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Fully conservative spectral Galerkin-Petrov method for the inhomogeneous Boltzmann equation

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Abstract

In this paper, we present an application of a Galerkin-Petrov method to the spatially one-dimensional Boltzmann equation. The three-dimensional velocity space is discretised by a spectral method. The space of the test functions is spanned by polynomials, which includes the collision invariants. This automatically insures the exact conservation of mass, momentum and energy. The resulting system of hyperbolic PDEs is solved with a finite volume method. We illustrate our method with two standard tests, namely the Fourier and the Sod shock tube problems. Our results are validated with the help of a stochastic particle method.

 $\label{eq:Keywords} \begin{array}{l} {\bf Keywords} \ {\rm Boltzmann} \ {\rm equation} \cdot {\rm Galerkin-Petrov} \ {\rm method} \cdot {\rm Orthogonal} \ {\rm polynomials} \cdot {\rm System} \ {\rm of} \ {\rm hyperbolic} \ {\rm equations} \cdot {\rm Finite} \ {\rm volume} \ {\rm method} \end{array}$

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1 Introduction

Numerically solving the Boltzmann equation has been a challenging problem for decades. Starting in the 1950s, first schemes had been proposed which were based on the Hilbert expansion or Monte Carlo integration of the collision operator. Different authors also developed stochastic particle methods. The most popular among these is the Direct Simulation Monte Carlo (DSMC), which was introduced by Bird in the 1960s, see his monograph [1]. The DSMC, or modifications of it, are still in use today. Although particle methods can be applied to large range of problems, their usage can cause difficulties when considering slow flows, which require many repetitions in order to damp the stochastic fluctuations.

That's why one is interested in competitive deterministic methods for the Boltzmann equation. Several schemes were designed, for example by using the Fourier representation of the collision operator, originally for Maxwell pseudo-molecules by

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Bobylev and Rjasanow [2], which was later extended in [3, 4] and by Ibragimov and Rjasanow [16]. More recently, these results were extended to general cross-sections [13, 12, 10] by Gamba and Tharkabhushanam and Gamba and Haack.

A spectral method based on trigonometric polynomials was presented in [21, 22, 23].

This work extends the ideas from [11] to the spatially inhomogeneous Boltzmann equation. Approaches similar to our method can be found in [18] and [9, 15] for two dimensions, both in velocity and space.

In [9], Fonn, Grohs and Hiptmair proposed a spectral scheme for the twodimensional spatially homogeneous Boltzmann equation. The particle density function is sought as a linear combination of basis functions consisting of polynomials, given in polar coordinates, multiplied with a Maxwellian weight. The homogeneous Boltzmann equation is discretised by a Galerkin ansatz with respect to a weighted inner product on $L^2(\mathbb{R}^3)$. The physical quantities related to the collision invariants are not conserved in general but only for a special choice of the weight function. The numerical effort of computing the discretised collision operator is reduced by exploiting the simple representation of spherical harmonics and their rotations in two dimensions, namely $Y_i(\varphi) = \exp(il\varphi)$. In [15], this ansatz was extended by Grohs, Hiptmair and Pintarelli to the two-dimensional inhomogeneous Boltzmann equation. Strang splitting is used to decouple the advection and collision step. In order to fulfil the conservation laws, two methods are presented, one by adding a basis of the collision invariants to the test functions, which leads to an overdetermined system of ODEs. The other possibility is adding a Lagrange multiplier which corrects the coefficients of the basis functions at each time step. The advection equation is solved by least squares method on the phase space combined with a continuous first order FEM.

Kitzler and Schöberl [18] use Galerkin-Petrov method in the velocity space and a Discontinuous Galerkin discretisation of the advection part for the two-dimensional inhomogeneous Boltzmann equation. The test functions are spanned by tensor products of (continuous) polynomials in the velocity variable and piecewise continuous polynomials in the space variables. The basis functions are obtained by multiplying the test functions with a Maxwellian weight, where the bulk velocity and temperature may depend on the spatial variable. This automatically insures exact conservation laws. The translation invariance together with the simple parametrisation of S^1 is used to reduce the numerical effort of the collision step.

This paper is organised as follows. In Section 2, we introduce our notation for the Boltzmann equation and give a formulation of the one-dimensional problems which are discussed in this paper. In Section 3, we investigate the semi-discretised Boltzmann equation which arise after an integration over the velocity space. This also includes a small section on the Burnett functions which are used for the construction of our basis and test functions. Section 4 gives some details of the implementation, in particular numerical integration over \mathbb{R}^3 and half-spaces as well as the formulation of boundary conditions and the discretisation of the hyperbolic system. In Section 5, we present the results of our scheme for two standard tests and different Knudsen numbers. Some concluding remarks can be found in Section 6

2 One-dimensional problems for the Boltzmann equation

We consider the spatially one-dimensional Boltzmann equation

$$\frac{\partial f}{\partial t}(t,x,v) + v_1 \frac{\partial f}{\partial x}(t,x,v) = \frac{1}{\mathrm{Kn}} Q(f,f)(v), \tag{1}$$

which models the time evolution of the particle density function

$$f: \mathbb{R}_{\geq 0} \times (0,1) \times \mathbb{R}^3 \to \mathbb{R}_{\geq 0}$$

of a gas located in (0, 1).

The right-hand side of equation (1) is called the collision integral or collision operator. It is given by

$$Q(g,h)(v) = \int_{\mathbb{R}^3} \int_{S^2} |u| \sigma\left(|u|, \frac{(u,e)}{|u|}\right) (g(v')h(w') - g(v)h(w)) \, \mathrm{d}S_e \, \mathrm{d}w,$$

where

$$u = v - w,$$

$$v' = \frac{1}{2} \left(v + w + |u|e \right),$$

$$w' = \frac{1}{2} \left(v + w - |u|e \right),$$

and σ denotes the differential cross-section which depends on the modelled gas interaction. Kn is called Knudsen number which is defined as the ratio of the mean free path $\lambda_{\rm MP}$ and a characteristic length L of the system

$$\mathrm{Kn} = \frac{\lambda_{\mathrm{MP}}}{L}.$$

The collision kernel $|u|\sigma(|u|, |u|^{-1}(u, e))$ can usually be expressed as

$$|u|\sigma\left(|u|,\frac{(u,e)}{|u|}\right) = |u|^{\lambda}b\left(\frac{(u,e)}{|u|}\right), \quad -3 < \lambda \le 1.$$

$$\tag{2}$$

This includes the case of variable hard spheres (VHS) as well as the Maxwell pseudo-molecules.

The weak formulation of the collision operator is particularly useful for our numerical scheme as in this form, the post-collision velocities v' and w' are transferred to the test function ψ .

