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Kinetic schemes and boundary conditions for moment equations

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Abstract. A numerical scheme for moment equations of kinetic theory, due to LeTallec & Perlat, is considered for the calculation of stationary heat transfer in the Grad 13 moment system and linearized extended thermodynamics of 14 moments. It is shown that the required distance of grid points must be considerably smaller than the mean free path. Thus, the kinetic scheme is useful only in the case of large Knudsen numbers. Results of the numerical calculation for 13 and 14 moments are compared with an analytical solution for heat transfer with 13 moments. The results indicate that the boundary conditions do not guarantee conservation of energy at the walls. In order to overcome this deficiency a modification of the boundary conditions is presented and discussed.

Keywords. Kinetic theory of gases, moments, boundary conditions.

1. Introduction

Recently Le Tallec & Perlat [1] proposed a numerical scheme for the moment equations of kinetic theory. The main ingredient of this *kinetic scheme* is the use of half-space moments of the phase density. A similar method was developed by Junk [2]. Within these schemes it is easy to formulate boundary conditions for the moments which follow directly from the boundary conditions for the phase density.

While Le Tallec & Perlat use their scheme for the entropy maximum closure [3], also known as Levermore system [4], the method can be applied to any moment method of kinetic theory which provides a normal solution of the phase density. Thus, the method may be used in the Grad moment method [5] as well as in kinetic theory based extended thermodynamics [6].

In the present paper we consider the most simple application: one-dimensional stationary heat transfer in a gas at rest, described by Grad's 13 moment system [5] and by linearized extended thermodynamics with 14 moments [6]. This problem is well suited for checking the numerical scheme, since the moment equations are analytically solvable in the 13 moment case.

For processes close to equilibrium, there is no difference in the results from

Grad's and Levermore's moment systems so that our results are strongly related to the Levermore system. The Grad closure provides explicit closure relations for moments, fluxes and half-space moments. This allows analytical considerations on the scheme which are not possible in the framework of the Levermore closure, in which the closure relations must be calculated numerically.

In particular, we tackle the question of the appropriate grid size for the numerical discretisation and show that the distance of grid points must be considerably less then the mean free path - a fact that was not recognized in [1] and [2]. Therefore, we consider only the case of large Knudsen numbers for our calculations.

The results indicate that the scheme does not preserve energy at the walls. We give arguments that this behavior should change, when a larger number of moments is taken into account. Moreover, we present a simple change of the boundary conditions which gives better results.

The paper is organized as follows: The next section gives a brief introduction to moment systems of kinetic theory. Section 3 deals with moment equations for 13 and 14 moments. These are presented and analytically solved for the case of stationary heat conduction in the 13 moment case. In Section 4 we present an alternative derivation of the scheme of Le Tallec & Perlat and the application of the scheme to the heat transfer problem. This section includes also a detailed discussion of the results. The above mentioned modification of the boundary conditions will be found in Section 5. The paper closes with our conclusions.

2. Moment systems of kinetic theory

2.1. Kinetic theory

We consider one-atomic ideal gases. The objective of kinetic gas theory is the determination of the phase density $f(x_i, t, c_i)$ which gives the number density of particles in the phase space element $d\mathbf{x}d\mathbf{c}$. Here, x_i, t denote space and time variables, respectively, and c_i is the velocity of a particle of mass m. The phase density is governed by the Boltzmann equation [7] [8],

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = \mathcal{S}(f) \ , \tag{1}$$

where the collision term $\mathcal{S}(f)$ accounts for the change of the phase density due to collisions among particles.

Once the phase density is known, one may calculate its moments, for instance the mass density ϱ, the momentum density ϱv_i and the energy density $\varrho\varepsilon$, given by

$$\varrho = m \int f \, d\mathbf{c} \ , \quad \varrho v_i = m \int c_i f \, d\mathbf{c} \ , \quad \varrho\varepsilon = \frac{3}{2}\varrho \frac{k}{m} T + \frac{\varrho}{2} v^2 = \frac{m}{2} \int c^2 f \, d\mathbf{c} \ .$$

In these definitions, k is Boltzmann's constant, v_i denotes the barycentric velocity of the gas and T denotes the temperature, which is *defined* here.

For the calculation of boundary value problems, one needs boundary conditions for the phase density f. The most simple model for these is due to Maxwell [7] [8]. He assumes that the fraction $(1-\theta)$ of the emerging particles has been reflected elastically at the wall. The remaining fraction θ is thermalized and leaves the wall in a Maxwellian distribution. θ is called accommodation coefficient. In this paper, we consider only the simplest case: full accommodation with $\theta = 1$. We choose the normal vector n_i of the wall so that it points inside the gas such that we have $n_k\left(c_k - v_k^W\right) \leq 0$ for the emerging particles and $n_k\left(c_k - v_k^W\right) \geq 0$ for the particles that leave the wall; v_k^W denotes the velocity of the wall.

Let f_N denote the phase density inside the gas. Then, we may write the phase density at the wall $\hat{f}$ according to Maxwells boundary conditions as

$$\hat{f} = \begin{cases} f_W, & n_k\left(c_k - v_k^W\right) \geq 0 \\ f_N, & n_k\left(c_k - v_k^W\right) \leq 0\ . \end{cases} \tag{2}$$

f_W is the Maxwellian of the thermalized particles,

$$f_W = f_M\left(\varrho_W, T_W, v_i^W\right) = \frac{\varrho_W}{m}\sqrt{\frac{m}{2\pi k T_W}}^3 e^{-\frac{m}{2kT_W}\left(c_k - v_k^W\right)^2}\ ,$$

where T_W denotes the temperature of the wall and ϱ_W is the density of the thermalized particles. ϱ_W has be to determined in order to ensure that the wall does not accumulate particles, a condition which may be written as

$$m\int_{n_k\left(c_k - v_k^W\right)\geq 0} \hat{f}\left(c_k - v_k^W\right) n_k d\mathbf{c} = -m\int_{n_k\left(c_k - v_k^W\right)\leq 0} \hat{f}\left(c_k - v_k^W\right) n_k d\mathbf{c}\ . \tag{3}$$

In the remainder of this paper we consider a gas at rest only, where the mean value of c_i vanishes, so that $\int f_N c_k n_k d\mathbf{c} = 0$. Of course, in this case also the wall is at rest, $v_k^W = 0$ and the condition (3) simplifies to

$$m\int_{n_k c_k \geq 0} f_W c_k n_k d\mathbf{c} = m\int_{n_k c_k \geq 0} f_N c_k n_k d\mathbf{c}\ . \tag{4}$$

2.2. Moments and moment equations

In moment methods one assumes that the state of the gas is satisfactorily described by a set of moments,

$$u_A = \int \psi_A\left(c_k\right) f\, d\mathbf{c}\ ,$$

where $\psi_A\left(c_k\right)$ is a vector of polynomials of the microscopic velocity. Which moments one has to take into account depends on the process under consideration.

