Grad's Moment Equations for Microscale Flows

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Abstract. Grad's moment equations are discussed for application to microscale flows in the transition regime. While Grad's 13 moment equations as well as Hilbert and Chapman-Enskog expansions of the Boltzmann equation cannot resolve the Knudsen boundary layer at the wall, this is different for moment theories with extended sets of moments. Since for channel flow with Knudsen numbers above 0.1 the Knudsen layer extends over the whole channel width, theories with more than 13 moments can be expected to give a more accurate description. Various sets of moment equations are considered for one-dimensional heat transfer in order to show the usefulness as well as the limitations of Grad's moment equations for microscale flows. In the linear case, the moment equations can be reduced to an eigenvalue problem, where the inverse eigenvalues determine the shape of the Knudsen boundary layer. The results give evidence that approaches with increasing moment number allow for the resolution of finer details of the Knudsen layer.

INTRODUCTION

In the microscale flow regime, distinguished by large Knudsen numbers but relatively small Mach numbers [1], the behavior of a gas cannot be described by the Navier-Stokes-Fourier theory satisfactorily. While the growing interest in the simulation of microscopic gas flows has revived the interest in higher order expansions of the Boltzmann equation, e.g. Hilbert expansions [2], or the Burnett equations [3][4], Grad's moment equations [5] only play a marginal role for the modeling of microscale flows. This is mostly due to the problem of assigning meaningful boundary values to higher moments. Despite this problem, there are two important reasons in favor of the Grad equations:

i.) The well-known set of 13 moment equations contains the Burnett equations, as can be seen by a second order expansion of the 13 moment equations in terms of the Knudsen number [6][7]. While the Burnett equations are ill-posed [8] (sometimes they are augmented [3][4] in order to overcome this deficiency), the Grad equations are well-posed for all values of the moments which are physically meaningful [9]. Moreover, they contain traces of all higher order contributions in the Knudsen number, a fact that might be an additional advantage.

ii.) The 13 moment equations as well as Hilbert expansions and Burnett equations cannot resolve the Knudsen boundary layer at the wall - jump and slip boundary conditions must account for Knudsen layer effects [2][1]. Theories with extended sets of moments, however, are capable of describing the main features of the Knudsen layer [10]. Since for channel flow with Knudsen numbers above 0.1 the Knudsen layer extends over the whole channel width, theories with more than 13 moments can be expected to give a more accurate description.

In this paper, we shall consider various sets of moment equations (up to 48 moments in the one-dimensional case) for one-dimensional heat transfer in order to show the usefulness as well as the limitations of Grad's moment equations for microscale flows.

In the linear case, the moment equations can be reduced to an eigenvalue problem, where the inverse eigenvalues determine the Knudsen layer. An increasing moment number allows for the resolution of finer details of the Knudsen layer. A theory with 26 moments gives a general description of Knudsen number effects, but fails in the description of a smaller layer (sub-Knudsen layer) at the wall, which, however, is captured when the number of moments is increased.

MOMENT SYSTEMS OF KINETIC THEORY

The goal of kinetic theory is to find the phase density f, defined such that $f d\mathbf{c}$ gives the number density of atoms with velocity in $(c_i, c_i + dc_i)$ at place x_i and time t. The macroscopic quantities density ρ, velocity v_i, density of internal

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energy $\rho\varepsilon$, pressure tensor $p_{\langle ij\rangle}$ and heat flux vector q_i of the gas are given by moments of the phase density, viz.

$$\rho = m\int f d\mathbf{c},\ \rho v_i = m\int c_i f d\mathbf{c},\ \rho\varepsilon = \frac{3}{2}\rho\frac{k}{m}T = \frac{m}{2}\int C^2 f d\mathbf{c},\ p_{\langle ij\rangle} = m\int C_{\langle i}C_{j\rangle} f d\mathbf{c},\ q_i = \frac{m}{2}\int C^2 C_i f d\mathbf{c} \qquad (1)$$

where m is the mass of one particle, k is Boltzmann's constant, and $C_i = c_i - v_i$ is the peculiar velocity; T is the gas temperature, defined by Eqn. $(1)_3$. The phase density is governed by the Boltzmann equation [11][12],

$$\frac{\partial f}{\partial t} + c_k\frac{\partial f}{\partial x_k} = S\left(f\right)\ , \qquad (2)$$