Theorem 2.1 For suitable $g, h, \psi : \mathbb{R}^3 \to \mathbb{R}$, the L^2 -inner product $(Q(g, h), \psi)_{L^2(\mathbb{R}^3)}$ can also be expressed as

$$\frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} g(v) h(w) \int_{S^2} |u|^{\lambda} \sigma\left(|u|, \frac{(u, e)}{|u|}\right) \left(\psi(v') + \psi(w') - \psi(v) - \psi(w)\right) \mathrm{d}S_e \,\mathrm{d}w \,\mathrm{d}v.$$

Proof. See [6].

As a direct consequence of Theorem 2.1 we get the following lemma. Lemma 2.2 For suitable $g, h : \mathbb{R}^3 \to \mathbb{R}$, we have

$$\int_{\mathbb{R}^3} Q(g,h)(v) \begin{pmatrix} 1\\v\\|v|^2 \end{pmatrix} \mathrm{d}v = 0.$$

Testing the Boltzmann equation with five functions, called collision invariants,

$$\psi_{0} : \mathbb{R}^{3} \to \mathbb{R}, v \mapsto 1,$$

$$\psi_{1} : \mathbb{R}^{3} \to \mathbb{R}, v \mapsto v_{1},$$

$$\psi_{2} : \mathbb{R}^{3} \to \mathbb{R}, v \mapsto v_{2},$$

$$\psi_{3} : \mathbb{R}^{3} \to \mathbb{R}, v \mapsto v_{3},$$

$$\psi_{4} : \mathbb{R}^{3} \to \mathbb{R}, v \mapsto |v|^{2},$$

we conclude the conservation of mass, momentum in all three directions and energy.

Proof. It is not hard to see that ψ_0, \ldots, ψ_4 fulfil

$$\psi(v') + \psi(w') = \psi(v) + \psi(w) \quad v, w \in \mathbb{R}^3, e \in S^2$$

The claim follows after an application of Theorem 2.1.

In order to get a well-defined problem for equation (1), initial and boundary conditions are imposed on the particle density function f. At the beginning, the particle density function is given by Maxwell distributions

$$f(0,x,v) = \frac{\rho_0(x)}{(2\pi T_0)^{\frac{3}{2}}} \exp\left(-\frac{|v-V_0(x)|^2}{2T_0(x)}\right), \quad x \in (0,1), \ v \in \mathbb{R}^3.$$
(3)

The boundaries can be opened, e.g. the shock tube, or closed in the case of the Fourier problem. For open boundaries, the particle density function has to fulfil inflow conditions

$$f(t, 0, v) = f_l(t, v), \quad t \ge 0, v \in \mathbb{R}^3_{\text{in}}(0)$$

$$f(t, 1, v) = f_r(t, v), \quad t \ge 0, v \in \mathbb{R}^3_{\text{in}}(1)$$
(4)

If the boundary conditions should model walls, i.e. the boundaries are closed, diffusely reflecting conditions are imposed on f,

$$f(t,0,v) = \left(\int_{\mathbb{R}^{3}_{\text{out}}(0)} f(t,0,w)|w_{1}|\,\mathrm{d}w\right) \frac{1}{2\pi T_{l}^{2}} \exp\left(-\frac{|v|^{2}}{2T_{l}}\right) \quad t \ge 0, v \in \mathbb{R}^{3}_{\text{in}}(0),$$

$$f(t,1,v) = \left(\int_{\mathbb{R}^{3}_{\text{out}}(1)} f(t,1,w)|w_{1}|\,\mathrm{d}w\right) \frac{1}{2\pi T_{r}^{2}} \exp\left(-\frac{|v|^{2}}{2T_{r}}\right) \quad t \ge 0, v \in \mathbb{R}^{3}_{\text{in}}(1),$$
(5)

where $\mathbb{R}^3_{in}(x) = \{v \in \mathbb{R}^3 : (v, n(x)) > 0\}$, $\mathbb{R}^3_{out}(x) = \{w \in \mathbb{R}^3 : (w, n(x)) < 0\}$ and $n(0) = (1, 0, 0)^{\top}$ and $n(1) = (-1, 0, 0)^{\top}$ denote the inner normals. This choice conserves the total mass of the gas.

3 Galerkin-Petrov method

The crucial part when solving the Boltzmann equation is the application of the collision operator. Every evaluation involves the computation of a five-fold integral. Furthermore, the operator is non-linear. However, the collision operator only acts on the velocity space and by the use its weak form, we can exploit its bilinear structure. In this formulation, the collision operator is descretised by a sequence of symmetric matrices which are independent of time and space as well as chosen initial and boundary conditions. Once these matrices are computed and stored, they can be used for different initial and boundary values as well as for different time-space integration schemes.

This motivates the following ansatz for the approximation $f^{(n)}$ of the particle density function

$$f^{(n)}(t, x, v) = \sum_{j=1}^{n} f_j(t, x)\varphi_j(v), \quad t \ge 0, \ x \in (0, 1), \ v \in \mathbb{R}^3,$$

where $(\varphi_j)_{j=1}^n$ are called basis or ansatz functions and $(f_j)_{j=1}^n$ is the coefficient vector.

Plugging this into the Boltzmann equation (1), we get the residual

$$R(t,x,v) = \sum_{j=1}^{n} \partial_t f_j(t,x)\varphi_j(v) + \partial_x f_j(t,x)v_1\varphi_j(v) - \sum_{k=1}^{n} \sum_{l=1}^{n} f_k(t,x)f_l(t,x)Q(\varphi_k,\varphi_l)(v),$$

for t > 0, $x \in (0, 1)$ and $v \in \mathbb{R}^3$. The coefficients $(f_j)_{j=1}^n$ are chosen such that for all t > 0 and $x \in (0, 1)$,

$$(R(t, x, -), \psi_i)_{L^2(\mathbb{R}^3)} = 0, \quad i = 1, \dots, n,$$
(6)

where the functions $(\psi_i)_{i=1}^n$ are called test functions. If $\psi_i = \varphi_i$ for $i = 1, \ldots, n$, this is the classical Galerkin method. However, choosing a set of test functions which includes the five collision invariants, the corresponding collision matrices vanish. We automatically conserve mass, momentum and energy.

For our method, the test functions are polynomials, including the collision invariants. The ansatz space is spanned by test functions multiplied with an Maxwellian weight. This choice of basis functions leads to consistent results in case of the steady-state and in the hydrodynamic limit, $\text{Kn} \rightarrow 0$.

3.1 Burnett functions

Our basis and test functions are derived from the Burnett functions, which were introduced in kinetic theory by Burnett in 1935 [5]. They were already used in [11] to construct basis and test functions. We adopt their main ideas with slight modifications regarding scaling factors.

