bar{\mu}_{k,p}^j\right). \tag{6.20}$$

Consider some positive sequence $\varepsilon_p \downarrow 0$ as $p \to \infty$. Using (6.18), for each p, we obtain that

$$\lim_{n\to\infty} P(d_{p,n} > \varepsilon_p) = 0. \tag{6.21}$$

Then, for each p, we can choose $n = n(p)$, such that

$$P(d_{p,n(p)} > \varepsilon_p) \leq \frac{1}{p^2}. \tag{6.22}$$

Consequently,

$$\sum_{p=1}^{\infty} P(d_{p,n(p)} > \varepsilon_p) < \infty. \tag{6.23}$$

Then, for almost all $\boldsymbol{\omega} \in \Omega$,

$$\lim_{n\to\infty} d_{p,n(p)}(\boldsymbol{\omega}) = 0. \tag{6.24}$$

Now, by Corollary 4.1, we conclude the proof of the Theorem. □

This theorem represents a space homogeneous reactive correspondent to the main result in the Babovsky-Illner simulation scheme for the classical Boltzmann equation (Theorem 7.1 of Ref. [5]).

Note that the numerical effort of the method is at most, $O(n \log n)$ (the dominant contribution being introduced by the random selections of Theorem 5.1.2, i.e. *(second selection) Step* 2). However, under additional conditions on $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}$, the sum (6.10) the numerical effort can be improved.

We consider the following simple case. Denote $\mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}} := \left\{\mathbf{w}' \in \mathbb{R}^{3|\boldsymbol{\alpha}|} | 0 < W_{\boldsymbol{\alpha}}(\mathbf{w}') - 2^{-1}(\sum_{n=1}^{N} \alpha_n m_n) V_{\boldsymbol{\alpha}}(\mathbf{w}')^2 - \sum_{n=1}^{N} \beta_n E_n\right\}$ (we recall that $W_{\boldsymbol{\alpha}}(\mathbf{w})$ is the energy defined in Section 2). By Lemma 3.1, $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}) \geq 0$ on $\mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}} \times \Omega_{\boldsymbol{\beta}}$. Suppose that in (6.2 -6.6), we have $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}) > 0$ on $\mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}} \times \Omega_{\boldsymbol{\beta}}$ for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M}$. Taking into account the form of the element $\mathrm{d}\mathbf{n}$ on $\Omega_{\boldsymbol{\beta}}$ in spherical coordinates (when (6.9) is obtained from (6.2 -6.6)) it follows easily that in (6.9), each function $q_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,\phi)$ can be constructed such that the set $\{\theta | q_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,\phi) = 0\}$ is finite and does not depend on the choice of $(\mathbf{w},\phi) \in \mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}} \times [0,2\pi)$. Consequently, for each $\boldsymbol{\beta} \in \mathcal{B}$, there is a measurable set $\Theta_{\boldsymbol{\beta}} \subset [0,\pi)^{3|\boldsymbol{\beta}|-5}$ such that $q_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,\phi) > 0$, for all $\mathbf{w} \in \mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}}$, $\theta \in \Theta_{\boldsymbol{\beta}}$, $\phi \in [0,2\pi)$, $\boldsymbol{\alpha} \in \mathcal{A}$. Denote

$$I_k(\phi;\mathbf{w},\theta) := \int_0^{\phi} q_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,\rho)\mathrm{d}\rho, \qquad \phi \in [0,2\pi)\,. \tag{6.25}$$

Then, for all $\mathbf{w} \in \mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}}$, $\theta \in \Theta_{\boldsymbol{\beta}}$, fixed, (6.25) defines an invertible map

$$[0,2\pi) \ni \phi \to I_k(\phi;\mathbf{w},\theta) \in [0, I_k(2\pi;\mathbf{w},\theta))\,, \tag{6.26}$$

with the inverse I_k^{-1}. In each integral of (6.9), with respect to $\mathrm{d}\phi$, we perform the change of variable $\phi = I_k^{-1}(y;\mathbf{w},\theta)$. Define

$$\tilde{H}_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,y) = H_{\boldsymbol{\alpha},\boldsymbol{\beta},k}(\mathbf{w},\theta,I_k^{-1}(y;\mathbf{w},\theta)). \tag{6.27}$$

