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A discontinuous Galerkin finite-element method for a 1D prototype of the Boltzmann equation

by

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A Discontinuous Galerkin Finite-Element Method for a 1D Prototype of the Boltzmann Equation

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ABSTRACT
To develop and analyze new computational techniques for the Boltzmann equation based on model or approximation adaptivity, it is imperative to have disposal of a compliant model problem that displays the essential characteristics of the Boltzmann equation and that admits the extraction of highly accurate reference solutions. For standard collision processes, the Boltzmann equation itself fails to meet the second requirement for d = 2, 3 spatial dimensions, on account of its setting in 2d, while for d = 1 the first requirement is violated because the Boltzmann equation then lacks the convergence-to-equilibrium property that forms the substructure of simplified models. In this article we present a numerical investigation of a new one-dimensional prototype of the Boltzmann equation. The underlying molecular model is endowed with random collisions, which have been fabricated such that the corresponding Boltzmann equation exhibits convergence to Maxwell-Boltzmann equilibrium solutions. The new Boltzmann model is approximated by means of a Discontinuous Galerkin (DG) finite-element method. To validate the one-dimensional Boltzmann model, we conduct numerical experiments and compare the results with Monte-Carlo simulations of equivalent molecular-dynamics models.

1. Introduction
Fluid-flow problems in the transitional molecular/continuum regime play an important role in many engineering applications, e.g., in hypersonic applications in aerospace engineering, in microfluidic devices and in many systems and processes in the high-tech industry. Furthermore, such problems are gaining further prominence with the perpetual trend towards miniaturization in science and engineering. In many applications, interest is restricted to a particular macroscale quantity of interest, i.e., a quantity that is independent of the characteristics of individual molecules, but rather depends on certain ensemble properties. Examples of such macroscale quantities are thrust, heat transfer at fluid/solid interfaces and flow rate.

The numerical simulation of flows in the transitional molecular/continuum regime and the determination of macroscale quantities from such simulations poses a fundamental challenge. In principle, a variety of flow models are available to serve as a basis for numerical simulations. The appropriateness of these flow models depends on the regime in which the flow resides, where the flow regime is identified by a scaling parameter known as the Knudsen number (Kn). The Knudsen number expresses the ratio of the mean free path between molecules and a typical length scale of observation. In the high Knudsen number regime (say Kn > 1), the length scale of observation essentially pertains to the behaviour of individual molecules. Accordingly, molecular-dynamics models, e.g., in the form of a Hamiltonian system, provide a meaningful description. In the low Knudsen number regime (say Kn < 0.1), the length scale of observation encapsulates large numbers of molecules, and the flow can be appropriately described by a continuum model, such as the Navier–Stokes and Euler equations. In the transitional regime, however, neither of the aforementioned models provides an adequate basis for numerical simulations. Continuum models are invalid in this regime or, at least, such models exhibit severe modeling errors. On the other hand, the number of molecules in the system is so large that it
1. Introduction

The transitional molecular/continuum regime is covered by the Boltzmann equation. The Boltzmann equation specifies the evolution of a one-molecule probability-density distribution in position/momentum space \([12, 23]\). The Boltzmann equation in fact encapsulates all conventional continuum models, in the sense that with appropriate scalings of the macroscopic length and time scales, limit solutions of the Boltzmann equation correspond to solutions of these continuum models \([3, 16, 21, 31, 32]\). Numerical approximation of the Boltzmann equation poses fundamental complications, however, on account of the high dimensional setting of the equation: for a problem with \(d\) spatial dimensions, the corresponding position/momentum domain of the Boltzmann equations is \(2d\)-dimensional. For conventional discretization methods for (integro-)differential equations, such as finite-difference and finite-element methods with uniform meshes, the number of unknowns in the discrete approximation increases by a factor of \(2^{2d}\) whenever the computational mesh is refined by a factor of 2. Notwithstanding successful applications to simplified problems (see, e.g., \([1, 17]\)), this computational complexity is prohibitive for practical applications. Current simulation methods for 2 and 3-dimensional problems are generally based on Bird’s Direct-Simulation-Monte-Carlo method \([6, 7]\) or its Nanbu extension \([2, 33]\). The computational complexity of DSMC methods depends sensitively on the Knudsen number, however, and the computational cost of the methods becomes prohibitive in the continuum limit.

A cogent alternative approximation method for the Boltzmann equation is provided by finite-element approximations of so-called moment-closure hierarchies of the Boltzmann equation \([22, 29, 30, 38]\). In a moment-closure hierarchy, the Boltzmann equation in \(2d\)-dimensions is represented by a hierarchy of hyperbolic systems in \(d\)-dimensions. The number of equations in each hyperbolic system depends on its rank in the hierarchy. The hyperbolic systems can in turn be approximated by a finite-element method; see, for instance, \([4, 28]\). An important property of moment-closure hierarchies, is that the (Maxwell-Boltzmann) equilibrium distributions that provide the connection between the molecular and continuum models of flows (cf., e.g., \([12]\)) are included in the coarsest model in the hierarchy. Accordingly, finite-element approximations of moment-closure hierarchies yield a very efficient approximation of the continuum limit.

In the context of a restricted interest to macroscale quantities, it is anticipated that substantial computational savings can be achieved by means of a goal-oriented adaptive-refinement strategy \([5, 20, 36]\). In goal-adaptive methods, the computational model is refined in such a manner that an optimal approximation of the quantity of interest is obtained. Based on the solution of a dual problem, the contribution of local errors in the solution to the quantity of interest is identified, and only the regions that yield a significant contribution to the error in the goal quantity are refined. One can therefore envisage a computational strategy based on finite-element approximations of moment-closure hierarchies, in which the hierarchical rank in the finite-element model is not globally fixed, but is instead locally adapted in accordance with the goal-error indicator.

To develop and investigate new computational techniques for the Boltzmann equation based on model or approximation adaptivity, it is imperative to have disposal of a model problem that displays the essential characteristics of the Boltzmann equation and, moreover, that admits the extraction of highly accurate reference solutions. The Boltzmann equation itself fails to meet the second requirement for \(d = 2, 3\), on account of its setting in \(2d\). For \(d = 1\), however, the first requirement is violated for standard collisions operators, e.g., corresponding to perfectly elastic collisions. In this case, the Boltzmann equation lacks the convergence-to-equilibrium property that provides the connection between molecular and continuum models, and that forms the substructure of simplified models.

In this article, we present a numerical investigation of a new one-dimensional prototype of the Boltzmann equation. The underlying molecular model is endowed with so-called random collisions, which are fabricated in such a manner that the corresponding Boltzmann equation exhibits Maxwell-
Boltzmann equilibrium solutions. Moreover, it can be shown that the prototype model satisfies an H-theorem. The collision operator in the Boltzmann equation assumes the typical form of an integral operator. The new Boltzmann model is approximated by means of a Discontinuous Galerkin (DG) finite-element method. To validate the one-dimensional Boltzmann model, we conduct numerical experiments and compare the results with Monte-Carlo simulations of equivalent molecular-dynamics models.

One-dimensional prototypes of the Boltzmann equation that exhibit a convergence-to-equilibrium property have been investigated previously. Notable examples are the Kac model [9, 26] and the Ianiro-Lebowitz model [11, 25]. The prototype that we present in this paper is reminiscent of these models, in that it is based on non-momentum-conserving random collisions. However, at variance with the model that we present, the molecular interactions in the Kac model are based on a random-walk (the Kac walk) and not on a mechanistic collision process. In the Ianiro-Lebowitz model, the randomness in the collision process pertains to the random selection between two distinct collision processes, viz., perfectly-elastic collision and velocity-sign-reversing collision. The model that we present is based on a single collision process which is inherently random on account of continuous dependence of the post-collision velocities on a random angle. We believe that our model therefore offers a closer similarity to the conventional Boltzmann equation in 2, 3-spatial dimensions in interpretation and properties of the collision mechanism. This closer similarity however comes at the expense of a profoundly more complicated collision operator than in the Ianiro-Lebowitz model.

In the context of the DG finite-element method that we consider in this paper, it is to be remarked that the numerical investigation of Boltzmann-type equations by means of DG finite-element methods has received only sparse attention. We allude to the recent work by Gamba and co-workers on the Boltzmann-Poisson equation [13], on the Vlasov-Poisson system [24] and on the Wigner-Fokker-Planck equation [19].

The remainder of this paper is organized as follows: Section 2 presents the molecular-dynamics model and elaborates the relation between the molecular-dynamics model and the Boltzmann equation. Section 3 is concerned with the derivation of the Boltzmann equation and the corresponding initial and boundary conditions. In Section 4 we present the DG finite-element formulation of the Boltzmann model. In addition, we address aspects related to the numerical approximation of the collision operator and iterative solution procedures for the nonlinear algebraic system of equations emanating from the finite-element approximations. In Section 5 we conduct numerical experiments to test the finite-element approximation and to exhibit the characteristics of the molecular-dynamics model and of the Boltzmann equation. Finally, Section 6 presents concluding remarks.

2. Molecular model

2.1 Impulsive differential equation

We first present a formal specification of the molecular model. We consider the motion of \( n \) molecules on an open unit interval \( \Omega = (0, 1) \), within a time interval \( T = (0, T) \). The molecules are identified by means of an index \( i \in \{1, 2, \ldots, n\} \). Without loss of generality, we assume that the molecules are sequentially indexed from left to right, i.e., \( 0 < x_i \leq x_{i+1} < 1 \). The molecules display a uniform motion, except at a countable number of moments, \( \{\tau_i\} \), at which hard collisions occur.

The molecular system is described by a system of so-called first-order impulsive differential equations; see [35, Ch. 15]. Denoting the position and velocity of each molecule by \( x_i : T \to \Omega \) and \( \xi_i : T \to \Xi := \mathbb{R} \), respectively, and collecting the positions and velocities in vectors \( \mathbf{x} = (x_1, \ldots, x_n) \) and \( \mathbf{\xi} = (\xi_1, \ldots, \xi_n) \), the motion of the molecules is governed by:

\[
\begin{align*}
(x', \xi') &= (\xi, m^{-1}b(\xi, x)) & \text{in } T \setminus \{\tau_i(x, \xi)\}, \\
(x(t^+), \xi(t^+)) &= (x(t^-), I(x(t^-), \xi(t^-))) & \text{at } t \in \{\tau_i(x, \xi)\}, \\
(x, \xi)(0) &= (x^0, \xi^0),
\end{align*}
\]

where \( \cdot' = \frac{d}{dt} \), \( (x^0, \xi^0) \in \Omega^n \times \Xi^n \) represent prescribed initial data, \( b = (b_1, \ldots, b_n) : T \times \Omega^n \to \Xi^n \) is a prescribed rate function for the hard collisions, and \( I : \Omega \times \Xi \to \Xi \) is a function which models the inelasticity of the collisions.
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Ω^n × Ξ^n → Ξ^n contains prescribed exogenous forces on the molecules, m is the molecule mass and \{τ_i(x, ξ)\} ⊂ T records the collision moments, i.e., all moments at which x_i = x_{i+1} and ξ_i > ξ_{i+1} for some i. Throughout, we shall assume the absence of exogenous forces and, accordingly, set b = 0. Moreover, for convenience, we set m = 2, so that the kinetic energy of a molecule with velocity ξ is ξ^2.