Definition 3.1 Given $k \in \mathbb{N}$, $l \in \mathbb{N}$ and $m \in \{-l, \ldots, l\}$, the (normalised) Burnett function $\psi_{k,l,m}$ is defined in spherical coordinates, $v = \rho e$, as

$$\psi_{k,l,m}: \mathbb{R}^3 \to \mathbb{R}, v \mapsto \sqrt{\frac{2k!}{\Gamma(k+l+\frac{3}{2})}} L_k^{(l+\frac{1}{2})} \left(\rho^2\right) \rho^l Y_{l,m}\left(e\right)$$

where $L_k^{(l+\frac{1}{2})}$ denotes the associated Laguerre polynomial of degree k and $Y_{l,m}$ the real-valued spherical harmonic, given by

$$Y_{l,m} = \begin{cases} \sqrt{2} \operatorname{Im}(Y_l^{|m|}), & m < 0\\ Y_l^0, & m = 0\\ \sqrt{2} \operatorname{Re}(Y_l^m), & m > 0. \end{cases}$$
(7)

Here, Y_l^m denotes the usual complex-valued spherical harmonic. **Remark 3.2** For $v \in \mathbb{R}^3 \setminus \{0\}$, $\rho \in [0, \infty)$ and $e \in S^2$ with $v = \rho e$ are uniquely given by

$$\rho = |v|, \quad e = \frac{v}{|v|}.$$

If v = 0, ρ is equal to 0, but e can be chosen arbitrarily. However, the Burnett functions are well-defined. This can be seen by a case distinction of $l \in \mathbb{N}$.

In the case of l = 0, $Y_{0,0}$ is a constant polynomial. Thus the value of $\psi_{k,0,0}$ does not depend on e for all $k \in \mathbb{N}$.

If l > 0, we have $\rho^l = 0^l = 0$ and $\psi_{k,l,m}(0) = 0$ for all $k \in \mathbb{N}$ and $m \in \{-l, \ldots, l\}$ independent of e.

Lemma 3.3 The Burnett functions are polynomials.

Proof. Let $k \in \mathbb{N}$, $l \in \mathbb{N}$ and $m \in \{-l, \ldots, l\}$. Then

$$\Phi_{k,l}: \mathbb{R}^3 \to \mathbb{R}, v \mapsto \sqrt{\frac{2k!}{\Gamma(k+l+\frac{3}{2})}} L_k^{(l+\frac{1}{2})} \left(|v|^2 \right)$$

is a polynomial as $v \mapsto |v|^2 = v_1^2 + v_2^2 + v_3^2$ is a polynomial. The spherical harmonic $Y_{l,m}$ is the restriction of a homogeneous polynomial $P_{l,m}$ of degree l on S^2 . Hence it holds for all $v = \rho e \in \mathbb{R}^3$

$$\rho^l Y_{l,m}\left(e\right) = P_{l,m}(v),$$

which completes the proof.

Lemma 3.4 For all $k, k' \in \mathbb{N}$, $l, l' \in \mathbb{N}$ and $m \in \{-l, \ldots, l\}$, $m' \in \{-l', \ldots, l'\}$, we have

$$\int_{\mathbb{R}^3} \exp(-|v|^2) \psi_{k,l,m}(v) \, \psi_{k',l',m'}(v) \, \mathrm{d}v = \delta_{kk'} \delta_{ll'} \delta_{mm'}.$$

Lemma 3.5 The collision invariants can be expressed as a linear combination of

Burnett functions, namely

$$\begin{split} \psi_{0,0,0}(v) &= \sqrt{\frac{1}{4\pi}}, \\ \psi_{0,1,-1}(v) &= \sqrt{\frac{3}{4\pi}}v_2, \\ \psi_{0,1,0}(v) &= \sqrt{\frac{3}{4\pi}}v_3, \\ \psi_{0,1,1}(v) &= -\sqrt{\frac{3}{4\pi}}v_1, \\ \psi_{1,0,0}(v) &= \sqrt{\frac{1}{4\pi}}\left(\frac{3}{2} - |v|^2\right). \end{split}$$

3.2 Basis and test functions

Starting with the Burnett functions, we construct our basis and test functions. In order to approximate a broader range of temperatures, we rescale the Burnett functions by a characteristic temperature T > 0.

Definition 3.6 For $k, l \in \mathbb{N}$, $m \in \{-l, \ldots, l\}$, we define

$$\psi_{k,l,m}^T : \mathbb{R}^3 \to \mathbb{R}, v \mapsto \frac{1}{T^{\frac{3}{4}}} \psi_{k,l,m}\left(\frac{v}{\sqrt{T}}\right),$$

the test function with indices k, l, m.

Definition 3.7 For $k, l \in \mathbb{N}, m \in \{-l, \ldots, l\}$, we define

$$\varphi_{k,l,m}^{T} : \mathbb{R}^{3} \to \mathbb{R}, v \mapsto \exp\left(-\frac{|v|^{2}}{2T}\right) \psi_{k,l,m}^{T}\left(v\right),$$

the basis function with indices k, l, m.

Lemma 3.8 For all $k, k' \in \mathbb{N}$, $l, l' \in \mathbb{N}$ and $m \in \{-l, \dots, l\}$, $m' \in \{-l', \dots, l'\}$, it holds

$$\int_{\mathbb{R}^3} \varphi_{k,l,m}^T(v) \, \varphi_{k',l',m'}^T(v) \, \mathrm{d}v = \delta_{kk'} \delta_{ll'} \delta_{mm'}.$$

If T = 1, we drop the superscript and simply write $\varphi_{k,l,m}$ and $\psi_{k,l,m}$ instead of $\varphi_{k,l,m}^T$ and $\psi_{k,l,m}^T$. In the following, we will often write φ_j^T and ψ_i^T , meaning that we implicitly choose an enumeration of the basis and test functions.

3.3 Semi-discretised Boltzmann equation

The set of indices used for the basis and also for the test functions are chosen from a sequence of increasing sets which are indexed by two integers, indicating the highest used degree for radial and spherical polynomials, that is for $K, L \in \mathbb{N}$ the indices are given by

$$I_{K,L} = \{(k,l,m) : k \in \{0,\dots,K\}, l \in \{0,\dots,L\}, m \in \{-l,\dots,l\}\}.$$
(8)

This insures that for all non-trivial choices of K and L, the collision invariants are always elements of the set of test functions.