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

Maxwell's boundary conditions for the phase density can be written as

$$\hat{f} = \begin{cases} \theta f_W + \left(1-\theta\right) f_N\left(-n_k C_k^W\right) & ,\quad n_k C_k^W \geq 0 \\ f_N & ,\quad n_k C_k^W \leq 0\ . \end{cases} \qquad (3)$$

where θ is the accommodation coefficient, i.e. the fraction of particles that is thermalized at the wall, and n_k is the normal of the wall, pointing towards the gas. f_N denotes the distribution directly at the wall, and $f_N\left(-n_k C_k^W\right)$ is the corresponding distribution of elastically reflected particles (i.e. same tangential velocity, but opposite normal velocity than f_N). f_W is the Maxwellian of the thermalized particles,

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

where T_W denotes the temperature of the wall, $C_i^W = c_i - v_i^W$, v_i^W is the velocity of the wall, and ρ_W is the density of the thermalized particles that follows from the condition that no particles are accumulated at the wall,

$$m\int_{n_k C_k^W \geq 0} \hat{f}\, C_k^W n_k\, d\mathbf{c} = -m\int_{n_k C_k^W \leq 0} \hat{f}\, C_k^W n_k\, d\mathbf{c}\ . \qquad (4)$$

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 $\rho, \rho v_i, \rho\varepsilon, p_{\langle ij\rangle}, q_i$ defined above.

Multiplication of the Boltzmann equation (2) by Ψ_A and subsequent integration over velocity space yields the moment equations

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

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

In Grad's moment method, the phase density is approximated as a series

$$f^{(\alpha)} = f_M\left(1 + \sum_A \Lambda_A^{(\alpha)}\left(u_B\right)\Psi_A^{(\alpha)}\right) \quad \text{with} \quad u_A = \int \Psi_A^{(\alpha)} f^{(\alpha)} d\mathbf{c}\ ; \qquad (6)$$

the coefficients $\Lambda_A^{(\alpha)}$ follow from the inversion of the last equation. f_M denotes the local Maxwellian,

$$f_M = \frac{\rho}{m}\sqrt{\frac{m}{2\pi k T}}^3 e^{-\frac{m}{2kT}\left(c_k - v_k\right)^2}\ .$$

From (6) one finds constitutive equations for fluxes and productions, viz.

$$F_{Ak}\left(x_i,t\right) = F_{Ak}\left(u_B\left(x_i,t\right)\right) \quad , \quad P_A\left(x_i,t\right) = P_A\left(u_B\left(x_i,t\right)\right) \ . \tag{7}$$

Thus, Grad's moment method provides a closed set of PDE's for the moments. We shall not give details of the calculations of the functions (7) which were performed with the computer algebra system *Mathematica*®, see [10] for more detail. For the productions, we have adopted the linearized collision term for Maxwell molecules, using a *Mathematica*® program that was developed by Au in the context of his thesis [13].

Following [10], we consider the following sets of moments as variables:

$$\Psi_A^{(\alpha)} = m\left\{1, c_i, c_i c_j, \ldots, c_{i_1} c_{i_2} \cdots c_{i_\alpha}, c^2 c_{i_1} c_{i_2} \cdots c_{i_{\alpha-1}}\right\} \quad , \ \alpha = 2, 3, \ldots, 11 \tag{8}$$

corresponding to $13\,(5)$, $26\,(8)$, $45\,(11)$, $71\,(15)$, $105\,(19)$, $148\,(24)$, $201\,(29)$, $265\,(35)$, $341\,(41)$, $430\,(48)$ moments; the numbers in brackets indicate the number of PDE's which must be solved in the one-dimensional case. For the moments, we adopt the notation

$$u^{(k)}_{\langle i_1 i_2 \ldots i_n\rangle} = m\int c^{2k} c_{\langle i_1 \cdots i_n\rangle} f \, d\mathbf{c} \quad \text{with} \quad u^{k}_{\langle i_1 i_2 \ldots i_n\rangle}\delta_{i_j i_k} = 0 \ ,$$

the angular brackets identify trace-free tensors. In the one-dimensional case, one needs to consider only the $x \cdots x$ parts of the trace free moments.