In Grad's 13 moment theory one has $\psi_A = m\left\{1, c_i, \frac{1}{2}c^2, c_{\langle i}c_{j\rangle}, \frac{1}{2}c^2 c_i\right\}$, i.e. the moments $\varrho, \varrho v_i, \varrho\varepsilon$ defined above plus the deviator of the momentum flux[1] and the energy flux, extended thermodynamics of 14 fields adds the full trace of the forth moment, $\psi_\Delta = mc^4$.

Multiplication of the Boltzmann equation (1) by ψ_A and subsequent integration over velocity space yields the moment equations

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} = P_A \quad , \quad \text{with} \quad F_{Ak} = \int \psi_A c_k f \, d\mathbf{c} \; , \; P_A = \int \psi_A \mathcal{S}(f) \, d\mathbf{c} \tag{5}$$

where we have introduced the fluxes of the moments F_{Ak} and the productions P_A. Note, that the productions of mass, momentum and energy vanish.

The equations $(5)_1$ do not form a closed system of partial differential equations for the moments since they contain the fluxes and the productions which are not a priori related to the moments. Here, a closure assumption is required, and it is obvious that a phase density of the form

$$f(x_k, t, c_k) = f(u_A(x_k, t), c_k) \tag{6}$$

serves for this purpose. A solution of this type is called "normal solution", and there are several methods to obtain it. Grad found his normal solution by an expansion around local equilibrium where the phase density is a Maxwellian. In the last years the method of maximizing the entropy [3] became more and more popular [4]. This method is equivalent to extended thermodynamics and we refer the interested reader to the textbook of Müller & Ruggeri for a detailed discussion of these topics [6].

One of the shortcomings of the moment theory is that it is not clear which boundary conditions one has to choose for moments without physical meaning, a problem which was addressed in [9]. The numerical scheme of Le Tallec & Perlat, discussed in Section 4 below, allows the use of boundary condition (2) for the phase density in its implementation. Thus, it should be possible to solve problems of kinetic theory with an arbitrary number of moments.

3. Extended thermodynamics with 13 and 14 moments

3.1. Moment equations

Extended thermodynamics of 14 variables chooses $\psi_A = m\big\{1, c_i, \frac{1}{2}c^2, c_{\langle i}c_{j\rangle}, \frac{1}{2}c^2 c_i, c^4\big\}$ or, equivalently, $\psi_A = m\left\{1, C_i, \frac{1}{2}C^2, C_{\langle i}C_{j\rangle}, \frac{1}{2}C^2 C_i, C^4\right\}$ where $C_i = c_i - v_i$ is the peculiar velocity. The second choice corresponds to the moments of the

[1] Brackets denote the traceless part of a symmetric tensor.

peculiar velocity

$$\varrho = m\int f\,d\mathbf{c} \qquad 0 = m\int C_i f\,d\mathbf{c} \qquad \frac{3}{2}\varrho\frac{k}{m}T = \frac{m}{2}\int C^2 f\,d\mathbf{c}$$
$$p_{ij} = m\int C_iC_j f\,d\mathbf{c} \quad q_i = \frac{m}{2}\int C^2C_i f\,d\mathbf{c} \quad \Delta = m\int C^4\left(f - f_M\right)\,d\mathbf{c}\;.$$

where we have introduced the pressure tensor p_{ij}, the heat flux q_i and the non-equilibrium part of the full trace of the forth moment Δ. f_M denotes the local Maxwellian, viz.

$$f_M = \frac{\varrho}{m}\sqrt{\frac{m}{2\pi kT}}^3\, e^{-\frac{m}{2kT}C^2}\;.$$

The trace of the pressure tensor defines the pressure

$$p = \frac{1}{3}p_{ii} = \varrho\frac{k}{m}T\;.$$

The corresponding normal solution for the phase density follows either from Grad's method [5] or from entropy maximization [3], [4], [6] and subsequent linearization around local thermal equilibrium as

$$f_{14} = f_M\left(1 + \frac{m^2}{8\varrho k^2T^2}\Delta - \frac{m^3}{12\varrho k^3T^3}\Delta C^2 + \frac{m^4}{120\varrho k^4T^4}\Delta C^4 - \right. \tag{7}$$
$$\left. + \frac{m^2}{2\varrho k^2T^2}p_{\langle jk\rangle}C_jC_k - \frac{m^2}{\varrho k^2T^2}q_kC_k\left(1 - \frac{1}{5}\frac{m}{kT}C^2\right)\right)\;.$$

The moment equations read

$$\frac{\partial\varrho}{\partial t} + \frac{\partial\varrho v_k}{\partial x_k} = 0\;, \tag{8}$$

$$\frac{\partial v_i}{\partial t} + v_k\frac{\partial v_i}{\partial x_k} + \frac{1}{\varrho}\frac{\partial p_{ik}}{\partial x_k} = 0\;, \tag{9}$$

$$\frac{3}{2}\varrho\frac{k}{m}\left(\frac{\partial T}{\partial t} + v_k\frac{\partial T}{\partial x_k}\right) + \frac{\partial q_k}{\partial x_k} + p_{kl}\frac{\partial v_k}{\partial x_l} = 0\;, \tag{10}$$

$$\frac{\partial p_{\langle ij\rangle}}{\partial t} + \frac{\partial p_{\langle ij\rangle}v_k}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2p_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} = -\alpha\varrho p_{\langle ij\rangle}\;, \tag{11}$$

$$\frac{\partial q_i}{\partial t} + v_k\frac{\partial q_i}{\partial x_k} + \frac{5}{2}p\frac{k}{m}\frac{\partial T}{\partial x_i} + \frac{kT}{m}\frac{\partial p_{\langle ik\rangle}}{\partial x_k} + \frac{1}{6}\frac{\partial\Delta}{\partial x_i}$$
$$+ \frac{7}{2}p_{\langle ik\rangle}\frac{k}{m}\frac{\partial T}{\partial x_k} - \frac{p_{\langle il\rangle}}{\varrho}\frac{\partial p_{lk}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i} = -\frac{2}{3}\alpha\varrho q_i\;, \tag{12}$$

$$\frac{\partial \Delta}{\partial t} + v_k \frac{\partial \Delta}{\partial x_k} + 8\frac{kT}{m}\frac{\partial q_k}{\partial x_k} + 8\frac{kT}{m} p_{\langle kl\rangle}\frac{\partial v_k}{\partial x_l} - 8\frac{q_k}{\varrho}\frac{\partial p_{\langle kl\rangle}}{\partial x_l} + 28\frac{k}{m} q_k \frac{\partial T}{\partial x_k} + \frac{7}{3}\Delta\frac{\partial v_k}{\partial x_k} = -\frac{2}{3}\alpha\varrho\Delta \,, \tag{13}$$

where α is a constant that follows by calculation of the collision production for Maxwell molecules. $\varrho\alpha$ is the collision frequency and the corresponding mean free path is given by $l = \sqrt{\frac{k}{m}T}/\varrho\alpha$. The first three equations are the equations of balance for the conserved quantities mass, momentum and energy.

