Convergence Study of Moment Approximations for Boundary Value Problems of the Boltzmann-BGK Equation

Manuel Torrilhon*

Center for Computational Engineering Science, RWTH Aachen University, Germany.

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Abstract. The accuracy of moment equations as approximations of kinetic gas theory is studied for four different boundary value problems. The kinetic setting is given by the BGK equation linearized around a globally constant Maxwellian using one space dimension and a three-dimensional velocity space. The boundary value problems include Couette and Poiseuille flow as well as heat conduction between walls and heat conduction based on a locally varying heating source. The polynomial expansion of the distribution function allows for different moment theories of which two popular families are investigated in detail. Furthermore, optimal approximations for a given number of variables are studied empirically. The paper focuses on approximations with relatively low number of variables which allows to draw conclusions in particular about specific moment theories like the regularized 13-moment equations.

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1 Introduction

The Boltzmann equation [4] describes the behavior of rarefied gases [3] on the basis of a probability density function defined on the phase space of particles including physical space and particle velocity. Moment methods have been originally explored by Harold Grad, see [9], to solve the Boltzmann equation in an approximate way. In moment approximations a polynomial expansion of the distribution function is used and the Boltzmann equation is projected onto polynomial basis functions of the velocity space yielding partial differential equations for the coefficients of the expansion.

Over the last decades moment theories have been investigated and further developed in various directions. Within the frame work of extended thermodynamics the
text book [19] demonstrates how moment approximations can be used to describe gas processes. Special mathematical properties of moment systems have been pointed out, e.g., in [15]. Moment equations come with the advantage that relatively low order approximations already give interesting results and there exist various particular moment equations which have been studied in detail, for example, Grad’s original 13-moment case [8] and Levermore’s 10-moment-closure [16]. A regularization technique that overcomes certain artefacts in moment closures have been suggested in [25] resulting in the regularized 13-moment-equations (R13), see also the text book [23]. Regularized moment equations have been subsequently derived based on the 10-moment-case in [17], the 26-moment-equations in [12] and used for high order approximation in a numerical context [2]. Attempts to develop low order moment equations that obey a physical entropy law or H-theorem are found in [10, 18, 21, 22, 26]. Modifications of the moment method for gases can also be found in [6, 14] with further developments in e.g., [20]. Moment approximations are also used in other kinetic contexts, see e.g., [7], for general kinetic equations, and [5] for applications to radiation therapy.

The central question when using moment approximations is: how many moments are needed to simulate a certain process with sufficient accuracy? Since there is no general mathematical theory which can be used to answer this question, empirical studies like in [1] are typically conducted to gain understanding into the convergence behavior of moment approximations for specific processes. However, in the context of boundary value problems no such study exists, and it remains entirely unclear how moment equations cope with exponential Knudsen layers at the wall. Various investigations on channel flows with low order moment systems can be found, e.g., in [11, 13, 28–30, 32, 34] but a detailed convergence study of moment systems for gases with increasing number of variables is missing. A model system with large number of variables is considered in [24].

This paper will consider large moment approximations applied to the linear BGK equation for two shear flow and two heat conduction scenarios in one space dimension. The focus will be on low order approximations and the result will allow to re-examine the capability and accuracy of existing moment theories.

The paper is organized as follows: The linear kinetic setting of four different boundary value problems is presented in Section 2, while the generic moment approximation approach for the linear setting is detailed in Section 3. The moment equations are specialized to the boundary value problems in Section 4 and the field solution of some exemplary cases are presented. Section 5 presents and discusses the empirical error analysis of the moment approximations of the four channel processes. The paper ends with a conclusion.

2 Kinetic problem statement

2.1 Equations

We will consider the BGK equation
\[
\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \frac{1}{\tau} (f_M - f) + S
\]  
(2.1)
as a model for the full Boltzmann equation [23] for monatomic, ideal gases. The distribution function of the particle velocities is given by \( f(x,t,c) \) where \( c \) is the velocity in the laboratory frame. The relaxation time \( \tau \) corresponds to an inverse collision frequency.