Plugging our basis and test functions into equation (6), we get a system of

$$n = (K+1)(L+1)^2$$

partial differential equations. Rewritten in matrix form, these equations read as

$$M^{T}\partial_{t}\mathbf{f} + D^{T}\partial_{x}\mathbf{f} = \frac{1}{\mathrm{Kn}}C^{T}(\mathbf{f}), \qquad (9)$$

where M^T is the mass matrix with entries

$$M^{T}[i,j] = \left(\varphi_{j}^{T}, \psi_{i}^{T}\right)_{L^{2}(\mathbb{R}^{3})}, \quad i,j = 1, \dots, n,$$

 D^T is the so-called flow matrix whose entries are given by

$$D^{T}[i,j] = \left(v_{1}\varphi_{j}^{T},\psi_{i}^{T}\right)_{L^{2}(\mathbb{R}^{3})}, \quad i,j = 1,\dots,n,$$

and the *i*-th component of $C^{T}(\mathbf{f})$ is

$$\mathbf{f}^{\top} Q_i^T \mathbf{f}, \quad i = 1, \dots, n.$$

Here, $(Q_i^T)_{i=1}^n$ denote the collision matrices. They are defined as

$$Q_i^T[k,l] = \left(Q(\varphi_k^T, \varphi_l^T), \psi_i^T\right)_{L^2(\mathbb{R}^3)}, \quad k, l, i = 1, \dots, n.$$

We drop the superscripts in case of T = 1.

It will be shown in the following that the system of PDEs in equation (9) can be expressed as

$$M\partial_t \mathbf{f} + T^{\frac{1}{2}} D \partial_x \mathbf{f} = T^{\frac{\lambda}{2} + \frac{3}{4}} \frac{1}{\mathrm{Kn}} C(\mathbf{f}), \tag{10}$$

exposing the dependence of the matrices on the characteristic temperature T.

Mass matrix

The entries of the mass matrix M^T can be rewritten as

$$M^{T}[i,j] = \int_{\mathbb{R}^{3}} \varphi_{j}^{T}(v)\psi_{i}^{T}(v) dv$$

=
$$\int_{\mathbb{R}^{3}} \varphi_{j}(v)\psi_{i}(v) dv$$

=
$$\int_{\mathbb{R}^{3}} \exp\left(-\frac{|v|^{2}}{2}\right)\psi_{j}(v)\psi_{i}(v) dv, \quad i, j = 1, \dots, n$$

Thus the mass matrix is independent of T. The last line in the earlier equation shows that the mass matrix is the Gramian of a weighted L^2 -inner product on \mathbb{R}^3 . Hence, it is symmetric and positive definite.

Flow matrix

The entries of the flow matrix D^{T} can be simplified to

$$D^{T}[i,j] = \int_{\mathbb{R}^{3}} \varphi_{j}^{T}(v)v_{1}\psi_{i}^{T}(v) dv$$

$$= T^{\frac{1}{2}} \int_{\mathbb{R}^{3}} v_{1}\varphi_{j}(v)\psi_{i}(v) dv$$

$$= T^{\frac{1}{2}} \int_{\mathbb{R}^{3}} v_{1} \exp\left(-\frac{|v|^{2}}{2}\right)\psi_{j}(v)\psi_{i}(v) dv, \quad i, j = 1, \dots, n$$

It can be seen from the last line of the above equation that D^T is symmetric.

Collision matrices

For the computation of the collision matrices, the weak form of the collision operator, as presented in Theorem 2.1, is used. Thus, for $i, k, l = 1, ..., n, Q_i^T[k, l]$ is given by

$$Q_i^T[k,l] = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \varphi_k^T(v) \,\varphi_l^T(w) \,q_i^T(v,w) \,\mathrm{d}w \,\mathrm{d}v, \tag{11}$$

where

$$q_i^T(v,w) = \frac{1}{2} \int_{S^2} |u|^{\lambda} b\left(\frac{(u,e)}{|u|}\right) \left(\psi_i^T(v') + \psi_i^T(w') - \psi_i^T(v) - \psi_i^T(w)\right) \mathrm{d}S_e, \ v,w \in \mathbb{R}^3.$$

As before, we scale the velocities with \sqrt{T} by applying the substitution

$$\mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^3 \times \mathbb{R}^3, (v, w) \mapsto (\sqrt{T}v, \sqrt{T}w),$$

which has Jacobian T^3 , on the integral in equation (11). The collision velocities transform as

$$\begin{split} \sqrt{T}u &= \sqrt{T}v - \sqrt{T}w,\\ \sqrt{T}v' &= \frac{1}{2} \left(\sqrt{T}v + \sqrt{T}w + |\sqrt{T}v - \sqrt{T}w|e \right),\\ \sqrt{T}w' &= \frac{1}{2} \left(\sqrt{T}v + \sqrt{T}w - |\sqrt{T}v - \sqrt{T}w|e \right), \end{split}$$

for all $v, w \in \mathbb{R}^3$, $e \in S^2$ and therefore

$$q_i^T(\sqrt{T}v,\sqrt{T}w) = T^{\frac{\lambda}{2} - \frac{3}{4}}q_i(v,w), \quad v, w \in \mathbb{R}^3.$$

Combining this with equation (11) yields

 $Q_i^T[k,l] = T^{\frac{\lambda}{2} + \frac{3}{4}} Q_i[k,l], \quad k, l, i = 1, \dots, n.$

The substitution

$$S^2 \to S^2, e \mapsto -e$$

shows that $q_i(v, w) = q_i(w, v), v, w \in \mathbb{R}^3$. Consequently, the collision matrices are symmetric.

Lemma 3.9 There exist a basis of \mathbb{R}^n , denoted by $(r_i)_{i=1}^n$, of generalised eigenvectors of D with respect to M and generalised eigenvalues $(\lambda_i)_{i=1}^n \subset \mathbb{R}$, such that

$$Dr_i = \lambda_i M r_i, \quad i = 1, \dots, n.$$
(12)

The generalised spectrum of D is point symmetric with respect to 0, i.e. if λ is a generalised eigenvalue of D, then $-\lambda$ is a generalised eigenvalue of D, too.

Proof. As D is symmetric and M is positive definite, the existence of the generalised eigensystem follows from standard theory. Let $r \in \mathbb{R}^n$ be a generalised eigenvector of D with respect to M and $\lambda \in \mathbb{R}$ be the corresponding generalised eigenvalue. We define $\tilde{r} \in \mathbb{R}^n$ by

$$\tilde{r}_i = c_i r_i, \quad i = 1, \dots, n$$

where

$$c_i = \begin{cases} 1, & l \text{ even} \\ -1, & l \text{ odd} \end{cases}, \quad i = h(k, l, m), \ i = 1, \dots, n \end{cases}$$

and $h: I_{K,L} \to \{1, \ldots, n\}$ is an enumeration of indices of the basis and test functions. Since the spherical harmonic $Y_{l,m}$ is even if l is even and odd otherwise, the test functions fulfil

