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Handbook of Numerical Methods for Hyperbolic Problems

Applied and Modern Issues

Volume Editors Rémi Abgrall and Chi-Wang Shu

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Applied and Modern Issues

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Editors' Introduction

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These two volumes represent the volumes 17 and 18 of Handbook of Numerical Analysis. It is entirely devoted to the numerical methods designed for approximating the solution of hyperbolic equations, or of equations that write as a sum of operators where the most important, in terms of the behaviour of the solution, is the hyperbolic one. An example is the Navier–Stokes equations with high Reynolds number where the solution behaviour is essentially dictated by the hyperbolic operator (here the Euler system), except in boundary layers because of the boundary conditions.

Hyperbolic partial differential equations appear often in applications. The most important application, already mentioned, is fluid dynamics, including specific flows such as multiphase flows, magnetohydrodynamics, water waves, etc. Other application areas include Maxwell equations, kinetic equations, traffic flow models and networks, etc. The solutions of hyperbolic partial differential equations often involve discontinuities, making mathematical analysis and numerical simulations difficult. In the past few decades there has been a large amount of literature in the design, analysis and application of various numerical algorithms for solving hyperbolic equations. The current volumes attempt to have experts in different types of algorithms write concise summaries so that the readers can find a variety of algorithms under different situations and become familiar with their relative advantages and limitations.

This is a formidable task. We had to make choices because the field has grown tremendously since the early ages dating back to von Neumann in the United States and researchers from the former Soviet Union such as Rusanov and Godunov. This field has grown up for various reasons. The demand on diverse high tech areas ranging from airplanes and rockets, to the nuclear and car industries as well as more recently the green industry, to name just a few, necessitates to master better and better tools to improve performance. If it was possible in the early ages to rely on analytical solutions and experimental facilities only, this is no longer the case because of various constraints: economical, technological (weight, etc.), energy consumption, etc. This evolution has needed improved algorithms, i.e., more and more accurate as well as more and more robust ones. Hence the research on algorithm has grown up and then exploded since the early 1970s.

In parallel, and also triggered by the same needs, computers have been more and more powerful from scalar, to vectors, then parallel and now massively parallel and hybrid architectures. This evolution of technology has also had a strong impact on the algorithms development.

Because of its success, it is now possible to compute more and more complicated problems, both in terms of geometry and physics.

There is still a lot to do to improve and understand the numerical methods designed for hyperbolic problems. The aim of these two volumes is to give a picture of the current state of the art.

In order to introduce the subject, we have asked Professor Dafermos from Brown University to provide a short summary on the theory of hyperbolic equations. Then, if one looks at the table of content, one would realize that we have tried to cover not only the classical topics, such as the finite volume method and the Riemann solvers that are the building blocks of many of the algorithms, but also less standard methods. Examples include algorithms for computing sharp transition propagated by linearly degenerate waves. Other examples are given by the ENO/WENO family. In that case we have tried to go over the classical description, by giving some analysis of the methods. Other high-order methods are also considered such as the discontinuous Galerkin (DG) ones, the more recent hybrid DG schemes, high-order finite element methods, front-tracking methods, methods for Lagrangian hydrodynamics, entropy stable schemes, etc. Time discretisation is also considered, as well as more specialized problems like the simulation of flows with low Mach numbers, level set techniques, numerical methods for Hamilton–Jacobi equations, etc.

Unfortunately, it is not possible, even in two quite thick volumes, to provide an exhaustive coverage of the state of the art. Even though the table of content seems to be exhaustive, many topics are still missing. For example, we have chosen to be quite restrictive on the subject of time stepping: there is no coverage on ADER and IMEX methods. The handling of problems with source terms is touched by chapters 5 and 6 (well-balanced schemes and asymptotic-preserving schemes), but there is no direct coverage on stiff source terms. If we have a chapter on methods for Cartesian meshes, there is no direct coverage on the application of immersed boundary methods. Similarly we have chosen to consider the problem of meshing in a specific way; there is no direct coverage on adaptive mesh refinement (AMR). The problem on boundary conditions is considered in chapter 2 this volume (volume 18) and chapter 19 previous volume (volume 17) of the handbook (SAT-SPB schemes and inverse Lax–Wendroff procedure), but much more could have been said. It was simply impossible to cover the whole field, and we apologize for this.

To end this introduction, we would like to thank all the contributors to these volumes, as well as the referees. Both have been extremely efficient.

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Chapter 15

Deterministic Solvers for Nonlinear Collisional Kinetic Flows: A Conservative Spectral Scheme for Boltzmann Type Flows

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Chapter Outline

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ABSTRACT

We present an overview of deterministic solvers for the Boltzmann and Landau equations inspired by their Fourier space representation as weighted convolutional forms, where the later can be obtained as a grazing collision limit of the former. This presentation offers an introduction to the area and elaborates on recent results for conservative spectral Lagrangian schemes applied to several applications ranging from homogeneous flows for Coulomb potentials given by the Landau equation by an approximating of a corresponding Boltzmann model with grazing transition scattering rates, to a full conservative approach for Vlasov–Poisson–Landau system for electron–ion dynamics. This conservative method is enforced by a Lagrangian constrained optimization problem that and conservation correction estimates that give place to semidiscrete error estimates and long-time convergence to statistical equilibrium states given by *Maxwellians* distributions.

Keywords: Nonlinear integral equations, Rarefied gas flows, Boltzmann and Landau Fokker Plank equations, Deterministic numerical approximations to kinetic equations, Conservative spectral methods

2010 MSC: 45E99, 35A22, 76X05, 76P05, 82C05, 65C20, 65C30

1 INTRODUCTION

1.1 Kinetic Evolution Models

The numerical solutions of kinetic evolution transport given by integral equations of Boltzmann type needs the underlying understanding of the problem to be approximated: the evolution of a probability density function usually described by a Hamiltonian particle transport encountering interactions. Thus, before we discuss different aspects of deterministic solvers for such models, we introduced the basic notions associated to kinetic transport evolution models.

Our starting point is to recall that complex particle model systems with exchangeability properties yield the propagation of chaos property, that is, the particle system can be models by the evolution of independent and identically distributed (iid) continuous random variables or probability density measures. These models appear in many contexts of classical and quantum statistical physics, and more recently in novel applications to social dynamics of multiagent interactions defined by some multiplicatively interacting stochastic processes. The models we shall be considered share is a unified general framework of material transport dynamics can be derived from the so-called *Master Equations* derived for the time evolution of a particle system modelled as being in exactly one of the countable number of admissible states at any given time, where switching between states are treated probabilistically when interactions occur. Such evolution is described by associating a probability density of states through discrete or continuous random variables. Interactions may be of "mean field" type when macroscopic forces depending on, either particle distribution averages, or particles of the same kind usually refer as *collisions*. Typical examples of "mean field" type interactions result in the so-called *collisionless* systems of transport models such as Vlasov–Poisson or Vlasov–Maxwell systems for plasma dynamics of charged particles.

However, when interactions due to *collisions* occur and the "switching" of states are described by a time-independent operator, the model represents a *kinetic evolution* and the process is *Markovian*. Such process may also include *birth and death* rates, meaning that probability density is injected in (birth) or taken away from (death) the system, and so the process is not in equilibrium. Examples of such models are the transport dynamics of classical kinetic collisional transport given by Boltzmann or Landau–Fokker–Plank type equations that may include mean field interactions to obtain a Vlasov–Poisson or Vlasov–Maxwell collisional plasma transport system (Chapman and Cowling, 1970; Graham and Méléard, 1999).

1.2 Binary Collisional Models and Double Mixing Convolution Forms

Rigorous justification of the propagation of chaos or *Stosszahlansatz* relies on contemporary ergodic theory and related areas in probability theory (Chapman and Cowling, 1970; Pulvirenti et al., 2014). We assume here its validity, implying that the system of N-particle interactions can be reduced to a closed form involving products of a single point probability density function (*pdf*) denoted by $f(x, v, t)$ solving a nonlocal, linear or multilinear structure in state space defined by $v \in \mathbb{R}^n$. In the case of binary interactions such *pdf* satisfies the following nonlocal weak form

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^d} f(x,v,t)\varphi(v)\mathrm{d}v &:= \int_{\mathbb{R}^d} Q(f,f)(x,v,t)\,\varphi(v)\mathrm{d}v \\ &= \kappa\int_{\mathbb{R}^d\times\mathbb{R}^d} f(x,v,t)f(x,v-u,t)\left(\int_{\Omega}(\varphi(v')-\varphi(v))B(u,\sigma)\mathrm{d}\sigma\right)\mathrm{d}u\mathrm{d}v\end{aligned} \tag{1}$$

where the $u = v - v_*$ is the relative position for any interacting states pairs (v, v_*) changing into (v', v'_*), for v fixed and v' determined by an *interaction law* with $v' = v'(v, v_*, \sigma)$ and $v'_* = v'_*(v, v_*, \sigma)$, with arbitrary $\sigma \in \Omega$ a manifold that determines the postcollisional relative position $u' = v' - v'_*$, for an arbitrary state $v_* \in \mathbb{R}^n$. Such manifold is the sphere S^{n-1} when the interaction correspond to particles characterized by indistinguishable spheres interacting by conserving centre of mass and local energies. The parameter κ quantifies the scaled mean free path in between interactions, and it is assumed to be or oder of unity in rarefied regimes. The material derivative d/dt refers to the Lagrangian formulation of Hamiltonian dynamics of mixing (x, v) states, as in classical to particle plasma physics, and they are viewed as the divergence-free dynamics of space-momentum mixing. The corresponding interacting pairs transition probability rates from (v, v_*) to (v', v'_*) are quantified by the collision kernel $B(u, \sigma)$. This equation is nonlocal and linear in the case when $f(x, v - u, t)$ is replaced by a know probability density. Thus, we define the *Kac Master equation* formulation as a *double mixing convolution* structure

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^N} f(x,v,t)\varphi(v)\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)(x,v,t)\,\varphi(v)\mathrm{d}v \tag{2}$$

$$= \kappa\int_{\mathbb{R}^d\times\mathbb{R}^d} f(x,v,t)f(x,v-u,t)G_{\varphi,B}(u,v)\mathrm{d}u\,\mathrm{d}v. \tag{3}$$

The weight function $G_{\varphi,B}(u, v)$ is a mixing form of premixing and postmixing positions in v-space that depends only on the state variable v and its relative position state u. This weight function models the σ-average of the interaction on the Ω manifold, i.e.

$$G_{\varphi,B}(u,v) = \int_{\Omega} (\varphi(v') - \varphi(v))\,B(v,u,\sigma)\mathrm{d}\sigma, \tag{4}$$

that depends on the σ-average of the test function φ on the exchange law of states multiplied to the transition probability interaction rates $B(u, \sigma)$. These weight functions $G_{\varphi,B}(u, v)$ are often nonlinear and encode most of the information about, not only, the dynamics of interactions but also the regularity of the solution to such equation as much the decay rate to equilibrium states. More precisely,

(1) The interaction law $v' = v'(v, v_*, \sigma)$; $v'_* = v'_*(v, v_* \sigma)$, microreversible or not, determines the space of *collision invariants*: all those $\varphi(v))$ that nullify the weight function $G_{\varphi,B}(u, v)$. These collision invariants select the properties of the stationary states.