A local source term \( S \) on the right-hand-side models external influences and will be discussed below. In this paper, the BGK equation is solved in a linearized form where the ground state is given by a absolute Maxwellian

\[
f_0(c) = \frac{\rho_0}{m} \frac{1}{(2\pi \theta_0)^{3/2}} \exp\left( -\frac{c^2}{2\theta_0} \right)
\]  
(2.2)
which is constant in space and time describing a gas at rest with density \( \rho_0 \), particle mass \( m \) and temperature \( \theta_0 \) (in energy density units). We are interested in the perturbation \( \tilde{f} \) of the distribution function \( f = f_0 + \varepsilon \tilde{f} \) such that the fields satisfy

\[
\rho(x,t) = \rho_0 + \varepsilon \tilde{\rho}(x,t), \quad v_i(x,t) = \varepsilon \tilde{v}_i(x,t), \quad \theta(x,t) = \theta_0 + \varepsilon \tilde{\theta}(x,t).
\]  
(2.3)
The linearized Maxwell distribution is than given by

\[
f_M(x,t,c) = \left( 1 + \frac{\tilde{\rho}}{\rho_0} + \varepsilon \frac{\tilde{v}_i c_i}{\theta_0} + \varepsilon \frac{\tilde{\theta}}{2\theta_0} \left( c_i^2 / \theta_0 - 3 \right) \right) f_0(c),
\]  
(2.4)
where the perturbed fields are computed up to first order in \( \varepsilon \) via

\[
\tilde{\rho} = m \int \tilde{f} \, dc, \quad \tilde{v}_i = \frac{m}{\rho_0} \int c_i \tilde{f} \, dc, \quad \tilde{\theta} = \frac{m}{3 \rho_0} \int \left( c_i^2 - 3 \theta_0 \right) \tilde{f} \, dc.
\]  
(2.5)

Boundary conditions are based on the accommodation model for the wall [23], which gives the incoming particles as a superposition of specularly reflected particles and accommodated particles which follow a given wall distribution function. We choose an inward-facing wall normal \( n \) with a corresponding velocity component \( c_n \). The wall does not move in the normal direction. We denote by \( f_{\text{wall}} \) the distribution function of the wall and \( f \) is the distribution of the gas just in front of the wall. The distribution function \( \bar{f} \) at the wall is then given by the accommodation model and reads

\[
\bar{f}(c) = \begin{cases} 
\chi f_{\text{wall}}(c) + \left( 1 - \chi \right) f(c^*), & c_n > 0, \\
f(c), & c_n < 0,
\end{cases}
\]  
(2.6)
where the velocity reflection \( c^* \) inverts the sign of the component normal to the wall \( c_n \). A boundary condition for \( f \) is derived from this by requiring \( f = \bar{f} \) at the wall. An alternative form of the kinetic boundary condition can be found by splitting the distribution function \( f \) into an odd and even part with respect to the normal velocity \( c_n \)

\[
f^{\text{(odd)}}(c) = \frac{1}{2} (f(c) - f(c^*)), \quad f^{\text{(even)}}(c) = \frac{1}{2} (f(c) + f(c^*)) , \quad f = f^{\text{(even)}} + f^{\text{(odd)}}.
\]  
(2.7)
Inserting this into (2.6) yields the relation
\[ f^{(\text{odd})} = \frac{\chi}{2-\chi} \left( f_{\text{wall}} - f^{(\text{even})} \right) \] for \( c_n > 0 \), \hspace{1cm} (2.8)
which defines the relevant incoming part of the distribution. In the linearized setting the wall distribution \( f_{\text{wall}} \) is given by
\[ f_{\text{wall}}(x,t,c) = \left( 1 + \varepsilon \frac{\rho_{\text{W}}}{\rho_0} + \varepsilon \frac{\nu_{\text{W}}}{\theta_0} + \varepsilon \frac{\theta_{\text{W}}}{2\theta_0} \left( c_i^2 / \theta_0 - 3 \right) \right) f_0(c), \] \hspace{1cm} (2.9)
where \( v_n^{(W)} = 0 \) because the wall is stationary with respect to the normal. The density of the wall distribution \( \rho_{\text{W}} \) follows from the requirement of zero mass flux through the wall. Throughout this paper we will use complete accommodation, that is, \( \chi = 1 \).

2.2 Channel setting

We consider a steady process in an infinitely long channel setup as depicted in Fig. 1. This setup can be viewed as a generic model geometry for many flow and heat conduction problems. In particular it already shows fundamental rarefaction effects, like parallel heat flux triggered from shear [25, 29]. The process within the channel is characterised by the specific driving forces as discussed below and the Knudsen number
\[ Kn = \frac{\tau}{\sqrt{\theta_0 L}} \] \hspace{1cm} (2.10)
based on the channel width and the BGK relaxation time scale. Rarefaction effects will be important for \( Kn \gtrsim 0.05 \).