The set of equations (8–13) reduces to Grad's 13 moment equations, if one sets $\Delta = 0$ and omits the last equation.

Note, that the equations (8–13) are not of the form $(5)_1$, due to the choice of moments of the peculiar velocity. This is of no concern here, because we are interested in problems with vanishing velocity only.

3.2. Stationary heat transfer with 13 and 14 moments

Let us consider the one-dimensional stationary heat transfer problem between two rigid walls at rest at $x = 0$ and $x = L$ with the temperatures

$$T(0) = T_0, \;\; T(L) = T_L \,.$$

Due to the one-dimensionality we have

$$v_i = [v, 0, 0] \,, \;\; p_{\langle ij\rangle} = \begin{bmatrix} p_{\langle 11\rangle} & 0 & 0 \\ 0 & -\frac{1}{2}p_{\langle 11\rangle} & 0 \\ 0 & 0 & -\frac{1}{2}p_{\langle 11\rangle} \end{bmatrix}, \;\; q_i = [q, 0, 0] \,.$$

In the case under consideration, all time derivatives and the velocity vanish. Thus, the mass balance (8) is identically fulfilled and the energy balance (10) reduces to $\frac{\partial q}{\partial x} = 0$. Equation (11) now reads $\frac{8}{15}\frac{\partial q}{\partial x} = -\alpha\varrho p_{\langle 11\rangle}$ and accordingly $p_{\langle ij\rangle}$ vanishes. The balance of momentum (9) now gives the constancy of the pressure, $p = const$, and this allows to introduce dimensionless quantities by

$$\hat{x} = \frac{x}{L} \,, \qquad \hat{T} = \frac{T}{T_0} \,, \qquad \hat{\Delta} = \frac{\Delta}{p\frac{k}{m}T_0} \,,$$

$$\hat{\varrho} = \frac{\varrho\frac{k}{m}T_0}{p} = \frac{1}{\hat{T}} \,, \qquad \hat{q} = \frac{q}{p\sqrt{\frac{k}{m}T_0}} \,, \qquad K_n = \frac{\sqrt{\frac{k}{m}T_0}^{\,3}}{\alpha L p} \,.$$

K_n, the ratio between the mean free path at T_0 and L, is the Knudsen number for the heat transfer problem. There remains the following simple system of ordinary non-linear differential equations

$$\frac{d\frac{5}{2}\hat{T} + \frac{\hat{\Delta}}{6}}{d\hat{x}} = -\frac{2}{3K_n}\frac{\hat{q}}{\hat{T}} \;\; , \;\; \frac{d28\hat{q}\hat{T}}{d\hat{x}} = -\frac{2}{3K_n}\frac{\hat{\Delta}}{\hat{T}} \;\text{ and }\; \hat{q} = const. \tag{14}$$

with the boundary conditions

$$\hat{T}\left(0\right)=1,\;\;\hat{T}\left(L\right)=\hat{T}_{L}\;.$$

Note that the heat flux $\hat{q}=const.$ enters these equations as a parameter while the constant pressure p determines the Knudsen number. The determination of $\hat{q}$ requires an additional boundary condition and in [9] this additional conditions was found my means of the statement that *the maximum of the local entropy production becomes minimal in stationary processes*. In the present context this statement is not needed since the numerical scheme implies boundary conditions for all moments.

We consider only the analytical solution for the 13 moment case - $\Delta=0$ - where (14) reduces to the law of Fourier

$$\hat{q}_{F}=-\frac{15}{4}K_{n}\hat{T}\frac{d\hat{T}}{d\hat{x}}=const$$

with the solution

$$\hat{T}=\sqrt{1+\left(\hat{T}_{L}^{2}-1\right)\hat{x}}\;. \tag{15}$$

In the case of small Knudsen numbers one has to consider the jump of the temperature at a wall which depends on the details of the wall-particle interaction. We consider the boundary condition (2) for gas and boundary at rest. The normal part of the energy flux $\frac{m}{2}\int c^{2}c_{i}fd\mathbf{c}$ has to be continuous at the wall, a condition which we may write as $\frac{m}{2}\int\hat{f}c^{2}c_{k}n_{k}d\mathbf{c}=\frac{m}{2}\int f_{N}c^{2}c_{k}n_{k}d\mathbf{c}$ or, with (2),

$$\frac{m}{2}\int_{n_{k}c_{k}\geq0}f_{W}c^{2}c_{k}n_{k}d\mathbf{c}=\frac{m}{2}\int_{n_{k}c_{k}\geq0}f_{N}c^{2}c_{k}d\mathbf{c}\;. \tag{16}$$

Now we consider Grad's 13 moments phase density with vanishing shear stresses, as it is appropriate in stationary heat transfer, viz.

$$f_{13}=\frac{\varrho}{m}\sqrt{\frac{m}{2\pi kT}}^{3}\;e^{-\frac{m}{2kT}c^{2}}\left(1-\frac{m^{2}}{\varrho k^{2}T^{2}}q_{k}C_{k}\left(1-\frac{1}{5}\frac{m}{kT}C^{2}\right)\right)\;,$$

where T is the temperature of the gas at the wall and ϱ is its density. We obtain from the conditions for conservation of mass and heat flux (4), (16)

$$\begin{aligned}\frac{1}{2}\varrho_{W}\sqrt{\frac{2}{\pi}}\sqrt{\frac{kT_{W}}{m}}&=\frac{1}{2}\varrho\sqrt{\frac{2}{\pi}}\sqrt{\frac{kT}{m}}\;,\\ \varrho_{W}\sqrt{\frac{2}{\pi}}\sqrt{\frac{kT_{W}}{m}}^{3}&=\varrho\sqrt{\frac{2}{\pi}}\sqrt{\frac{kT}{m}}^{3}+\frac{1}{2}q_{k}n_{k}\;.\end{aligned}$$

Elimination of the density ϱ_W yields for the temperature jump between wall and gas

$$\frac{T_W - T}{T} = \frac{1}{2}\sqrt{\frac{\pi}{2}}\frac{q_k n_k}{p\sqrt{\frac{kT}{m}}} \,.$$

We denote the dimensionless temperatures of the gas at the walls by ϑ_0 and ϑ_L and find for the jumps at $\hat{x} = 0, \hat{x} = 1$

$$\frac{1 - \vartheta_0}{\vartheta_0} = \frac{1}{2}\sqrt{\frac{\pi}{2}}\frac{\hat{q}}{\sqrt{\vartheta_0}} \quad , \quad \frac{\hat{T}_L - \vartheta_L}{\vartheta_L} = -\frac{1}{2}\sqrt{\frac{\pi}{2}}\frac{\hat{q}}{\sqrt{\vartheta_L}} \,. \tag{17}$$

The corresponding temperature function and heat flux are

$$\hat{T} = \sqrt{\vartheta_0^2 + \left(\vartheta_L^2 - \vartheta_0^2\right)\hat{x}} \quad , \quad \hat{q} = -\frac{15}{8}K_n\left(\vartheta_L^2 - \vartheta_0^2\right) \,, \tag{18}$$

where ϑ_0 and ϑ_L follow from (17) with $(18)_2$. In the remainder of the paper we shall calculate the stationary heat transfer problem with numerical methods and we shall use Equation (18) as a benchmark.