(2) Propagation of chaos assumption and time irreversibility: *decorrelation before* the next interaction is encoded in the difference $\varphi(v') - \varphi(v)$ of the weight function and presets stability for the flow. In particular, when the interaction is microreversible and the transition probability rate function $B(u, \sigma)$ has symmetric properties consistent with such microreversibility, then setting $\varphi(v) = \log f(v)$, the monotonicity of the logarithmic function yields the H-theorem (Cercignani et al., 1994)

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^N} f(x,v,t)\log(v)\,\mathrm{d}v \int_{\mathbb{R}^d} Q(f,f)(x,v,t)\log(v)\mathrm{d}v$$
$$= \int_{\mathbb{R}^d\times\mathbb{R}^d} f(x,v,t)f(x,v-u,t)\left[\int_{\Omega} (\log(v') - \log(v))B(v,u,\sigma)\mathrm{d}\sigma\right]\mathrm{d}u\,\mathrm{d}v \leq 0. \tag{5}$$

In the particular case of elastic interactions conserving centre of mass and local energy, both items *(1)* and *(2)* imply that the only stationary state is a Gaussian distribution in v-space, called the equilibrium Maxwellian distribution, defined by the moments corresponding to the collision invariants associated with the initial data $f_0(v) \geq 0$ for a.e. $v \in \mathbb{R}^d$ and $\int_{\mathbb{R}^d} f_0(v)(1+|v|^2)\,\mathrm{d}v < \infty$. In the limit as $t \to +\infty$, we expect that $f(v, t)$ converges to the *equilibrium Maxwellian* distribution, i.e.

$$f(t,v) \to M[m_0, u_0, T_0](v) := m_0(2\pi T_0)^{-d/2} \exp\left(-\frac{|v-u_0|^2}{2T_0}\right), \tag{6}$$

where, if $m_0 > 0$ is the density mass, and the *moments or observables* are defined by

$$m_0 := \int_{\mathbb{R}^d} f_0(v)\,\mathrm{d}v, \quad u_0 := \frac{1}{m_0}\int_{\mathbb{R}^d} f_0(v)\,\mathrm{d}v, \quad T_0 := (\mathrm{d}m_0)^{-1}\int_{\mathbb{R}^d} |v-u_0|^2 f_0(v)\,\mathrm{d}v$$

while $f(v, t) = 0$ for a.e. $(v,t) \in \mathbb{R}^d \times \mathbb{R}^+$ if $m_0 = 0$. The quantities m_0, u_0 and T_0 are the density mass, mean and variance, associated to probability density $f(v, t)$.

(3) The transition probability interaction rate operator $B(u, \sigma)$, or *collision kernels*, encodes not only regularity but also quantitative properties of solutions, as well as decay rates to equilibrium. For example, in the classical particle physics dynamics case, the dependence of $|u| = |v - v_*|$ relates to intermolecular potentials rates between pairs of interacting particles. In addition, the dependence on σ encodes the rate of collisions depending on the direction of the phase variables before and after the interaction.

(4) *The double mixing convolution structure is changed into a weighted convolution by the Fourier transform:* We observed in Gamba and Tharkabhushanam (2009) that if the interaction law satisfies that the post–pre difference of states $v' - v$ depends only on the relative variable $u = v - v_*$ and σ, i.e., $v' - v = \omega(u, \sigma)$ (like in most particle systems of elastic or inelastic interactions) then, when testing the collisional integral with $\varphi(v) = \exp(-iv\cdot\zeta)$ in (1) and (2), it yields an identity for the Fourier transformed equation just in the v-variable, classically defined by $\hat{\ }(\zeta) = \mathcal{F}_{v\to\zeta}(f(v))(\zeta) = (2\pi)^{d/2}\int_{\mathbb{R}^d} e^{-i\zeta\cdot v} f(v)\mathrm{d}v$, to obtain

$$\hat{Q}(f,f)(\zeta) = \frac{1}{(\sqrt{2\pi})^d}\int_{\mathbb{R}^d} e^{-i\zeta\cdot v} Q(f,f)(v)\mathrm{d}v = \kappa\int_{\mathbb{R}^d} \mathcal{F}(f(v)f(v-\mathbf{u}))(\zeta)\mathcal{G}_B(\zeta,u)\mathrm{d}u$$
$$\text{with the weight function} \quad \mathcal{G}_B(\zeta,u) = \int_{\sigma\in\Omega} [e^{-i\frac{1}{2}\zeta\cdot\omega(u,\sigma)} - 1]B(u,\sigma)\,\mathrm{d}\sigma. \tag{7}$$

Consequently, $\hat{Q}(f,f)(\zeta)$ is also a *weighted convolution* of $\hat{f}(\zeta)$. In particular, the Boltzmann evolution in Fourier space is

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{f}(\zeta) = \hat{Q}(f,f)(\zeta) = \kappa\int_{\xi\in\mathbb{R}^d} \hat{G}_B(\zeta,\xi)\hat{f}(\xi)\hat{f}(\xi-\zeta)\mathrm{d}\xi \quad \text{with} \quad \hat{G}_B(\zeta,\xi) = \mathcal{F}_{u\to\xi}\mathcal{G}_B(\zeta,u). \tag{8}$$

Remark. Both $\mathcal{G}_B(\zeta, u)$ and $\hat{G}_B(\zeta, \xi)$ can be viewed as *symbol* of the multilinear integral operator (as the analogue to symbols of PDE's).

1.3 Classical Elastic Collisional Transport Theory: The Boltzmann Equation

Eqs. (1) and (2) are exactly the weak (or Maxwell) formulation of the collisional Boltzmann equation for elastic, inelastic interaction or collisional dynamics given by

$$
\begin{aligned}
&v' = v + \frac{\beta}{2}(|u|\sigma - u) \text{ and } v'_* = v - \frac{\beta}{2}(|u|\sigma - u) \text{with relative velocity } \ u = v - v_*,\\
&\qquad B(u,\sigma) = |u|^\lambda\, b(\hat{u}\cdot\sigma), \text{with } d < \lambda \leq 1,\ \ \hat{u} = \frac{u}{|u|} \text{ and}\\
&\qquad \cos\theta = \frac{(\hat{u},\sigma)}{|u|}, \text{ with } \theta \text{ the scattering angle, } \ 1/2 < \beta \leq 1,
\end{aligned}
\tag{9}
$$

with the scattering direction $\sigma = u'/|u|$ the scattering direction given by the postcollisional relative velocity u'. The classical elastic case if for $\beta = 1$ (i.e. local energy conservation). In particular $v' - v = \frac{\beta}{2}(|u|\sigma - u) = \omega(u,\sigma)$.

In addition, a standard assumption is that the space dynamics in between the interactions evolve according to Hamiltonian dynamics for the evolving pair in x-space/v-phase space given by $(x(t), v(t)$, position and velocity, respectively, when

$$
\dot{x} = \partial_v H(x,v), \text{ and } \dot{v} = -\partial_x H(x,v) \tag{10}
$$

we have the following classical dynamics of *rarefied* transport associated to the Liouville equation in between interactions and the collisional or interacting nonlocal form given by the Masters equation framework, written in strong form.

Two important cases in the space inhomogeneous setting are *binary* and *linear* interactions, discussed next.

(i) *The nonlinear Boltzmann transport equation for binary interactions*: modelling monoatomic gases corresponds to binary collisional forms with Hamiltonian dynamics (10) between interactions defined for $f = f(x, v, t)$, written in strong form, is

$$
\begin{aligned}
&\frac{\partial f}{\partial t} + v\cdot\nabla_x f = Q(f,f)(x,v,t)\\
&\quad = \kappa \int\int_{(u,\sigma)\in\mathbb{R}^d\times S^{d-1}} B_\lambda(|u|,\hat{u}\cdot\sigma)\left[J_\beta f(x,{}'v,t) f(x,{}'v - {}'u,t)\right.\\
&\quad \left. - f(x,v,t) f(x,v-u,t)\right] \mathrm{d}\sigma \mathrm{d}u
\end{aligned}
\tag{11}
$$

with $B_\lambda(|u|,\hat{u}\cdot\sigma)=|u|^\lambda b(\hat{u}\cdot\sigma)$ with $-d<\lambda\leq 1$, where $'v$ denotes a pre-collisional state with respect to v. The term $J_\beta=\dfrac{\partial(v,v_*)}{('v,'v_*)}$ is the Jacobian of the "post" to "pre"-variable transformation and $|J_1|=1$. The angular function $b(\hat{u}\cdot\sigma)=b(\cos\theta)$ may or may not be an integrable function on the sphere S^{d-1}. If integrable, i.e., $\int_{S^{d-1}}b(\hat{u}\cdot\sigma)\,\mathrm{d}\sigma<K$, we will say it satisfies the *Grad cut-off assumption*.

(ii) *The linear Boltzmann equation* (Forward Kolmogorov equation): The strong formulation of linear evolution of $f=f(x,k,t)$, a *pdf*, given by

$$D_t f=Q(f)(x,k,t)=\int S_{k,k'}(k\leftarrow k')f'\mathrm{d}k'-f(x,k,t)\int S_{k',k}(k'\leftarrow k)\mathrm{d}k'. \quad (12)$$

When the Hamiltonian dynamics are included, as for the case of charged transport with a repulsive potential $\Phi(x,t)$, this linear (12) models the dynamics of electron transport along an electronic band energy surface $\varepsilon(k)$ given by the Hamiltonian $H=\varepsilon(k)-\Phi(x)$ according to (10). It yields the material derivative

$$D_t f=\partial_t f+\frac{1}{\hbar}\partial_k\varepsilon(k)\cdot\partial_x f+\frac{1}{\hbar}\partial_x\Phi(x,t)\cdot\partial_k f \quad (13)$$

corresponding to $\dot{x}=\frac{1}{\hbar}\partial_k\varepsilon(k)$ and $\dot{v}=\frac{1}{\hbar}\partial_x\Phi(\vec{x})=-\frac{q}{\hbar}\vec{E}(k,t)$. In addition, the potential function Φ, with its corresponding electric field $qE(x,t)=-\partial_x\Phi(x,t)$, takes into account mean field effects of the total system, and is determined by the Poisson equation for charges. The band energy function $\varepsilon(k)$ is an eigenvalue of the Bloch decomposition associated to the quantum crystallographic calculation. These equations model *hot electron collisional transport along divergence-free surfaces* ($\varepsilon(k)$, $\Phi(x,t)$) in nano-scale semiconductor devices where magnetic forces are negligible.

Both types of collisional models, nonlinear *(i)* and linear *(ii)*, appear in problems that range from electron/hole transport in a crystal lattice with a linear collisional transport (Cheng et al., 2009, 2012; Morales Escalante and Gamba, 2016; Morales-Escalante et al., 2015), to classical gas dynamics problems (Aoki et al., 1993; Aristov, 2001; Bobylev et al., 2000; Brilliantov and Pöschel, 2004; Chapman and Cowling, 1970; Gamba and Tharkabhushanam, 2009, 2010; Gamba et al., 2004; Munafo et al., 2014; Sone, 2007); to flow of self-interacting particle systems, network dynamics in social, economic and information systems (Bobylev et al., 2009; Duffie et al., 2009; Ringhofer, 2010).

1.4 Deterministic Solvers for Integral Equations of Boltzmann Type

In recent years, there has been a development of deterministic solvers for kinetic transport equations, whole first high-dimensional simulations were performed by Monte Carlo sampling methods for particle systems (Bird, 1994). There are essentially three alternatives to Monte Carlo approach for the computation of the Boltzmann equation: conservative finite element methods, conservative Spectral–Lagrangian methods and discrete velocities methods (DVM). Recent references for the conservative spectral methods can be found in Alonso et al. (2016) and Cheng et al. (2009). While in this review presentation we shall focus mostly on the conservative spectral method for nonlinear binary interactions, the linear collisional transport as in the case of collisional plasma simulations for semiconductor transport or Vlasov–Poisson–Maxwell dynamics can be performed by discontinuous Galerkin schemes, where conservation and positivity propagation is achieved by enhancing basis functions for conservation and reconstruction fluxes for positivity. This is possible for linear collisional forms that have only one conserve quantity: density mass. See this type of work in Cheng et al. (2009, 2012), Morales-Escalante et al. (2015), Morales Escalante and Gamba (2016) and references therein.

The propagation of numerical positivity for a probability distribution function $f(v, t)$ defined in all v-space while having its numerical mass, mean and variance preserved for each time step remains a very difficult task. The available reconstruction methods for conservation while preserving positivity propagation that worked so well in the Vlasov–Boltzmann equation for linear interactions (Cheng et al., 2012) fail to work in the nonlinear collisional setting as they yield overdetermined systems of discrete equations with no available solutions to guaranty such properties.