In equation (2.1b), we have introduced the condensed notation \( t^\pm = \lim_{\epsilon \to \pm 0} t \) for the one-sided limits from below (−) and above (+). We restrict our considerations to functions for which these limits are well defined.

Equation (2.1b) directly imposes continuity of positions at collisions. The effect of collisions on the velocity is represented by the impuls operator \( I = (I_1, \ldots, I_n) : \Omega^n × Ξ^n → Ξ^n \). The velocity of non-colliding particles is continuous at collisions, while the post-collision velocity of colliding particles depends on their pre-collision velocity according to a certain collision process. These conditions give rise to the following specification of the impuls operator:

\[
I_i : (x^-, ξ^-) \mapsto ξ^+_i = \begin{cases} I_>(ξ^-, ξ^+_{i+1}) & \text{if } x^-_i = x^+_{i+1}, ξ^-_i > ξ^+_{i+1}, \\ I_<(ξ^-, ξ^-_{i-1}) & \text{if } x^-_i = x^-_{i-1}, ξ^-_i < ξ^-_{i-1}, \\ ξ^-_i & \text{otherwise.} \end{cases} \tag{2.2}
\]

In (2.2), \( I_>(ξ, ζ) \) (resp. \( I_<(ξ, ζ) \)) corresponds to the post-collision velocity of a molecule with pre-collision velocity ξ that sustains a collision on its right (resp. left) side with a molecule with velocity ζ < ξ (resp. ζ > ξ). Perfectly elastic collision are for instance represented by:

\[
I_>(ξ, ζ) = ζ, \quad I_<(ξ, ζ) = ζ. \tag{2.3}
\]

We furthermore stipulate that molecules diverge after collision. This translates into the requirement that for all ξ > ζ it holds that \( I_>(ξ, ζ) < I_<(ξ, ζ) \).

Molecule-boundary collisions occur when \( x_1(t^-) = 0 \) and \( ξ_1(t^-) < 0 \) or \( x_0(t^-) = 1 \) and \( ξ_0(t^-) > 0 \). Molecule-boundary interactions are represented by a map \( (x_i(t^-), ξ_i(t^-)) \mapsto (x_i(t^+), ξ_i(t^+)) \) with \( i ∈ \{1, n\} \). In particular, we consider specular reflection

\[
(x^-_i, ξ^-_i) \mapsto (x^+_i, ξ^+_i) = (x^-_i, -ξ^-_i), \tag{2.4}
\]

and periodicity:

\[
(x^-_i, ξ^-_i) \mapsto (x^+_i, ξ^+_i) = (x^-_i \mod 1, ξ^-_i), \tag{2.5}
\]

where \( x \mod 1 = \{s ∈ (0, 1) : x = z + s, z ∈ Ξ \} \) denotes the modulo of x with divisor 1. Let us note that for periodic molecule-boundary interactions, the set \( \{x_1(t), \ldots, x_n(t)\} \) is not sequentially ordered, but it is a cyclic permutation of an ordered set instead. The assumption that the molecules are sequentially indexed can be upheld, if we regard cyclic permutations of ordered sets as an equivalence class. In Sections 3 and 5, we shall also consider random molecule-boundary interactions, viz.,

\[
(x^-_i, ξ^-_i) \mapsto (x^+_i, ξ^+_i) = (x^-_i, ξ^+_i), \tag{2.6}
\]

with ζ a random variable.

It is to be noted that if the molecules are initially indexed from left to right, i.e., \( 0 < x^0_i < x^0_{i+1} < 1 \), then the aforementioned post-collision-divergence stipulation ensures that the positions remain ordered according to \( 0 ≤ x_i(t) ≤ x_{i+1}(t) ≤ 1 \), respectively ordered under cyclic permutation for periodic molecule-boundary interactions.

2.2 Non-deterministic setting and equilibrium distributions

Let us consider a non-deterministic specification of the initial conditions. We denote by \( \Sigma := Ω × Ξ \) the phase space of the individual molecules, and by \( \Sigma^n \) the phase space of the ensemble of molecules. The elements of \( \Sigma \) and \( \Sigma^n \) will be denoted by \( σ := (x, ξ) \) and \( σ \), respectively. Formally, a non-deterministic
specification of the initial conditions consists of a probability-density function \( \rho_0 : \Sigma^n \to [0, \infty] \) that assigns to each subset \( \omega \subset \Sigma^n \) the probability that the initial states \( \sigma := (\sigma_1, \ldots, \sigma_n) \) reside in \( \omega \):

\[
P(\sigma \in \omega) = \int_{\omega} \rho_0(\sigma) \, d\sigma.
\]

The probability distribution of a molecular system evolves under the Liouville equation; see, e.g., \([14, 37]\). The evolution can alternatively be described by duality according to:

\[
\int_{\Sigma^n} \Psi(\sigma) \, \rho(t, \sigma) \, d\sigma = \int_{\Sigma^n} \Psi(S_t \sigma) \, \rho_0(\sigma) \, d\sigma,
\]

for all sufficiently smooth observables (or test functions, i.e., infinitely differentiable functions with compact support) \( \Psi : \Sigma^n \to \mathbb{R} \), where \( S_t \sigma \) is the state of the system at time \( t \) corresponding to the initial condition \( \sigma \). Equation (2.8) expresses that \( \rho \) is constant along trajectories of the molecular system.

Suppose that instead of general observables, we restrict our interest to so-called macroscale quantities,

\[
\Psi(\sigma) = \frac{1}{n} \sum_{i=1}^{n} \psi(\sigma_i),
\]

for any sufficiently smooth function \( \psi : \Sigma \to \mathbb{R} \). It then holds that

\[
\int_{\Sigma^n} \Psi(\sigma) \, \varrho(t, \sigma) \, d\sigma = \frac{1}{n} \sum_{i=1}^{n} \int_{\Sigma^n} \psi(\sigma_i) \, \varrho(t, \sigma) \, d\sigma \\
= \frac{1}{n} \sum_{i=1}^{n} \int_{\Sigma} \psi(\sigma_i) \left( \int_{\Sigma^{n-1}} \varrho(t, \sigma) \prod_{j \neq i} d\sigma_j \right) \, d\sigma_i = \int_{\Sigma} \psi(\sigma) \, f(t, \sigma) \, d\sigma,
\]

where the (one-molecule) phase-space density \( f : \Sigma \to [0, \infty] \) is defined by

\[
f(t, \sigma) := \frac{1}{n} \sum_{i=1}^{n} \int_{\Sigma^{n-1}} \varrho(t, \sigma|_{\sigma_i=\sigma}) \prod_{j \neq i} d\sigma_j,
\]

with, in particular, \( \sigma|_{\sigma_i=\sigma} = (\sigma_1, \ldots, \sigma_{i-1}, \sigma, \sigma_{i+1}, \ldots, \sigma_n) \). In view of its form (2.11), the function \( f \) is also often referred to as a (one-molecule) marginal distribution. Equation (2.10) conveys that all macroscale quantities can be directly determined on the basis of the one-molecule phase-space density. The evolution of the one-molecule phase-space density associated with a molecular system is governed by the corresponding Boltzmann equation, i.e., the Boltzmann equation provides a specification of \( f \) without reference to the underlying solution of the Liouville equation via (2.11). It is to be remarked, however, that the Boltzmann equation of a molecular system can in general only be derived under certain simplifying assumptions, e.g., molecular chaos; see, e.g., \([12, 23]\). The solution of the Boltzmann equation then forms an approximation to the one-molecule phase-space density defined by (2.11).

An important property of many molecular systems pertains to the existence of so-called (Maxwell-Boltzmann) equilibrium distributions. The existence of such distributions in fact underlies the connection between kinetic flow models and continuum flow models such as the Euler and Navier–Stokes equations. For many kinetic flow models, the corresponding one-molecule phase-space density possesses the following convergence property:

\[
\lim_{T \to \infty} T^{-1} \int_{0}^{T} \int_{\Sigma} f(t, \sigma) \psi(\sigma) \, d\sigma \, dt = \int_{\Sigma} M(\sigma) \psi(\sigma) \, d\sigma
\]

(2.12)
for all test functions \( \psi \), where \( \mathcal{M} : \Sigma \to [0, \infty] \) conforms to:
\[
\mathcal{M}(x, \xi) = \alpha \exp \left( -\beta |\xi - v|^2 \right),
\]
for certain constants \( \alpha > 0, \beta \geq 0 \) and \( v \in \mathbb{R}^d \). The convergence-to-equilibrium property of molecular systems is closely connected to mixing-behavior; see [14] and also [27, §20.5].

2.3 Random collisions
A fundamental difference between molecular systems with perfectly elastic collisions in 1-spatial dimension and in 2- or 3-spatial dimensions is that the 1-dimensional system is non-mixing, whereas the higher dimensional systems are. This deficiency of the 1-dimensional system follows immediately from (2.3): denoting by \( \xi^-, \zeta^- \) and \( \xi^+, \zeta^+ \) the pre- and post-collision velocities of two colliding molecules, the elastic-collision process in 1 dimension is characterized by:
\[
(\xi^-, \zeta^-) \mapsto (\xi^+, \zeta^+) = (\zeta^-, \xi^-).
\]
(2.14)
Therefore, the (unordered) set of molecular velocities, \( \{\xi_i(t)\}_{i=1}^n \), is time invariant and the 1-dimensional system does not display mixing behavior. Consequently, the 1-dimensional molecular system with perfectly-elastic collisions does not exhibit convergence to equilibrium.

To introduce mixing in the 1-dimensional molecular system, we endow the system with random collisions. To this end, we define \( I_\Rightarrow \) and \( I_\Leftarrow \) in the impuls operator \( I \) in (2.2) as
\[
I_\Rightarrow (\xi, \zeta) = |\xi, \zeta| \cos(\alpha + \pi/4), \quad I_\Leftarrow (\xi, \zeta) = |\xi, \zeta| \sin(\alpha + \pi/4),
\]
(2.15)
where \( |\xi, \zeta| = \sqrt{\xi^2 + \zeta^2} \) and \( \alpha \) is a random variable which assumes values in the interval \([0, \pi]\) subject to a sinusoidal probability-density distribution; see Figure 1 for an illustration. Let us remark that, alternatively, according to the transformation formula for integrals (see, e.g., [27, Thm. 1.101]), \( \alpha \) in (2.15) can be replaced by \( \arccos(-s) \), with \( s \) a uniformly distributed random variable in the interval \([-1, 1]\). The random-collision process (2.15) has been constructed such that solutions of the corresponding stochastic impulsive differential equation (2.1) convergence to equilibrium distributions of the form (2.13) as time progresses (in an appropriate sense). A numerical investigation of this convergence-to-equilibrium property is presented in Section 5.3.

A collision process is perfectly elastic if and only if it conserves energy and momentum. Recalling that perfectly elastic collisions are non-mixing in 1-dimension, one of the conservation properties must be abandoned in the random-collision process to introduce mixing behavior. The random-collision process corresponding to (2.15) complies with conservation of energy and violates conservation of momentum. Considering the (generic) collision between two particles with pre-collision velocities \( \xi \) and \( \zeta \), \( \xi > \zeta \), the post-collision velocities are \( I_\Rightarrow (\xi, \zeta) \) and \( I_\Leftarrow (\zeta, \xi) \), respectively. Conservation of energy then follows from the identities:
\[
(I_\Rightarrow (\xi, \zeta))^2 + (I_\Leftarrow (\zeta, \xi))^2 = (\xi^2 + \zeta^2) \cos^2(\alpha + \pi/4) + (\xi^2 + \zeta^2) \sin^2(\alpha + \pi/4) = \xi^2 + \zeta^2.
\]
(2.16)
Similarly, it can be shown that the collision does not generally conserve momentum.