$$u^{(k)}_{\langle n\rangle} = u^{(k)}_{\langle \underbrace{xx\cdots x}_{n-times}\rangle} = \int \psi^{(k)}_{\langle n\rangle} f \, d\mathbf{c} \quad , \quad F^{(k)}_{\langle n\rangle} = \int \psi^{(k)}_{\langle n\rangle} c_x f \, d\mathbf{c} \quad , \quad P^{(k)}_{\langle n\rangle} = \int \psi^{(k)}_{\langle n\rangle} S \, d\mathbf{c} \tag{9}$$

so that the one-dimensional moment equations read

$$\frac{\partial u^{(k)}_{\langle n\rangle}}{\partial t} + \frac{\partial F^{(k)}_{\langle n\rangle}}{\partial x} = P^{(k)}_{\langle n\rangle} \ . \tag{10}$$

The choice (8) of moments corresponds to the set of variables

$$u^{(k)}_{\langle n-2k\rangle} \ , \ {\scriptstyle k=0,\ldots,\left\|\frac{n}{2}\right\|} \ , \ {\scriptstyle n=0,\ldots,\alpha} \ ; \ u^{(k)}_{\langle \alpha+1-2k\rangle} \ , \ {\scriptstyle k=1,\ldots,\left\|\frac{\alpha+1}{2}\right\|} \ . \tag{11}$$

where

$$\left\|\frac{n}{2}\right\| = \begin{cases} \frac{n}{2} & n \ even \\ \frac{n-1}{2} & n \ uneven \end{cases}$$

It is customary to introduce the non-equilibrium part of the moments

$$w^{(k)}_{\langle i_1 i_2 \ldots i_n\rangle} = m\int c^{2k} c_{\langle i_1 \cdots i_n\rangle}\left(f - f_M\right) d\mathbf{c} \quad , \quad w^{(k)}_{\langle n\rangle} = \int \psi^{(k)}_{\langle n\rangle}\left(f - f_M\right) d\mathbf{c}$$

According to this definition, the $w^{(k)}_{\langle n\rangle}$ vanish in equilibrium. Due to the definitions of density, velocity, and temperature, we have $w^{(0)} = 0$, $w^{(0)}_i = 0, w^{(1)} = 0$ also in non-equilibrium. Thus, we can replace the set of variables (11) by the set

$$\rho = u^{(0)}_{\langle 0\rangle} \quad , \quad v_i = u^{(0)}_{\langle i\rangle}\Big/u^{(0)}_{\langle 0\rangle} \quad , \quad T = u^{(1)}_{\langle 0\rangle}\Big/3u^{(0)}_{\langle 0\rangle}\frac{k}{m} \ , \tag{12}$$

$$w^{(k)}_{\langle n-2k\rangle} \ , \ {\scriptstyle k=0,\ldots,\left\|\frac{n}{2}\right\|} \ , \ {\scriptstyle n=2,\ldots,\alpha} \ , \ \{k,n\} \neq \{1,2\} \ ; \ w^{(k)}_{\langle \alpha+1-2k\rangle} \ , \ {\scriptstyle k=1,\ldots,\left\|\frac{\alpha+1}{2}\right\|} \ .$$

STEADY STATE HEAT TRANSFER

We consider one-dimensional steady heat transfer between two parallel walls at rest. In this case, the gas will be at rest as well, so that $v_i = u^{(0)}_{\langle 1 \rangle} = 0$.

Dimensionless variables are introduced as follows: The length scale is defined by the wall distance L, and we choose a temperature T_0 as the measure for temperature, e.g. the temperature of a wall, or in the middle between the walls. A reference pressure p_0 defines the scale for the density as $\rho_0 = p_0 / \frac{k}{m} T_0$. The velocity scale is given by $\sqrt{\frac{k}{m} T_0}$ and defines also the time scale by $L / \sqrt{\frac{k}{m} T_0}$. Altogether, we introduce the following dimensionless quantities:

$$\hat{x} = \frac{x}{L} \quad , \quad \hat{t} = \frac{\sqrt{\frac{k}{m} T_0}\, t}{L} \quad , \quad \hat{c}_i = \frac{c_i}{\sqrt{\frac{k}{m} T_0}} \quad , \quad \hat{T} = \frac{T}{T_0} \quad , \quad \hat{u}^{(k)}_{\langle n \rangle} = \frac{u^{(k)}_{\langle n \rangle}}{p_0 \sqrt{\frac{k}{m} T_0}^{2k+n-2}} \quad , \quad \hat{w}^{(k)}_{\langle n \rangle} = \frac{w^{(k)}_{\langle n \rangle}}{p_0 \sqrt{\frac{k}{m} T_0}^{2k+n-2}} \; .$$