We can choose some measurable sets

$$\mathcal{C}_{\boldsymbol{\alpha}\boldsymbol{\beta}} \subseteq \mathbb{R}^{3|\boldsymbol{\alpha}|} \times [0,\pi)^{3|\boldsymbol{\beta}|-5} \times \mathbb{R}_+, \text{ for } \boldsymbol{\alpha} \in \mathcal{A}, \boldsymbol{\beta} \in \mathcal{B},$$

such that, (6.9) takes the following form

$$\int_{\mathbb{R}^3} \varphi(\mathbf{v})\mathrm{d}\bar{\mu}_k^j(\mathbf{v}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A},\boldsymbol{\beta}\in\mathcal{B}} \int_{\mathcal{C}_{\boldsymbol{\alpha}\boldsymbol{\beta}}} (\varphi \circ \tilde{H}_{\boldsymbol{\alpha},\boldsymbol{\beta},k})(\mathbf{w},\theta,y)\mathrm{d}\bar{\mu}_{\boldsymbol{\alpha}}^{j-1}(\mathbf{w})\mathrm{d}\theta dy. \tag{6.28}$$

For applications it is important to observe that the conclusion remains the same if weaker conditions are imposed on $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}$, e. g. if one supposes that for each $\boldsymbol{\alpha},\boldsymbol{\beta} \in \mathcal{M}$, $r_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}) > 0$ on $\mathcal{D}_{\boldsymbol{\alpha}\boldsymbol{\beta}} \times \Omega_{\boldsymbol{\beta}}$ except a countable set, etc.

Obviously, (6.28) has the form (6.10), but has the important property that if $\bar{\mu}_k^{j-1}$, for $k = 1, \ldots, N$ are HSPM, after *Step* 1 *(first selection)* the output measures are also a HSPM.

In order to obtain $\bar{\mu}_k^j$, for $k = 1, \ldots, N$ as HSPM with the same number of terms as $\bar{\mu}_k^{j-1}$, we can apply the following immediate corollary of Theorem 5.1.2, which introduces a numerical complexity of only $O(n)$.

COROLLARY **6.1** *Suppose that there is a positive measure μ on $\mathbb{R}^m$, absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^m$, such that*

$$\frac{1}{m_n} \sum_{l=1}^{m_n} \mu_{n,l} \rightharpoonup \mu, \text{ as } n \to \infty. \tag{6.29}$$

Define $\mu_{n,i}(\boldsymbol{\omega}) := \mu_{n,l}|_{l=\tilde{c}_{n,i}(\boldsymbol{\omega})}$ for all $\boldsymbol{\omega} \in \Omega$, all $i \in \mathcal{I}_n$ and $n \in \mathbb{N}^*$. Let $\mathbb{N}^* \ni n \to k_n \in \mathbb{N}^*$ be a sequence such that $k_n \leq m_n$, for all $n \in \mathbb{N}^*$ and

$$\sum_{n=1}^{\infty} \frac{1}{k_n^2} < \infty. \tag{6.30}$$

Then, for $P-$almost all $\boldsymbol{\omega}$,

$$\sigma_{3,n}(\boldsymbol{\omega}) := \frac{1}{k_n} \sum_{i=1}^{k_n} \mu_{n,i}(\boldsymbol{\omega}) \rightharpoonup \mu \text{ as } n \to \infty. \tag{6.31}$$

Further we can proceed as in the scheme constructed before, but without applying Theorem 5.1.2. Instead we apply Corollary 6.1. The scheme reduces to iterations alternating with selections, and the conclusion of Theorem 6.1 remains valid. The numerical effort becomes $O(n)$.

Finally remark that if (2.18) reduces the classical Boltzmann equation, for the one-component simple gas, then the sum in the r.h.s of (6.28) can be compressed to a unique term as in Ref. [4]. In general, this is not possible in the case of gas mixtures.

7. Concluding Remarks

From the above analysis, it follows that besides a convenient existence theory, only the conservation of the total mass is needed to introduce the numer-

ical scheme described here. The other properties (e.g. detailed balance, H-Theorem) of the Wang-Chang-Uhlenbeck-de Boer and Ludwig and Heil system of equations play no role in this algorithm. Note that, the numerical scheme can also be used and when the detailed balance does not hold, e.g., for models where we ignore some recombination processes (as in the situation when we consider the collisional dissociation, but neglect the recombination by triple collisions Ref. [24]).

We discuss possible generalizations as well as some limitations of the results.

1^0 In the case of non-reacting gas mixtures one can obtain similar numerical schemes for the space-dependent equation (2.10), in the frame of the theory of existence of solutions of Ref. [17]. This can be done by adapting directly the spatial cell homogenization method of Ref. [5].