For the application of the kinetic scheme we shall follow Le Tallec & Perlat and solve the stationary problem by time stepping. Thus, we need a set of instationary equations. We reduce the equations (8)–(13) due to our knowledge of the stationary results. First of all, the pressure deviator vanishes in one-dimensional stationary heat conduction and we may ignore $p_{\langle ik\rangle}$ and its balance equation (11) from the beginning. Moreover the velocity will vanish, $v = 0$, while the pressure will be constant, $p = \varrho\frac{k}{m}T = const.$ If we impose these conditions from the beginning, we have to ignore the balance equations of mass and momentum. The remaining equations read

$$\begin{aligned} \frac{\partial \frac{3}{2}p\ln T}{\partial t} + \frac{\partial q}{\partial x} &= 0 \,, \\ \frac{\partial q}{\partial t} + \frac{\partial \frac{5}{2}p\frac{k}{m}T + \frac{\Delta}{6}}{\partial x} &= -\frac{2}{3}\alpha\frac{p}{\frac{k}{m}T}q \,, \\ \frac{\partial \Delta + 30\frac{k}{m}pT}{\partial t} + \frac{\partial 28\frac{k}{m}qT}{\partial x} &= -\frac{2}{3}\alpha\frac{p}{\frac{k}{m}T}\Delta \,, \end{aligned} \tag{19}$$

where $(19)_1$ was used to rewrite $(19)_3$ in a form appropriate for the numerical scheme.

4. Kinetic scheme of Le Tallec & Perlat

4.1. Derivation

We present our own derivation of the numerical scheme. While Le Tallec & Perlat start from the Boltzmann equation, our argument is based on the moment equations plus the definitions of moments, fluxes and productions, and the knowledge of the normal solution. We consider one-dimensional processes so that the moment equations (5) read

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_A}{\partial x} = P_A \tag{20}$$

with $F_A = F_{A1}$. For the discretisation in space we consider an interval $x \in (0, L)$ divided in n parts of length $\Delta x = L/n$, with center points $x^i, i = 1, \ldots, n$. Integration of (20) along Δx gives

$$\frac{\partial u_A^i}{\partial t} + \frac{1}{\Delta x} \int_{x^i - \frac{\Delta x}{2}}^{x^i + \frac{\Delta x}{2}} \frac{\partial F_A}{\partial x} dx = P_A^i \tag{21}$$

where

$$u_A^i = \frac{1}{\Delta x} \int_{x^i - \frac{\Delta x}{2}}^{x^i + \frac{\Delta x}{2}} u_A dx \quad \text{and} \qquad P_A^i = \frac{1}{\Delta x} \int_{x^i - \frac{\Delta x}{2}}^{x^i + \frac{\Delta x}{2}} P_A dx \; .$$

Thus, the interval around x^i is associated with one value u_A^i and the normal solution for the phase density in Δx is determined by this value, $f^i = f\left(u_A^i, c_k\right)$. We consider the integral in (21) which yields

$$\int_{x^i - \frac{\Delta x}{2}}^{x^i + \frac{\Delta x}{2}} \frac{\partial F_A}{\partial x} dx = F_A^{i+\frac{1}{2}} - F_A^{i-\frac{1}{2}} \; ,$$

where $F_A^{i\pm\frac{1}{2}} = F_A\left(x^i \pm \frac{\Delta x}{2}\right)$ denote the fluxes at the borders of the interval. We consider the definition $(5)_2$ and decompose the flux into its parts due to particles travelling in positive or negative x-direction, respectively,

$$F_A^{i+\frac{1}{2}} = \int \psi_A c_x f^{i+\frac{1}{2}} \, d\mathbf{c} = \int_{c_x \geq 0} \psi_A c_x f^{i+\frac{1}{2}} \, d\mathbf{c} + \int_{c_x \leq 0} \psi_A c_x f^{i+\frac{1}{2}} \, d\mathbf{c} \; . \tag{22}$$

Here, the first integral describes the flux of ψ_A from x^i towards x^{i+1} and the second integral gives the flux from x^{i+1} into x^i.

The key step of the method is the assumption that the flux out of x^i is determined by the state in cell i, while the flux into the cell i is determined by the state in the neighboring cell, $i + 1$. This assumption may be written as

$$\int_{c_x \geq 0} \psi_A c_x f^{i+\frac{1}{2}} \, d\mathbf{c} \simeq A_A^i \quad , \quad \int_{c_x \leq 0} \psi_A c_x f^{i+\frac{1}{2}} \, d\mathbf{c} \simeq B_A^{i+1}$$

where the half-fluxes in positive and negative direction, A_A^i and B_A^i, are defined as

$$A_A^i = \int_{c_x \geq 0} \psi_A c_x f^i \, d\mathbf{c} \quad , \quad B_A^i = \int_{c_x \leq 0} \psi_A c_x f^i \, d\mathbf{c} \; . \tag{23}$$

Now, (22) reads

$$F_A^{i+\frac{1}{2}} = A_A^i + B_A^{i+1} \tag{24}$$

and we obtain the space discretized moment equations as

$$\frac{\partial u_A^i}{\partial t} + \frac{1}{\Delta x}\left(A_A^i + B_A^{i+1} - A_A^{i-1} - B_A^i\right) = P_A^i \quad , \; i = 1, \ldots, n \; . \tag{25}$$

In order to show that the above discretisation is of first order in space we expand

$$u_A^i = u_A \; , \quad A_A^i = A_A \; , \quad A_A^{i\pm1} = A_A \pm \frac{\partial A_A}{\partial x}\Delta x + \frac{\partial^2 A_A}{\partial x^2}\frac{(\Delta x)^2}{2} \quad , \quad \text{etc.} \tag{26}$$

and obtain with $A_A + B_A = F_A$ from (25)

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_A}{\partial x} - \frac{\Delta x}{2}\frac{\partial^2 (A_A - B_A)}{\partial x^2} = P_A + \mathcal{O}\left((\Delta x)^2\right) \; . \tag{27}$$

The original equations are recovered, if Δx is small and we shall discuss the appropriate value of Δx below.

Following Le Tallec & Perlat, we consider discrete times $t^j = j\Delta t$ with time step Δt and use a semi-implicit discretisation of (25), viz.

$$u_A^{i,j+1} - \Delta t P_A^{i,j+1} = u_A^{i,j} - \frac{\Delta t}{\Delta x}\left(A_A^{i,j} + B_A^{i+1,j} - A_A^{i-1,j} - B_A^{i,j}\right) \; , \tag{28}$$

$i = 1, \ldots, n \; ; \;\; j = 0, 1, \ldots$ where $u_A^{i,j} = u_A\left(x^i, j\Delta t\right)$ etc.