For easier notation, the hats will be omitted in the sequel. The dimensionless productions contain the Knudsen number, i.e. the ratio between the mean free path of the particles and the wall distance L, given by

$$\mathrm{Kn} = \frac{\sqrt{\frac{k}{m} T_0}^3}{L p_0 \gamma} \; . \tag{13}$$

γ is a constant that follows from the calculation of the collision production for Maxwell molecules and is related to heat conductivity κ by $\gamma = \frac{15}{4} \left(\frac{k}{m} \right)^2 \frac{T}{\kappa}$, see [10].

Before studying general systems, we consider the balance equations for the first 13 moments, see Eqns. (1). In the one-dimensional steady state case they read

$$0 = 0 \;\; , \;\; \frac{\partial \left(\rho T + w^{(0)}_{\langle 2 \rangle} \right)}{\partial x} = 0 \;\; , \;\; \frac{\partial q}{\partial x} = 0 \;\; , \;\; \frac{\partial \left(\frac{4}{15} w^{(1)}_{\langle 1 \rangle} + w^{(0)}_{\langle 3 \rangle} \right)}{\partial x} = -\frac{w^{(0)}_{\langle 2 \rangle}}{\mathrm{Kn}} \;\; , \;\; \frac{\partial \left(\frac{1}{3} \left(15 \rho T^2 + w^{(2)}_{\langle 0 \rangle} \right) + w^{(1)}_{\langle 2 \rangle} \right)}{\partial x} = -\frac{2}{3} \frac{w^{(1)}_{\langle 1 \rangle}}{\mathrm{Kn}}$$

Here, $u^{(0)}_{\langle 2 \rangle} = w^{(0)}_{\langle 2 \rangle}$ is the $\langle xx \rangle -$component of the pressure tensor, $\frac{1}{2} u^{(1)}_{\langle 1 \rangle} = \frac{1}{2} w^{(1)}_{\langle 1 \rangle}$ is the $\langle x \rangle$ component of the heat flux, and $15 \rho T^2 + w^{(2)}_{\langle 0 \rangle} = u^{(2)}_{\langle 0 \rangle}$ is the trace of the fourth-order moment. Integration of the second equation (the moment equation) yields

$$\rho = \frac{1 - w^{(0)}_{\langle 2 \rangle}}{T} \; , \tag{14}$$

when we set the constant of integration equal to unity ($= p_0$ in proper units). It follows that the density is not an independent variable. From the third equation (the energy equation) follows that the heat flux is a constant

$$\frac{1}{2} w^{(1)}_{\langle 1 \rangle} = q = const.$$

that must be determined from the boundary conditions. Then, with Eqn. (14), the fifth equation can be written as

$$\frac{5}{2} \left(1 - w^{(0)}_{\langle 2 \rangle} \right) T + \frac{1}{6} w^{(2)}_{\langle 0 \rangle} + \frac{1}{2} w^{(1)}_{\langle 2 \rangle} = \frac{5}{2} K - \frac{2}{3} \frac{q}{\mathrm{Kn}} x$$

where K is another constant of integration. This equation can be used to eliminate temperature as an independent variable,

$$T = \frac{K - \frac{4}{15} \frac{q}{\mathrm{Kn}} x - \frac{1}{15} w^{(2)}_{\langle 0 \rangle} - \frac{1}{5} w^{(1)}_{\langle 2 \rangle}}{1 - w^{(0)}_{\langle 2 \rangle}} \; . \tag{15}$$

It follows that density, temperature and heat flux are not variables anymore, and are replaced by the constants of integration $\hat{p}_0 = 1$, q, K. The remaining variables are denoted by

$$w_{\{j\}} = \begin{cases} w^{(k)}_{\langle n-2k \rangle} \quad , \quad k{=}0,\ldots,\left\| \frac{n}{2} \right\| \; , \; n{=}2,\ldots,\alpha \;\; , \{k,n\} \neq \{1,2\} \;\; , \{k,n\} \neq \{1,3\} \\ \\ w^{(k)}_{\langle \alpha+1-2k \rangle} \quad , \quad k{=}1,\ldots,\left\| \frac{\alpha+1}{2} \right\| \; . \end{cases}$$