$$\psi_i(-v) = c_i \psi_i(v), \quad v \in \mathbb{R}^3, \ i = 1, \dots, n.$$

Let $i \in \{1, \ldots, n\}$. We have

$$\begin{split} (D\tilde{r})_i &= \sum_{j=1}^n D[i,j]\tilde{r}_j = \sum_{j=1}^n \int_{\mathbb{R}^3} v_1 \exp\left(-\frac{|v|^2}{2}\right) \psi_i(v)\psi_j(v) \,\mathrm{d}v\,\tilde{r}_j \\ &= \sum_{j=1}^n \int_{\mathbb{R}^3} -v_1 \exp\left(-\frac{|v|^2}{2}\right) c_i\psi_i(v)c_j\psi_j(v) \,\mathrm{d}v\,\tilde{r}_j \\ &= -c_i \sum_{j=1}^n D[i,j]c_j\tilde{r}_j = -c_i \sum_{j=1}^n D[i,j]r_j \\ &= -c_i \lambda \sum_{j=1}^n M[i,j]r_j = -\lambda \sum_{j=1}^n c_i M[i,j]c_j\tilde{r}_j \\ &= -\lambda \sum_{j=1}^n \int_{\mathbb{R}^3} \exp\left(-\frac{|v|^2}{2}\right) c_i\psi_i(v)c_j\psi_j(v) \,\mathrm{d}v\,\tilde{r}_j \\ &= -\lambda \sum_{j=1}^n \int_{\mathbb{R}^3} \exp\left(-\frac{|v|^2}{2}\right) \psi_i(v)\psi_j(v) \,\mathrm{d}v\,\tilde{r}_j \\ &= -\lambda (M\tilde{r})_i. \end{split}$$

The generalised spectrum of D with respect to M in case of K = 9, L = 9, i.e. n = 1000, is shown in Figure 1.

We can now decouple the left-hand side. Following the notation of Lemma 3.9, let R denote the matrix whose columns are the generalized eigenvectors $(r_i)_{i=1}^n$ and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$. Equation (12) reads as

$$DR = MR\Lambda. \tag{13}$$



Figure 1: Generalised spectrum of D with respect to M for K = 9, L = 9, i.e. n = 1000.

Substituting f = Rg in equation (10), we get, after an application of equation (13),

$$\partial_t g + T^{\frac{1}{2}} \Lambda \partial_x g = T^{\frac{\lambda}{2} + \frac{3}{4}} \frac{1}{\mathrm{Kn}} R^{-1} M^{-1} C(Rg).$$
(14)

Initial and boundary conditions of the coefficient vector are obtained by minimising the L^2 -error which occurs when plugging the approximation $f^{(n)}$ into equations (3) and (4) or (5).

As the basis functions are orthonormal, we have

$$\mathbf{f}(0,x) = \left(\left(f_0(x,-), \varphi_i^T \right)_{L^2(\mathbb{R}^3)} \right)_{i=0}^n.$$

Let us assume that there is an approximation of the outgoing flux σ_{out} at the boundaries in case of diffuse reflection. If we impose inflow conditions, $\sigma_{out} = 1$.

As the boundary conditions are only imposed on \mathbb{R}^3_{in} , we minimise the L^2 -error on this half-space. Therefore, for all t > 0 and boundary points x, $\mathbf{f}(t, x)$ has to fulfil the linear system

$$M_{\rm in}^T \mathbf{f}(t, x) = \sigma_{\rm out} b^T(t, x), \tag{15}$$

where

$$M_{\rm in}^T[i,j] = \int_{\mathbb{R}^3_{\rm in}} \varphi_j^T(v) \varphi_i^T(v) \,\mathrm{d}v, \quad i,j = 1,\dots, n$$

and

$$b^{T}(t,x)_{i} = \int_{\mathbb{R}^{3}_{\text{in}}} f_{\text{in}}(t,x,v)\varphi_{i}^{T}(v) \,\mathrm{d}v, \quad i = 1,\dots, n.$$

 $M_{\rm in}^T$ can be simplified to

$$M_{\rm in}^T[i,j] = \int_{\mathbb{R}^3_{\rm in}} \varphi_j(v)\varphi_i(v)\,\mathrm{d}v, \quad i,j=1,\ldots,n,$$

meaning that this matrix is independent of T. $M_{\rm in}$ is symmetric and positive definite. The approximation of the outgoing fluxes is discussed in Section 4.

4 Numerical realisation

The computation the matrices from Section 3 involves three types of integrals,

$$\int_{\mathbb{R}^3} \exp\left(-\frac{|v|^2}{2}\right) p(v) \,\mathrm{d}v,$$
$$\int_{S^2} p(e) \,\mathrm{d}S_e$$

and

$$\int_{H} \exp\left(-\frac{|v|^2}{2}\right) p(v) \,\mathrm{d}v,$$

where H is a half-space, given by $H = \{v \in \mathbb{R}^3 : (v, n) > 0\}$ with $n \in S^2$, and p is polynomial in three variables.

As the Burnett functions are given in spherical coordinates, the integrals over \mathbb{R}^3 and H are rewritten as

$$\int_{\mathbb{R}^3} \exp\left(-\frac{|v|^2}{2}\right) p(v) \,\mathrm{d}v = \int_{(0,\infty)} \rho^2 \exp\left(-\frac{\rho^2}{2}\right) \int_{S^2} p(\rho e) \,\mathrm{d}S_e \,\mathrm{d}\rho$$

and

$$\int_{H} \exp\left(-\frac{|v|^2}{2}\right) p(v) \,\mathrm{d}v = \int_{(0,\infty)} \rho^2 \exp\left(-\frac{\rho^2}{2}\right) \int_{S^2} p(\rho e) \mathbb{1}_{[0,1]}\left((e,n)\right) \,\mathrm{d}S_e \,\mathrm{d}\rho.$$
(16)

The radial integrals are approximated by a Gauß quadrature generated by the weight function

$$w: [0,\infty) \to [0,\infty), \rho \mapsto \rho^2 \exp\left(-\frac{\rho^2}{2}\right).$$

This quadrature rule is sometimes referred as Gauß-Maxwell quadrature [24]. The integrals over the sphere are approximated by the Lebedev quadrature [19].

Although the Lebedev quadrature is suitable for the integration over S^2 , it fails if one integrates over half-spheres as demanded in (16). In this case, we express pas a linear combination of spherical harmonics. The integral over the sphere is now reduced to integrals such as

$$\int_{S^2} \mathbb{1}_{[0,1]} ((e,n)) |(e,n)|^{\beta} Y_{l,m}(e) \, \mathrm{d}S_e, \quad l \in \mathbb{N}_0, \ |m| \le l,$$

and $\beta \in \{0, 1\}$, which can be computed with the Funk-Hecke theorem [7]. The case $\beta = 0$ refers to projections an half-spaces, whereas integrals with $\beta = 1$ are needed for the computation of outflows.

Theorem 4.1 (Funk-Hecke) Let $Y_{l,m}$ be a spherical harmonic of degree $l \in \mathbb{N}$, and $g \in L^1([-1,1])$. For all $n \in S^2$ it holds:

$$\int_{S^2} g((n,e))Y_l(e) \,\mathrm{d}S_e = 2\pi \,Y_l(n) \left(\int_{[-1,1]} g(x)P_l(x) \,\mathrm{d}x\right),$$

where P_l is the Legendre polynomial of degree l.