2 THE LANDAU AND BOLTZMANN OPERATORS RELATION THROUGH THEIR DOUBLE MIXING CONVOLUTIONAL FORMS

The *binary interaction* problem is the focus of the rest of this chapter. Its particular conservation and positivity propagation involves the preservation of several averaged quantities that are difficult to approximate while keeping the approximate solution positive throughout the flow computational time. Our goal is to present a method for numerically solve the Boltzmann equation with a constrained minimization problem that secures the $d + 2$ collision invariants conservation property and converge to the unique equilibrium Maxwellian characterized by the moments of initial state $f_0(v)$.

The Landau–Fokker–Plank equation (Landau, 1937; Landau and Lifschitz, 1980) is a limiting model for the Boltzmann equation used to describe binary elastic collisions (9) *that only result in very small deflections of particle trajectories*. Such limit is necessary in the case for *Coulomb potentials of the form* $|u|^{-3}$, where the classical formulation of the Boltzmann operator is not well posed. However, without loss of generality, one can consider the general form of a potential $|u|^{\lambda}$, with $-3 \leq \lambda \leq 1$ in the grazing collision regime. In particular, the strong form of the Landau–Fokker–Planck equation, written in $3 - d$ (omitting the variables x and t for simplicity), is

$$
\begin{aligned}
\partial_t f(v) &= Q_L(f,f)(v) \\
&= \kappa \,\mathrm{div}_v \left(\int_{\mathbb{R}^3} |u|^{\lambda+2} \left(I - \frac{u \otimes u}{|u|^2} \right) (f(v-u)\nabla_v f(v) - f(v)(\nabla_v f)(v-u))\mathrm{d}u \right) \\
&= \kappa \,\mathrm{div}_v \left(\mathcal{D}_{ij}(v) \nabla_v f(v) - \mathcal{E}_i f(v) \right),
\end{aligned}
\tag{14}
$$

with $\mathcal{D}_{ij}(v) := \int_{\mathbb{R}^3} |u|^{\lambda+2} \left(I - \frac{u \otimes u}{|u|^2} \right) f(v-u)\mathrm{d}u$ and $\mathcal{E}_i(v) = \int_{\mathbb{R}^3} |u|^{\lambda+2} \left(I - \frac{u \otimes u}{|u|^2} \right)$ $(\nabla_v f)(v-u)\mathrm{d}u$.

Written in weak form, this operator is a *double mixing convolution*

$$
\begin{aligned}
&\int_{\mathbb{R}^3} Q_L(f,f)\phi(v)\mathrm{d}v \\
&\quad = \kappa \int_{\mathbb{R}^6} f(v) f(v-u) \left(-4|u|^{\lambda} u \cdot \nabla\phi + |u|^{\lambda+2} \left(I - \frac{u \otimes u}{|u|^2} : D^2\phi \right) \right) \mathrm{d}v\mathrm{d}u,
\end{aligned}
\tag{15}
$$

with a local weight function $G_L(u,v) = \left(-4|u|^{\lambda} u \cdot \nabla\phi + |u|^{\lambda+2} \left(I - \frac{u \otimes u}{|u|^2} : D^2\phi \right) \right)$.

Its Fourier transform takes the form of the weighted convolution (Gamba and Haack, 2014)

$$
\hat{Q}_L(f,f)(\zeta) = \kappa \int_{\mathbb{R}^3} \mathcal{F}\{f(v)f(v-u)\}(\zeta) \left(4i|u|^{\lambda}(u\cdot\zeta) - |u|^{\lambda+2}|\zeta^{\perp}|^2 \right) \mathrm{d}u, \tag{16}
$$

where $\zeta^{\perp} = \zeta - (\zeta \cdot u)/|u|^2 u$, the orthogonal component of ζ to u. Thus, the corresponding representation with weight function $\mathcal{G}_L(u,\zeta)$, as in (7), is now given by the local functions in (u,ζ)-space, the weight function is $\mathcal{G}_L(u,\zeta) = |u|^{\lambda}(4i(u\cdot\zeta) - |u|^2|\zeta^{\perp}|^2)$.

Applying the Fourier transform to the difference of the Boltzmann (1), (9), (11) and Landau operators (1) and (16), as done in Gamba and Haack (2014), yields the difference of *weighted convolutions*

$$
(\hat{Q}_B - \hat{Q}_L)(f,f)(\zeta) = \int_{u\in\mathbb{R}^3} (\mathcal{G}_B(\zeta,u) - \mathcal{G}_L(\zeta,u))\, \mathcal{F}(f(v)f(v-u))(\zeta)\mathrm{d}u, \tag{17}
$$

where $\mathcal{G}_B(\zeta,u)$ is represented in (7) for the case of classical elastic interactions, with an angular dependence of $\sigma \in S^2$. Considering a collision cross section that separates in a potential part depending on powers of $|\mathbf{u}|$ and an angular part $b(\hat{u}\cdot\sigma)$, yields

$$\mathcal{G}_B(\zeta,u) = \int_{\sigma\in S^2} [e^{-i\frac{1}{2}\zeta\cdot\omega(u,\sigma)} - 1]\,|u|^{\lambda} b(\hat{u}\cdot\sigma)\,\mathrm{d}\sigma, \quad \text{with} \quad v' - v = \frac{1}{2}(|u|\sigma - u). \tag{18}$$

In order to be able to handle the approximation analysis and actual computations it is necessary to perform the following fundamental decomposition for spherical integrations of the weight function $\mathcal{G}_\sigma(\zeta,u)$, associated to the Fourier transform of the Boltzmann collision operator. This decomposition is done splitting the "polar" direction to the relative velocity u parametrized by the θ-angular parameter, and the corresponding azimuthal direction integration parametrized by a ϕ-angular parameter. The weight function $\mathcal{G}_\sigma(\zeta,u)$ form in (18) can be written as

$$\mathcal{G}_B(\zeta,u) = 2\pi|u|^{\lambda}\int_0^{\pi} b_\varepsilon(\cos\theta)\sin\theta\left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot u} J_0\left(\frac{|u|\sin\theta|\zeta^{\perp}|}{2}\right) - 1\right)\mathrm{d}\theta, \tag{19}$$

with J_0 is the 0th Bessel function of first kind (see Abramowitz and Stegun, 1964, 9.2.21).

Remark. This formulation of the collisional integral does not separate the gain and loss terms. Cancellation potential singularity is possible in the grazing collision limit where the states v and v' are infinitesimally closed.

Defining σ with a pole in the direction of u, parametrized by $\sigma = \cos\theta\frac{u}{|u|} + \sin\theta\omega$, $\omega \in S^{d-2}$,

$$\mathcal{G}_B(\zeta,u) = |u|^{\lambda}\int_0^{\pi}\int_{S^{d-2}} b(\cos\theta)\sin\theta\left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot u} e^{-i\frac{1}{2}|u|\sin\theta(\zeta\cdot\omega)} - 1\right)\mathrm{d}\theta\mathrm{d}\omega. \tag{20}$$

In the relevant case $d = 3$, the right-hand side of (20) can be written (see Gamba and Haack, 2014 for the calculation)

$$2\pi|u|^{\lambda}\int_0^{\pi} b(\cos\theta)\sin\theta\left(e^{i\frac{1}{2}(1-\cos\theta)\zeta\cdot u} J_0\left(\frac{|u|\sin\theta|\zeta^{\perp}|}{2}\right) - 1\right)\mathrm{d}\theta. \tag{21}$$

The isotropic case when $b(\cos\theta)$ is constant, ζ can be used instead of u as the polar direction for σ, and so the weight (20) is a sinc-function (Gamba and Tharkabhushanam, 2009).

Finally, let $\widehat{G_b}$ be the Fourier transform of G_b. By symmetry, $\widehat{G_b}$ is real valued. Then, the convolution weights $\hat{G}_b(\zeta,\xi)$ from (8), written in $3-d$, where the integration with respect to u is performed in spherical coordinates $(r,\eta) \in \mathbb{R}^+ \times S^2$,

$$\begin{aligned}\hat{G}_b(\xi,\zeta) &= 2\pi\int_{\mathbb{R}^3} |u|^{\lambda} e^{-i\xi\cdot u}\int_0^{\pi} b(\cos\theta)\sin\theta\left[e^{\frac{i\zeta}{2}\cdot u(1-\cos\theta)} J_0\left(\frac{1}{2}|u||\zeta^{\perp}|\sin\theta\right) - 1\right]\mathrm{d}\theta\mathrm{d}u \\ &= 2\pi\int_0^{\infty}\int_{S^2} r^{\lambda+2}\int_0^{\pi} b(\cos\theta)\sin\theta\left[e^{-ir(\xi-\frac{\zeta}{2}(1-\cos\theta))\cdot\eta} J_0\left(\frac{1}{2}r|\zeta^{\perp}|\sin\theta\right) - e^{-ir\xi\cdot\eta}\right] \\ &\quad\times \mathrm{d}\theta\mathrm{d}\eta\mathrm{d}r.\end{aligned}$$

Taking γ the polar angle with respect to ζ direction for the integration in $\eta \in S^2$

$$\hat{G}_b(\xi,\zeta) = 4\pi^2 \int_0^\infty r^{\lambda+2} \int_0^\pi \int_0^\pi b(\cos\theta)\sin\theta \sin\gamma J_0\left(r\left| \xi - \frac{\xi\cdot\zeta}{|\zeta|^2}\zeta \right| \sin\gamma \right)$$
$$\times \left[\cos\left(r(\xi - \frac{\zeta}{2}(1-\cos\theta)) \cdot \frac{\zeta}{|\zeta|}\cos\gamma \right) J_0\left(\frac{1}{2} r|\zeta|\sin\gamma\sin\theta \right) \right. \quad (22)$$
$$\left. - \cos\left(r\xi \cdot \frac{\zeta}{|\zeta|}\cos\gamma \right) \right] \mathrm{d}\theta \mathrm{d}\gamma \mathrm{d}r,$$

This function can be precomputed. This is the actual weight in the *weighted convolutional* form in Fourier space (8).

2.1 The Grazing Collision Limit

This identity (21) developed in Gamba and Haack (2014) is used to get a detailed expansion of $e^{-i\frac{1}{2}\zeta\cdot(|u|\sigma-u)} - 1$ in powers of $\zeta\cdot(|u|\sigma - u)$, combined with the grazing collisions ansatz of short-range cut-off potentials such as of Rutherford-type potential satisfying the following properties (Villani, 1998): the family of angular kernels $b_\varepsilon(\theta) = c_\varepsilon\, b(\theta)\, 1_{\theta\geq\varepsilon}$, for $\varepsilon > 0$, satisfy

G1. $\int_{S^2} b(\hat{u}\cdot\sigma)\mathrm{d}\sigma$ unbounded but $\lim_{\varepsilon\to 0} 4\pi\int_0^\pi b_\varepsilon(\cos\theta)\sin^2\frac{\theta}{2}\sin\theta\mathrm{d}\theta = \Lambda_0 < \infty$.
G2. $\int_0^\pi b_\varepsilon(\cos\theta)(1-\cos\theta)^{2+k}\sin\theta\mathrm{d}\theta \to 0$ for $k\geq 0$,
G3. $b_\varepsilon(\theta) \to 0$ uniformly on $\theta > \theta_0$; $\forall\theta_0 > 0$;

We note that the elastic interaction relation (9) implies $|v'-v|^2 = |u|^2\sin^2\frac{\theta}{2}$, yielding an angular singularity cancellation by means of the grazing collision ansatz *G1*. The constant c_ε depends on the singularity of the angular function $b(\theta)$ and $c_\varepsilon \to 0$ and $\varepsilon \to 0$. Hence conditions *G2* and *G3* indicate the interaction is "grazing", meaning that, as $\varepsilon \to 0$, then because of the cut-off $\theta \to 0$ and so $v \approx v_*$.