3. The Boltzmann equation
In a non-deterministic setting, the expectation of macroscale quantities of the molecular system can be determined from the corresponding one-molecule phase-space density; see Section 2.2. The one-molecule phase-space density in principle evolves under the Boltzmann equation of the molecular system. In this section, we present the Boltzmann equation associated with the molecular system (2.1) and the random-collision process (2.15).
3. The Boltzmann equation

Figure 1: Illustration of the random collision process: The random collision maps the pre-collision velocities $\xi^-, \zeta^-$ ($\xi^- > \zeta^-$) to the post-collision velocities $\xi^+ = I_\succ (\xi^-, \zeta^-)$ and $\zeta^+ = I_\prec (\zeta^-, \xi^-)$ with $I_\prec$ according to (2.15). The dashed line indicates the probability density $p(\alpha) = \frac{1}{2} \sin(\alpha)$.

3.1 Integro-differential evolution equation

To provide a setting for the Boltzmann equation, we recall that $\Sigma = \Omega \times \Xi$ denotes the position-velocity product domain. We denote the class of all suitable probability-density functions on $\Sigma$ by

$$\mathcal{D} = \left\{ f : \Sigma \to [0, \infty] : f \geq 0 \text{ a.e.}, \int_{\Sigma} f(\sigma) \, d\sigma = 1 \right\},$$

where $\sigma$ represents Lebesgue measure. Typically, functions in $\mathcal{D}$ have to satisfy further requirements, e.g. with respect to their behavior as $|\xi| \to \infty$, but these will not be further explored here. The evolution of the one-molecule phase-space density $f : T \to \mathcal{D}$ is governed by the Boltzmann equation:

$$f'(t) + \xi \nabla f(t) - \varepsilon^{-1} Q(f(t), f(t)) = 0 \quad t \in T,$$

(3.1)

where $\cdot'$ denotes the temporal derivative, $\nabla(\cdot)$ denotes the spatial derivative in the sense of distributions, $Q(\cdot, \cdot)$ is a bilinear operator referred to as the (normalized) collision operator, and $\varepsilon$ is a positive scaling parameter called the Knudsen number. In particular, in the current setting, it holds that $\varepsilon = 1/(n - 1)$. For readers less familiar with kinetic models, it is to be noted that the transport velocity $\xi$ in (3.1) is an independent variable. The collision operator generally assumes the form of an integral operator, rendering the Boltzmann equation of integro-differential type. The collision operator corresponding to the random-collision process (2.15) is elaborated in the next section.

3.2 Random-collision operator

The collision operator is obtained by the standard heuristic derivation; see, e.g., [12, 23]. A collision is conceived of as the annihilation of the pre-collision state and the production of a post-collision state. Accordingly, the collision operator can be separated in a loss ($L$) and a gain ($G$) component:

$$Q(f, g) := G(f, g) - L(f, g),$$

(3.2)

Given a one-molecule phase-space density $f \in \mathcal{D}$, the collision rate of molecules with state $(x, \xi)$ and molecules with state $(x, \zeta)$ is itself a random variable characterized by the probability-density function
3. The Boltzmann equation

\[ f(x, \xi) f(x, \zeta) |\xi - \zeta|. \]

If we distinguish between the cases \( \xi > \zeta \) and \( \xi < \zeta \), the loss terms associated with these types of collisions can be represented by \( L_>(f, f) \) and \( L_<(f, f) \), respectively, where:

\[
L_>(f, g) : (x, \xi) \mapsto \int_\xi^\infty f(x, \xi) g(x, \xi) |\xi - \zeta| d\zeta, \quad L_<(f, g) : (x, \xi) \mapsto \int_\xi^\infty f(x, \xi) g(x, \xi) |\xi - \zeta| d\zeta.
\]

(3.3)

The loss operator \( L \) is simply the sum of \( L_> \) and \( L_< \). It is to be noted, however, that the integrands of both integrals in (3.3) are identical and that the integration does not involve the arguments of \( f \).

Hence, \( L \) can be written in the compact form:

\[
L(f, g) : (x, \xi) \mapsto f(x, \xi) \int_\xi^\infty g(x, \xi) |\xi - \zeta| d\zeta.
\]

(3.4)

To facilitate the derivation of the gain term, we first restrict ourselves to post-collision states with \( \xi^+ < \zeta^+ \); cf. Figure 1. Denoting by \( \Xi^+ = \{(\xi^+, \zeta^+) \in \mathbb{R}^2 : \xi^+ < \zeta^+\} \) the aggregate of all post-collision velocities, we consider the probability \( P_B \) that a post-collision state occurs in the bounded subset

\[
B = \{(\xi^+, \zeta^+) = (s \cos(\theta + \pi/4), s \sin(\theta + \pi/4)) : r < s < r + \delta r, \alpha < \theta < \alpha + \delta \alpha \} \subset \Xi^+,
\]

with \((r, \delta r, \alpha, \delta \alpha) \in (0, \infty) \times (0, \infty) \times (0, \pi) \times (0, \pi)\) subject to the condition that \( B \subset \Xi^+ \) and \( B \neq \emptyset \), but otherwise arbitrary. For convenience, we fix \( x \in \Omega \). Denoting by \( h : \Xi^+ \to [0, \infty] \) the probability-density function associated with the post-collision velocities, it holds that

\[
P_B = \frac{1}{2} \sin \theta \int_B f(x, \xi) f(x, \zeta) |\xi^- - \zeta^-| d\xi^- d\zeta^- = \int_0^{\pi} \int_0^{\alpha+\delta \alpha} h(s \cos(\theta + \pi/4), s \sin(\theta + \pi/4)) s \sin \eta \sin \eta \sin \theta \sin \delta r \sin \alpha \sin \delta \alpha ds \sin \eta \sin \theta \sin \delta \alpha. \]

(3.5)

where the second identity follows from a transformation to polar coordinates. On account of the energy-conservation property, only pre-collision velocities in the semi-circular set \( C \),

\[
C = \{(\xi^-, \zeta^-) \in \mathbb{R}^2 : \xi^- > \zeta^-, |\xi^- - \zeta^-| \in (r, r + \delta r)\},
\]

can lead to post-collision velocities in \( B \). Recalling the sinusoidal probability density of the post-collision velocities, we then obtain

\[
P_B = \frac{1}{2} \int_0^{\pi} \int_0^{\alpha+\delta \alpha} f(x, \xi) f(x, \zeta) |\xi^- - \zeta^-| d\xi^- d\zeta^- = \frac{1}{2} \sin \theta \int_0^{\alpha+\delta \alpha} \int_0^{\pi} f(x, s \cos(\pi/4)) f(x, s \sin(\pi/4)) \sqrt{2} s \sin \eta \sin \eta \sin \theta \sin \delta r \sin \alpha \sin \delta \alpha ds \sin \theta ds \sin \eta \sin \delta \alpha. \]

(3.6)

The second identity in (3.6) follows from a transformation to polar coordinates and the trigonometric relation \( \cos \eta \sin \eta = -\sqrt{2} \sin(\eta - \pi/4) \). Because \( r, \delta r, \alpha \) and \( \delta \alpha \) are essentially arbitrary, Equations (3.5) and (3.6) imply

\[
h(\xi^+, \zeta^+) = \frac{1}{2} \int_0^{\pi} f(x, -|\xi^- + \zeta^-| \cos(\alpha + \pi/4)) f(x, -|\xi^+ + \zeta^+| \sin(\alpha + \pi/4)) \sin \alpha ds \sin \alpha ds. \]

(3.7)

The gain generated by collisions with \( \xi > \zeta \) is obtained by integrating the post-collision probability density \( h \) in (3.7) over \( \zeta < \xi \). The result can be expressed as \( G_>(f, f) \) with

\[
G_>(f, g) : (x, \xi) \mapsto \int_\xi^\infty \frac{1}{2} \int_0^{\pi} f(x, s \cos(\pi/4)) f(x, s \sin(\pi/4)) \sqrt{2} s \sin \eta \sin \eta \sin \theta \sin \delta r \sin \alpha \sin \delta \alpha ds \sin \theta ds. \]

(3.8a)
In a similar manner, it can be shown that the gain generated by collisions with \( \xi < \zeta \) can be expressed as \( G_{<}(f,f) \) with

\[
G_{<}(f,g) : (x,\xi) \mapsto \int_{-\infty}^{\infty} \frac{1}{2} \xi - \zeta | f(x,|\xi|,\cos(\alpha + \pi/4)) g(x,|\xi|,\sin(\alpha + \pi/4)) | \sin \alpha \, d\nu. \quad (3.8b)
\]

The gain operator \( G \) consists of the sum of \( G_{>}, \) and \( G_{<} \).

An important property of the collision operator \( Q = G_{>} + G_{<} - L_{>} - L_{<} \), which we report without proof, is that

\[
\int_{-\infty}^{\infty} \psi(\xi) Q(f(x,\xi),f(x,\xi)) \, d\xi = 0 \quad \text{a.e. } x \in \Omega,
\]

for all \( f \in D \), if \( \psi \) resides in the space of collision invariants, \( \text{span}\{1,\cdot\} \). Equation (3.9) implies that collisions are mass and energy conserving. It then follows that solutions of the Boltzmann equation \( (3.1) \) satisfy

\[
\frac{d}{dt} \int_{\Sigma} \psi(\xi) f(t,x,\xi) \, dx \, d\xi = \int_{-\infty}^{\infty} \psi(\xi) \frac{\partial}{\partial \xi} f(t,0,\xi) \, d\xi - \int_{-\infty}^{\infty} \psi(\xi) \frac{\partial}{\partial \xi} f(t,1,\xi) \, d\xi,
\]

for all \( \psi \in \text{span}\{1,\cdot\} \).

### 3.3 Auxiliary conditions

The Boltzmann equation \((3.1)\) must be equipped with suitable initial and boundary conditions. To specify the boundary conditions, we note that \( \Sigma = \Omega \times \Xi \) is a strip with boundary \( \partial \Sigma = \partial \Omega \times \Xi \). The boundary therefore consist of two disjoint parts, \( \Gamma_0 = \{x = 0\} \times \Xi \) and \( \Gamma_1 = \{x = 1\} \times \Xi \). As a necessary condition for stability, a boundary condition must be provided at inflow boundaries, i.e., the parts of the boundary where \( \xi \nu_x < 0 \) with \( \nu_x \) the \( x \)-component of the outward unit normal vector on \( \partial \Sigma \). In particular, it holds that \( \nu_x = -1 \) (resp. \( \nu_x = 1 \)) on \( \Gamma_0 \) (resp. \( \Gamma_1 \)). Hence, we can partition \( \Gamma_0 \) in an inflow boundary \( \Gamma_0^- = \{x = 0\} \times \{\xi > 0\} \) and an outflow boundary \( \Gamma_0^+ = \Gamma_0 \setminus \Gamma_0^- \). Similarly, we split \( \Gamma_1 \) in \( \Gamma_1^- = \{x = 1\} \times \{\xi < 0\} \) and \( \Gamma_1^+ = \Gamma_1 \setminus \Gamma_1^- \). Moreover, we define \( \Gamma^\pm = \Gamma_0^\pm \cup \Gamma_1^\pm \). A suitable boundary condition for \((3.1)\) is provided by:

\[
f = f^b \quad \text{at } \Gamma^-,
\]

where \( f^b \) is a (possibly time-dependent) non-negative prescribed function. An appropriate initial condition for \((3.1)\) is provided by a specification of the one-molecule probability-density function at \( t = 0 \):

\[
f(0) = f^0,
\]

with \( f^0 \) a prescribed probability density in \( D \).