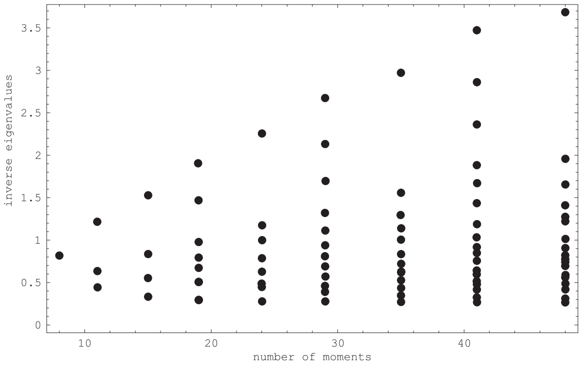

FIGURE 1. Inverse eigenvalues λ_α for moment theories with various number of moments α, as defined in Eqn. (8). Only positive values are shown.

where the index j is a suitable counter for the variables.

Closer examination shows that the remaining moment equations are of the form

$$\frac{\partial F_{\{k\}}\left(qx,q,w_{\{j\}}\right)}{\partial x}=P_{\{k\}}\left(qx,q,w_{\{j\}}\right)\ .$$

We are interested only in linear deviations from equilibrium where $q_{|E}=w_{\{j\}|E}=0$, the index E refers to evaluation in equilibrium. Then, we can expand the equations in first order in the non-equilibrium variables to obtain

$$A_{ki}\frac{dw_{\{i\}}}{dx}=B_kq+C_{ki}\frac{w_{\{i\}}}{\mathrm{Kn}} \tag{16}$$

where the matrices A_{ki} , C_{ki} and the vector B_k are given by

$$A_{ki}=\left[\frac{\partial F_{\{k\}}}{\partial w_{\{i\}}}\right]_{|E}\quad,\quad B_k=\left[\frac{\partial P_{\{k\}}}{\partial q}-\frac{\partial F_{\{k\}}}{\partial qx}\right]_{|E}\quad,\quad C_{ki}\frac{1}{\mathrm{Kn}}=\left[\frac{\partial P_{\{k\}}}{\partial w_{\{i\}}}\right]_{|E}$$

Note that $\left[P_{\{k\}}\right]_{|E}=0$, and $\det C\neq 0$ since the conservation laws are not anymore among the equations that we consider. Also, we have made the occurrence of the Knudsen number Kn explicit.

The solutions of the equations (16) read

$$w_{\{i\}}=-\mathrm{Kn}C_{ik}^{-1}B_kq+\sum_\alpha \tilde{w}_{\{i\}}^{\alpha}\exp\left[\frac{\lambda_\alpha x}{\mathrm{Kn}}\right] \tag{17}$$

where the λ_α are the inverse eigenvalues of $C_{ik}^{-1}A_{kj}$, i.e. the solutions of

$$\det\left[C_{ik}^{-1}A_{kj}-\frac{1}{\lambda}\delta_{ij}\right]=0\ .$$

Of course, only non-zero eigenvalues are of interest here. Note that the entries in $C_{ik}^{-1}B_k$ are mostly zero, but not when $w_{\{i\}}$ refers to a vector variable $w_{\langle 1\rangle}^{(k)}$. $\tilde{w}_{\{i\}}^{\alpha}$ are the amplitudes that must be determined from boundary conditions. Figure 1 shows the inverse eigenvalues λ for the moment systems defined in (8). For each positive value λ_α (shown), there is a corresponding value with negative sign (not shown).

KNUDSEN BOUNDARY LAYERS

We proceed with the interpretation of the above result, Eqn. (17). Linearizing Eqn. (15) and combining it with Eqn. (17) yields for the temperature

$$T=K-\frac{4}{15}\frac{q}{\mathrm{Kn}}x+\sum_\alpha\left\{A_\alpha\sinh\left[\frac{\lambda_\alpha}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]+B_\alpha\cosh\left[\frac{\lambda_\alpha}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]\right\} \tag{18}$$