An application of Theorem 4.1 yields for the earlier equation

$$\int_{S^2} \mathbb{1}_{[0,1]} \Big((e,n) \Big) \left| (e,n) \right|^{\beta} Y_{l,m} \, \mathrm{d}S_e = 2\pi Y_{l,m}(n) \int_{[0,1]} x^{\beta} P_l(x) \, \mathrm{d}x.$$

The one-dimensional integrals can be computed analytically,

$$\int_{[0,1]} P_l(x) \, \mathrm{d}x = \begin{cases} 1, & l = 0\\ 0, & l > 0 \text{ even} \\ \binom{1/2}{(l+1)/2}, & l > 0 \text{ odd} \end{cases},$$

and

$$\int_{[0,1]} x P_l(x) \, \mathrm{d}x = \begin{cases} \frac{1}{2}, & l = 0\\ \frac{1}{3}, & l = 1\\ 0, & l > 1 \text{ odd }, \\ \frac{1}{3} \binom{3/2}{l/2 + 1}, & l > 1 \text{ even} \end{cases}$$

where

$$\binom{\alpha}{k} = \prod_{i=0}^{k-1} \frac{\alpha - i}{i+1}, \quad \alpha \in \mathbb{R}, \, k \in \mathbb{N},$$

denotes the generalised binomial coefficient.

By the use of these quadratures, one can compute the matrices from Section 3.3. Most of the time is spent on the computation of the collision matrices. That's why we will address their computation in further detail.

Computation of the collision matrices

In this Section, we follow the approach from [11]. In contrast to [11], we use a Gauß-Maxwell quadrature for the computation of the radial integrals. Let us fix $K \in \mathbb{N}$, the maximal degree of Laguerre polynomials, and $L \in \mathbb{N}$, the maximal degree of spherical harmonics. We choose the indices of our basis and test functions as

$$I_{K,L} = \{(k,l,m) : k \in \{0,\ldots,K\}, l \in \{0,\ldots,L\}, m \in \{-l,\ldots,l\}\},\$$

which has

$$n = (K+1)(L+1)^2$$

elements.

Let N_{GM} denote the order of Gauß-Maxwell quadrature $(\rho_i, w_i^{\text{GM}})_{i=1}^{N_{\text{GM}}}$ and N_{L} the order of the Lebedev quadrature $(e_j, w_j^{\text{L}})_{j=1}^{N_{\text{L}}}$. To compute an entry of a collision matrix, let $k, l, i \in \{1, \ldots, n\}$ and let $(k_v, l_v, m_v), (k_w, l_w, m_w), (k_i, l_i, m_i)$ be the corresponding indices for the basis and test functions. A straightforward approximation

of equation (11) yields

$$Q_{i}[k, l] \approx (4\pi)^{2} \sum_{i_{v}=1}^{N_{\text{GM}}} \omega_{i_{v}}^{\text{GM}} \rho_{i_{v}}^{l_{v}} L_{k_{v}}^{(l_{v}+\frac{1}{2})}(\rho_{i_{v}}^{2}) \times \\ \sum_{j_{v}=1}^{N_{\text{L}}} \omega_{j_{v}}^{\text{L}} Y_{l_{v}m_{v}}(e_{j_{v}}) \times \\ \sum_{i_{w}=1}^{N_{\text{GM}}} \omega_{i_{w}}^{\text{GM}} \rho_{i_{w}}^{l_{w}} L_{k_{w}}^{(l_{w}+\frac{1}{2})}(\rho_{i_{w}}^{2}) \times \\ \sum_{j_{w}=1}^{N_{\text{L}}} \omega_{j_{w}}^{\text{L}} Y_{l_{w}m_{w}}(e_{j_{w}})(q_{L})_{i}(v_{i_{v},j_{v}}, w_{i_{w},j_{w}}),$$

where $v_{i_v,j_v} = \rho_{i_v} e_{j_v}$, $w_{i_w,j_w} = \rho_{i_w} e_{j_w}$ and

$$(q_L)_i(v_{i_v,j_v}, w_{i_w,j_w}) = 4\pi \frac{C_\lambda}{2} \sum_{j=1}^{N_L} \omega_j^L |v_{i_v,j_v} - w_{i_w,j_w}|^\lambda b \left(\frac{(v_{i_v,j_v} - w_{i_w,j_w}, e_j)}{|v_{i_v,j_v} - w_{i_w,j_w}|} \right) \times \left(\psi_i(v'_{i_v,j_v,i_w,j_w}(e_j)) + \psi_i(w'_{i_v,j_v,i_w,j_w}(e_j)) - \psi_i(v_{i_v,j_v}) - \psi_i(w_{i_w,j_w})) \right),$$

with

$$v_{i_{v},j_{v},i_{w},j_{w}}'(e_{j}) = \frac{1}{2} \left(v_{i_{v},j_{v}} + w_{i_{w},j_{w}} + |v_{i_{v},j_{v}} - w_{i_{w},j_{w}}|e_{j} \right),$$

$$w_{i_{v},j_{v},i_{w},j_{w}}'(e_{j}) = \frac{1}{2} \left(v_{i_{v},j_{v}} + w_{i_{w},j_{w}} - |v_{i_{v},j_{v}} - w_{i_{w},j_{w}}|e_{j} \right).$$

However, this form is not used for the computation of the matrix entries. Due to the product structure of the Burnett functions, there are some repetitive parts which have to be computed only once. Storing them reduces the computational effort.

Let us define the three arrays $P_{\rm GM}$, $P_{\rm L}$ and $P_{\rm Q}$. The first array $P_{\rm GM}$ is given by

$$(P_{\mathrm{GM}})_{k,l,i} = \omega_i^{\mathrm{GM}} \rho_i^l L_k^{(l+\frac{1}{2})}(\rho_i^2),$$

for k = 0, ..., K, l = 0, ..., L and $i = 1, ..., N_{GM}$. The entries of the second array are

$$(P_{\mathrm{L}})_{l,m,j} = \omega_j^{\mathrm{L}} Y_{l,m}(e_j),$$

for l = 0, ..., L, m = -l, ..., l and $j = 1, ..., N_{\rm L}$. The entries of the third array $P_{\rm Q}$ are computed as

$$(P_{\mathbf{Q}})_{i_v,j_v,i_w,j_w,i} = (q_L)_i (v_{i_v,j_v}, w_{i_w,j_w}),$$

for $i_v, i_w = 1, ..., N_{\text{GM}}$ and $j_v, j_w = 1, ..., N_{\text{L}}$.