If we insist that the boundary conditions comply with \textit{conservation of mass}, i.e., that probability-density functions subject to \((3.1)\) and the boundary conditions remain normalized at one, then we must impose the ancillary condition that the right member of \((3.10)\) vanishes for \( \psi = 1 \). In this case, it is generally not possible to maintain \((3.11)\) with \( f^b \) as prescribed data, independent of \( f \). We will be concerned with three types of mass-conserving boundary conditions, consistent with specular reflection, periodicity and random reflection in the molecular model; see Equations \((2.4)\)–\((2.6)\). The specular-reflection boundary condition is given by:

\[
f(t)|_{\Gamma_0^-} = f(t)|_{\Gamma_0^+} \circ S_- \text{ on } (0,\infty) \quad \text{and} \quad f(t)|_{\Gamma_1^-} = f(t)|_{\Gamma_1^+} \circ S_- \text{ on } (-\infty,0),
\]

for \( t \in T \), with \( S_-(\cdot) = -\cdot \). Periodicity in the molecular model corresponds to the boundary condition:

\[
f(t)|_{\Gamma_0^-} = f(t)|_{\Gamma_1^+} \text{ on } (0,\infty) \quad \text{and} \quad f(t)|_{\Gamma_0^+} = f(t)|_{\Gamma_1^-} \text{ on } (-\infty,0),
\]
for $t \in T$. Random reflection in the molecular model translates into a prescribed probability-density profile $f^b : \Gamma^- \to [0, \infty)$ in the Boltzmann model. The corresponding boundary condition is given by

$$\bar{f} = \lambda(f) f^b$$

with $\lambda(f) = \frac{\int_{\Gamma^+} f(\xi) \xi \, d\xi}{\int_{\Gamma^-} f^b(\xi) \xi \, d\xi}$ at $\Gamma^-$, \hspace{1cm} (3.15)

for $t \in T$. The ratio $\lambda(f)$ can be conceived of as a scaling parameter to comply with (3.10). It is to be noted that for the three types of boundary conditions in Equations (3.13)–(3.15), the boundary condition at the inflow boundary depends on the solution at the outflow boundary. One easily verifies that the specular-reflection boundary condition (3.13) and the periodic boundary condition (3.14) are energy conserving, in the sense that these conditions eliminate the right member of (3.10) for $\psi = 1$. Moreover, the specular-reflection boundary condition (3.13) and the periodic boundary condition (3.14) indeed eliminate the right member of (3.10) for $\psi = (\cdot)^2$.

4. Numerical aspects

4.1 DG finite-element method

In this section, we consider the approximation of the Boltzmann equation (3.1) and the corresponding auxiliary conditions by means of a space/time Discontinuous Galerkin (DG) finite-element method. Assuming that $f(x, \xi)$ vanishes sufficiently fast as $|\xi| \to \infty$, we truncate the velocity domain $\Xi$ to a bounded subset and extend $f$ by zero outside $\Sigma = \Omega \times \Xi$. Let us denote by $X$ either $T, \Omega$ or $\Xi$. We cover $X$ with open subintervals $\{\Delta_i^X\}_{i=1}^n$ such that $\Delta_i^X < \Delta_{i+1}^X$ and

$$\text{int}(\Delta^X_1 \cup \Delta^X_2 \cup \cdots \cup \Delta^X_n) = X.$$ 

These coverings serve as a basis for a regular partition of the space-velocity-time cylinder $\Theta = T \times \Sigma$ into a collection $\mathcal{K}$ of hexahedral element domains:

$$\mathcal{K} = \{\kappa \subset \Theta : \kappa = \Delta_i^T \times \Delta_j^\Omega \times \Delta_k^\Xi, (i, j, k) \in \{1, \ldots, n_T\} \times \{1, \ldots, n_\Omega\} \times \{1, \ldots, n_\Xi\}\}.$$ \hspace{1cm} (4.1)

The interior and boundary faces of the elements in $\mathcal{K}$ are collected in the sets

$$\mathcal{F}^0 = \{\gamma \subset \Theta : \gamma = \text{int}(\partial \kappa_0 \cap \partial \kappa_1), (\kappa_0, \kappa_1) \in \mathcal{K} \times \mathcal{K}, \kappa_0 \neq \kappa_1\},$$

$$\mathcal{F}^\partial = \{\gamma \subset \partial \Theta : \gamma = \text{int}(\partial \kappa \cap \partial \Theta), \kappa \in \mathcal{K}\},$$

respectively, without repetition. The collection of all faces is denoted by $\mathcal{F} = \mathcal{F}^0 \cup \mathcal{F}^\partial$. Moreover, we introduce collections of $t$-faces and $x$-faces according to:

$$\mathcal{F}_t = \{\gamma \subset \mathcal{F} : (t_0, x_0, \xi_0) \in \gamma \land (t_1, x_1, \xi_1) \in \gamma \Rightarrow t_0 = t_1\},$$

$$\mathcal{F}_x = \{\gamma \subset \mathcal{F} : (t_0, x_0, \xi_0) \in \gamma \land (t_1, x_1, \xi_1) \in \gamma \Rightarrow x_0 = x_1\},$$

without repetition. We use the notation $\mathcal{F}_t^0(= \mathcal{F}_t \cap \mathcal{F}^0)$ to denote the interior $t$-faces. A similar connotation holds for $\mathcal{F}_t^\partial, \mathcal{F}_x^0$ and $\mathcal{F}^\partial_x$.

The DG finite-element approximation of the solution to (3.1) consists of an element-wise tensor-product polynomial approximation. In particular, we define the DG approximation space of order $p \geq 0$ subordinate to the mesh $\mathcal{K}$ by:

$$H_{\mathcal{K}, p}(\Theta) = \{f \in L^2(\Theta) : f|_{\kappa} \in \mathcal{P}^p(\kappa), \kappa \in \mathcal{K}\},$$ \hspace{1cm} (4.2)

where $\mathcal{P}^p(\kappa) = \{f \in L^2(\kappa) : f : (t, x, \xi) \mapsto w_1(t) w_2(x) w_3(u), w_i \text{ is polynomial of degree } \leq p\}$. Whenever $\mathcal{K}$ and $p$ are evident or irrelevant for the presentation, they will be suppressed. In (4.2), we have assumed that the order of approximation is isotropic and uniform on $\mathcal{K}$. However, this assumption is nonessential and can be discarded without further consequences.
Moreover, to weakly enforce the auxiliary conditions, we replace \( f \) by \( f_\nu + f_\xi \) on \( \partial \kappa \). Upon separating the integral into a sum of contributions of the element domains and invoking the divergence theorem, we obtain:

\[
\sum_{\kappa \in K} \int_{\partial \kappa} (f_\nu + f_\xi \upsilon_\kappa) w \, dS - \int_\kappa f (w' + \nabla w) \, d\Theta - \int_\kappa Q(f, f) w \, d\Theta = 0,
\]

where \( \upsilon_\kappa \) and \( \upsilon_{\kappa} \) represent the temporal and spatial components of the outward unit normal vector on \( \partial \kappa \), respectively. For each element, the element-edge integral in the left-most term of (4.3) can be separated into a sum of contributions of faces \( \gamma \subset \partial \kappa \), \( \gamma \in F_t \cup F_x \). To stabilize the DG formulation and to weakly enforce temporal continuity, we replace \( f \) and \( f_\xi \) at interior faces by the upwind fluxes:

\[
f^- : \bigcup_{\gamma \in F_t^0} \gamma \to \mathbb{R}, \quad f^- : (t, x, \xi) \mapsto \lim_{\epsilon \to 0} f(t - \epsilon, x, \xi),
\]

\[
\varphi : \bigcup_{\gamma \in F_x^0} \gamma \to \mathbb{R}, \quad \varphi : (t, x, \xi) \mapsto \lim_{\epsilon \to 0} f(t, x - \epsilon \text{sign}(\xi), \xi) \xi.
\]

Moreover, to weakly enforce the auxiliary conditions, we replace \( f \) and \( f_\xi \) at faces \( \gamma \subset \{ t = 0 \} \times \Sigma \) and \( \gamma \subset \Gamma^- \) by their specification according to the initial and boundary conditions. After a rearrangement of the element-edge integrals, and restricting \( f \) to approximations in \( H(\Theta) \), we obtain the DG formulation:

\[
f \in H(\Theta) : \quad a(f, w) = b(w) \quad \forall w \in H(\Theta),
\]

where the semilinear form \( a : H(\Theta) \times H(\Theta) \to \mathbb{R} \) and the linear form \( b : H(\Theta) \to \mathbb{R} \) are defined by

\[
a(f, w) = \sum_{\gamma \in F_t^0} \int_{\gamma} f^- [w] \, d\gamma + \sum_{\gamma \in F_x^0} \int_{\gamma} \upsilon_{\gamma} [w] \, d\gamma + \sum_{\gamma \in F_x^0} \int_{\gamma} \nabla \cdot [w] \, d\gamma + \sum_{\gamma \subset \{ t = 0 \} \times \Sigma} \int_{\gamma} f_\xi \upsilon_\xi w \, d\gamma
\]

\[
- \sum_{\kappa \in K} \int_{\kappa} f (w' + \nabla w) \, d\kappa - \sum_{\kappa \in K} \int_{\kappa} Q(f, f) w \, d\kappa
\]

\[
b(w) = \sum_{\gamma \subset \{ t = 0 \} \times \Sigma} \int_{\gamma} f_\xi w \, d\gamma - \sum_{\gamma \subset \Gamma^-} \int_{\gamma} f_\xi^b \upsilon_\xi w \, d\gamma
\]

with the jump operator \([\cdot] : H(\Theta) \to L^2(\bigcup_{\gamma \in F_x^0} \gamma)\) according to:

\[
\forall w \in H(\Theta), \quad [w] : (t, x, \xi) \mapsto \begin{cases} w(t^-, x, \xi) - w(t^+, x, \xi) & \text{if } (t, x, \xi) \in \bigcup_{\gamma \in F_t^0} \gamma, \\ w(t, x^-, \xi) - w(t, x^+, \xi) & \text{if } (t, x, \xi) \in \bigcup_{\gamma \in F_x^0} \gamma. \end{cases}
\]

In the above formulation, we have assumed that the boundary conditions conform to (3.11). The formulation extends mutatis mutandis to the boundary conditions (3.13)–(3.15).