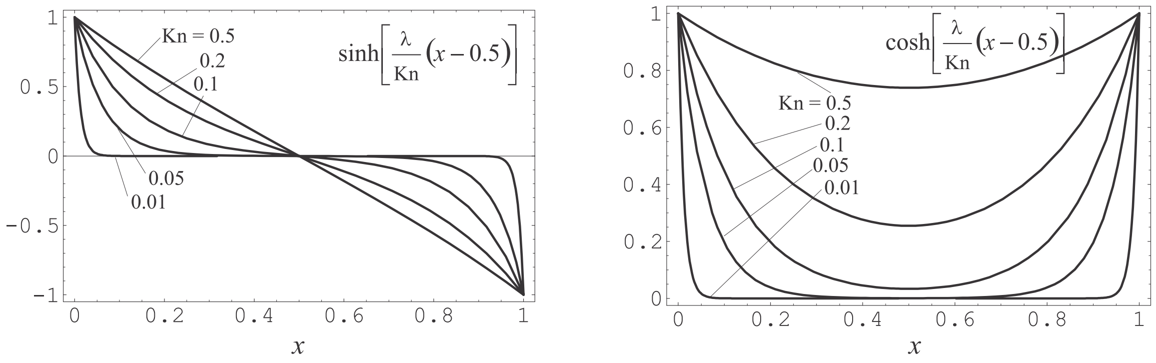

FIGURE 2. The functions $\sinh\left[\frac{\lambda}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]$ and $\cosh\left[\frac{\lambda}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]$ for a variety of Knudsen numbers (normalized).

where now the sum is taken only over the positive values λ_α, and A_α, B_α are new constants that must be determined from boundary conditions. The first two terms, $K-\frac{4}{15}\frac{q}{\mathrm{Kn}}x$, are the usual solution of the linearized Fourier law, i.e. a straight temperature curve. The additional terms are the corrections of the Fourier law due to microscale effects. Figure 2 shows the functions $\sinh\left[\frac{\lambda}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]$ and $\cosh\left[\frac{\lambda}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]$ for a variety of Knudsen numbers. For the Figure, we chose the value for $\alpha=3$ (26 moments), $\lambda=0.818$. Note, that the values for λ vary between 0.25 and 3.6.

It can be seen that for small Knudsen numbers ($\mathrm{Kn}\leq 0.01$) these terms affect only the region close to the wall, while they are zero in the interior. Thus, we find the Knudsen boundary layers at the walls. For larger Knudsen numbers, however, these terms contribute to the temperature profile everywhere in $[0,1]$, and it follows that the boundary layer extends over the whole space between the walls. This is the case already for Knudsen numbers above 0.05.

From Figure 1 we see that moment systems with more moments have a wider spectrum of eigenvalues, and thus can resolve more details of the Knudsen layer. Larger values of λ refer to smaller boundary layers, while smaller values refer to wider layers.

Grad's 13 moment theory uses the moments (1) as variables, and the quantities $w^{(2)}_{\langle 0\rangle}, w^{(1)}_{\langle 2\rangle}$ are not variables, but follow from the constitutive theory as $w^{(2)}_{\langle 0\rangle}=w^{(1)}_{\langle 2\rangle}=0$. Therefore, the 13 moment theory does not exhibit Knudsen layer effects, but leads to the Fourier solution $T=K-\frac{4}{15}\frac{q}{\mathrm{Kn}}x$.

The 26 moment theory gives just one non-zero eigenvalue, corresponding to $\lambda=\sqrt{\frac{245}{366}}=0.818$. Therefore the 26 moment theory is capable of describing the basic features of the boundary layer, but the description is not very accurate. See the next section for a closer examination of the 26 moment case.

For large enough Knudsen numbers we can expand the temperature (18) to obtain

$$T=K-\frac{4}{15}\frac{q}{\mathrm{Kn}}x+\sum_{\alpha}\left\{A_\alpha\frac{\lambda_\alpha}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)+B_\alpha\right\} \tag{19}$$

and we see that the microscale corrections add linear functions $\left\{A_\alpha\frac{\lambda_\alpha}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)+B_\alpha\right\}$ to the temperature. Here it becomes most obvious that the Fourier law ($q=\frac{15}{4}\mathrm{Kn}\frac{\partial T}{\partial x_i}$ in the linear, dimensionless case) is not valid in the microscale regime.