2^0 In the case of reacting gas mixtures, one can also obtain similar numerical schemes for the space-dependent equation (2.10). To this end, the adaptation of the spatial cell homogenization method of Ref. [5] is not as straightforward as it appears. This is due to the collisions that produce new particles in a given spacial cell. For this purpose, we need "to establish" the space position in the cell for each "new born" particle and at the same time, to keep the control on convergence.

3^0 Assumption (3.13) replaces in the reactive model the boundedness condition on the collision law used in Ref. [4, 5]. This condition is essential for the control of the positivity of the solutions in the time-discretized equation (4.1). Indeed, Assumption (3.13) is restrictive from an analytical point of view. Nevertheless, for practical purposes, it is satisfactory for those models where the high energy-tail of the gas consists of very few molecules (see Ref. [7]).

The existence of unique positive solutions to (2.10) and (2.18) can be proved for more general transition functions $K_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ (see Ref. [18]). The simulation scheme can be also extended in this respect, but the (possible) singularities of $K_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ must not destroy the continuity of the functions $r_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ and $p_{\boldsymbol{\alpha},\boldsymbol{\beta}}$ (necessary for the convergence in the weak sense of the measures).

4^0 One can improve the approximation algorithm as follows. Instead of assigning to each species the same number of terms in HSPM, one can fix a given number of terms n for all the species. Then, when we apply the selection algorithm given by Theorem 5.1.2 (or Corollary 6.1), we can allocate to each species a number of terms "proportional" to its mass, such that the total number of terms for all the species to be (approximative) n. The same is also valid for the approximation of the initial data. By example if we designate by n_k the number of terms corresponding to the species $k = 1, \ldots, N$, then

we define

$$n_k := \left[\left[\left[n \cdot \frac{m_k \int_{\mathbb{R}^3} f_k^0(\mathbf{v})\mathrm{d}\mathbf{v}}{\sum_{l=1}^{N} m_l \int_{\mathbb{R}^3} f_l^0(\mathbf{v})\mathrm{d}\mathbf{v}} \right]\right]\right]. \tag{7.1}$$

5^0 In this numerical scheme there are three essential sources of approximation errors.

1. The errors from the approximation of the initial data.
2. The errors produced by the time discretization.
3. The errors introduced by stochastic selections.

The contribution of the stochastic errors over the time discretized scheme can be illustrated as it follows. Giving, for the chemical species $k = 1, \ldots, N$, an initial data, say $\nu_k^{0,0}$ of the form (2.22) the algorithm follows the computational chain

$$\nu_k^{0,0} \to \nu_k^{1,1} \to \nu_k^{2,2} \to \ldots \to \nu_k^{T_\Delta - 1, T_\Delta - 1} \to \nu_k^{T_\Delta, T_\Delta} \tag{7.2}$$

corresponding to the diagonal of the scheme

$$\begin{array}{ccccccccccc}
\nu_k^{0,0} & \longrightarrow & \nu_k^{0,1} & \longrightarrow & \nu_k^{0,2} & \longrightarrow & \ldots & \longrightarrow & \nu_k^{0,T_\Delta-1} & \longrightarrow & \nu_k^{0,T_\Delta} \\
 & & \wr\!\!\!\wr & & & & & & & & \\
 & & \nu_k^{1,1} & \longrightarrow & \nu_k^{1,2} & \longrightarrow & \ldots & \longrightarrow & \nu_k^{1,T_\Delta-1} & \longrightarrow & \nu_k^{1,T_\Delta} \\
 & & & & \wr\!\!\!\wr & & & & & & \\
 & & & & \nu_k^{2,2} & \longrightarrow & \ldots & \longrightarrow & \nu_k^{2,T_\Delta-1} & \longrightarrow & \nu_k^{2,T_\Delta} \\
 & & & & & & & & \vdots & & \vdots \\
 & & & & & & & & \wr\!\!\!\wr & & \\
 & & & & & & & & \nu_k^{T_\Delta-1,T_\Delta-1} & \longrightarrow & \nu_k^{T_\Delta-1,T_\Delta} \\
 & & & & & & & & & & \wr\!\!\!\wr \\
 & & & & & & & & & & \nu_k^{T_\Delta,T_\Delta}
\end{array} \tag{7.3}$$

Here, the horizontal chains represent the exact iterations of the time discretized equations, such that for each $j = 0, \ldots, T_\Delta - 1$ and $p = j+1, \ldots, T_\Delta$ the measure $\nu_k^{j,p}$ is given as $(p-j)$ - th iteration for the input data $\nu_k^{j,j}$. In addition, $\nu_k^{j,j}$ is provided by random selection form $\nu_k^{j-1,j}$, for $j = 1, \ldots, T_\Delta$.