### 4.2 Evaluation of the collision term

The element-domain and edge integrals in (4.5a) can be evaluated by standard quadrature formulas. However, the intrinsic integrals in the collision operator require special attention. Let us consider, for instance, the loss term (3.4). In the implementation of the semi-linear form (4.5a), the loss term must be evaluated at quadrature points \( \{ \xi_q \} \). For each \( \xi_q \), the integrand in (3.4) is \( C^0 \) continuous, regardless of the smoothness of \( f \), on account of the \( |u - v| \) term. Hence, straightforward application of a quadrature formula will not generally yield an accurate approximation of the integral. If, instead, the contributions \( L_\infty \) and \( L_\infty \) according to (3.3) are evaluated separately, then the integrand of each of
these integrals is smooth, and the integrals can be accurately approximated by a quadrature formula. A similar observation holds for the gain term \( G \), and its constituents \( G_\rightarrow \) and \( G_\leftarrow \) in (3.8).

To evaluate the gain-term components \( G_\rightarrow \) and \( G_\leftarrow \), we require the inner-most \( \alpha \)-integral over \( \alpha \in (0, \pi) \) for each combination of quadrature points \((\xi_q, \zeta_r)\). If \( f \) is sufficiently smooth, the integrand of this integral is smooth, and the integral can be accurately approximated by a high-order quadrature formula. The disadvantage of this approach is, however, that the approximation is generally inaccurate if the smoothness assumption on \( f \) is violated. In particular, if \( f \) corresponds to a DG finite-element approximation, then it is too irregular for a high-order quadrature formula. Moreover, the accuracy of the approximation to the integral is essentially fixed, independent of the mesh and the order of the finite-element approximation space \( H_{K,p}(\Theta) \). Hence, if the mesh is refined, then the error incurred by the integration procedure inhibits convergence.

An alternative approach to evaluate the \( \alpha \)-integral, is to partition the interval \( \Pi = (0, \pi) \) in subintervals \( \Delta^\Pi \), in such a manner that the sets \( \{ \pm |\xi| \sin(\Delta^\Pi + \pi/4) \} \) and \( \{ \pm |\xi| \cos(\Delta^\Pi + \pi/4) \} \) are contained within the elements \( \kappa \in K \), and then evaluate the contributions of these subintervals separately by a quadrature formula of sufficiently high order. More precisely, recalling from the previous section the covering \( \{ \Delta^\Pi \} \) of \( \Xi \) which underlies the mesh \( K \), for each combination of quadrature points \((\xi_q, \zeta_r)\) and \( \chi \in \{ \pm \sin, \pm \cos \} \), we define the collections of subintervals:

\[
\Delta^\Pi = \left\{ \text{the smallest collection of subsets } \Delta^\Pi \subset \Pi : \text{int}(\cup \Delta^\Pi) = \Pi, \right. \\
\left. \quad \alpha \chi(\Delta^\Pi + \pi/4) \subseteq \Delta^\Pi_i \text{ for some } i \in \{1, \ldots, n_\Xi \} \right\},
\]

where \( \alpha = |\xi_q, \zeta_r| \); see Figure 2 for an illustration. Next, we construct the set of integration intervals by taking the collective intersections of the intervals in \( \Delta^\Pi \) for the various \( \chi \):

\[
\Delta^\Pi_\chi = \left\{ \Delta^\Pi : \bigcap \Delta^\Pi_i \subseteq \Delta^\Pi_\chi \right\}.
\]

The set \( \Delta^\Pi_\chi \) is the smallest collection of subsets \( \Delta^\Pi \subset \Pi \) that covers \( \Pi \) and such that \( \Delta^\Pi \) is included in some subinterval \( \Delta_\chi \in \Delta^\Pi \) for all \( \chi \in \{ \pm \sin, \pm \cos \} \). Finally, we partition the \( \alpha \)-integrals in the gain-term components \( G_\rightarrow \) and \( G_\leftarrow \) in sums of contributions from the intervals in \( \Delta^\Pi_\chi \), and evaluate these contributions by standard quadrature. For instance, for the \( \alpha \)-integral pertaining to \( G_\leftarrow (f, f) \) in (3.8b),

\[
\int_0^\pi \sum_{\Delta^\Pi \in \Delta^\Pi_\chi} f(x, |\xi| |\zeta| \cos(\alpha + \pi/4)) f(x, |\xi| |\zeta| \sin(\alpha + \pi/4)) \sin \alpha \, d\alpha
\]

The advantage of this approach is that the quadrature is applied on integration subintervals in which \( f \) is smooth. Moreover, the accuracy of the approximation to the integral converges as the mesh is refined, as the integration subintervals are refined accordingly.

### 4.3 Iterative solution procedure

The space/time DG formulation (4.4) translates into a sequence of nonlinear algebraic systems, corresponding to the space/time slabs \( \Theta_\chi = \Delta^T_\chi \times \Sigma \). Newton-type solution approaches for these nonlinear systems are impaired by the non-locality of the collision term. As a result of this non-locality, consistent linearizations of (4.4) give rise to highly dense matrices. Therefore, we opt for a solution procedure based on Picard iteration, in which we treat the non-local parts of the collision operator explicitly.
4. Numerical aspects

\[ \alpha \rightarrow u \rightarrow a_0 \pi \]

Figure 2: Partition of \((0, \pi)\) into a collection \(\mathcal{T}_K^{\sin}\) of non-overlapping subintervals \(\Delta_i^{\Pi}\) according to (4.6).

To elaborate the Picard iteration procedure, let us consider the Boltzmann equation in the integro-differential form (3.1) with the collision operator partitioned in gain and loss components according to (3.2):

\[ f'(t) + \xi \nabla f(t) - \varepsilon^{-1} G(f(t), f(t)) + \varepsilon^{-1} L(f(t), f(t)) = 0. \quad (4.7) \]

The bilinear operator \(G(\cdot, \cdot)\) is non-local in both arguments. The bilinear operator \(L(\cdot, \cdot)\) is local in its first argument and non-local in its second argument; see (3.4). A Picard-iteration approach based on a partition of the collision operator in local and non-local components reads as follows: Given an initial approximation \(f_0\), solve

\[ f_k'(t) + \xi \nabla f_k(t) + \varepsilon^{-1} L(f_{k-1}(t), f_k(t)) = \varepsilon^{-1} G(f_{k-1}(t), f_{k-1}(t)), \quad (4.8) \]

for \(k = 1, 2, \ldots\), subject to the auxiliary conditions. One easily verifies that a fixed point of the recursive relation (4.8) indeed satisfies (4.7). It is to be noted that the Picard iteration (4.8) is in fact applied locally within each time slab \(\Theta_i\), \(i = 1, 2, \ldots, n_T\). The subproblem corresponding to each time step is subject to initial conditions of the form (3.12) and boundary conditions of the form (3.11), or similar; cf. Section 3.3.

Under some ancillary assumptions, elaborated below, the linear subproblems in the Picard iteration (4.8) in conjunction with the initial and boundary conditions form a so-called Friedrichs’ system and, hence, they are well posed [15, 18]. To elaborate the classification as a Friedrichs’ system, we consider (4.8) within a space-time slab \(\Theta_i\) and we introduce the following notation:

\[ (y_1, y_2, y_3) = (t, x, \xi), \quad (\mathcal{A}^1, \mathcal{A}^2, \mathcal{A}^3) = (1, y_3, 0), \quad \mathcal{D} = \sum_{k=1}^{3} \nu_k \mathcal{A}^k, \]

\[ \mathcal{K}(y_1, y_2, y_3) = \varepsilon^{-1} \int_{-\infty}^{\infty} f_{k-1}(y_1, y_2, \zeta) |y_3 - \zeta| \, d\zeta, \quad b = \varepsilon^{-1} G(f_{k-1}(t), f_{k-1}(t)), \quad (4.9) \]

where \((\nu_1, \nu_2, \nu_3) = (\nu_t, \nu_x, \nu_\xi)\) represents the outward unit normal to the boundary \(\partial \Theta_i\). In addition, we define the operators \(A_1, A_0\) and \(A\) according to

\[ A_1 f = \sum_{k=1}^{3} \mathcal{A}^k \frac{\partial f}{\partial y_k}, \quad A_0 f = \mathcal{K} f \quad \text{and} \quad A = A_1 + A_0, \]
5. Numerical experiments and results

which enables us to condense Equation (4.8) into:

$$Af_k = b.$$  \hspace{1cm} (4.10)

Furthermore, we recast the auxiliary conditions into

$$\left(\mathcal{M} - \mathcal{D}\right)f\big|_{\partial\Theta_i} = d,$$  \hspace{1cm} (4.11)

where $\mathcal{M} = |\mathcal{D}|$ and $d \in \mathbb{R}$ represent (compatible) boundary data. It is to be noted that condition (4.11) is trivially satisfied at outflow boundaries, i.e., whenever $\mathcal{D} \geq 0$: the left member of (4.11) vanishes independent of $f$, while the compatibility condition on the boundary data imposes $d = 0$. The $\mathcal{A}^k$ in (4.9) reside in $L^\infty(\Theta_i)$ and, hence, $\mathcal{A}^k \in L^\infty(\partial\Theta_i)$. Additionally, we assume that $\mathcal{N}$ is also sufficiently regular, in particular, $\mathcal{N} \in L^\infty(\Theta_i)$, which translates into some ancillary regularity requirements on the sequence of approximations $f_k$. The equation (4.10) in conjunction with the auxiliary conditions (4.11) form a Friedrichs’ system if there exists a positive constant $\mu_0$ such that the following stipulations hold:

(F1) $\mathcal{A}^k$ is symmetric ($k = 1, 2, 3$);

(F2) $\mathcal{N} + \mathcal{N}^T - \sum_{k=1}^3 \partial_{y_k} \mathcal{A}^k \geq \mu_0$ a.e. in $\Theta_i$;

(F3) $\mathcal{M} + \mathcal{M}^T \geq 0$ a.e. on $\partial\Theta_i$;

(F4) $\ker(\mathcal{D} - \mathcal{M}) + \ker(\mathcal{D} + \mathcal{M}) = \mathbb{R}$ a.e. on $\partial\Theta_i$.

The symmetry of $\mathcal{A}^1$, $\mathcal{A}^2$, $\mathcal{A}^3$ in condition (F1) is obvious in the scalar case under consideration. The conditions (F3) and (F4) are a straightforward consequence of the definition of $\mathcal{M}$. Condition (F2) translates into ancillary conditions on $f_{k-1}$. However, condition (F2) can be removed by considering $\exp(-\mu_1 t)f(t)$ instead of $f(t)$, in which case (F2) holds with $\mu_0 = \mu_1$.

A comprehensive analysis of the convergence of the sequence of approximations (4.8) is beyond the scope of this work. Instead, the convergence behaviour of the Picard iteration is examined on the basis of numerical experiments in Section 5.

5. Numerical experiments and results

To exhibit the properties of the Boltzmann model, we conduct numerical experiments on the basis of the DG finite-element method outlined in Section 4. For comparison, we also consider realizations of the underlying molecular model of Section 2. In Section 5.1, we first examine some aspects related to the numerical approximation of the Boltzmann equation by means of the DG finite-element method. In particular, we consider the convergence behavior of the Picard iteration method and the convergence behavior of the finite-element approximation under mesh refinement. Section 5.3 is concerned with the convergence-to-equilibrium property of the Boltzmann model. Next, in Section 5.4, we compare results of the Boltzmann equation and of the underlying stochastic molecular-dynamics model. Finally, we consider in Section 5.5 a heat transfer problem, in which the Boltzmann equation and the underlying molecular model are supplied with boundary conditions corresponding to a time-dependent boundary temperature.