This is equation (32) of [1]. The solution of the numerical scheme (28) for the variables $u_A^i, \; i = 1, \ldots, n$ requires

i.) Constitutive equations for the half fluxes and the productions

$$A_A^i = A_A^i\left(u_B^i\right), \;\; B_A^i = B_A^i\left(u_B^i\right), \;\; P_A^i = P_A^i\left(u_B^i\right) \; ;$$

these follow from the definitions (23), (5) and the normal solution $f^i = f\left(u_A^i, c_k\right)$.

ii.) Initial values for the moments, $u_A^{i,0}$

iii.) Boundary conditions, i.e. the half fluxes A_A^0 and B_A^{n+1} which follow from the boundary conditions for the phase density. According to the boundary condition (2), these are the half fluxes of the Maxwellians f_W.

4.2. Kinetic scheme for stationary heat transfer

We consider the scheme for the equations (19). Indeed, in the space derivatives of these equations we find fluxes of the moments[2], viz.

$$
\begin{aligned}
q = F_\varepsilon &= \frac{m}{2}\int c^2 c_x f_{14}\, d\mathbf{c}\,, \\
\frac{5}{2}p\frac{k}{m}T + \frac{\Delta}{6} = F_q &= \frac{m}{2}\int c^2 c_x c_x f_{14}\, d\mathbf{c}\,, \\
28\frac{k}{m}qT = F_\Delta &= \frac{m}{2}\int c^4 c_x f_{14}\, d\mathbf{c}\,,
\end{aligned}
$$

so that we can apply the numerical scheme (28) to the set of equations (19). We introduce the abbreviations

$$
\delta = \sqrt{\frac{k}{m}T_0}\frac{\Delta t}{\Delta x} \quad \text{and} \quad n = \frac{L}{\Delta x}
$$

and use the same dimensionless quantities as in Section 3 to obtain the following scheme

$$
\begin{aligned}
T^{i,j+1} &= T^{i,j}\exp\left\{-\frac{2}{3}\delta\left(A_\varepsilon^{i,j} + B_\varepsilon^{i+1,j} - A_\varepsilon^{i-1,j} - B_\varepsilon^{i,j}\right)\right\}\,, \\
q^{i,j+1}\left(1+\frac{2}{3}\frac{\delta}{nK_n}\frac{1}{T^{i,j+1}}\right) &= q^{i,j} - \delta\left(A_q^{i,j} + B_q^{i+1,j} - A_q^{i-1,j} - B_q^{i,j}\right)\,, \qquad (29) \\
\Delta^{i,j+1}\left(1+\frac{2}{3}\frac{\delta}{nK_n}\frac{1}{T^{i,j+1}}\right) &= \Delta^{i,j} - 30\left(T^{i,j+1} - T^{i,j}\right) - \\
&\quad - \delta\left(A_\Delta^{i,j} + B_\Delta^{i+1,j} - A_\Delta^{i-1,j} - B_\Delta^{i,j}\right)\,,
\end{aligned}
$$

where i runs from 1 to n. The quantities A and B are dimensionless half fluxes of the phase density (7), given by

$$
\begin{aligned}
A_\varepsilon &= \frac{1}{2}q + \sqrt{\frac{2}{\pi}}\sqrt{T}\left(1+\frac{1}{40}\frac{\Delta}{T}\right) \\
B_\varepsilon &= \frac{1}{2}q - \sqrt{\frac{2}{\pi}}\sqrt{T}\left(1+\frac{1}{40}\frac{\Delta}{T}\right) \\
A_q &= \frac{5}{4}T\left(1+\frac{1}{15}\frac{\Delta}{T}\right) + \frac{9}{5}\sqrt{\frac{2}{\pi}}\sqrt{T}q
\end{aligned}
$$

[2] Note, that in a gas at rest $C_i = c_i$ holds.

$$B_q = \frac{5}{4}T\left(1+\frac{1}{15}\frac{\Delta}{T}\right) - \frac{9}{5}\sqrt{\frac{2}{\pi}}\sqrt{T}q$$
$$A_\Delta = 14Tq + 12\sqrt{\frac{2}{\pi}}\sqrt{T}^3 + \frac{3}{2}\sqrt{\frac{2}{\pi}}\sqrt{T}\Delta$$
$$B_\Delta = 14Tq - 12\sqrt{\frac{2}{\pi}}\sqrt{T}^3 - \frac{3}{2}\sqrt{\frac{2}{\pi}}\sqrt{T}\Delta$$

It remains to determine the boundary conditions, i.e. the values of A_A^0 and B_A^{n+1}. We denote the Maxwellians of the particles that leave the walls by f_0, f_L, and have

$$A_A^0 = \int_{c_x\geq 0} \psi_A c_k f_0 \, d\mathbf{c} \quad \text{and} \quad B_A^{n+1} = \int_{c_x\leq 0} \psi_A c_k f_L \, d\mathbf{c} \ ,$$

with

$$f_0 = \frac{\varrho_0}{m}\sqrt{\frac{m}{2\pi k T_0}}^3 e^{-\frac{m}{2kT_0}c^2} \ , \quad f_L = \frac{\varrho_L}{m}\sqrt{\frac{m}{2\pi k T_L}}^3 e^{-\frac{m}{2kT_L}c^2} \ .$$

T_0 and T_L are the temperatures of the walls and the densities ϱ_0, ϱ_L follow from the requirement that the walls do not accumulate particles (4),

$$\int_{c_x\geq 0} c_x f_0 \, d\mathbf{c} = -\int_{c_x\leq 0} c_x f^1 d\mathbf{c} \ , \quad \int_{c_x\leq 0} c_x f_L \, d\mathbf{c} = -\int_{c_x\geq 0} c_x f^{n+1} \, d\mathbf{c} \ .$$

After some straightforward calculations we find

$$A_\varepsilon^0 = \sqrt{\frac{2}{\pi}}\sqrt{\frac{1}{T^1}}\left(1-\frac{1}{120}\frac{\Delta^1}{T^1}\right)$$
$$B_\varepsilon^{n+1} = -\sqrt{\frac{2}{\pi}}\sqrt{\frac{T_{W_L}^2}{T^n}}\left(1-\frac{1}{120}\frac{\Delta^n}{T^n}\right)$$
$$A_q^0 = \frac{5}{4}\sqrt{\frac{1}{T^1}}\left(1-\frac{1}{120}\frac{\Delta^1}{T^1}\right)$$
$$B_q^{n+1} = \frac{5}{4}\sqrt{\frac{T_{W_L}^3}{T^n}}\left(1-\frac{1}{120}\frac{\Delta^n}{T^n}\right)$$
$$A_\Delta^0 = 12\sqrt{\frac{2}{\pi}}\sqrt{\frac{1}{T^1}}\left(1-\frac{1}{120}\frac{\Delta^1}{T^1}\right)$$
$$B_\Delta^{n+1} = -12\sqrt{\frac{2}{\pi}}\sqrt{\frac{T_{W_L}^4}{T^n}}\left(1-\frac{1}{120}\frac{\Delta^n}{T^n}\right)$$

With these formulae, our numerical scheme for the calculation of one-dimensional stationary heat transfer is complete. The above equations give the scheme for extended thermodynamics with 14 moments. The scheme for Grad's theory of 13 moments is obtained by setting $\Delta = 0$ and omission of equation $(29)_3$.