A δ, ε-family of admissible angular singularities: In the sequel, we consider the $d = 3$ dimensional space. Introducing ε and δ reference parameters, in the notation of the *ε-grazing and δ-singular* angular function $b_\varepsilon^\delta(\cos\theta)\sin^{d-2}\theta$, define the functions $H_\delta(x)$ as the antiderivative from the area differential of the angular part of the differential cross section as follows

$$b_\varepsilon^\delta(\hat{u}\cdot\sigma)\mathrm{d}\sigma = -\frac{1}{2\pi H_\delta(\sin(\varepsilon/2))}\frac{1}{\sin^{4+\delta}(\theta/2)}\sin(\theta)1_{\theta\geq\varepsilon}\,\mathrm{d}\theta\mathrm{d}\omega$$
$$= -\frac{4}{2\pi H_\delta(\sin(\varepsilon/2))}\frac{1}{x^{1+\delta}}\frac{1}{x^2}\,1_{x\geq\sin(\varepsilon/2)}\mathrm{d}x\mathrm{d}\omega\,, \quad (23)$$

for $x = \sin(\theta/2)$. Thus, equating the last term above to the right-hand side of relation (21), one can explicitly calculate $H_\delta(x)$ as the antiderivative of $x^{-(1+\delta)}$, to obtain

$$H_\delta(x) = -\frac{x^{-\delta}}{\delta}, \text{ for } \delta > 0 \text{ and } H_0(x) = \log x, \text{ for } \delta = 0; \tag{24}$$

where the choice of the exponent δ must satisfy condition *G3*, for $H_\delta(x)$.

Finally, an expansion of the weight $\mathcal{G}_{b_\varepsilon^\delta}(u,\zeta)$ as calculated in (21), which recovers an ε and $\sin(\theta/2)$ free term, labelled $\mathcal{G}_L(u,\zeta)$ in Gamba and Haack (2014), so that the following theorem holds

Theorem 1. *Assume that f_ε^δ satisfies*

$$|\mathcal{F}\{f_\varepsilon^\delta(\mathbf{v},t) f_\varepsilon^\delta(\mathbf{v}-\mathbf{u})\}(\zeta)| \le \frac{A(\zeta,t)}{1+|\mathbf{u}|^{3+a}}, \tag{25}$$

with $A(\zeta,t)$ uniformly bounded by $k(1+|\zeta|)^{-3}$, k constant, and $a > 0$. Moreover, assume the angular scattering cross section $b_\varepsilon^\delta(\cos\theta)\sin\theta^{d-2}$ satisfies conditions $G1$, $G2$ and $G3$ with H_δ from (24), with $0 \le \delta < 2$, and $\lambda = -3$. Then, the rate of convergence from the Boltzmann with grazing collisions to the Landau collision operator is given by

$$\|\widehat{Q_L}(f_\varepsilon^\delta, f_\varepsilon^\delta) - \widehat{Q_{b_\varepsilon^\delta}}(f_\varepsilon^\delta, f_\varepsilon^\delta)\|_{L^\infty} \le O\left(\frac{\left|1 + (|\log(\sin(\varepsilon/2))| - 1)\, 1_{\{\delta=1\}}\right|}{|H_\delta(\sin(\varepsilon/2))|}\right) \to_{\varepsilon\to 0} 0. \tag{26}$$

The proof of this statement can be found in Gamba and Haack (2014), but basically consists in showing

$$\mathcal{G}_\sigma(u,\zeta) = \mathcal{G}_L(u,\zeta) + O(b_\varepsilon) \text{ and } \int_{\mathbb{R}^d} O(b_\varepsilon)\mathcal{F}(f(v)f(v-u))(\zeta)\mathrm{d}u \to_{\varepsilon\to 0} 0, \tag{27}$$

if $|\mathcal{F}\{f_\varepsilon^\delta(\mathbf{v},t) f_\varepsilon^\delta(\mathbf{v}-\mathbf{u})\}(\zeta)|$ satisfies conditions (25), uniformly in time. This estimate will ensure the asymptotics of solutions to the Boltzmann equation for Coulombic interactions in the grazing collision limit to solutions of the Landau equation. It is important to observe that the rate of decay in ε depends on the choice of the angular singularity in b_ε^δ. In addition, it is numerically observed different entropy decay rates to equilibrium depending on the singularity strength measure by δ in the angular function $b_\varepsilon^\delta(\hat{u}\cdot\sigma)\sin^{d-2}\theta$.

The numerical implementations of a comparison of the Boltzmann equation for grazing collision limits and the corresponding reduced Landau equation were extensively performed in Gamba and Haack (2014). The conservative spectral method (see Sections 3 and 4) was implemented, where the weight function (22) was precomputed. Numerical simulations of such comparisons for different cross sections are in Fig. 1.

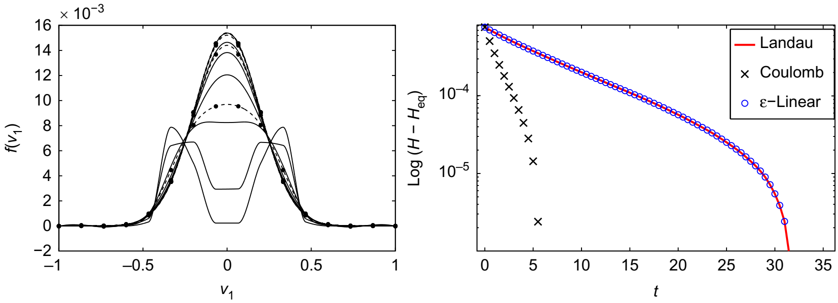

FIG. 1 Comparisons of solutions to Boltzmann using Rutherford cross section (Villani, 1998) and to Landau equations. *Left*: Slice of the distribution marginal function at times $t = 0$, 9, 36, 81, 144, 225, 900. *Solid lines*: Spline reconstruction of Landau equation solution. *Dashed lines* with *solid circles*: Spline reconstruction of Boltzmann equation. $\varepsilon = 10^{-4}$, $N = 16$. *Right*: Convergence of entropy to equilibrium: Log of entropy decay for Boltzmann solution with the Rutherford cross section (24) with $\delta = 0$ with crosses, and with ε-linear cross section with $\delta = 1$ with *circles*, and Landau solution with *solid curve*. $N = 16$, $\varepsilon = 10^{-4}$. When calculating the entropy H, we exclude grid points where the distribution is negative. *From Gamba, I.M., Haack, J.R., 2014. A conservative spectral method for the Boltzmann equation with anisotropic scattering and the grazing collisions limit. J. Comput. Phys. 270, 40–57.*

3 A CONSERVATIVE SPECTRAL METHOD FOR THE COLLISIONAL FORM

The following approach and its approximation analysis and error estimates for the solutions to the Cauchy problem Boltzmann equation were introduced in Alonso et al. (2016), Gamba and Tharkabhushanam (2009) and Gamba and Tharkabhushanam (2010) inspired by the work in Bobylev and Rjasanow (1999) and Pareschi and Russo (2000). We present here a short version of the strategy to be used. We recall the definition of the Lebesgue's spaces $L^p_k(\Omega)$ and the Hilbert spaces $H^\alpha_k(\Omega)$ for a measurable set Ω (for the purpose of this discussion without loss of generality Ω is either $(-L, L)^d$ or $\mathbb{R}^d$ most of the time.)

$$L^p_k(\Omega) := \left\{ f : \|f\|_{L^p_k(\Omega)} := \left(\int_\Omega \left| f(v)\langle v\rangle^k \right|^p \mathrm{d}v \right)^{\frac{1}{p}} < \infty \right\}, \text{ with } p \in [1, \infty),\ k \in \mathbb{R},$$

$$H^\alpha_k(\Omega) := \left\{ f : \|f\|_{H^\alpha_k(\Omega)} := \left(\sum_{\beta \le \alpha} \| D^\beta f \|^2_{L^2_k(\Omega)} \right)^{\frac{1}{2}} < \infty \right\}, \text{ with } \alpha \in \mathbb{N}^d,\ k \in \mathbb{R},$$

where $\langle v\rangle := \sqrt{1 + |v|^2}$. The standard definition is used for the case $p = \infty$,

$$L_k^\infty(\Omega) := \left\{ f : \|f\|_{L_k^\infty(\Omega)} := \operatorname{esssup}\left| f(v)\langle v\rangle^k \right| < \infty \right\}, \text{ with } k \in \mathbb{R}.$$

It will be commonly used the following shorthand to ease notation when the domain Ω is clear from the context

$$\|\cdot\|_{L_k^p(\Omega)} = \|\cdot\|_{L_k^p} = \|\cdot\|_{p,k},$$

and the subindex k will be omitted in the norms for the classical spaces L^p and H^α. What follows is short presentation of the extended work in Alonso et al. (2016).

3.1 Choosing a Computational Cut-Off Domain Ω_L

Because the computation of this problem entices to numerically solve the evolution of a probability distribution function defined in the whole $\mathbb{R}^d$-space, it is relevant to discuss the choice of a computational cut-off domain in such a way that the numerical error for the flow evolution is negligible regarding this choice of computational window. This discussion is actually independent of the choice computational scheme and applies to existing as well new approaches such as the recently developed in Zhang and Gamba (2016). The following result is rigorous and applied to the Boltzmann equation for hard potentials, that is (11) with $1 \geq \lambda > 0$. Hence, for any $f(v, t)$ solution of the elastic homogeneous Boltzmann equation lying in $\mathcal{C}(0, T; H^\alpha(\mathbb{R}^d))$, with a given initial state $f(v,0) = f_0(v) \in H^\alpha(\mathbb{R}^d)$. A natural question to ask is: can one secure the propagation of regularity and tail decay for the solution of the Boltzmann problem, uniformly in time? What are good functional spaces for probability distribution functions that are solutions of the Boltzmann flow problem? These questions have been recently addressed in Bobylev et al. (2004) and Gamba et al. (2009) and provide an answer in a suitable form for any computational approach of the space homogeneous elastic Boltzmann equation.

To address this problem, we introduce the following notation for exponentially weighted integrable functions. Define

$$L^1_{(r,2)}(\mathbb{R}^d) := \left\{ g : \|g\|_{L^1_{(r,2)}} := \int_{\mathbb{R}^d} |g(y)|\, e^{r|y|^2} \mathrm{d}y < \infty \right\}, \text{ with } r > 0, \tag{28}$$

and analogous definition for the spaces $L^p_{(r,2)}(\mathbb{R}^d)$ with $p \in (1, \infty]$. These functional spaces are comprise of nonnegative elements in $L^1_{(r,2)}(\mathbb{R}^d)$ that are Gaussian (or Maxwellian) weighted regular probability densities, meaning that the probability density g not only has all its moments bounded but also grow as the moments of a Gaussian distribution. That also means the probability density $g(y)$ decays like $e^{-r|y|^2}$ with rate r for large $|y|$ in the sense of L^1. In particular, one may view r^{-1} as the corresponding Gaussian or Maxwellian *tail temperature* of the density.

The following rigorous result was obtained for the elastic homogenous Boltzmann initial value problem (Gamba et al., 2009) that shows if $f_0(v) \in L^1_{(r_0,2)}(\mathbb{R}^d)$, then solution $f(v,t) \in L^1_{(r,2)}(\mathbb{R}^d_v)$, for some $0 < r \le r_0$, uniformly in t, where r only depends on a number k'-moments of the initial state f_0, with $k' > 2$, as well as on the scattering kernel B (i.e. on the potential rate λ and the angular function $b(\hat{u}\cdot\sigma)$). In addition, if the angular cross section satisfies $b(\hat{u}\cdot\sigma) \in L^{1+}(\mathbb{S}^{d-1})$, then the propagation of $f(v,t) \in L^\infty_{(\bar{r},2)}(\mathbb{R}^d)$, with $0 < \bar{r} \le r \le r_0$, for all time $t > 0$ was also shown in Gamba et al. (2009), provided the initial data $f_0(v) \in L^\infty_{(r_0,2)}(\mathbb{R}^d)$. As a consequence, for any given initial state $f_0 \in L^1_{e^{\alpha|v|^2}}(\mathbb{R}^d)$ or $f_0 \in L^\infty_{e^{\alpha|v|^2}}(\mathbb{R}^d)$, there exists a rate $\beta = \beta(k'(f_0), \lambda, b)$, for which these exponentially weighted L^1 and L^∞ norms propagate uniformly in time.