The above computational chain shows that one can expect that the errors due to the random selections increase when the timestep Δt decreases. Indeed,

such a behavior was observed in numerical applications Ref. [13, 12]. Some theoretical estimations on the errors Ref. [12] prove that the probabilistic errors ε behave like

$$\varepsilon \sim \frac{1}{\Delta t \cdot \sqrt{n}}. \tag{7.4}$$

Consequently, when we decrease the timestep (to improve the errors for the time discretization, Proposition 4.1.b) we shall increase the number of terms for the initial approximation, in order to keep the stochastic errors in acceptable limits.

8. Appendix

Proof of Lemma 3.1.

Let $n \in \mathbb{N}^*$ and let $a_1, \ldots, a_n > 0$, be some constants. Consider the positive quadratic form defined on $\mathbb{R}^{3n}$ by

$$T := T(\mathbf{v}_1, \ldots, \mathbf{v}_n) = \sum_{i=1}^{n} a_i \mathbf{v}_i^2, \tag{8.1}$$

where $\mathbf{v}_i \in \mathbb{R}^3$, for all $i = 1, \ldots, n$. One introduces the Jacobi-type transformation

$$\mathbb{R}^{3n} \ni (\mathbf{v}_1, \ldots, \mathbf{v}_n) \to (\underline{V}, \xi) \in \mathbb{R}^3 \times \mathbb{R}^{3n-3}, \tag{8.2}$$

where

$$\underline{V} := (\sum_{i=1}^{n} a_i)^{-1} \sum_{i=1}^{n} a_i \mathbf{v}_i, \tag{8.3}$$

and $\xi := (\xi_1, \ldots, \xi_{n-1})$, with

$$\xi_i := \left[\frac{1}{a_{i+1}} + \frac{1}{\sum\limits_{j=1}^{i} a_j} \right]^{-\frac{1}{2}} \left[\mathbf{v}_{i+1} - \frac{\sum\limits_{j=1}^{i} a_j \mathbf{v}_j}{\sum\limits_{j=1}^{i} a_j} \right], \tag{8.4}$$

for $i = 1, \ldots, n-1$.

By (8.2), the form T takes the form

$$T = T(\underline{V}, \xi) = \left(\sum_{i=1}^{n} a_i \right) \cdot \underline{V}^2 + \xi^2. \tag{8.5}$$

Define

$$W_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}) := W_{\boldsymbol{\alpha}}(\mathbf{w}) - \frac{1}{2}\left(\sum_{n=1}^{N}\alpha_n m_n\right)\cdot V_{\boldsymbol{\alpha}}(\mathbf{w})^2 - \sum_{n=1}^{N}\beta_n E_n, \tag{8.6}$$

and

$$t_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}) := \begin{cases} [W_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w})]^{1/2} & \text{if} \quad W_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}) \geq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{8.7}$$

Now, consider the form on $\mathbb{R}^{3|\boldsymbol{\beta}|}$,

$$T_{\boldsymbol{\beta}}(\mathbf{u}) := W_{\boldsymbol{\beta}}(\mathbf{u}) - \sum_{n=1}^{N}\beta_n E_n \tag{8.8}$$

and a corresponding Jacobi-type transformation as in (8.2),

$$\mathbb{R}^{3|\boldsymbol{\beta}|} \ni \mathbf{u} \to (\underline{V}, \xi) \in \mathbb{R}^3 \times \mathbb{R}^{3|\boldsymbol{\beta}|-3}, \tag{8.9}$$

with $\xi := (\xi_1, \ldots, \xi_{|\boldsymbol{\beta}|-1})$, where $\xi_i \in \mathbb{R}^3$, for all $i = 1, \ldots, |\boldsymbol{\beta}| - 1$. Denote by $\Delta_{\boldsymbol{\beta}}$ the Jacobian determinant of the transformation. Let ξ be represented in spherical coordinates on $\mathbb{R}^{3|\boldsymbol{\beta}|-3}$, $\xi = r\mathbf{n}$, with $(r, \mathbf{n}) \in [0, \infty) \times \Omega_{\boldsymbol{\beta}}$. Consider the inverse map

$$\mathbb{R}^3 \times \mathbb{R}_+ \times \Omega_{\boldsymbol{\beta}} \ni (\underline{V}, r, \mathbf{n}) \to \mathbf{u}(\underline{V}, r, \mathbf{n}) \in \mathbb{R}^{3|\boldsymbol{\beta}|} \tag{8.10}$$

of the transformation $\mathbf{u} \to (\underline{V}, r, \mathbf{n})$ and set

$$\mathbf{u}_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n}) := \mathbf{u}(\underline{V}, r, \mathbf{n})|_{\,\underline{V}=V_{\boldsymbol{\alpha}}(\mathbf{w}), r=t_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w})}. \tag{8.11}$$