The approximation of the matrix entry of the collision matrix is now given by

$$Q_{i}[k, l] \approx (4\pi)^{2} \sum_{i_{v}, i_{w}=1}^{N_{\rm GM}} \sum_{j_{v}, j_{w}=1}^{N_{\rm L}} (P_{\rm GM})_{k_{v}, l_{v}, i_{v}} (P_{\rm L})_{l_{v}, m_{v}, j_{v}} (P_{\rm GM})_{k_{w}, l_{w}, i_{w}} (P_{\rm L})_{l_{w}, m_{w}, j_{w}} (P_{Q})_{i_{v}, j_{v}, i_{w}, j_{w}, i_{w}, j_{w}, i_{w}, j_{w}, j_{$$

The numerical effort for computing $P_{\rm GM}$ and $P_{\rm L}$ is sublinear in the number of basis functions and linear in the number of quadrature nodes. The computation time is



Figure 2: Approximation of the solution by a piecewise constant function. To fulfil boundary conditions, the dashed cells, called ghost cells, are added to the discretisation.

negligible to the time spend on computing $P_{\rm Q}$. This is the crucial part of the numerical integration as its computation involves $N_{\rm GM}^2 N_{\rm L}^2$ evaluations of the spherical integrals, leading to $N_{\rm GM}^2 N_{\rm L}^3$ evaluations of the integrand which itself is rather expensive due to the computation of the collision velocities and the transformation from Cartesian to spherical coordinates in order to evaluate the test function ψ_i . However, the computation of the entries of $P_{\rm Q}$ can readily be parallelised. The same holds true if one computes the entries of Q_i using the three precomputed arrays $P_{\rm GM}$, $P_{\rm L}$ and $P_{\rm Q}$.

Numerical solution of the PDE system

For the solution of the PDE system in (14), we follow a finite volume approach. Each component of \mathbf{g} is approximated a function which is constant on every cell of the spatial discretisation as depicted in Figure 2. The outgoing flow at the walls is approximated by

$$\int_{\mathbb{R}^{3}_{\text{out}}} f^{(n)}\left(t, x_{\frac{1}{2}}, v\right) |(v, n)| \, \mathrm{d}v = \sum_{i=1}^{n} f_{i}\left(t, x_{\frac{1}{2}}\right) \int_{\mathbb{R}^{3}_{\text{out}}} \varphi_{i}^{T}(v) |(v, n)| \, \mathrm{d}v,$$

for the left wall,

$$\int_{\mathbb{R}^{3}_{\text{out}}} f^{(n)}\left(t, x_{N_{x}-\frac{1}{2}}, v\right) |(v, n)| \, \mathrm{d}v = \sum_{i=1}^{n} f_{i}\left(t, x_{N_{x}-\frac{1}{2}}\right) \int_{\mathbb{R}^{3}_{\text{out}}} \varphi_{i}^{T}(v) |(v, n)| \, \mathrm{d}v,$$

for the right wall. Here, N_x denotes the number of cells in (0, 1). The number of ghost cells depends on the choice of the flux reconstruction at the cell interfaces. If one uses the simple upwind scheme, adding a ghost cell at each side suffices. Reconstructing the flux with a higher order scheme like WENO [20] means that we have to add further ghost cells, depending on the used stencil. Their values are set to the solution of the linear system (15).

5 Numerical results

In this section, we present results obtained by our method for the hard spheres model. The collision kernel is given by

$$|u|\sigma\left(|u|,\frac{(u,e)}{|u|}\right) = \frac{1}{4\pi}|u|.$$

To validate our computations, we compare them with a stochastic simulation, carried out with the Direct Simulation Monte Carlo (DSMC).



Figure 3: Sketch of the one-dimensional Fourier problem. We seek the particle density function along the axis labeled by x. T_l , T_r are the temperatures of the walls, T_0 is the initial temperature of the gas.

5.1 Fourier problem

We choose diffusely reflecting walls at the left and the right boundary, cf. (5). We seek for the steady state solution. Initially, the gas is in equilibrium state. The parameters of the Maxwellians in equation (3) are constant, $\rho_0 = 1$, $V_0 = (0, 0, 0)^{\top}$ and $T_0 = 1.25$. The left wall has temperature $T_l = 1.0$, the right wall $T_r = 1.5$. The characteristic temperature of the basis and test functions T is set to 1.25. This situation is depicted in Figure 3.

We compare the results for three different Knudsen numbers, Kn = 1.0, 0.25, 0.025. The final time t_f is chosen such that on average, a particle has crossed the interval (0, 1) ten times. It can be calculated as $t_f \approx 6.32$. The number of cells N_x for both the stochastic and the deterministic method is 512. The DSMC solutions were obtained by 20 000 repetitions and 1024 particles per cell in the beginning.

The time step size τ of the deterministic method is chosen as

$$\tau = \mathrm{CFL} \frac{1}{N_x} \frac{1}{\max_{i=1,\dots,n} |\lambda_i|},\tag{17}$$

where where CFL is the Courant number and $(\lambda_i)_{i=1}^n$ are the generalised eigenvalues of D with respect to M. In our tests, CFL was set to 0.5. The fluxes are approximated by the fifth order WENO5 scheme [17]. The resulting system of ODEs is integrated by an explicit third order strong stability-preserving Runge-Kutta method [14].

The final densities and temperatures for the stochastic method and several choices of K and L, c.f. Table 1, are shown in Figure 6 for Kn = 1.0, in Figure 8 for Kn = 0.25 and in Figure 10 for Kn = 0.025, respectively. They are also plotted near the walls in Figures 7, 9 and 11 for the Knudsen numbers 1.0, 0.25 and 0.025, respectively. Plots of the final particle densities restricted to a straight line for the Knudsen numbers 1.0, 0.25 and 0.025 can be found in Figures 12a, 12b and 12c, respectively. In Figure 5, a contour plot of the particle density function for Kn = 0.25 restricted to the plane $\{v \in \mathbb{R}^3 : v_3 = 0\}$ is shown.

Table 1: Number of basis and test functions for different choices of parameters. The set $I_{K,L}$ is defined in equation (8).

\overline{K}	L	$ I_{K,L} $
3	3	64
3	5	144
3	7	256

The lower the Knudsen number, the better our method performs compared to the stochastic solution. For Knudsen numbers above 1.0, free flow is dominating over the collision interaction. This leads to almost discontinuous solutions of the Boltzmann equation, especially close to the walls, where only the inflowing particles are affected by the boundary conditions. Due to the lack of sufficient interaction for Kn = 1.0, these streams of different temperatures are not well mixed. Therefore the particle density functions have different asymptotic behaviour towards $\pm \infty$. These functions cannot be approximated well with our basis functions, c.f. Figure 12a. That's why the highest errors in Figures 6a and 6b appear near the walls.