This propagation property secures a stable numerical simulation of the Boltzmann equation, provided the numerical preserving the conservation laws or corresponding collision invariants hold. This property yields the convergence to the analytic solution of the initial value problem and its long-time behaviour converges to the equilibrium Maxwellian, as defined in (6). In fact we showed that it is sufficient to choose the domain $\Omega_L = (-L, L)^d$ large enough such that, at least, most of the mass and energy of the solution f will be contained in it throughout the simulation. One possible strategy for choosing the size of the simulation domain is as follows: assume without loss of generality a bounded initial datum f_0 with compact support and having zero momentum $\int f_0\, v = 0$. Then,

$$f_0(v) \le C_0\, m_0 (2\pi T_0)^{-d/2}\, e^{-\frac{r_0|v|^2}{2T_0}}, \tag{29}$$

where $m_0 := \int f_0\, \mathrm{d}v$ is the initial mass, $T_0 := \int f_0 |v|^2\, \mathrm{d}v$ is the initial temperature, and $r_0 \in (0, 1]$ and $C_0 \ge 1$ are the stretching and dilating constants. The aforementioned analytical results secure that for some $r := r(f_0, \lambda, b) \in (0, r_0]$ and $C := C(f_0, \lambda, b) \ge 1$

$$f(t,v) \le C_0\, m_0 (2\pi T_0)^{-d/2}\, e^{-\frac{r|v|^2}{2T_0}} =: M(f_0, C, r),\ t > 0.$$

A simple criteria to pick the segment length L of the simulation domain Ω_L are to ensure that most of the mass and kinetic energy (or variance) of f will remain in it throughout the numerical simulation. In other words, we want that, for some small number $\mu << 1$,

$$\int_{\Omega_L^c} f(v,t)\langle v\rangle^2 \mathrm{d}v \le \int_{\Omega_L^c} M(f_0, C, r)\langle v\rangle^2 \mathrm{d}v \le \mu \int_{\Omega_L} f_0(v)\langle v\rangle^2 \mathrm{d}v = \mu(m_0 + T_0).$$

where μ is chosen to be understood as a domain cut-off error tolerance that *remains uniform in time* and solely depends on the initial state and Ω_L. Equivalently, one needs to choose the size of L, or equivalently the measure of Ω_L, such that

$$(m_0+T_0)^{-1}\int_{\Omega_L^c} M(f_0,C,r)\langle v\rangle^2 \mathrm{d}v \le \mu \approx 0 \tag{30}$$

In order to minimize the computation effort, one should pick the smallest of such domains, that is, Ω_{L_*} $L_* = \min\{L>0: \mathrm{supp}(f_0)\subset\Omega_L,\ \Omega_L^c \text{ satisfaces(30)}\}$.

The choice of μ in (30) depends on the knowledge of precise values for the constants C and r not so easy to determine for a generic initial data, Hence, in order to avoid overestimating the size of Ω_L, the simulation domain, it is best to set $r_0 = r = 1$ and choose $C = C_0 \ge 1$ as the smallest constant satisfying (29) (which always exists for any compactly supported and bounded f_0), and set

$$\max\left\{f_0,\ m_0\ (2\pi T_0)^{-d/2}\ e^{-\frac{|v|^2}{2T_0}}\right\} \le M(f_0,C,1),$$

with equality if and only if f_0 is the equilibrium Maxwellian as in (6) (in such a case $C = 1$). Then the use of classical *Normal Table for log-normal distributions* yields the error μ incurred in the simulation as a function of the chosen Ω_L, uniformly in time, for any simulation of the Boltzmann collisional model homogeneous in x-space.

Remark. In this deterministic approach, as much as with Monte Carlo methods like the Bird scheme (Bird, 1994), the x-space inhomogeneous Hamiltonian transport for nonlinear collisional forms is performed by time operator-splitting algorithms. That means, depending on the problem, the computational v-domain Ω_L can be updated with respect to the characteristic flow associated to underlying Hamiltonian dynamics.

3.2 Fourier Series, Projections and Extensions

In the implementation of any spectral method the single most important analytical tool is the Fourier transform defined by $\hat{f}(\zeta) := (2\pi)^{d/2}\int_{\mathbb{R}^d} f(v)e^{-i\zeta\cdot v}\mathrm{d}v$, defined for any $f\in L^1(\mathbb{R}^d)$. Our goal is to approximate the collisional form in Fourier space, given by the weighted convolution in Fourier space (8), by making use on the approximant Fourier series in a rather simple and convenient way. Indeed, fixing a domain of work $\Omega_L := (-L, L)^d$ for $L > 0$, recall that for any $f \in L^2(\Omega_L)$ the *Fourier series* of f, denoted from now on by f_L is given by $f_L \sim 1/((2L)^d)\sum_{k\in\mathbb{Z}^d}\hat{f}_L(\zeta_k)e^{i\zeta_k\cdot v}$, where $\zeta_k := \dfrac{2\pi k}{L}$ are the spectral modes and $\hat{f}_L(\zeta_k)$ is the Fourier transform of f_L evaluated in such modes.

Next, define the operator $\Pi^N : L^2(\Omega_L) \to L^2(\Omega_L)$ as

$$\left(\Pi^N f_L\right)(v) := f_L^{\Pi}(v) = \left(\frac{1}{(2L)^d}\sum_{|k|\le N}\hat{f}_L(\zeta_k)e^{i\zeta_k\cdot v}\right)\mathbf{1}_{\Omega_L}(v), \tag{31}$$

that is, the *orthogonal projection* on the "first N" basis elements and see that for any integer α the derivative operator commutes with the projection operator. In Ω_L

$$\partial^\alpha\left(\Pi^N f_L\right)(v) = \left(\frac{1}{(2L)^d}\sum_{|k|\le N}\widehat{\partial^\alpha f}(\zeta_k)e^{i\zeta_k\cdot v}\right)\mathbf{1}_{\Omega_L}(v) = \left(\Pi^N\partial^\alpha f\right)(v). \tag{32}$$

The Parseval's theorem implies $\left\|\Pi^N f_L\right\|_{L^2(\Omega_L)} \le \|f_L\|_{L^2(\Omega_L)}$ for any N; and $\left\|\Pi^N f_L - f_L\right\|_{L^2(\Omega_L)} \searrow 0$ as $N\to\infty$. Because of the decay properties described in the procedure of choosing the computational domain Ω_L, we can avoid the expected aliasing effect for a classical Fourier approximation by series by using the classical extension theorem in Sobolev spaces as follows.

3.2.1 The Extension Operator

For fixed $\alpha_0 \ge 0$ we introduce the *extension operator* $\mathrm{E}: L^2(\Omega_L)\to L^2(\mathbb{R}^d)$ such that $\mathrm{E}: H^\alpha(\Omega_L)\to H^\alpha(\mathbb{R}^d)$ holds for any $\alpha \le \alpha_0$. The construction of such operator (Stein, 1970) is well known having the following properties:

E1. Linear and bounded, with $\|\mathrm{E}f\|_{H^\alpha(\mathbb{R}^d)} \le C_\alpha \|f\|_{H^\alpha(\Omega_L)}$ for $\alpha\le\alpha_0$.

E2. $\mathrm{E}f = f$ a.e. in Ω_L. Furthermore, denoting $f^\pm$ the positive and negative parts of f one has $(\mathrm{E}f)^\pm = \mathrm{E}f^\pm$, a.e. in $\mathbb{R}^d$.

E3. Outside Ω_L the extension is constructed using a reflexion of f near the boundary $\partial\Omega_L$. Thus, for any $\delta \ge 1$ we can choose an extension with support in $\delta\Omega_L$, the dilation of Ω_L by δ, and $\|\mathrm{E}f\|_{L^p(\delta\Omega_L\setminus\Omega_L)} \le C_0 \|f\|_{L^p(\Omega_L\setminus\delta^{-1}\Omega_L)}$ for $1\le p\le 2$, where the constant C_0 is independent of the support of the extension.

E4. In particular, properties E2 and E3 imply that for any $\delta \ge 1$, there is an extension such that $\|\mathrm{E}f\|_{L^p_k(\mathbb{R}^d)} \le 2C_0\delta^{2k}\|f\|_{L^p_k(\Omega_L)}$ for $1\le p\le 2$, $k\ge 0$.

The case $\delta = 1$ is only possible using an extension by zero, that is, when $(Ef)(v) = f(v)1_{\Omega_L}(v)$, and so α_0 is restricted to zero.

3.3 A Conservative Spectral Method for the Homogeneous Boltzmann Equation

After the cut-off domain Ω_L has been fixed, the projection operator is applied to both sides of Eq. (8) to obtain

$$\frac{\partial\Pi^N f}{\partial t}(v,t) = \Pi^N Q(f,f)(v,t), \text{ in } (0,T]\times\Omega_L.$$

Hence, for such a domain Ω_L and sufficiently large number of modes N, it is expected that the approximation $\Pi^N Q(f,f) \sim \Pi^N Q(\Pi^N f, \Pi^N f)$, in $(0, T] \times \Omega_L$ will be valid, leading to pose and solve the problem

$$\frac{\partial g}{\partial t}(v,t) = \Pi^N Q(g,g)(v,t), \text{ in } (0,T] \times \Omega_L,$$

with initial condition $g_0 = \Pi^N f_0$, and expect that it should be a good approximation to $\Pi^N f$. In other words we define the numerical solution to be $g_N := g$ and expect to show that this discrete solution will be a good approximation to the solution of the Boltzmann problem in the cut-off domain, that is, $g \approx f$ in Ω_L, provided the number of modes N used is sufficiently large. This formalism has been shown in Alonso et al. (2016), under some assumptions for the space homogeneous Boltzmann equation. To this end, we much study a modified problem, namely, the convergence towards f of the solution g of the semidiscrete problem

$$\frac{\partial g}{\partial t}(v,t) = Q_c(g,g)(v,t) \quad \text{in} \quad (0,T] \times \Omega_L, \tag{33}$$

with initial condition $g_0 := g_0^N = \Pi^N f_0$. The operator $Q_c(g)$ is defined as the $L^2(\Omega_L)$-closest function to $\Pi^N Q(\mathrm{E}g,\ \mathrm{E}g)$ having null mass, momentum and energy. Since the gain collision operator is global in velocity, it turns out that a good approximation to f will be obtained as long as Ω_L and N are sufficiently large. The extension operator E has a subtle job to do in the approximation scheme which is related precisely to the global behaviour of the gain collision operator. Since solutions of the approximation problem (33) lie in Ω_L, they are truncated versions of f. The gain operator does not possess higher derivatives *in* Ω_L when acting on truncated functions due to the singularity created in the boundary $\partial\Omega_L$. The extension smooths out the gain collision operator at the price of extending the domain. In the case of discontinuous solutions where only L^2-error estimate is expected, the correct extension to use in the scheme is the extension by zero. We discuss this more carefully in the following sections.

Before continue with the discussion, we are now in position to summarize the main results on convergence, error estimates and asymptotic behaviour. These statements are stated in the following theorem. Rigorous proofs can be found at Alonso et al. (2016).

Theorem 2 (Error estimates and convergence to the equilibrium Maxwellian). *Fix an initial nonnegative initial data* $f_0 \in \left(L_2^1 \cap L^2\right)(\mathbb{R}^d)$. *Then, for any time* $T > 0$ *there exist a lateral size* $L := L(T, f_0)$ *and a number of modes* $N_0 := N(T, L, f_0)$ *such that*

1. ***Semidiscrete existence and uniqueness:*** *The semidiscrete problem* (33) *has a unique solution* $g \in \mathcal{C}\left(0,T;L^2(\Omega_L)\right)$ *for any* $N \geq N_0$.
2. ***L_k^2-error estimates:*** *if* $f_0 \in (L^1 \cap L^2)_{k'+k+\frac{1}{2}}(\mathbb{R}^d)$ *for some* $k', k \geq 0$, *then*

$$\sup_{t\in[0,T]} \|f-g\|_{L_k^2(\Omega_L)} \leq CL^{-\lambda k'} e^{cT}, \text{ for any } N \geq N_0,$$

where $N_0 := N(T, L, f_0, k)$, $C := C(k, f_0)$, $c := c(k, f_0)$ *and* f *is the solution of the Boltzmann equation* (11).