In the numerical experiments below, the domain $\Sigma = \Omega \times \Xi$ in all cases corresponds to $\Sigma = (0, 1) \times (-8, 8)$. The truncation of the velocity domain has been selected such that its effect on the results is negligible. Further, we remark for completeness that the integrals in the finite-element method are approximated by a quadrature rule of order $q = p + 1$ for all terms except the collision integral, for which we use $q = p + 2$. Here $p$ denotes the polynomial order of the finite-element space; see also Equation (4.2).

In the sequel, we will frequently refer to (drifting) Maxwellians. To facilitate the exposition, we introduce the notation:

$$\mathcal{M}_{e,v}(\xi) = \left(2\pi(e - v^2)\right)^{-1/2} \exp\left(-\frac{(\xi - v)^2}{2(e - v^2)}\right), \quad |v| < \sqrt{e},$$  \hspace{1cm} (5.1)
5. Numerical experiments and results

5.1 Numerical approximation of the Boltzmann equation

5.1.1 Convergence of the Picard-iteration process

The Picard iteration process (4.8) relies on a disassembly of the collision operator into a local component, which is treated implicitly, and a nonlocal component, which is treated explicitly. To assess the convergence behavior of this iterative process, we consider (4.8) subject to the initial condition \( f(0) = M_{2,1} \) and periodic boundary conditions (3.14), and provided with the initial estimate \( f_0 = M_{2,1} \). Let us note that the initial estimate and all subsequent approximations \( f_k \) are spatially homogeneous, i.e. \( x \)-independent. The transport term \( \xi \nabla (\cdot) \) therefore vanishes identically.

Because we will consider different values of the Knudsen number, for each \( \varepsilon > 0 \) we denote by \( \{ f_{\varepsilon}^k \}_{k \in \mathbb{Z}^+} \) the corresponding sequence of iterates generated by (4.8). Furthermore, \( r_{\varepsilon,\delta t}^k \) denotes the norm of the residual of the \( k \)-th iterate on the time interval \( t \in (0, \delta t) \) according to:

\[
r_{\varepsilon,\delta t}^k = \left( \int_0^{\delta t} \left\| \partial_t f_{\varepsilon}^k(t) - \varepsilon^{-1} Q(f_{\varepsilon}^k(t), f_{\varepsilon}^k(t)) \right\|_{L^2(\Sigma)}^2 \, dt \right)^{1/2}.
\]

(5.2)

Figure 3 plots the residual reduction \( r_{\varepsilon,\delta t}^k / r_{\varepsilon,\delta t}^0 \) versus the iteration counter \( k \), for fixed time-interval duration \( \delta t = 2^{-7} \) and Knudsen numbers \( \varepsilon \in \{2^{-10}, 2^{-9}, \ldots, 2^{-4}\} \) (solid line, right to left) and for \( \varepsilon = 2^{-7} \) and time-interval durations \( \delta t \in \{2^{-10}, 2^{-9}, \ldots, 2^{-4}\} \) (symbols, left to right).

where \( e \) and \( v \) are referred to as the energy and drift, respectively. For \( v \neq 0 \), the distribution in (5.1) is called a drifting Maxwellian with energy \( e \).

Figure 3 indicates that the residual reduction is invariant under the transformation \( (\varepsilon, \delta t) \mapsto (\varepsilon/c, \delta t/c) \) for any positive constant \( c \) and, therefore, that the dependence of \( r_{\varepsilon,\delta t}^k / r_{\varepsilon,\delta t}^0 \) on \( \varepsilon \) and \( \delta t \) is in fact parametrized by \( \delta t / \varepsilon \). This is confirmed by a scaling argument; see Appendix A.

Let us remark that the convergence behavior in Figure 3 is representative for the general behavior of the iterative process, and that similar behavior is observed for other test cases.

5.2 Convergence of the DG finite-element approximation

To validate the implementation of the DG finite-element method for the one-dimensional Boltzmann model, we examine the convergence behavior of the finite-element approximation under mesh refine-
ment. To this end, we consider the Boltzmann equation (3.1) with nonhomogeneous data,

\[ f'(t) + \xi \nabla f(t) - Q(f(t), f(t)) = \Lambda(t) := \tilde{f}'(t) + \xi \nabla \tilde{f}(t) - Q(\tilde{f}(t), \tilde{f}(t)) \]  

subject to the auxiliary conditions

\[ f(0) = \tilde{f}(0), \quad f(t)|_{\Gamma_-} = \tilde{f}(t)|_{\Gamma_-}, \]

where

\[ \tilde{f}(t, x, \xi) = \frac{\sin^2 \left( \frac{\pi(x-t)}{\sqrt{2}\pi(t+1)} \right)}{\sqrt{2}\pi(t+1)} \exp \left( - \frac{\xi^2}{2(t+1)} \right). \]

Note that the Knudsen number has been set to \( \epsilon = 1 \) in (5.3a). Evidently, the data in (5.3) has been constructed such that \( \tilde{f} \) satisfies (5.3). Let us remark that the evaluation of the collision operator in the right member of (5.3a) is nontrivial, which poses restrictions on the reference solutions \( f \) that can be considered.

We consider the DG finite-element approximation (4.4) of the initial-boundary-value problem (5.3) on the space-velocity-time cylinder \( \Theta = T \times \Omega \times \Xi = (0, 1) \times (0, 1) \times (-8, 8) \). We regard a sequence of meshes \( \{K_h\} \) composed of \( (n_T, n_\Omega, n_\Xi) = h^{-1}(1, 1, 1) \) elements with \( h^{-1} \in \{6, 8, 10, \ldots\} \), and approximation orders \( p = 1, 2 \). Denoting by \( \mathbf{f}_{h,p} \) the DG approximation in \( H_{K_h,p}(\Theta) \), Figure 4 plots the norm of the error in the approximation, \( \|\mathbf{f}_{h,p} - \mathbf{f}\|_{L^2(\Theta)} \), versus the reciprocal mesh parameter, \( h^{-1} \).

In addition, Figure 4 plots the norm of the error in the gain and loss terms,

\[ \|G(\mathbf{f}_{h,p}, \mathbf{f}_{h,p}) - G(\bar{f}, \bar{f})\|_{L^2(\Theta)} \quad \text{and} \quad \|L(\mathbf{f}_{h,p}, \mathbf{f}_{h,p}) - L(\bar{f}, \bar{f})\|_{L^2(\Theta)}. \]

From Figure 4 we observe that \( \|\mathbf{f}_{h,p} - \mathbf{f}\|_{L^2(\Theta)} \leq Ch^{p+1} \) for some constant \( C > 0 \) as \( h \to 0 \), which implies that the DG finite-element approximation yields optimal convergence in the \( L^2 \)-norm; see, e.g., [8, 15, 34]. Remarkably, for \( p = 1 \), the gain and loss terms converge at the same rate as the approximation itself, while for \( p = 2 \), the convergence rate of the gain and loss terms exceeds that of the approximation. A further investigation of this superconvergence property of the gain and loss terms for \( p = 2 \) is beyond the scope of this treatise.

5.3 Convergence to equilibrium

The collision process (2.15) has been constructed such that solutions of the Boltzmann equation approach a non-drifting Maxwellian \( \mathcal{M}_{2,0} \) as \( t \to \infty \), provided that suitable boundary conditions are imposed. To examine the convergence-to-equilibrium property, we consider DG finite-element approximations of the Boltzmann equation (3.1), provided with periodic boundary conditions (3.14) and the space-homogeneous initial condition \( f(0) = \mathcal{M}_{2,1} \).

Figure 5 plots the \( L^2 \)-norm of the deviation of the DG finite-element approximation from equilibrium, \( \|f_{h,p}(t) - \mathcal{M}_{2,0}\|_{L^2(\Sigma)} \), versus time, for Knudsen numbers \( \epsilon \in \{1/9, 1/4, 1/2, 1\} \). The left panel of Figure 5 presents results for \( p = 1 \) and mesh parameter \( h \in \{1/40, 1/20, 1/10\} \). The right panel presents results for \( p = 2 \) and \( h \in \{1/6, 1/12, 1/24\} \). From Figure 5 it can be observed that \( f_{h,p}(t) \) converges exponentially to \( \mathcal{M}_{2,0} \) as \( t \) increases, until the discretization error in \( f_{h,p}(t) \) becomes dominant.

The dominance of the discretization error for large \( t \) is corroborated by the fact that for sufficiently small \( h \), \( \|f_{h,p}(t) - \mathcal{M}_{2,0}\|_{L^2(\Sigma)} \) reduces by approximately \( 2^{-(p+1)} \) if \( h \) is reduced by a factor of 2; cf. also Section 5.2. Furthermore, Figure 5 shows that the rate of convergence to equilibrium increases with decreasing \( \epsilon \), i.e., as the number of molecules in the system increases. By means of a similar scaling argument as in Appendix A, it can be shown that the convergence rate is in fact proportional to \( \epsilon^{-1} \). It is noteworthy that the observed exponential decay to equilibrium as time progresses agrees with Cercignani’s conjecture [10, 39].
Figure 4: Convergence of the finite-element approximation: discretization error $\|f_{h,p} - \bar{f}\|_{L^2(\Theta)}$ versus the reciprocal mesh parameter $h^{-1}$, for $p = 1$ (left) and $p = 2$ (right). In addition, the plots present the error in the gain term, $\|G(f_{h,p}, f_{h,p}) - G(\bar{f}, \bar{f})\|_{L^2(\Theta)}$, (dashed) and in the loss term, $\|L(f_{h,p}, f_{h,p}) - L(\bar{f}, \bar{f})\|_{L^2(\Theta)}$ (dash-dot).

Figure 5: Convergence to equilibrium: $L^2$-norm of the deviation of the DG approximation from equilibrium, $\|f_{h,p}(t) - M_{2,0}\|_{L^2(\Sigma)}$, versus $t$, for $p = 1$, $h \in \{1/40, 1/20, 1/10\}$ (left) and $p = 2$, $h \in \{1/24, 1/12, 1/6\}$ (right), and for $\varepsilon = 1$ (continuous), $\varepsilon = 1/2$ (dashed), $\varepsilon = 1/4$ (dash-dot) and $\varepsilon = 1/9$ (dots). Numbers next to curly brackets indicate reduction factor.
5. Numerical experiments and results

5.4 Comparison of the Boltzmann equation and molecular dynamics

We consider the Boltzmann equation (3.1) with $\epsilon = 1/9$, provided with specular-reflection boundary conditions (3.13) and the initial condition $f(0) = f^0$ with space-inhomogeneous initial data:

$$f^0(x, \xi) = \begin{cases} \frac{(\pi/4)^2 \sin(\pi x) \sin\left((\pi/4)(\xi + 1)\right)}{0} & \text{if } (x, \xi) \in [0, 1] \times [-1, 3]; \\ \text{otherwise}; \end{cases}$$

(5.5)

see Figure 7 for an illustration. Note that the Knudsen number $\epsilon = 1/9$ corresponds to $n = 10$ molecules. We compare the finite-element approximation of the solution of the above initial-boundary-value problem with a Monte-Carlo simulation of the underlying molecular-dynamics (MD) model, i.e., of the stochastic impulsive differential equation (2.1) with collision process (2.15). The MD model is furnished with specular-reflection boundary conditions according to (2.4). For the Monte-Carlo process, we consider a sequence of random initial data, $\{(x^0, \xi^0)\}_{j=1}^m$, and a corresponding sequence of solutions of Equation (2.1), $\{(x(t), \xi(t))\}_{j=1}^m$. Each initial datum consists of a pair of $n$-tuples of random positions, $x^0_j = (x^0_{1j}, \ldots, x^0_{nj})$, and velocities, $\xi^0_j = (\xi^0_{1j}, \ldots, \xi^0_{nj})$. The initial positions $x^0_{ij}:= (x^0_{ij})$ are (realizations of) random variables with values in $(0, 1)$ with probability-density distribution $(2/\pi) \sin(\pi r)$. The initial velocities $\xi^0_{ij}$ are random variables with values in $(-1, 3)$ with probability-density distribution $(8/\pi) \sin((\pi/4)(r + 1))$. Hence, the pairs $(x^0_{ij}, \xi^0_{ij})$ have distribution $f^0$ according to (5.5).