4.3. The appropriate grid-size

Now we ask for the number of grid points n which is required in order to have a good agreement between the discretized equations and the original equations. We consider the stationary case of (29) and expand the half fluxes up to second order in Δx, see (26), (27). We obtain with $\Delta x = \frac{1}{n}$ in dimensionless formulation

$$\begin{aligned} \frac{dq}{dx} - \sqrt{\frac{2}{\pi}} \frac{d^2\sqrt{T}\left(1+\frac{1}{40}\frac{\Delta}{T}\right)}{dx^2}\frac{1}{n} &= 0 \,, \\ \frac{d\left(\frac{5}{2}T+\frac{1}{6}\Delta\right)}{dx} - \frac{9}{5}\sqrt{\frac{2}{\pi}}\frac{d^2\sqrt{T}q}{dx^2}\frac{1}{n} &= -\frac{2}{3}\frac{1}{K_n}\frac{q}{T} \,, \\ \frac{d28Tq}{dx} - 12\sqrt{\frac{2}{\pi}}\frac{d^2\left(\sqrt{T}^3+\frac{1}{8}\sqrt{T}\Delta\right)}{dx^2}\frac{1}{n} &= -\frac{2}{3}\frac{1}{K_n}\frac{\Delta}{T} \,. \end{aligned} \tag{30}$$

For $n \to \infty$ the original equations (14) are recovered. But which finite value of n is large enough to guarantee that the additional terms may be neglected? We consider the energy balance $(30)_1$ where we insert the heat flux according to $(30)_2$,

$$\begin{aligned} &\frac{d}{dx}\left(T\frac{d\left(\frac{15}{4}T+\frac{1}{4}\Delta\right)}{dx}\right) \\ &\quad + \sqrt{\frac{2}{\pi}}\left[-\frac{27}{10}\frac{d}{dx}\left(T\frac{d^2\sqrt{T}q}{dx^2}\right)\frac{1}{n} + \frac{d^2\sqrt{T}\left(1+\frac{1}{40}\frac{\Delta}{T}\right)}{dx^2}\frac{1}{K_n n}\right] = 0 \,. \end{aligned}$$

In this equation both terms in the square brackets must vanish. Since q is of order $\mathcal{O}(K_n)$, the first term is of order $\mathcal{O}\left(\frac{K_n}{n}\right)$ and will vanish as $\frac{1}{n}$ for Knudsen numbers smaller than 1. The second term, however, is of order $\mathcal{O}\left(\frac{1}{K_n n}\right)$ and will vanish only, if $n \gg \frac{1}{K_n}$ .The Knudsen number is the ratio of the mean free path l and the macroscopic length L, $K_n = l/L$, and n defines the grid size, $\Delta x = L/n$ so that the above condition indicates that the grid size must be considerably smaller then the mean free path,

$$\Delta x \ll l \,. \tag{31}$$

This condition is a restriction to the applicability of the kinetic scheme. Only for problems involving distances of few mean free paths, one may consider the kinetic scheme as an appropriate tool for the numerical solution of moment equations. Since one will need extended moment methods mostly in case of large Knudsen numbers, this restriction may not be severe. Note, however, that the condition (31) is violated in the applications to Couette flow in [1].

In order to avoid misunderstanding, we state that the restriction (31) is characteristic for the kinetic schemes but not for the system (19). Indeed, if one considers

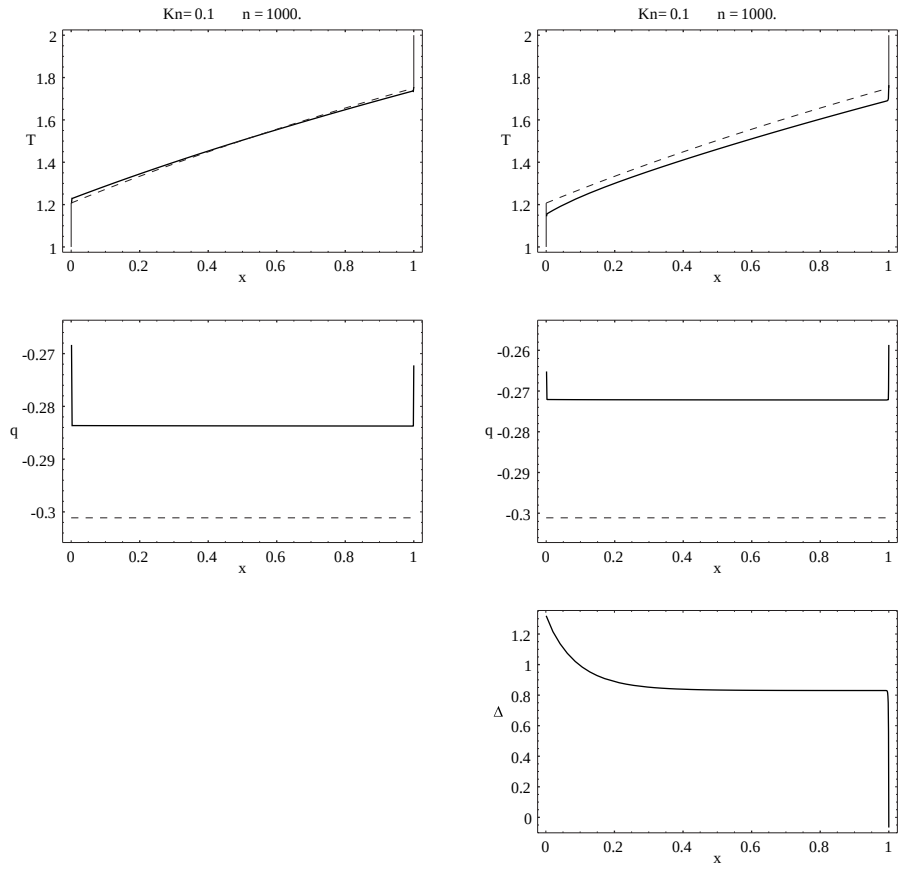

Figure 1.
Stationary heat transfer with 13 (left column) and 14 (right column) moments, $K_n = 0.1$: temperature T, heat flux q and fourth moment Δ according to the numerical scheme (28) (continuous) in comparison with exact solution of 13 moment case (18) (dashed).

the stationary case of (19) and performs a second order discretisation in space, i.e. $\frac{\partial q}{\partial x} = (q^{i+1} - q^{i-1})/(2\Delta x)$ etc., one finds that $K_n/n^2 \ll 1$ has to hold. Clearly, this restriction is less severe then (31).

4.4. Results and discussion

We consider a large Knudsen number, $K_n = 0.1$ with $n = 1000$ grid points and $\delta = 0.2$. As initial conditions we choose $q = 0$, $\Delta = 0$ and random temperatures between the two wall temperatures which were chosen as $T_0 = 1$ and $T_L = 2$, respectively.