Hilbert and Chapman-Enskog expansions of the Boltzmann equation rely on series expansions with the Knudsen number as smallness parameter of the type $\phi=\phi_0+\phi_1\mathrm{Kn}+\phi_2\mathrm{Kn}^2+\ldots$ The boundary layer term $\exp\left[\frac{\lambda_\alpha x}{\mathrm{Kn}}\right]$ in Eqn. (17) cannot be expanded in this manner, and we conclude that both methods are not capable of resolving the Knudsen layer. Therefore, these methods can only be used for small boundary layers, which can be considered as jumps at the walls [2].

Here, it is also interesting to note that the 2nd order Chapman-Enskog expansion - the Burnett equations - yields the Fourier law for temperature independently of the model for interatomic collisions. The result for pressure, however, depends on the interaction potential: pressure is constant for Maxwell molecules, but has a small contribution of order $O\left(\mathrm{Kn}^2\right)$ for other potentials, in particular for hard spheres.

THE 26 MOMENT SYSTEM

In Ref. [10], we have used the method of kinetic schemes [15][16] to solve the heat transfer problem for moment equations. This numerical method uses halfspace fluxes of the moments in velocity space, and allows a direct implementation of the boundary conditions (3). The results obtained agree very well with direct solutions of the Boltzmann equation by Ohwada [17], when the number of moments is sufficiently large. In order to understand the requirement of large moment numbers better, one has to recall that the moment method assumes a moment solution (6) in all space points, i.e. a series. According to the boundary condition (3), the phase density at the wall is a discontinuous function of the microscopic velocity. A series in polynomials, which pictures this discontinuity sufficiently, will require a large number of expansion coefficients, i.e. moments. Since the kinetic schemes indeed use a discontinuous phase density at the walls, they can only give reliable results when many moments are considered. This is the reason why the results with 26 moments in Ref. [10] show spurious boundary layers which stem from the numerical method.

Nevertheless, the set of 26 moments can give results which agree better with the solutions of larger moment systems than solutions of the Fourier law. For the linear 26 moment case (8 one-dimensional equations), we obtain the solution

$$T = K - \frac{4}{15}\frac{q}{\mathrm{Kn}}\left(x-\frac{1}{2}\right) - \frac{26}{35}\sigma \ , \ \ \sigma = w_{\{1\}} = A\sinh\left[\frac{\lambda_\alpha}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right] + B\left(\cosh\left[\frac{\lambda_\alpha}{\mathrm{Kn}}\left(x-\frac{1}{2}\right)\right]-1\right)$$

$$w_{\{2\}} = -\frac{366}{245}\mathrm{Kn}\frac{dw_{\{1\}}}{dx} \ , \ w_{\{3\}} = 0 \ , \ \ w_{\{4\}} = \frac{61}{7}w_{\{1\}}$$

where $\sigma = w^{(0)}_{\langle 2\rangle}$ is the anisotropic stress, see [10] (the other 3 equations are $\rho = \frac{1-\sigma}{T}$, $v = 0$, $q = const.$). The solution contains the constants of integration K, q, A, B and thus four boundary conditions are required to solve the problem.

It is not possible to get an accurate fit to the kinetic scheme results for the three quantities T, q, σ at the same time: only two of these can be fitted well, and the third one will not match the kinetic scheme solutions. Obviously, the contributions of other eigenvalues λ_α are important for the proper determination of T and σ. Nevertheless, we show some results which follow from an approach to the boundary conditions that goes back to the work of Grad [5].

The idea for the boundary conditions is to assume that the phase density at the wall is given by Grad's phase density, where the coefficients are determined such that some fluxes perpendicular to the wall have the same value with the wall phase density $\hat{f}$ as given by Eqn. (3) and with Grad's phase density, Eqn. (6). Thus, we have the boundary conditions

$$F_{Ak}n_k = \int \Psi_A c_k n_k \hat{f}\, d\mathbf{c} = \int \Psi_A c_k n_k f\, d\mathbf{c} \implies \int_{c_k n_k \geq 0} \Psi_A c_k n_k \left(f - f_W\right) d\mathbf{c} = 0 \ \text{ for some } A. \tag{20}$$

For the solution of heat transfer with 26 moments four boundary conditions are required, and thus we can only use two conditions of this type at each of the two boundaries. With 26 moments in the one dimensional case we have

$$\Psi_A = \left\{1, c_x, c^2, c_x^2 - \frac{1}{3}c^2, c^2 c_x, \left(c_x^2 - \frac{3}{5}c^2\right)c_x, c^4, c^2\left(c_x^2 - \frac{1}{3}c^2\right)\right\} \ .$$