To enable a comparison of the DG finite-element approximation of the Boltzmann equation and the Monte-Carlo simulation of the MD model, we first extract from the sequence of solutions $\{x(t), \xi(t)\}_{j=1}^m$ an equivalent time-dependent probability-density function in the DG approximation space. To this end, let $V_{K,p}(\Sigma)$ denote the trace of $H_{K,p}(\Theta)$ for some fixed $t \in T$. We construct the $L^2$-representation $\tilde{f}_m : T \rightarrow V_{K,p}(\Sigma)$ of $\{(x, \xi)\}_{j=1}^m$ according to:

$$\tilde{f}_m(t) \in V_{K,p}(\Theta) : \quad (w, \tilde{f}_m(t))_{L^2(\Sigma)} = \frac{1}{mn} \sum_{j=1}^m \sum_{i=1}^n w(x_{i,j}(t), \xi_{i,j}(t)) \quad \forall w \in V_{K,p}(\Sigma),$$

(5.6)

with $m$ the number of samples in the Monte-Carlo process. The function $\tilde{f}_m(t)$ can be conceived of as the Riesz representation (in $L^2(\Sigma)$) of the functional $w \mapsto \sum_{i,j} w(x_{i,j}(t), \xi_{i,j}(t))$.

Figure 6 (left) plots the $L^2$-norm of the deviation between the $L^2$-representation of the Monte-Carlo simulation of the MD model, $f_m(t)$, and the corresponding equilibrium distribution, $\mathcal{M}_{\epsilon,0}$, versus time, for sample sizes $m \in \{10^2, 10^3, 10^4\}$. The energy of the equilibrium distribution is $e = 5 - 32/\pi^2$, in accordance with the energy associated with the initial data $f^0$ in (5.5). In addition, Figure 6 (left) plots the $L^2$-norm of the deviation between the DG finite-element approximation of the Boltzmann solution with mesh parameter $h = 1/24$ and approximation order $p = 2$, and the equilibrium distribution. It is to be remarked that the same finite-element space has been used to construct the $L^2$-representation of $\{(x, \xi)\}_{j=1}^m$. Figure 6 (right) plots the $L^2$ norm of the difference between the $L^2$-representation of the Monte-Carlo MD results, $\tilde{f}_m(t)$, and the finite-element approximation of the Boltzmann equation, $f_{h,p}(t)$, versus time, for sample sizes $m \in \{10^2, 10^3, 10^4\}$.

Figure 6 (left) shows that the $L^2$-norm of the deviation between the Monte-Carlo MD results and the equilibrium distribution approaches a constant as $t$ increases, modulo relatively small fluctuations. The deviation between $\tilde{f}_m(t)$ for large $t$ and $\mathcal{M}_{\epsilon,0}$ decreases by a factor of approximately $\sqrt{10}$ if the sample size, $m$, in the Monte-Carlo process is increased by a factor of 10. This behavior can be explained as follows: Denoting by $W_1, W_2, \ldots$ a sequence of uncorrelated random variables with expectation $\langle W \rangle$ and variance $\text{Var}(W)$, it holds for any $\epsilon > 0$ that:

$$P\left(\left|\frac{1}{m} \sum_{k=1}^m (W_k - \langle W \rangle)\right| \geq \epsilon\right) \leq \frac{\text{Var}(W)}{\epsilon^2 m} \quad \forall m \in \mathbb{N};$$
Figure 6: Comparison of the Boltzmann equation and MD: \((\text{left})\) \(L^2\)-norm of the deviation from equilibrium of Monte-Carlo MD with sample sizes \(m \in \{10^2, 10^3, 10^4\}\) (solid) and of the DG approximation of the Boltzmann solution (dashed); \((\text{right})\) \(L^2\)-norm of the difference between MD and the DG approximation of the Boltzmann solution. Numbers next to curly brackets indicate reduction factor.

see [27, Thm. 5.14]. In particular, the sequence \(\{W_k\}_{k \in \mathbb{N}}\) therefore satisfies the weak law of large numbers. By complementarity, and setting \(\bar{\epsilon} = \sqrt{\text{Var}(W)} / \epsilon m\), we obtain:

\[
P \left( \left| \frac{1}{m} \sum_{k=1}^{m} (W_k - \langle W \rangle) \right| \leq \frac{\sqrt{\text{Var}(W)}}{\sqrt{\epsilon m}} \right) \geq 1 - \epsilon. \quad (5.7)
\]

To each \(w \in V_{K,p}(\Sigma)\) and fixed \(t \in T\) in the right member of (5.6), we can associate a sequence of random variables \(W_k = w(x_{i(k),j(k)}(t), \xi_{i(k),j(k)}(t))\), with \(k \mapsto (i(k), j(k))\) a suitable re-indexation scheme. Assuming that these \(W_k\) are independent and, therefore, uncorrelated, the right member of (5.6) converges to its expectation at rate \(1/\sqrt{m}\) in the sense of (5.7).

It moreover appears from Figure 6 \((\text{left})\) that for \(m = 10^3\), the sampling error in the Monte-Carlo process is much larger than the discretization error in the DG finite-element approximation of the Boltzmann solution. Figure 6 \((\text{right})\) conveys that the sampling error in the Monte-Carlo MD results is essentially uniform in time.

An interesting observation pertaining to Figure 6 \((\text{left})\) is that the convergence to equilibrium of the Boltzmann solution proceeds via two regimes. Initially, for \(t \in (0, \bar{t})\) with \(\bar{t} \approx 1\), the Boltzmann solution displays fast convergence. In the asymptotic regime, \(t \in (\bar{t}, \infty)\), convergence occurs more slowly. Of course, the convergence to equilibrium of the DG finite-element approximation eventually ceases on account of discretization errors. In Figure 6 \((\text{left})\), this occurs at \(t \approx 8\). The initial fast-convergence regime is associated with convergence of the Boltzmann solution to a local (in space) Maxwellian, which can be identified as an effect of collisions. The asymptotic slow-convergence regime corresponds to convergence to the global Maxwellian, and is dominated by transport. Figure 7 shows snapshots of the Boltzmann solution and of the \(L^2\)-representation of the Monte-Carlo MD results at times \(t \in \{0, 1/4, 1, 10\}\). The snapshot at \(t = 0\) corresponds to the initial condition. The snapshot at \(t = 1/4\) corresponds to the fast-convergence regime. At \(t = 1\), the convergence to local Maxweillians is essentially completed. The snapshot at \(t = 10\) shows the steady state solution, corresponding to the DG finite-element approximation of the equilibrium distribution \(\mathcal{M}_{e,0}\).
Figure 7: Snapshots at $t \in \{0, 1/4, 1, 10\}$ (top to bottom) of the evolution of the finite-element approximation of the Boltzmann equation (left) and of the $L^2$-representation of Monte-Carlo MD (right) for the spatially-inhomogeneous initial data (5.5); cf. also Figure 6.
5.5 Heat transfer

Finally, we compare the Boltzmann equation and Monte-Carlo MD for a test case corresponding to heat transfer at a boundary. To this end, we define a time-dependent energy according to:

$$e(t) = \begin{cases} 
1 + \sin\left(\frac{\pi t}{\ell}\right) & 0 < t \leq \frac{\ell}{2} \\
\frac{1}{2} & \frac{\ell}{2} < t \leq \ell
\end{cases}$$

(5.8)

for some heat-up time $\ell > 0$. We consider the Boltzmann equation with $\epsilon = 1/9$, provided with the initial condition (3.12) with data $f^0 = M_{1,0}$, the time-dependent random-reflection boundary condition (3.15) with $\bar{f}^0(t) = M_{\epsilon(t),0}$ at the left inflow boundary, $\Gamma_0^-$, and the reflection boundary condition (3.13) at $\Gamma_1^-$. One may note that the initial condition is compatible with the boundary conditions, as $\bar{f}^0(0) = f(0)|_{\Gamma_0^-}$ and, moreover, $f(0)|_{\Gamma_1^+} = f(0)|_{\Gamma_1^-} \circ S_-$, in accordance with (3.13).

We approximate the solution to the aforementioned initial-boundary-value problem by means of the DG finite-element method on an approximation space with polynomial order $p = 2$ and mesh parameter $h = 1/24$ and time step $\delta t = 1/10$. The energy that is transferred from the boundary $\Gamma_0$ to the domain during the time interval $(0,t)$ is in principle given by both sides of the identity:

$$\int_{\Sigma} \xi e f(t,x,\xi) \, dx \, d\xi - \int_{\Sigma} \xi f^0(x,\xi) \, dx \, d\xi = \int_0^t \int_0^\infty \xi^3 f^b(s,\xi) \, d\xi \, ds + \int_0^t \int_{-\infty}^0 \xi^3 f(s,0,\xi) \, d\xi \, ds;$$

(5.9)

cf. Equation (3.10). For the finite-element approximation, the identity (5.9) only holds up to quadrature errors and errors induced by the truncation of the velocity domain. However, the differences between the left and right members of (5.9) were in all cases negligible.

The Monte-Carlo MD computation of the heat-transfer problem is similar to that in Section 5.4, with $f^0$ now according to $f^0 = M_{1,0}$ and the specular-reflection map (2.4) at the left boundary replaced by the random-reflection map (2.6), with $\zeta$ a time-dependent random variable. In particular, the post-collision velocity at the boundary, $\zeta_i$, is a random variable with values in $\mathbb{R}_+$ with probability-density distribution

$$\mathcal{R}(t) : \xi \mapsto c(t) \xi M_{\epsilon(t),0}(\xi),$$

(5.10)

where $c(t)$ is a normalization constant. The distribution $\mathcal{R}$ in (5.10) is referred to as a Rayleigh distribution. It is to be noted that the Rayleigh distribution corresponds to the probability density of the flux. In the MD model, the energy that is transferred from the boundary $\Gamma_0$ to the domain during the time interval $(0,t)$ is determined by $\sum_i \xi_i^2(t) - \sum_i \xi_i^2(0)$, in analogy with the left member of (5.9).