3. ***H^α-error estimates:*** *For the smooth case $f_0 \in \left(L^1_2 \cap H^{\alpha_0}_q\right)(\mathbb{R}^d)$, with $\alpha_0 > 0$ and $q = \max\{k' + k, 1 + \frac{d}{2\lambda}\}$, with k' ≥ 2, it follows for any $\alpha \leq \alpha_0$*

$$\sup_{t\in[0,T]} \|f - g\|_{H^\alpha_k(\Omega_L)} \leq C_{k'} e^{c_k T}\left(O\left(\frac{L^{\lambda k + |\alpha_0|}}{N^{|\alpha_0| - |\alpha|}}\right) + O\left(L^{-\lambda k'}\right)\right), \text{ for any } N \geq N_0,$$

where $N_0 := N(T, L, f_0, k, \alpha)$. And finally,

4. ***Convergence to the equilibrium Maxwellian**: for every $\delta > 0$ there exist a simulation time $T := T(\delta) > 0$, corresponding lateral size $L := L(T, f_0)$ and baseline number of modes $N_0 := N_0(T, L, f_0, \alpha)$ such that for any $\alpha \leq \alpha_0$*

$$\sup_{t\in[\frac{T}{2},T]} \| \mathcal{M}_0 - g\|_{H^\alpha(\Omega_L)} \leq \delta, \;\; N \geq N_0,$$

where $\mathcal{M}_0$ is the equilibrium Maxwellian (6) having the same mass, momentum and kinetic energy of the initial configuration $f_0(v)$.

The sketch of the proof of Theorem 2, presented next, relies on the control problem that enforces conservation at the numerical level.

3.4 Conservation Method—An Extended Isoperimetric Problem

This is the procedure that secures the conservation of the necessary collision invariants. This procedure is posed as a standard $L^2(\Omega_L)$-optimization problem. Therefore, due to the truncation of the velocity domain the projection of $Q(f, f)$, namely $\Pi^N Q(f, f)$, does not preserve mass, momentum and energy. In order to accomplish these conservation properties, the problem is posed as constraints in a optimization problem to a conserved state. We denote, for the sake of brevity,

$$Q_u(f)(v) := \Pi^N(Q(\mathrm{E}f, \mathrm{E}f)\, \mathbf{1}_{\Omega_L})(v). \tag{34}$$

The indicator function $\mathbf{1}_{\Omega_L}(v)$ is due to the fact that the domain of $Q(\mathrm{E}f, \mathrm{E}f)$ most likely be larger than Ω_L, and thus the extension operator helps to avoid introducing spurious nonsmoothness within the domain Ω_L due to the domain cut-off, as described in Section 3.2.

The conservation optimization problem consists into minimize, in the Banach space

$$\mathcal{B}^e = \left\{X \in L^2(\Omega_L) : \int_{\Omega_L} X = \int_{\Omega_L} Xv = \int_{\Omega_L} X|v|^2 = 0\right\},$$

the functional, defined for a computed and unconserved collision operator $Q_u(f)$, by

$$\mathcal{A}^e(X) := \int_{\Omega_L} (Q_u(f)(v) - X)^2 \mathrm{d}v. \tag{35}$$

In other words, minimize the L^2-distance to the projected collision operator subject to mass, momentum and energy conservation. The following lemma plays is fundamental for error estimates as well as the convergence to the equilibrium Maxwellian (6).

Lemma 1 (Elastic Lagrange estimate). *The problem* (35) *has a unique minimizer given by*

$$X^{\star} = Q_u(f)(v) - \frac{1}{2}\left(\gamma_1 + \sum_{j=1}^{d} \gamma_{j+1} v_j + \gamma_{d+2}|v|^2\right),$$

where γ_j, for $1 \le j \le d+2$, are Lagrange multipliers associated with the elastic optimization problem. Furthermore, these Lagrange multipliers are given by

$$\gamma_1 = O_d \rho_u + O_{d+2} e_u; \;\; \gamma_{j+1} = O_{d+2} \mu_u^j, \;\; j = 1, 2, \ldots, d; \;\; \gamma_{d+2} = O_{d+2} \rho_u + O_{d+4} e_u.$$

The parameters ρ_u, e_u, μ_u^j are defined below in (38) *and $O_r := O(L^{-r})$ only depends inversely on diameter $|\Omega_L|$. The minimized objective function is*

$$\begin{aligned} \mathcal{A}^e(X^*) = \|Q_u(f) - X^*\|^2_{L^2(\Omega L)} &\le C(d)\left(2\gamma_1^2 L^d + \left(\sum_{j=1}^{d} \gamma_{j+1}^2\right) L^{d+2} + \gamma_{d+2}^2 L^{d+4}\right) \\ &\le \frac{C(d)}{L^d}\left(\rho_u^2 + \frac{e_u^2}{L^{d+1}} + \sum_{j=2}^{d+1} \mu_j^2\right) \end{aligned} \tag{36}$$

The proof of this lemma is constructive and very fundamental. When the objective function is an integral equation and the constraints are integrals, the optimization problem can be solved by forming the Lagrangian functional and finding its critical points. Indeed, set for all $j = 1, 2, \ldots, d$,

$$\psi_1(X) := \int_{\Omega_L} X(v) \mathrm{d}v; \;\; \psi_{j+1}(X) := \int_{\Omega_L} v_j X(v) \mathrm{d}v; \;\; \psi_{d+2}(X) := \int_{\Omega_L} |v|^2 X(v) \mathrm{d}v,$$

and define

$$\mathcal{H}(X, X', \boldsymbol{\gamma}) := \mathcal{A}^e(X) + \sum_{i=1}^{d+2} \gamma_i \psi_i(X) = \int_{\Omega_L} h(v, X, X', \boldsymbol{\gamma}) dv.$$

then, introduced $h(v, X, X', \boldsymbol{\gamma}) := (Q_u(f)(v) - X(v))^2 + \left(\gamma_1 + \sum_{j=1}^{d} \gamma_{j+1} v_j + \gamma_{d+2}|v|^2\right) X(v)$. In order to find the critical points compute $D_X\mathcal{H}$ and $D_{\gamma_j}\mathcal{H}$ and note that the derivatives $D_{\gamma_j}\mathcal{H}$ just retrieve the constraint integrals. Hence, for multiple independent variables v_j and a single dependent function $X(v)$ the Euler–Lagrange equations are

$$D_2 h(v, X, X', \boldsymbol{\gamma}) = \sum_{j=1}^{d} \frac{\partial D_3 h}{\partial v_j}(v, X, X', \boldsymbol{\gamma}) = 0.$$

We used the fact that h is independent of X'. This gives the following equation for the conservation correction in terms of the Lagrange multipliers

$$
\begin{aligned}
&2(X(v)-Q_u(f)(v))+\gamma_1+\sum_{j=1}^{d}\gamma_{j+1}v_j+\gamma_{d+2}|v|^2=0,\\
&\text{and therefore,}\quad X^\star(v)=Q_u(f)(v)-\frac{1}{2}\left(\gamma_1+\sum_{j=1}^{d}\gamma_{j+1}v_j+\gamma_{d+2}|v|^2\right).
\end{aligned}
\tag{37}
$$

Letting $g(v,\gamma)=\gamma_1+\sum_{j=1}^{d}\gamma_{j+1}v_j+\gamma_{d+2}|v|^2$ and substituting (37) into the constraints $\psi_j(X^\star) = 0$ yields

$$
\begin{aligned}
\rho_u &:= \int_{\Omega_L} Q_u(f)(v)\mathrm{d}v=\frac{1}{2}\int_{\Omega_L} g(v,\gamma)\mathrm{d}v\\
\mu_u^j &:= \int_{\Omega_L} v_j Q_u(f)(v)\mathrm{d}v=\frac{1}{2}\int_{\Omega_L} v_j g(v,\gamma)\mathrm{d}v,\quad j=1,2,\ldots,d,\\
e_u &:= \int_{\Omega_L} |v|^2 Q_u(f)(v)\mathrm{d}v=\frac{1}{2}\int_{\Omega_L} |v|^2 g(v,\gamma)\mathrm{d}v.
\end{aligned}
\tag{38}
$$

Identities (38) form a $d + 2$ by $d + 2$ system of linear equations that can be uniquely solved. Indeed, solving for the critical γ_0, γ_{j+1}, $j = 1, 2, \ldots, d$ and γ_{j+2} yields

$$
\gamma_1=O_d\rho_u+O_{d+2}e_u;\quad \gamma_{j+1}=O_d\mu_u^j;\quad \gamma_{d+2}=O_{d+2}\rho_u+O_{d+4}e_u,
\tag{39}
$$

where $O_r := O(L^{-r})$. In particular, O_r depends inversely on $|\Omega_L|$. Substituting these values of critical Lagrange multipliers (39) into (37) gives explicitly the critical $X^\star(v)$. Moreover, the objective function $\mathcal{A}^e(X)$ can be computed at its minimum as

$$
\begin{aligned}
\mathcal{A}^e(X^\star)=\| Q_u(f)-X^\star \|^2_{L^2(\Omega_L)} &= \int_{\Omega_L}(Q_u(f)(v)-X^\star(v))^2\mathrm{d}v\\
&=\frac{1}{4}\int_{\Omega_L}\left(\gamma_1+\sum_{j=1}^{d}\gamma_{j+1}v_j+\gamma_{d+2}|v|^2\right)^2\mathrm{d}v.
\end{aligned}
$$

Upon simplification, taking $\Omega_L=(-L,L)^d$ and expressing the Lagrange multipliers $\gamma_j, j=1\ldots d+2$ in terms of the unconserved moments ρ_u, $\mu_{u,j+1}, j=1\ldots d$ and e_u from relation (39), one obtains

$$
\begin{aligned}
\| Q_u(f)-X^* \|^2_{L^2(\Omega_L)} &\le C(d)\left(2\gamma_1^2L^d+\frac{2}{d}\left(\sum_{j=1}^{d}\gamma_{j+1}^2\right)L^{2d-1}+\gamma^2{}_{d+2}L^{d+4}\right)\\
&\le \frac{1}{L^d}\,O\left(\left(\rho_u+\frac{e_u}{L^{(d+1)/2}}\right)^2+\sum_{j=1}^{d+1}\mu_{j+1}^2\right),
\end{aligned}
$$

which is just an $O(L^{-d})$ proportional to these unconserved moments that are shown to be uniformly bounded in time in Lemma 3 in Section 4.2. In a sense this result is better described as an *isomoment* estimate, which yields estimate (36). The strict convexity of $\mathcal{A}^e$ implies that this critical point is the unique minimizer. This results clearly shows that the last estimate secures, after a few iterations of the conservation algorithm (to be fully described in the next section) that, for a fixed L and a number of modes N the solution of the minimization problem will converge to an approximate of the collision operator whose first $d + 2$ moments are null. This is the tool that will allows us to construct error estimates for the approximation to the true solution to the Boltzmann equation and the numerically calculated one for the spectral-conserved algorithm. In addition these *conservation correction estimates* from Lemma 2 in (42), provide the necessary tool to prove that the numerical solution converges to the equilibrium Maxwellian (6) (see Alonso et al., 2016 for details.) □

Summarizing, we are now in conditions to define the *conserved projection operator* $Q_c(f)$ as follows.