![Figure 1: Schematic channel setup for linear shear flow and heat conduction experiments. The flow may be triggered from moving walls or external acceleration. Heat conduction is induced by different wall temperatures or external heat sources.](image)

The channel extension is along the \( x \)-direction but the fields vary only across the channel in \( y \)-direction. We assume the channel position to be symmetric with respect to the
x-axis, such that \( y \in [-L/2, L/2] \). Furthermore, we assume that the steady velocity profile points only in \( x \)-direction with component \( v_x(y) \).

Note that another popular test case is Kramers’ problem, see for example [34] which considers only a single wall and a pre-described bulk flow at infinity. This setting is strongly related to Couette flow below and the convergence and accuracy results are expected to be similar.

### 2.2.1 Shear flow

Inside the channel a flow can be generated by two effects. One effect are walls moving at different velocities which leads to plane Couette flow. The wall velocities enter the kinetic equations through the wall distribution function (2.9) of the boundary conditions. The steady flow can also be induced from an external acceleration \( a_i \). In the linearized setting of the BGK equation it suffices to model this influence as a source term

\[
S = -\varepsilon a_i \frac{\partial f_0(c)}{\partial c_i} = \varepsilon \frac{a_i c_i}{\theta_0} f_0(c)
\]

such that the transfer equation for momentum becomes

\[
\rho_0 \partial_t \tilde{v}_i + \rho_0 \partial_x \tilde{\theta} + \theta_0 \partial_x \tilde{\rho} + \partial_x \tilde{\sigma}_{ij} = \rho_0 a_i
\]

in linearized but three-dimensional form with \( \tilde{\sigma}_{ij} \) a stress tensor perturbation. The acceleration is assumed to be orientated along the channel with only non-vanishing component \( a_x \). In principle, the acceleration may depend on the variable \( y \) and act on the flow differently across the channel. In the constant case the process corresponds to acceleration-driven Poiseuille flow.

In this paper we will consider two cases of linear shear flow:

- **Couette flow** where the walls move in opposite directions with speed \( v_W^{(0,1)} = \pm \bar{v}_W / 2 \) and no acceleration is acting \( a_x = 0 \).

- **Poiseuille flow** where the walls are kept at rest \( v_W^{(0,1)} = 0 \) and the flow is accelerated by the acceleration \( a_x = a = \text{const} \) in \( y \).

To gain a better insight into channel flows based on the BGK equation Fig. 2 shows three exemplary cases of shapes of distribution function (sections at \( c_z = 0 \)) as they occur in the linearized BGK solution for Couette flow at \( Kn = 0.5 \). The walls move in opposite directions such that the velocity profile for \( v_x \) becomes point-symmetric. The left plot in Fig. 2 shows the contours of the distribution in the center of the channel where \( v_x = 0 \). At this point the flow is closest to an equilibrium distribution, but the shear \( \sigma_{xy} \) distorts the distribution function. The deviation from a Maxwellian increases towards the walls (middle and right plot in the figure) where the distribution function becomes discontinuous in velocity space. In the outer right picture the upper half of the distribution is given by the wall distribution, a Maxwellian shifted by the velocity of the wall to the right. The lower part represents particles from the interior of the channel which are in a clear non-equilibrium state.
2.2.2 Normal heat conduction

Heat conduction across the channel in normal direction can be generated from a temperature difference of the walls or an external heat source along the channel width. In the linearized setting the equations for the heat conduction problem decouple from those of the shear flow and both scenarios can be solved and investigated independently. The source term for the BGK equation has the form

\[ S = \epsilon_r \frac{r(x)}{3 \rho_0 \theta_0} \left( \frac{c_i^2}{\theta_0} - 3 \right) f_0(c) \]  

such that the transfer equation for energy reads

\[ \frac{3}{2} \rho_0 \partial_t \tilde{\theta} + \rho_0 \theta_0 \partial_i \tilde{v}_i + \partial_i \tilde{q}_i = r \]  

in the linearized but three-dimensional case with \( \tilde{q}_i \); a perturbation of the heat flux. The heating source \( r \) depends on space in general. In a nonlinear setting flow and heat conduction are coupled, for example, through the dissipation rate \( \sigma_{ij} \partial_i v_j \). When evaluated for Poiseuille flow the dissipation rate shows a parabolic shape across the channel.