Figure 1 shows the stationary results for 13 and 14 moments (50000 iterations)

in comparison to the analytical result (18). In the 13 moment case (left column of Fig.1) we find considerable agreement between the results for the temperature. The heat flux, however, is not constant at the boundaries, but jumps. The values of the temperature jumps do not agree between numerical and analytical solution and also the constant value of the heat flux differs by 5% from the analytical solution.

In the present problem the heat flux should be constant due to the conservation of energy. The jumps correspond to an energy supply at the boundaries. Also in the case of 14 moments, the results for the heat flux imply jumps at the walls, see right column of Fig.1.

In [1], the authors find a similar jump for the shear stress in the case of Couette flow which contradicts the conservation of momentum. The authors suggest that the jumps become smaller with an increasing number of grid points and will eventually vanish for $n \to \infty$. This is in contradiction to our findings for the heat flux which indicate that the jumps change only slightly with the number of grid points. E.g. for the jump at the left wall, we find in the 14 moments case $q^1 - q^2 = \{0.007729, 0.006971, 0.006931, 0.006904\}$ with $n = \{100, 1000, 2000, 5000\}$.

The explanation for this difference is found in the equations of the scheme for the cells at the walls (stationary case): the number of grid points n appears only in the combination $\frac{1}{nK_n}$. It follows that the grid size has no influence in case that condition (31) is fulfilled. As we said before, (31) is violated for the calculations in [1] and this is the reason for the changes of the jumps with the grid size.

It is interesting that the jumps are smaller in the 14 moment case. This might give some hope that a larger number of moments will give better results. Indeed, it should be kept in mind that one will need many moments - not only 13 or 14 - in processes with large Knudsen numbers. In order to understand this better, one has to consider that the moment method assumes a normal solution (6) in all space points. According to the boundary condition (2), the phase density at the wall is a discontinuous function of the microscopic velocity. Of course, one might think of a normal solution, e.g. a series in Hermite polynomials, which pictures this discontinuity sufficiently. Most probably, this will require a large number of expansion coefficients, i.e. moments. Once one considers a sufficient number of moments to resolve the discontinuity in velocity space, one may expect to have conservation of energy and momentum at the walls. From our results for the cases with 13 and 14 moments we conclude that these numbers are not sufficient, although, as pointed out above, the jump in the heat flux is smaller for the 14 moment case.

Obviously, one will find remainders of the Maxwellian, and therefore a discontinuous phase density, within a distance of some mean free path of the wall. Thus, in any case, one will need a large number of moments, at least in the vicinity of the wall. We like to emphasize, that this is a question of the number of moments, *and not* of the form of the phase density: Also the Levermore closure of Ref. [1] does not describe a discontinuous phase density.

5. Modified boundary conditions

Now, we present a modification of the boundary conditions which may support our arguments about the number of moments. We recall, that the phase density $\hat{f}$, given by (2), is discontinuous in velocity space and that we shall need many moments in order to approximate the discontinuity. The idea of our modification is to construct a phase density $\bar{f}$ at the boundary which is not discontinuous at the walls, but an approximation of the original phase density $\hat{f}$. Speaking about moment theories, we have to consider $\bar{f}$ to be a good approximation, if a certain number of its moments agree with the moments of $\hat{f}$, which we denote by

$$\hat{u}_A = \int \psi_A\left(c_k\right) \hat{f}\, d\mathbf{c}$$

Of course, considering a moment theory with the normal solution $f\left(u_A, c_k\right)$, we choose this normal solution also at the wall, so that we have

$$\bar{f} = f\left(\hat{u}_A, c_i\right) \ .$$

The half fluxes from the walls, A_A^0 and B_A^{n+1}, respectively, have now to be calculated from the phase density $\bar{f}$. We obtain in dimensionless form

$$\begin{aligned}
A_\varepsilon^0 &= \frac{1}{2}\hat{q}_0 + \sqrt{\frac{2}{\pi}}\hat{p}_0\sqrt{\hat{T}_0}\left(1 + \frac{1}{40}\frac{\hat{\Delta}_0}{\hat{p}_0\hat{T}_0}\right) \\
B_\varepsilon^{n+1} &= \frac{1}{2}\hat{q}_L - \sqrt{\frac{2}{\pi}}\hat{p}_L\sqrt{\hat{T}_L}\left(1 + \frac{1}{40}\frac{\hat{\Delta}_L}{\hat{p}_L\hat{T}_L}\right) \\
A_q^0 &= \frac{5}{4}\hat{p}_0\hat{T}_0\left(1 + \frac{1}{15}\frac{\hat{\Delta}_0}{\hat{p}_0\hat{T}_0}\right) + \frac{9}{5}\sqrt{\frac{2}{\pi}}\sqrt{\hat{T}_0}\hat{q}_0 \\
B_q^{n+1} &= \frac{5}{4}\hat{p}_L\hat{T}_L\left(1 + \frac{1}{15}\frac{\hat{\Delta}_L}{\hat{p}_L\hat{T}_L}\right) - \frac{9}{5}\sqrt{\frac{2}{\pi}}\sqrt{\hat{T}_L}\hat{q}_L \\
A_\Delta^0 &= 14\hat{T}_0\hat{q}_0 + 12\sqrt{\frac{2}{\pi}}\hat{p}_0\sqrt{\hat{T}_0}^3 + \frac{3}{2}\sqrt{\frac{2}{\pi}}\sqrt{\hat{T}_0}\hat{\Delta}_0 \\
B_\Delta^{n+1} &= 14\hat{T}_L\hat{q}_L - 12\sqrt{\frac{2}{\pi}}\hat{p}_L\sqrt{\hat{T}_L}^3 - \frac{3}{2}\sqrt{\frac{2}{\pi}}\sqrt{\hat{T}_L}\hat{\Delta}_L
\end{aligned}$$

$\hat{p}_0$, $\hat{T}_0$, $\hat{p}_L$, $\hat{T}_L$ etc. are the dimensionless moments of $\hat{f}$ at $x = 0$ and $x = L$, respectively. Due to lack of space, their values will not be presented in this paper. Figure 2 presents the results for stationary heat transfer with 13 and 14 moments and Table 1 shows the average heat flux $q = \sum_{i=2}^{n-1} q^i$ as well as the jumps at the walls $q^1 - q$, $q^n - q$. Also here, we find a jump in the heat flux, but it is considerably