Lowering the Knudsen number leads to a higher importance of the collisions. The collision operator smoothes the particle density function. Moreover, the higher impact of the collisions also reduces the distance in which the particles preserve their temperatures given by the boundary conditions. The different temperatures of particles emerging from the walls and the rest of the gas are mixed. This leads to more symmetric particle density functions which can be approximated well by our basis function, c.f. Figure 12c.

Therefore, our method shows a very good agreement with the stochastic simulation in case of Kn = 0.025.

5.2 Shock tube problem

As a second example, we consider a Sod-like shock tube problem [25]. The parameters of the initial Maxwellians are piecewise constant, cf. Figure 4,

$$\begin{pmatrix} \rho_l \\ V_l \\ T_l \end{pmatrix} = \begin{pmatrix} 8 \\ (0,0,0)^\top \\ 1 \end{pmatrix}, \quad \begin{pmatrix} \rho_r \\ V_r \\ T_r \end{pmatrix} = \begin{pmatrix} 1 \\ (0,0,0)^\top \\ 1 \end{pmatrix}.$$
(18)

We show the results for three different Knudsen numbers, Kn = 0.1, 0.01, 0.001 and compare them with a stochastic solution at the time

$$t_f = 0.14.$$

For the DSMC solution, we chose 512 cells with a typical number of 1024 particles per cell. For the Galerkin-Petrov method, the index set for our basis functions is given by $I_{3,3}$. For the characteristic temperature we choose T = 1. Increasing the radial or the spherical degree hardly changes the results. We use 512 cells in space. The system of ODEs is integrated with a adaptive Runge–Kutta–Fehlberg method [8] to address the stiffness which is caused by the small Knudsen numbers in this example.



Figure 4: Sketch of the initial situation of the shock tube problem. Two areas of different densities and same bulk velocities and temperatures are separated by diaphragm (dashed line), which is removed at t = 0.

The four physical quantities density, bulk velocity, temperature and pressure at the end time t_f are shown in Figures 13, 14 and 15 for the Knudsen numbers 0.1, 0.01 and 0.001, respectively.

The results of the Galerkin-Petrov method are in good agreement with those from the DSMC method for all three Knudsen numbers.

Comparing the results from the Boltzmann equation with the exact solution of the Euler equations, one can clearly see the differences between them become smaller when lowering the Knudsen number, which is conform to the Hilbert expansion. The best agreement is observed in the rarefaction wave and shock discontinuity. Due to a non-vanishing (numerical and) physical viscosity, the edges of the solutions of the Boltzmann equation are smeared out.

However near the contact discontinuity, the solutions of the Boltzmann equation and the Euler equations differ even for small Knudsen numbers. This can be seen best by studying the bump in the bulk velocity, which is located at the contact discontinuity. Generated at t = 0 by the removal of the diaphragm, it travels with the speed of the contact discontinuity, which seems to be independent of the Knudsen number.

Our numerical experiments indicate that, in contrast to the solution of the Euler equations, the bulk velocity is not constant around the contact discontinuity, but slightly lower left from the bump and larger at the right. This means that the two discontinuities are travelling with different speeds.

6 Conclusion

The Galerkin-Petrov method presented in this paper is fully conservative independent of the time stepping method. Most of the computation time is spent on the collision matrices. However, their computation can be easily parallelised. Furthermore, having computed them for a specific choice of basis and test functions, they can be reused for different problems, as they are independent of the initial and boundary conditions, the characteristic temperature or the spatial and temporal discretisation. This leads to a very fast deterministic method, as a computation of the collision operator is



Figure 5: Contour plot of the final particle density function for Kn = 0.25 and K = 3, L = 3 at x = 0.25 in the (v_1, v_2) -plane.

reduced to the evaluation of several quadratic forms. Depending on the problem, one can obtain very good results with around 100 basis functions.



Figure 6: Comparison of different sets of basis functions for Kn = 1.0. K is set to 3; L takes the values 3, 5 and 7. The stochastic curves are added for reference. The deterministic curves are obtained with $N_x = 512$ and τ chosen as in equation (17). Figure 6a shows the density at the time t_f , whereas in Figure 6b, the temperature at the time t_f is shown.



Figure 7: Comparison of different sets of basis functions for Kn = 1.0 near the walls. *K* is set to 3; *L* takes the values 3, 5 and 7. The stochastic curves are added for reference. The deterministic curves are obtained with $N_x = 512$ and τ chosen as in equation (17). Figures 7a and 7b show the density at the time t_f near the left and the right wall, respectively. Figures 7c and 7d show the temperature at the time t_f near the left and the right wall, respectively.



Figure 8: Comparison of different sets of basis functions for Kn = 0.25. K is set to 3; L takes the values 3, 5 and 7. The stochastic curves are added for reference. The deterministic curves are obtained with $N_x = 512$ and τ chosen as in equation (17). Figure 8a shows the density at the time t_f , whereas in Figure 8b, the temperature at the time t_f is shown.



Figure 9: Comparison of different sets of basis functions for Kn = 0.25 near the walls. *K* is set to 3; *L* takes the values 3, 5 and 7. The stochastic curves are added for reference. The deterministic curves are obtained with $N_x = 512$ and τ chosen as in equation (17). Figures 9a and 9b show the density at the time t_f near the left and the right wall, respectively. Figures 9c and 9d show the temperature at the time t_f near the left and the right wall, respectively.



Figure 10: Comparison of different sets of basis functions for Kn = 0.025. K is set to 3; L the values 3, 5 and 7. The stochastic curves are added for reference. The deterministic curves are obtained with $N_x = 512$ and τ chosen as in equation (17). Figure 10a shows the density at the time t_f , whereas in Figure 10b, the temperature at the time t_f is shown.



Figure 11: Comparison of different sets of basis functions for Kn = 0.025 near the walls. K is set to 3; L takes the values 3, 5 and 7. The stochastic curves are added for reference. The deterministic curves are obtained with $N_x = 512$ and τ chosen as in equation (17). Figures 11a and 11b show the density at the time t_f near the left and the right wall, respectively. Figures 11c and 11d show the temperature at the time t_f near the left and the right wall, respectively.



Figure 12: Comparison of the final particle density function for K = 3, L = 3 with the stochastic particle density function at x = 0.25 for the Knudsen numbers 1.0, 0.25 and 0.025.



Figure 13: Numerical solution of the shock tube problem at t_f obtained with DSMC and the Galerkin-Petrov method for Kn = 0.1. The exact solution of the Euler equations is shown by dashed lines.



Figure 14: Numerical solution of the shock tube problem at t_f obtained with DSMC and the Galerkin-Petrov method for Kn = 0.01. The exact solution of the Euler equations is shown by dashed lines.



Figure 15: Numerical solution of the shock tube problem at t_f obtained with DSMC and the Galerkin-Petrov method for Kn = 0.001. The exact solution of the Euler equations is shown by dashed lines.

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