In this paper we will consider two cases of linear heat conduction:

- **Heat conduction between walls** where the walls are kept at different temperature \( \theta_{W}^{(0,1)} = \theta_0 \pm \tilde{\theta}_W \) and no local heat source \( r = 0 \).
- **Poisseuille heat conduction** where the walls are kept at ground state temperature \( \theta_{W}^{(0,1)} = \theta_0 \) and the channel is heated by \( r = \alpha \gamma^2 \).

Both setting can be considered the heating analogs of the shear flow problems described above.
3 Moment approximations

We will solve the linearized BGK equation by means of moments. That is, we assume the distribution can be approximated by

\[ f_N(x,t,c) = \left( 1 + \varepsilon \varphi_N(x,t,c) \right) f_0(c), \]  

(3.1)

where \( \varphi_N \) is a polynomial in the velocity \( c \) with coefficients depending on space \( x \) and time \( t \), in general. This approach goes back to Harold Grad [8], [9]. When using spherical coordinates for the velocity \( c = cv \), with amplitude \( c \) and a direction vector from the unit sphere \( v \in S^2 \), we can write an orthonormal expansion of the polynomial as

\[ \varphi_N(x,t,c) = \sum_{n=0}^{N} \sum_{i=0}^{M_n} w_i(s) L^s_n(x,t) \left( \frac{c^2}{2\theta_0} \right)^{n+1/2} v_{i_1,\ldots,i_n}, \]  

(3.2)

with coefficients \( w_i(s) \), see [19] and [31]. These coefficients are directly related to the moments of the distribution function which is why the expansion approach is called moment approximation. In the expansion, the sum in \( n \) and \( s \) is explicit, but additionally doubled indices \( i_m \in \{1,2,3\} \) are summed over (summation convention). The upper limits of the sum will be discussed below. The tensor \( v_{i_1,\ldots,i_n} \) is constructed from the direction vector \( v \) by

\[ v_{i_1,\ldots,i_n} = v_{(i_1} v_{i_2} \cdots v_{i_n)} = \frac{(-1)^n}{(2n-1)!!} \|x\|^{n+1} \partial_{i_1} \partial_{i_2} \cdots \partial_{i_n} \left( \frac{1}{\|x\|} \right), \]  

(3.3)

where \( x \) is a position vector, see [33]. As a result \( v_{i_1,\ldots,i_n} \) is a fully symmetric and deviatoric (tracefree) tensor of \( n \)-th degree containing in total \( 2n+1 \) independent components, see [23]. When the position \( x \) in (3.3) is written in explicit spherical coordinates based on a radius and two angles, the components of \( v_{i_1,\ldots,i_n} \) can be written as a superposition of spherical harmonics. Hence, the independent components correspond to \( 2n+1 \) spherical harmonic functions at level \( n \). In view of this, the index \( N \) in (3.2) represents the highest degree of anisotropy that is modeled by the expansion. On each level \( n \) of anisotropy the radial dependence is modeled by the polynomials

\[ L^s_n(\xi) = 2^{n/2} \sqrt{\Gamma(n+\frac{3}{2})\Gamma(n+s+\frac{1}{2})} \frac{\xi^s}{n!s!} \sum_{p=0}^{\min(s, n)} (-1)^p \frac{\Gamma(n+p+3/2)}{\Gamma(n+p+3/2)} \left( \frac{s}{p} \right) \xi^{p+s/2} \]  

(3.4)

which are related to associated Laguerre polynomials.

The polynomials in (3.2) are chosen such that they satisfy an orthonormality relation of the form

\[ A_{i_1,\ldots,i_n} \int_{\mathbb{R}^3} L^s_n \left( \frac{c^2}{2\theta_0} \right) v_{i_1,\ldots,i_n} L^r_m \left( \frac{c^2}{2\theta_0} \right) v_{j_1,\ldots,j_m} f_0(c) \, dc = \begin{cases} 0 & \text{if } (n,s) \neq (m,r), \\ A_{i_1,\ldots,i_n} & \text{else}, \end{cases} \]  

(3.5)
where $A_{i_1i_2\cdots i_n}$ is an arbitrary tensor that is contracted with the $i$-indices in the integral. Due to the deviatoric nature of $v_{i_1i_2\cdots i_n}$ only the deviatoric parts of $A_{i_1i_2\cdots i_n}$ remain as indicated by the angular brackets in (3.5). For the same reason we consider the coefficients $w_{i_1i_2\cdots i_n}^{(s)}$ in the expansion (3.2) to be tracefree.