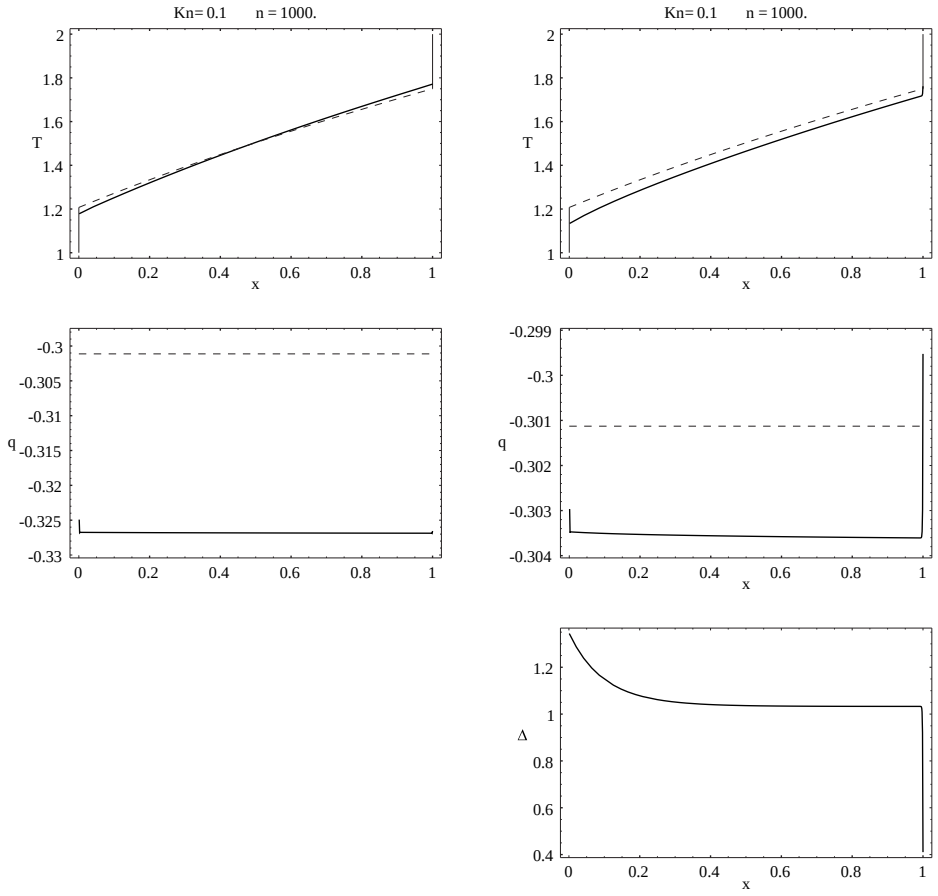

Figure 2.
Stationary heat transfer with 13 (left column) and 14 (right column) moments with modified boundary conditions, $K_n = 0.1$.

smaller than in the original scheme, where it was about 5% (note the different scale of Figures 1 and 2). With the new boundary conditions, we find a jump in the heat flux of ca. 0.6% for 13 moments and of ca. 1.3% in the 14 moment case. Thus, our modified boundary conditions need no further input to exhibit the conservation of energy. We conclude that the violation of the conservation law for energy seems to be a question of the boundary conditions and not of the discretisation method.

However, the temperature curve of the 13 moment case does not match the analytical solution. This discrepancy is due to the fact, that the new boundary conditions are only an approximation of the original ones. The approximation will be better, if more moments are taken into account.

Table 1.
Heat flux q and its jumps $q^1 - q$, $q^n - q$, for the various methods (wall temperatures $T_{W_0} = 1$, $T_{W_L} = 2$, $Kn = 0.1$, 10^3 gridpoints, 5 10^4 iterations)

	q	$q^1 - q$	$q^n - q$
ET13 analytic	−0.3011	0	0
ET13 kin. scheme	−0.2837	0.01535	0.01147
ET14 kin. scheme	−0.2722	0.006971	0.01349
ET13 modified BC	−0.3268	0.001907	0.0002741
ET14 modified BC	−0.3036	0.0005942	0.004036

Table 2.
Heat flux q and its jumps $q^1 - q$, $q^n - q$, for the various methods (wall temperatures $T_{W_0} = 1$, $T_{W_L} = 2$, $Kn = 0.01$, 10^4 gridpoints, 7 10^5 iterations).

	q	$q^1 - q$	$q^n - q$
ET13 analytic	−0.051641	0	0
ET13 kin. scheme	−0.05108	0.002503	0.002296
ET14 kin. scheme	−0.05059	0.001560	0.001680
ET13 modified BC	−0.05238	0.0002164	0.0001016
ET14 modified BC	−0.05152	0.0001677	0.0002664

We also give a brief account of results obtained with different parameters. Table 2 shows the average heat flux q and the jumps at the walls for $K_n = 0.01$ and the wall temperatures $T_{W_0} = 1$, $T_{W_L} = 2$. In order to have proper results, we had to take 10^4 grid points, the corresponding computing times were several hours. Again, the jumps are one order of magnitude smaller with the modified boundary conditions. Also here, the result with 14 moments and modified boundary conditions matches best with the analytical result. We do not show the corresponding temperature curves, since all four results have no visible differences to the analytical solution.

Table 3.
Heat flux q and its jumps $q^1 - q$, $q^n - q$, for the various methods (wall temperatures $T_{W_0} = 1$, $T_{W_L} = 1.1$, $Kn = 0.1$, 10^3 gridpoints, 5 10^4 iterations).

	q	$q^1 - q$	$q^n - q$
ET13 analytic	−0.02615	0	0
ET13 kin. scheme	−0.02501	0.001185	0.001148
ET14 kin. scheme	−0.02416	0.0007385	0.0008101
ET13 modified BC	−0.02776	0.00008635	0.00007118
ET14 modified BC	−0.02597	0.00008583	0.0001344

In Table 3, we have printed the same quantities for $K_n = 0.1$, but a smaller temperature difference, $T_{W_0} = 1$, $T_{W_L} = 1.1$. Once again, we have a difference of one order of magnitude in the jumps between the original and the modified boundary conditions and the 14 moments solution with the modified boundary conditions is closest to the analytical solution.

6. Conclusions

The kinetic scheme of Le Tallec & Perlat provides a tool to solve moment equations of kinetic theory. In particular it allows the calculation of boundary value problems with an arbitrary number of moments. The method is based on half space moments of the phase density and the boundary conditions for these follow directly from the boundary conditions for the phase density.

Unfortunately, as was shown, the method is restricted to distances of some mean free paths only, since the grid size must be considerably smaller than the mean free path.

Moreover, the results of [1] and the present paper indicate the violation of the conservation laws for energy and momentum. Clearly, this shades some doubt on the usefulness of the method which should be studied in greater detail in order to understand its deficiencies. As was pointed out above, it is probable, although not sure, that a higher number of moments will improve the results. This will be considered in future work.

In many cases, one will be satisfied with approximate solutions obtained by a theory with a low number of moments. We presented a modification of the boundary conditions which may be used in these cases. The modification seems to be very natural for the use in moment equations: the discontinuous phase density at the wall is replaced by a normal solution which agrees with the original phase density in the moments under consideration only. Here, the conservation of energy is well fulfilled without further assumptions. The results for the 13 moment case deviate from the analytical solution due to the approximative character of the new boundary conditions and one may expect, again, better results for an increasing number of moments. Calculations with many moments are planned for the future.

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