We chose the heat flux ($\Psi_3 c_x$) and one other flux ($\Psi_A c_x$) to be continuous at both walls. The choice of the second flux has considerable influence on the results. Due to space restrictions, we only show results for $A = 4$ and $A = 5$ for Kn $= 0.5$, see Figure 3 which shows temperature T on the left, and stress σ on the right. Obviously, the choice $A = 5$ gives a better result for the temperature than $A = 4$, and both give better results than the Fourier law. This is also so for the heat flux, which follows from the kinetic schemes as $q_{ks} = -0.0507365$, with $A = 5$ as $q_5 = -0.0525366$, with $A = 4$ as $q_4 = -0.0543537$ and with the Fourier law as $q_F = -0.0559726$. However, a good match for temperature and heat flux corresponds to a large deviation for the stresses, as can be seen in the right figure ($\sigma = 0$ for the Fourier case, not drawn). Altogether we may say that the 26 moment case gives a reasonable improvement to the Fourier law. While temperature curve and heat flux match quite well with the kinetic scheme results, the 26 moment case at least allows to compute an anisotropic stress in steady state heat transfer, albeit its value is wrong.

In Figure 3, we have highlighted a small region close to the wall, denoted as *sub-Knudsen layer*. Apparently, the temperature in this region is affected by larger values of λ_α which describe smaller boundary layers. This region cannot be described with the 26 moment case at all. The sub-Knudsen layer corresponds to larger values of the inverse eigenvalues λ_α that arise only when a larger number of moments is considered. The sub-Knudsen layer is quite small and its details may be ignored.

Similar results can be expected for more general flow phenomena. In steady state Couette flow a velocity boundary layer can be observed, as well as a heat flux in the direction of the flow that can be seen in molecular dynamics, but not

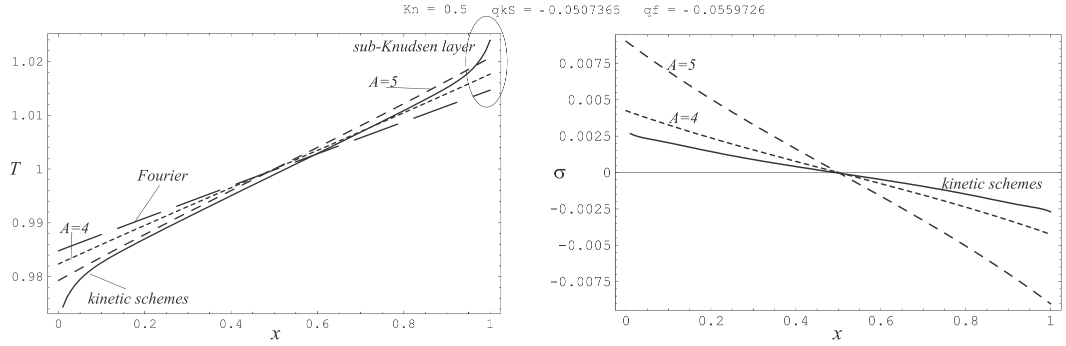

FIGURE 3. Dimensionless temperature and stress for stationary heat transfer: kinetic scheme simulations (continuous); 26 moments case with boundary conditions (20) (A=4: small dashes, A=5: dashes); and Fourier law predictions (large dashes). Kn=0.5, temperatures at left and right are 0.95, 1.05, respectively.

within the Navier-Stokes-Fourier theory [18]. This heat flux parallel to the flow is a linear microscale effect, similar to the non-vanishing stress σ that we have observed in steady heat transfer.

We conclude that the 26 moment case can describe microscale effects that can not be described by the Navier-Stokes-Fourier equations, the Burnett equations, or Hilbert expansions, such as boundary layers, anisotropic stresses induced by heatflow, or heatflow induced by stresses. However, due to the low number of moments considered, predictions of the 26 moment system cannot be expected to stand in perfect agreement with solutions of the Boltzmann equation. Also, it must be noted that moment methods allow the proper resolution of shock structures only if the flow speed is below the maximum wave velocity of the theory, which grows with the number of moments [9]. Therefore, the use of the 26 moments theory is restricted to Mach numbers not larger than 1.1 .

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