Definition. For any fixed $f \in L^2(\Omega_L)$ the *conserved projection operator* $Q_c(f)$ is defined as the minimizer of problem (E) That is,

$$Q_c(f) := X^{\star}. \tag{40}$$

From Lemma 1, the minimized objective function (36) in the elastic optimization problem depends only on the nonconserved moments ρ_u, μ_u^j, and e_u of $Q_u(f)$. These quantities are to be approximating the $d + 2$ dimensional zero vector, therefore, the conserved projection operator is a perturbation of $Q_u(f)$ by a second order polynomial. Denoting the moments of a function f by

$$m_k(f) := \int_{\mathbb{R}^d} |f(v)|\,|v|^{\lambda k}\,\mathrm{d}v. \tag{41}$$

Lemma 2 (Conservation correction estimate). *Fix $f \in L^2(\Omega_L)$, then the accuracy of the conservation minimization problem is proportional to the spectral accuracy. That is, for any $k, k' \geq 0$ and $\delta > 1$ there exists an extension E such that*

$$\begin{aligned} \| (Q_c(f) - Q_u(f))|v|^{\lambda k}\|_{L^2(\Omega_L)} \leq \frac{C}{\sqrt{k+\mathrm{d}}} L^{\lambda k} \,\| Q(\mathrm{E}f, \mathrm{E}f) - Q_u(f)\|_{L^2(\Omega_L)} \\ + \frac{\delta^{2\lambda k'}}{\sqrt{k+\mathrm{d}}} O_{(d/2+\lambda(k'-k))}(m_{k'+1}(f) m_0(f) + Z_{k'}(f)), \end{aligned} \tag{42}$$

where C is a universal constant and $\mathrm{Z}_{k'}(f)$ depending on the moments up to order k'.

3.5 Discrete in Time Conservation Method: Lagrange Multiplier Method

In this section we consider the discrete version of the conservation scheme. For such a discrete formulation, the conservation routine is implemented as a Lagrange multiplier method where the conservation properties of the discrete distribution are set as constraints. Let $M = N^d$, the total number of Fourier modes. For elastic collisions, $\rho = 0$, $\mathbf{m} = (m_1, \ldots, m_d) = (0, \ldots, 0)$ and $e = 0$ are conserved. Let $\omega_j > 0$ be the integration weights for $1 \leq j \leq M$ and define

$$\mathbf{Q}_u = \begin{pmatrix} Q_{u,1} & Q_{u,2} & \cdots & Q_{u,M} \end{pmatrix}^T$$

as the distribution vector at the computed time step, and

$$\mathbf{Q}_c = \begin{pmatrix} Q_{c,1} & Q_{c,2} & \cdots & Q_{c,M} \end{pmatrix}^T$$

as the corrected distribution vector with the required moments conserved. For the elastic case, let

$$\mathbf{C}^e_{(d+2)\times M} = \begin{pmatrix} \omega_j \\ v_1\,\omega_j \\ \cdots \\ v_d\,\omega_j \\ |v_j|^2\,\omega_j \end{pmatrix} \quad 1 \leq j \leq M, \tag{43}$$

be the integration matrix, and $\mathbf{a}^e_{(d+2)\times 1} = \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}t}\rho & \frac{\mathrm{d}}{\mathrm{d}t}m_1 & \cdots & \frac{\mathrm{d}}{\mathrm{d}t}m_{\mathrm{d}} & \frac{\mathrm{d}}{\mathrm{d}t}e \end{pmatrix}^T$ be the vector of conserved quantities (note that $\mathbf{a}^e$ is null $d + 2$-dimensional null vector in the case of elastic theory, but may not be in general). With this notation in mind, the discrete conservation method can be written as a constrained optimization problem: find $\mathbf{Q}_c$ such that is the unique solutions of

$$\mathcal{A}(\mathbf{Q}_c) = \left\{ \min \|\mathbf{Q}_u - \mathbf{Q}_c\|_2^2 : \mathbf{C}^e\mathbf{Q}_c = \mathbf{a}^e \text{ with } \mathbf{C}^e \in \mathbb{R}^{d+2\times M},\, \mathbf{Q}_u \in \mathbb{R}^M,\, \mathbf{a}^e \in \mathbb{R}^{d+2} \right\}.$$

The Lagrange multiplier is used to solve the minimization problem $\mathcal{A}(\mathbf{Q}_c)$. Let $\boldsymbol{\gamma} \in \mathbb{R}^{d+2}$ be the Lagrange multiplier vector. Then the scalar objective function to be optimized is given by

$$\mathrm{L}(\mathbf{Q}_c, \boldsymbol{\gamma}) = \sum_{j=1}^{M} \left|Q_{u,j} - Q_{c,j}\right|^2 + \boldsymbol{\gamma}^T(\mathbf{C}^e\mathbf{Q}_c - \mathbf{a}^e). \tag{44}$$

Eq. (44) can be solved explicitly for the corrected distribution value and the resulting equation of correction be implemented numerically in the code. Indeed, taking the derivative of $\mathrm{L}(\mathbf{Q}_c, \boldsymbol{\gamma})$ with respect to $Q_{c,j}$, for $1 \leq j \leq M$ and γ_i, for $1 \leq i \leq d + 2$

$$\frac{\partial \mathrm{L}}{\partial Q_{c,j}} = 0, \ \ j = 1, \ldots, M \ \ \Rightarrow \ \ \mathbf{Q}_c = \mathbf{Q}_u + \frac{1}{2}(\mathbf{C}^e)^T \boldsymbol{\gamma}. \tag{45}$$

Moreover,

$$\frac{\partial \mathrm{L}}{\partial \gamma_i} = 0, \ \ i = 1, \ldots, d+2 \ \ \Rightarrow \ \ \mathbf{C}^e \mathbf{Q}_c = \mathbf{a}^e,$$

retrieves the constraints. Hence, one needs to solve for $\boldsymbol{\gamma}$ the following equation

$$\mathbf{C}^e (\mathbf{C}^e)^T \boldsymbol{\gamma} = 2(\mathbf{a}^e - \mathbf{C}^e \mathbf{Q}_u). \tag{46}$$

Now, since $\mathbf{C}^e(\mathbf{C}^e)^T$ is symmetric and $\mathbf{C}^e$ is an integration matrix, then $\mathbf{C}^e$ is also positive definite. As a consequence, the inverse of $\mathbf{C}^e(\mathbf{C}^e)^T$ exists and one can compute the value of $\boldsymbol{\gamma}$ simply by

$$\boldsymbol{\gamma} = 2(\mathbf{C}^e (\mathbf{C}^e)^T)^{-1} (\mathbf{a}^e - \mathbf{C}^e \mathbf{Q}_u).$$

Substituting $\boldsymbol{\gamma}$ into (45) and recalling that $\mathbf{a}^e = \mathbf{0}$ for the elastic case,

$$\mathbf{Q}_c = \mathbf{Q}_u + (\mathbf{C}^e)^T \left(\mathbf{C}^e (\mathbf{C}^e)^T\right)^{-1} (-\mathbf{C}^e \mathbf{Q}_u) = \left[\mathbb{I} - (\mathbf{C}^e)^T \left(\mathbf{C}^e (\mathbf{C}^e)^T\right)^{-1} \mathbf{C}^e\right] \mathbf{Q}_u : \\ = \Lambda_N(\mathbf{C}^e)\, \mathbf{Q}_u, \tag{47}$$

where $\mathbb{I} = N \times N$ identity matrix. In the sequel, we regard this conservation routine as *Conserve*. Thus,

$$Conserve(\mathbf{Q}_u) = \mathbf{Q}_c = \Lambda_N(\mathbf{C}^e)\, \mathbf{Q}_u. \tag{48}$$

Define D_t to be any time discretization operator of arbitrary order. Then, the discrete problem that we solve reads

$$D_t \mathbf{f} = \Lambda_N(\mathbf{C}^e)\, \mathbf{Q}_u. \tag{49}$$

Thus, multiplying (49) by $\mathbf{C}^e$ it follows the conservation of observables

$$D_t(\mathbf{C}^e \mathbf{f}) = \mathbf{C}^e D_t \mathbf{f} = \mathbf{C}^e \Lambda_N(\mathbf{C}^e)\, \mathbf{Q}_u = 0, \tag{50}$$

where we used the commutation $\mathbf{C}^e D_t = D_t \mathbf{C}^e$ valid since $\mathbf{C}^e$ is independent of time, see Gamba and Tharkabhushanam (2009) for additional comments.

4 LOCAL EXISTENCE, CONVERGENCE AND REGULARITY FOR THE SEMIDISCRETE SCHEME

In this section we enunciate L^1_k and L^2_k estimates for the approximation solutions $\{g_N\}$ of the problem (33) in the elastic case. The reader must refer to reference Alonso et al. (2016) for rigorous details. For the purpose of this presentation we use several well-known results that require different integrability properties for the angular kernel b, by assuming $b(\hat{u} \cdot \sigma)$ bounded from $\sigma \in S^{d-1}$ like it is the case for hard spheres in three dimensions (generalization for $b \in L^1(\mathbb{S}^{d-1})$ can be made at the cost of technical work). What is important that we work with hard potentials and so $1 \geq \lambda > 0$ in (9). The theory for Maxwell molecules $\lambda = 0$ needs a slightly different approach.

Recall that we have imposed conservation of mass, momentum and energy by building the operator $Q_c(g)$ with a constrained minimization procedure. Thus,

$$\int_{\Omega_L} g(v,t)\psi(v)\mathrm{d}v = \int_{\Omega_L} g_0(v)\psi(v)\mathrm{d}v$$

for any collision invariant $\psi(v) = \{1, v, |v|^2\}$. However, due to velocity truncation, the approximating solution g in general may be negative in some small portions of the domain. This is precisely the technical difficulty that we have to overcome. In Section 4.1, we present the statement of the proof of convergence of the proposed approximation in the number of modes N in a time interval $(0, T(L)]$ where $T(L)$ is a time depending on the lateral size L of the velocity domain Ω_L. We find a control on the negative mass that can be formed in such interval characterized in terms of L. In Sections 4.2 and 4.3, we improve the estimates assuming that the approximating solutions behaves well, that is, its negative mass does not increases too fast in the time interval in question.

4.1 Local Existence

Since the natural space to study the spectral scheme is $L^2(\Omega_L)$, thus we start proving that the problem is well posed in this space. Due to velocity truncation, we do not have the standard a priori estimates in L^1 that help in the theory, however, the constrain method permits to extend the time where the scheme gives an accurate solution of the original Boltzmann problem.

Proposition 1. *Let $g_0 \in L^2(\Omega_L)$ and fix the domain $(0, T(L)] \times \Omega_L$ with $T(L) \sim \left(L^{d+2(\lambda+1)} \| g_0\|_{L^2(\Omega_L)}\right)^{-1}$. Then the approximating problem (33) has a unique solution $g \in \mathcal{C}\left(0,T(L);L^2(\Omega_L)\right)$ with initial condition g_0.*[a] *In addition, the approximating sequence $\{g_N\}$ to solutions of (33), with initial condition $g_{0N} = \Pi^N g_0$, converges strongly in $\mathcal{C}\left(0,T(L);L^2(\Omega_L)\right)$ as $N \to \infty$. In particular,*

$$\sup_{t\in[0,T(L)]} \| Q(\mathrm{E}g_N,\mathrm{E}g_N) - Q_u(g_N)\|_{L^2(\Omega_L)} \to 0 \;\text{ as }\; N \to 0, \tag{51}$$

and the strong limit $\bar{g}$ is the unique solution of the equation

$$\frac{\partial \bar{g}}{\partial t} = Q(E\bar{g},E\bar{g})\boldsymbol{I}_{\Omega_L} - \frac{1}{2}\left(\bar{\gamma}_1 + \sum_{j=1}^{d}\bar{\gamma}_{j+1}v_j + \bar{\gamma}_{d+2}|v|^2\right), \quad \bar{g}(0) = g_0. \tag{52}$$

The coefficients of the quadratic polynomial are given in Lemma 1 with parameters (38) evaluated at $Q(E\bar{g},E\bar{g})$. Furthermore, the negative mass of g is quantified as

$$\sup_{t\in[0,T(L)]} \| g^- \|_{L^2(\Omega_L)} = \| g_0^- \|_{L^2(\Omega_L)} + O_{d/2+\lambda+2} \| g_0\|_{L^2(\Omega_L)}. \tag{53}$$

[a]Note that g actually depends on N since Q_c depends on N. We omit this dependence to ease notation.