Obviously, for all $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{M}$ such that (2.6) is satisfied, we have

$$V_{\boldsymbol{\beta}}(\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n})) = V_{\boldsymbol{\alpha}}(\mathbf{w}) \qquad W_{\boldsymbol{\beta}}(\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n})) = W_{\boldsymbol{\alpha}}(\mathbf{w}). \tag{8.12}$$

Define

$$\begin{aligned} p_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n}) &:= 2^{-1}\Delta_{\boldsymbol{\beta}} \cdot t_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w})^{3|\boldsymbol{\beta}|-5} K_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{u}_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n}), \mathbf{w}), \\ r_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n}) &:= 2^{-1}\Delta_{\boldsymbol{\beta}} \cdot t_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w})^{3|\boldsymbol{\beta}|-5} K_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{w}, \mathbf{u}_{\boldsymbol{\beta}\boldsymbol{\alpha}}(\mathbf{w}, \mathbf{n})). \end{aligned} \tag{8.13}$$

From (8.12), one obtains property i) of the Lemma 3.1. Property ii) follows from the definitions introduced in (8.7) and (8.13).

The limits (3.6) and (3.7), can be obtained from (3.3) and (3.4). We start the computation with the integral upon d$\mathbf{u}$, by choosing $(\underline{V}, r, \mathbf{n})$ as new integration variables such that $\mathbf{u} = \mathbf{u}(\underline{V}, r, \mathbf{n})$. Since $\mathbf{f}_{\boldsymbol{\alpha}} \in C_c(\mathbb{R}^{3|\boldsymbol{\alpha}|})$ and $\mathbf{f}_{\boldsymbol{\beta}} \in C_c(\mathbb{R}^{3|\boldsymbol{\beta}|})$, using the properties of $K_{\boldsymbol{\alpha},\boldsymbol{\beta}}$, δ_ε^3, δ_η and $\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}$, we obtain (3.6) and (3.7) by repeated application of Lebesgue's dominated convergence theorem.

Using a similar argument as in the proof (3.6), for all $f \in C_c(\mathbb{R}^{3|\boldsymbol{\beta}|})$ and $\varphi \in C_b(\mathbb{R}^{3|\boldsymbol{\alpha}|})$, we get

$$\begin{aligned} &\lim_{\eta\to 0}\lim_{\varepsilon\to 0}\int_{\mathbb{R}^{3|\boldsymbol{\alpha}|}\times\mathbb{R}^{3|\boldsymbol{\beta}|}} \varphi(\mathbf{w})\sigma^{\varepsilon,\eta}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{u},\mathbf{w})f(\mathbf{u})\mathrm{d}\mathbf{w}\mathrm{d}\mathbf{u} \\ &= \int_{\mathbb{R}^{3|\boldsymbol{\alpha}|}\times\boldsymbol{\Omega}_{\boldsymbol{\beta}}} \varphi(\mathbf{w})p_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n})f(\mathbf{u}_{\boldsymbol{\beta},\boldsymbol{\alpha}}(\mathbf{w},\mathbf{n}))\mathrm{d}\mathbf{w}\mathrm{d}\mathbf{n}, \end{aligned} \tag{8.14}$$

giving the left side of (3.9). To obtain the right side of (3.9), we repeat the procedure, but first we perform the integral upon d$\mathbf{w}$ in the left side of (8.14) (using the change of variables induced by the Jacobi-type transformation $\mathbb{R}^{3|\boldsymbol{\alpha}|} \ni \mathbf{w} \to (\underline{V}, \xi) \in \mathbb{R}^3 \times \mathbb{R}^{3|\boldsymbol{\alpha}|-3}$, associated to the form $T_{\boldsymbol{\alpha}}(\mathbf{w}) = W_{\boldsymbol{\alpha}}(\mathbf{w}) - \sum_{n=1}^N \boldsymbol{\alpha}_n E_n$, and then taking the representation of $\xi \in \mathbb{R}^{3|\boldsymbol{\alpha}|-3}$ in spherical coordinates). □

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