Figure 8 plots the energy in the domain versus time for heat-up times $\ell \in \{2^1, 2^5, 2^9\}$, for the finite-element approximation of the Boltzmann solution and the Monte-Carlo MD computation with sample size $m = 10^4$. For short heat-up times, a significant discrepancy between the heat transfer obtained from the Boltzmann equation and from Monte-Carlo MD is observed, which imparts that the random-reflection map (2.6) in the MD process and the random-reflection boundary condition (3.15) in the Boltzmann equation are not equivalent. The discrepancy in the heat transfer is particularly emphatic at large deviations from equilibrium. For slow heating ($\ell = 2^0$), the system is at all times close to equilibrium, and the discrepancy between the Boltzmann approximation and Monte-Carlo MD is negligible.

The discrepancy between the heat transfer in the Boltzmann model and in the Monte-Carlo MD computations ultimately emanates from differences in the energy-fluxes at the boundary. To examine the difference in the energy fluxes, we compare in Figure 9 averaged Rayleigh distributions associated with both models on the time interval $T = (0,T)$, according to:

$$\langle \xi f(\cdot,0,\xi) \rangle_T = \frac{1}{T} \int_0^T \xi f(t,0,\xi) \, dt.$$

(5.11)
6. Conclusion

We presented a numerical investigation of a new one-dimensional prototype of the Boltzmann equation. The one-dimensional model is intended as a platform for developing efficient new numerical approximation methods for the Boltzmann equation, based on discretization or model adaptivity. The molecular model that underlies the one-dimensional Boltzmann equation is of stochastic-impulsive-differential-equation type. The molecular model is endowed with a random-collision process, which has been fabricated in such a manner that solutions of the corresponding Boltzmann equation exhibit convergence to Maxwell-Boltzmann equilibrium distributions. The collision operator in the Boltzmann equation assumes the typical form of an integral operator.

We presented a Discontinuous Galerkin finite-element approximation method for the Boltzmann model. Special attention was required for the numerical evaluation of the intrinsic integrals in the collision operator, on account of potential non-smoothness of the integrands, and to ensure that the approximation of the collision operator converges sufficiently fast under mesh refinement. We moreover proposed a Picard-type iterative solution procedure for the nonlinear algebraic systems emanating from the finite-element approximation of the Boltzmann equation, based on a partition of the collision operator in local and non-local components. The explicit treatment of the non-local components bypasses the complications of non-locality, such as highly-dense matrices. We showed that under suitable boundary conditions, the linear systems in the Picard procedure correspond to Friedrichs’ systems.

Figure 8: Heat transfer at a boundary: energy in the domain versus time for the finite-element approximation of the Boltzmann equation (solid) and the Monte-Carlo MD simulation (dashed) with $m = 10^4$, for heat-up times $t \in \{2^1, 2^3, 2^6\}$. The dotted line indicates the boundary energy $e(t)$ according to (5.8).

Figure 9 (left) displays the average Rayleigh distribution over the time interval $T = (0, 4)$ for fast heating ($t = 2$). Figure 9 (right) displays the average Rayleigh distribution over the time interval $T = (0, 40)$ for slow heating ($t = 2^9$). It can be observed that the Rayleigh distribution of the Boltzmann model and of the Monte-Carlo MD model coincide at the inflow ($\xi > 0$), in accordance with the equivalence of the imposed boundary data in the two models. At the outflow ($\xi < 0$), the time-averaged Rayleigh distributions of the two models also coincide for slow heating, but not for fast heating. For fast heating, the Monte-Carlo MD model displays a minutely increased probability at higher outflow velocities (approximately in the range of velocities between $-6$ and $-3$), which corresponds to a higher outflux of energy in the molecular model than in the Boltzmann model. Accordingly, the heat transfer from the boundary into the domain is slower in the molecular model than in the Boltzmann model.
Numerical experiments were conducted to validate the one-dimensional Boltzmann model and its approximation by means of the Discontinuous Galerkin method. The numerical experiments exhibited that the convergence behavior of the Picard-iteration process deteriorates with decreasing Knudsen number and increasing time step in the numerical time-integration procedure. More precisely, we established that the residual reduction is parametrized by the ratio of the time step over the Knudsen number. The numerical experiments moreover conveyed that the DG method yields optimal convergence in the $L^2$-norm for smooth solutions. Exponential decay to equilibrium was observed, in accordance with Cercignani’s conjecture.

A comparison of the Discontinuous-Galerkin approximation of the Boltzmann model and a Monte-Carlo computation of the underlying molecular model for space-inhomogeneous initial data and specular-reflection boundary conditions imparted that the two models are equivalent, in the sense that the Monte-Carlo computation converges to the Boltzmann solution as the number of samples increases, and the Discontinuous-Galerkin approximation converges to the Boltzmann solution as the mesh is refined or the order of approximation is increased. It was verified that the convergence rate of the Monte-Carlo computation is $1/\sqrt{m}$, with $m$ the number of samples, in accordance with convergence theory in the context of the weak law of large numbers. The numerical results moreover conveyed that for spatially inhomogeneous initial data, the convergence to equilibrium proceeds via an initial fast convergence regime, in which the Boltzmann solution converges to a spatially local Maxwellian, and a subsequent slow convergence regime, corresponding to convergence to the global Maxwellian.

Finally, we considered a test case corresponding to heat transfer at a boundary, to illustrate the complexities in extracting boundary conditions for the Boltzmann equation from a molecular-dynamics boundary condition. We observed that the Boltzmann model and the Monte-Carlo molecular-dynamics model display close agreement for slow heating, but not for fast heating. The difference between the results appears to be induced by an inconsistency in the boundary conditions of the molecular-dynamics model and its representation in the Boltzmann model, which manifests itself at larger deviations from equilibrium.
Therefore, provided that the identity holds for \( k \) of the presentation, we define \( \hat{\rho}_k(t) := \partial_t f_k^\varepsilon(t) + \xi \nabla f_k^\varepsilon(t) - \varepsilon^{-1}Q(f_k^\varepsilon(t), f_k^\varepsilon(t)) = \partial_t f_k^\varepsilon(t) - \varepsilon^{-1}Q(f_k^\varepsilon(t), f_k^\varepsilon(t)). \) (A.1)

The second identity follows from the spatial homogeneity (\( x \)-independence) of \( f_k^\varepsilon \). The objective is to prove that for each \( \varepsilon > 0 \), \( \delta t > 0 \) and \( \varepsilon > 0 \), the following identity holds:

\[
\frac{\int_0^{\delta t/c} \|\hat{\rho}_k^{\varepsilon/c}(t)\|_{L^2(\Sigma)}^2 \, dt}{\int_0^{\delta t/c} \|\hat{\rho}_0^{\varepsilon/c}(t)\|_{L^2(\Sigma)}^2 \, dt} = \frac{\int_0^{\delta t} \|\hat{\rho}_0^{\varepsilon}(t)\|_{L^2(\Sigma)}^2 \, dt}{\int_0^{\delta t} \|\hat{\rho}_0^{\varepsilon}(t)\|_{L^2(\Sigma)}^2 \, dt}.
\]

(A.2)

By multiplying the identity (4.8) by a positive constant \( c \), we obtain:

\[
c \partial_t f_k^\varepsilon(t) + (\varepsilon/c)^{-1}L(f_k^\varepsilon(t), f_k^\varepsilon(t)) = (\varepsilon/c)^{-1}G(f_k^\varepsilon(t), f_k^\varepsilon(t)).
\]

Note that the transport term in (A.3) again vanishes on account of spatial homogeneity. To facilitate the presentation, we define \( \tilde{t} = t/c \) and \( \hat{f}_k^{\varepsilon,c}(\tilde{t}) = f_k^\varepsilon(\tilde{t}) \). From (A.3) and the chain rule, it follows that

\[
\partial_t \hat{f}_k^{\varepsilon,c}(\tilde{t}) + (\varepsilon/c)^{-1}L(\hat{f}_k^{\varepsilon,c}(\tilde{t}), \hat{f}_k^{\varepsilon,c}(\tilde{t})) = (\varepsilon/c)^{-1}G(\hat{f}_k^{\varepsilon,c}(\tilde{t}), \hat{f}_k^{\varepsilon,c}(\tilde{t})).
\]

(A.4)

Noting the similarity between (A.4) and (4.8), we infer that

\[
f_k^{\varepsilon/c}(\tilde{t}) = f_k^\varepsilon(\tilde{t}), \quad k = 1, 2, \ldots,
\]

(A.5)

provided that the identity holds for \( k = 0 \), i.e. for the initial estimate. By virtue of the \( t \)-independence of \( f_0^{\varepsilon/c} = f_0^\varepsilon = M_{2,1} \), this provision indeed holds.

From (A.1) and (A.5) we obtain the chain of identities:

\[
\hat{\rho}_k^{\varepsilon/c}(t) = \partial_t f_k^{\varepsilon/c}(t) - (\varepsilon/c)^{-1}Q(f_k^{\varepsilon/c}(t), f_k^{\varepsilon/c}(t)) = \partial_t f_k^\varepsilon(\tilde{t}) - (\varepsilon/c)^{-1}Q(f_k^\varepsilon(\tilde{t}), f_k^\varepsilon(\tilde{t})) = c((f_k^\varepsilon)'(\tilde{t}) - \varepsilon^{-1}Q(f_k^\varepsilon(\tilde{t}), f_k^\varepsilon(\tilde{t}))) = c\hat{\rho}_k^\varepsilon(\tilde{t}).
\]

Therefore,

\[
\int_0^{\delta t/c} \|\hat{\rho}_k^{\varepsilon/c}(t)\|_{L^2(\Sigma)}^2 \, dt = \int_0^{\delta t/c} c^2\|\hat{\rho}_k^\varepsilon(\tilde{t})\|_{L^2(\Sigma)}^2 \, dt = c \int_0^{\delta t} \|\hat{\rho}_0^\varepsilon(s)\|_{L^2(\Sigma)}^2 \, ds,
\]

from which (A.2) follows straightforwardly.

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A. Scaling of the residual reduction
Consider the Picard iteration process (4.8), subject to the initial condition \( f(0) = M_{2,1} \) and periodic boundary conditions (3.14), and provided with the initial estimate \( f_0 = M_{2,1} \). For each \( \varepsilon > 0 \), let \( \{f_k^\varepsilon\}_{k \in \mathbb{Z}_+} \) denote the corresponding sequence of approximations generated by (4.8). With each \( \varepsilon > 0 \) and the corresponding sequence of approximations \( \{f_k^\varepsilon\}_{k \in \mathbb{Z}_+} \), we associate the sequence of residuals \( \{\rho_k^\varepsilon\}_{k \in \mathbb{Z}_+} \) according to

\[
\rho_k^\varepsilon(t) := \partial_t f_k^\varepsilon(t) + \xi \nabla f_k^\varepsilon(t) - \varepsilon^{-1}Q(f_k^\varepsilon(t), f_k^\varepsilon(t)) = \partial_t f_k^\varepsilon(t) - \varepsilon^{-1}Q(f_k^\varepsilon(t), f_k^\varepsilon(t)).
\]

Note that the transport term in (A.3) again vanishes on account of spatial homogeneity. To facilitate

\[
\int_0^{\delta t/c} \|\rho_k^{\varepsilon/c}(t)\|_{L^2(\Sigma)}^2 \, dt = \int_0^{\delta t/c} c^2\|\rho_k^\varepsilon(\tilde{t})\|_{L^2(\Sigma)}^2 \, dt = c \int_0^{\delta t} \|\rho_k^\varepsilon(s)\|_{L^2(\Sigma)}^2 \, ds,
\]

References

A. Scaling of the residual reduction


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