4.2 Uniform Propagation of Numerical Unconserved Moments

We assume now that a solution $g \in \mathcal{C}\big(0,T;L^2(\Omega_L)\big)$ for problem (33) with initial condition $g_0 \in L^2(\Omega_L)$ exists. The *conservation scheme* and the following stability condition implies that moments up to order 2 are controlled by the initial datum.

4.2.1 Stability Condition

We denote $T_\epsilon \in [0, T]$ the time where the smallness relation for the negative mass and energy of g and the boundedness of sequence $\{g_N\} := \{g\}$ in L^2 holds, that is for some fixed $\epsilon > 0$,

$$\sup_{t\in[0,T_\epsilon]} \frac{\int_{\{g<0\}} |g(v,t)|\langle v\rangle^2 \mathrm{d}v}{\int_{\{g\geq 0\}} g(v,t)\langle v\rangle^2 \mathrm{d}v} \leq \epsilon, \quad \sup_{N\in\mathbb{Z}^+} \sup_{t\in[0,T_\epsilon]} \| g(t)\|_{L^2(\Omega_L)} < \infty. \tag{54}$$

Remark. This stability condition even holds for the scheme to compute the Boltzmann equation with an anisotropic grazing-Coulomb collision cross section (23) as shown in Fig. 2 in the grazing collision limit approximating the Landau equation. The conservation Spectral–Lagrangian scheme secures that after 800 mean free times, the value of $\epsilon < 0.05$ in the relation (54), meaning that the relative proportion of negative energy is very small, and so the solutions keeps essentially positive, and so stabilizes the scheme.

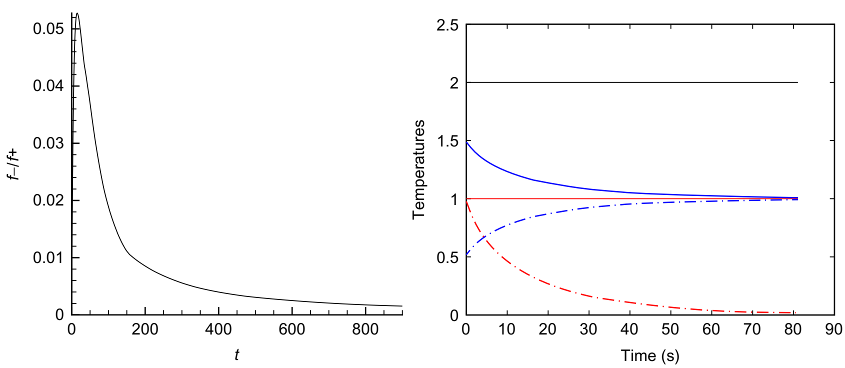

FIG. 2 *Left:* Ratio of energy in negative grid points to energy in positive grid points from the stability condition (54). The grazing parameter is $\varepsilon = 10^{-4}$, $N = 16$. *Right*: Temperatures evolution for the a benchmark component plasma system: *solid blue*, ion temperature T_i; *dash-dot blue*, electron temperature T_e; *solid black*, total conserved temperature $\overline{T} = T_i + T_e$; *dash-dot red*, temperature difference $|T_i - T_e|$ evolution. *Left panel from Gamba, I.M., Haack, J.R., 2014. A conservative spectral method for the Boltzmann equation with anisotropic scattering and the grazing collisions limit. J. Comput. Phys. 270, 40–57. Right panel from Zhang, C., Gamba, I.M., 2016. A Conservative Scheme for Vlasov Poisson Landau Modeling Collisional Plasmas. arXiv:1605.05787 (e-prints, section 7.1.2).*

Indeed, for $k = \{0, 2\}$

$$\int_{\Omega_L} |g||v|^k = \int_{\Omega_L} g_0|v|^k - 2\int_{\Omega_L} g^-|v|^k \leq \int_{\Omega_L} g_0|v|^k$$

$$+2\epsilon\int_{\Omega_L} g^+|v|^k \leq \int_{\Omega_L} g_0|v|^k + 2\epsilon\int_{\Omega_L} |g||v|^k.$$

Hence, choosing $\epsilon \leq 1/4$ it follows

$$\int_{\Omega_L} |g(v,t)||v|^k \mathrm{d}v \leq 2\int_{\Omega_L} g_0|v|^k \mathrm{d}v, \quad \text{for } t \in [0,T_\epsilon], \quad k = 1,2; \tag{55}$$

and the following lemma holds.

Lemma 3 (Numerical moments bounds). *For any lateral size $L > 0$ and moment $k > 0$ there exist an extension E and a number of modes $N_0(T_\epsilon, L, k)$ such that*

$$\sup_{t\in[0,T_\epsilon]} \| g\|_{L^1_k(\Omega_L)} \leq C_k\left(\| g_0\|_{L^1_2}, m_{k'}(g_0)\right), \quad \forall N \geq N_0, \tag{56}$$

with $C_k(\cdot)$ a constant depending only on k, $\| g_0\|_{L^1_2}$, and $m_{k'}(g_0)$ with $k' = \max\{k, k_0\}$. The number $k_0 > 0$ it is uniquely determined by $\| g_0\|_{L^1_2}$.

The proof of this fundamental results relies on the *conservative scheme* estimate

$$\int_{\Omega_L} g(w,t)|v-w|^2 \mathrm{d}w = \int_{\Omega_L} g_0(w)|v-w|^2 \mathrm{d}w. \tag{57}$$

and condition (54) to obtain an uniform lower bound for the collision operator negative part. The following result implies stability of the conservative scheme as well as convergence to the equilibrium Maxwellian. This lower bound is shown in Alonso et al. (2016) with the assumption that the entropy $\int g(v) \log g(v)\, \mathrm{d}v$ is bounded, since the numerical approximant $g(v)$ may not be positive at all its point of definition.

Lemma 4 (Lower bound for the discrete collision frequency). *Assume the uniform propagation of some moment $\frac{2+\mu}{\lambda}$, and that $\sup_{t\in[0,T_\epsilon]}\int_{\Omega_L} |g(w,t)||w|^{2+\mu} dw \leq C(g_0) < \infty$ for some $\mu > 0$. Then,*

$$\left(g * |u|^\lambda\right)(v) \geq C(g_0)\langle v\rangle^\lambda, \tag{58}$$

with $C(g_0) > 0$ depending only on the mass, energy and the $\frac{2+\mu}{\lambda}$-moment of g_0.

4.3 Uniform L^2_k Integrability Propagation

The result from Lemma 4 is fundamental to obtain the following weighted Sobolev estimates for the approximate solution to the collisional equation.

Lemma 5 (L_k^2-propagation estimates). *For any lateral size $L > 0$ and moment $k > 0$ there exist an extension E and a number of modes $N_0(T_\epsilon, L, k)$ such that*

$$\sup_{t\in[0,T_\epsilon]} \| g\|_{L_k^2(\Omega_L)} \le \max\left\{\| g_0\|_{L_k^2(\Omega_L)},\, C_k(m_k(g_0))\right\},\ \ N\ge N_0.$$

Moreover, the negative mass of g can be estimated as

$$\sup_{t\in[0,T_\epsilon]} \| g^-\|_{L^2(\Omega_L)} \le e^{C\left(\|g_0\|_{L_2^1(\Omega_L)}\right)T_\epsilon} \left(\| g_0^-\|_{L^2(\Omega_L)} + O_{\mathrm{d}/2+\lambda k}\,\widetilde{C}_k(m_{k+1}(g_0))\,\max\{1,T_\epsilon\}\right),\ \ N\ge N_0.$$

The constants C_k and $\widetilde{C}_k$ are independent of the asymptotic parameters T_ϵ, L and N.

The nest results gather the necessary information to estimate the propagation of higher order Sobolev regularity for the approximate solution, if initially so.

4.4 Uniform Semidiscrete H_k Sobolev Regularity Propagation

At last, we obtain the extend the discrete L_k^2 integrability estimates from Lemma 5 to the derivatives of g. Indeed, the follow result has been shown as well.

Lemma 6 *Assume $g_0 \in H_{k+2}^{\alpha}(\Omega_L)$ with $\alpha \in [0, \alpha_0]$ and $k \ge 0$. For any lateral size $L > 0$ there exist an extension E_{α_0} and a number of modes $N_0(T_\epsilon, L, k, \alpha)$ such that*

$$\sup_{t\in[0,T_\epsilon]} \| g\|_{H_k^{\alpha}(\Omega_L)} \le \max\left\{\| g_0\|_{H_{k+2}^{\alpha}(\Omega_L)}, C_k(m_k(g_0))\right\},\ \ N\ge N_0,$$

where $C_k(\cdot)$ depends on k and the k-moment of g_0.

Remark. The initial restriction $\alpha \in [0, \alpha_0]$ is due to the fact that in general $Q(\mathrm{E}g, \mathrm{E}g)$ possesses at most α_0 derivatives.

Finally, gathering the results of Sections 3.4 and 3.5, with the results of global existence, L_k^1 and L_k^2 moment estimates, as well the higher order Sobolev regularity estimates form (6) of last section as well as spectral accuracy for the collisional integral shown in Gamba and Tharkabhushanam (2009), one can obtain both error estimates for the spectral scheme in the case of smooth and nonsmooth initial data, and convergence to the equilibrium Maxwellian (6). The first result removes the small negative mass and energy assumption (54) needed for the a priori estimates throughout the previous section. The results hold for any initial state $f_0(v)$ associated to the Cauchy problem for the Boltzmann equation, assumed to be $L^2(\mathbb{R}^d)$ and nonnegative (see Alonso et al., 2016 for rigorous details).

5 FINAL COMMENTS AND CONCLUSIONS

The conservative spectral Lagrangian method for the Boltzmann equation was applied for a system of such equations in the modelling of a multienergy level gas (Munafo et al., 2014). In this case, the formulation of the numerical method accounts for both elastic and inelastic collisions. It was also be used for the particular case of a mixture of monatomic gases without internal energy. The conservation of mass, momentum and energy during collisions is enforced through the solution of constrained optimization problem to keep the collision invariances associated to the mixtures (see Munafo et al., 2014, section 4.3). The effectiveness have been compared with the results obtained by means of the DSMC method and excellent agreement has been observed. More recently this conservative spectral Lagrangian approach has been implemented for a system of electron–ions in plasma modelled by a 2×2 system of Poisson–Vlasov–Landau equations (Zhang and Gamba, 2016), implemented by time-splitting methods staggering the time steps for advection of the Vlasov–Poisson system and the collisional system including recombinations. The constrained optimization problem is applied to the collisional step in a revised version from Gamba and Tharkabhushanam (2009) where the matrix $\mathbf{C}^{\mathbf{e}}$ defined in (43) was calculated in Fourier space given by the Fourier of the collision invariant polynomials to obtain a more accurate formulation. The benchmarking for the constrained optimization implementation for the mixing problem was done for an example of a space homogeneous system where the explicit decay the difference for electron and ion temperatures is known (Zhang and Gamba, 2016, section 7.1.2). Yet the used scheme captures the total conserved temperature being the sum of the Ions and electron temperatures, respectively (see Fig. 2, right side).

To end, we point out that the conservative spectral Lagrangian scheme for approximating solutions for the Boltzmann equation for elastic interactions converges to the equilibrium Maxwellian (6) if the equation is scalar, as is it shown in Theorem 2, part 4. One should note that it is the conservation subscheme the one that enforces the convergence to the equilibrium Maxwellian state by enforcing the collision invariants. This is exactly how the Boltzmann and H-theorems (Cercignani et al., 1994) work: the equilibrium Maxwellian (6) is proven to be the stationary state due to the conservation properties combined with the elastic collision law.

In other words for the case of inelastic collision (when the collision invariants are just $d + 1$) or for space inhomogeneous multicomponent Boltzmann systems flow models, it is not correct to assume that the stationary state is a Maxwellian distribution density (i.e. a Gaussian in v-space) as, for instance, asymptotic preserving schemes assume. Just the enforcing the conserved quantities for the system by the constrain minimization problem, the *Conservation Correction Estimate* of Lemma 2 will select the correct equilibrium states for each of the system components.

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