3.1 Moment variables

A concrete moment theory based on the expansion (3.2) is chosen by specifying what coefficients in the sum should be considered. This selection process is constrained by various mathematical and physical considerations. In the nonlinear setting Galilean invariance of the final system of evolution equations for the coefficients requires that if $w_{i_1i_2\cdots i_n}^{(0)}$ is included than also $w_{i_1i_2\cdots i_n}^{(n/2-p/2)}$ with $p = 0, 1, \cdots, n$ must be included [19], in order to construct a full non-tracefree moment [31]. Rotational symmetry also suggests that all components of a single tensor are included. We will follow this framework and characterize a moment theory by the tuple

$$(M_0, M_1, M_2, \cdots, M_N) \quad \text{with} \quad M_0 \geq M_1 \geq \cdots \geq M_N \quad (3.6)$$

which specifies the number $M_n$ of tensor variables selected on each level $n = 0, \cdots, N$. The resulting coefficients are obtained by projection of the distribution function with the basis functions

$$\psi(c) \in \left\{ L_{n_s}^{(n)} \left( \frac{c^2}{2\theta_0} \right) v_{i_1i_2\cdots i_n} \right\} \quad 0 \leq n \leq N, \quad 0 \leq s \leq M_n \quad (3.7)$$

as defined above such that

$$w_{i_1i_2\cdots i_n}^{(s)}(x,t) = m \int_{\mathbb{R}^3} L_{n_s}^{(n)} \left( \frac{c^2}{2\theta_0} \right) v_{i_1i_2\cdots i_n} f_N(x,t,c) \, dc. \quad (3.8)$$

This essentially defines the coefficient as moments of the distribution. The first few coefficients $w_{i_1i_2\cdots i_n}^{(s)}$ can be linked to the linearized physical quantities and we note for future reference

$$\tilde{\rho} = \rho_0 w^{(0)}, \quad \tilde{\vartheta}_i = \frac{\sqrt{\theta_0}}{\rho_0} w_i^{(0)}, \quad \tilde{\theta} = -\sqrt{\frac{2}{3}} w^{(1)}, \quad \tilde{\vartheta}_{ij} = \sqrt{2} w_{ij}^{(0)}, \quad \tilde{\vartheta}_{ij}^{(1)} = -\sqrt{\frac{5}{2}} w_i^{(1)}. \quad (3.9)$$

The set of variables can be visualized in a diagram spanning $s$ and $n$ as shown in Fig. 3, where each point represents a traceless tensor of degree $n$ with $2n+1$ independent components. The plots in the figure show two typical orderings of theories. The left diagram shows the theories in which complete moments of the type $\int c_{i_1}c_{i_2}\cdots c_{i_n} f \, dc$ are included subsequently but each split into traces and tracefree parts represented by the dots along the lines in the figure. These theories are called full moment theories. The smallest non-trivial moment system of this type is Levermore’s 10-moment-case, which considers the ten fields of density, velocity, temperature and stress deviator. Including the complete...
Figure 3: Left: All variables below and on an indicated line constitute a full moment theory where only complete tensors are considered. Right: All variables below and on an indicated line constitute an ordered moment theory where successive fluxes of fluxes are considered.

third moment gives G20, with the fourth moment G35, etc. The second diagram shows theories where the next one always includes the neglected fluxes of the previous one. These are called ordered moment theories. It starts with the conservation laws of mass, momentum and energy as equations for density, velocity and temperature and includes stress and heat flux to obtain Grad’s 13-moment-case. Including the flux variables of G13 yields G26, after which comes G45, etc. Both approaches are popular when moment methods are used, the first one for example in [15] and [17], for the second one see [23]. Fig. 3 also shows the tuple representation (3.6) of each theory. The entries in the tuples can easily be identified with the number of dots in the columns of the diagram.

Note, that there exists no statement about what ordering or what selection of moments gives especially accurate results. It is the aim of this paper to study the convergence behavior empirically to guide the way to a potentially general theory of moment approximations.

3.2 Moment equations

Inserting the ansatz (3.1) of the distribution with the expansion (3.2) into the BGK equation (2.1) and projecting subsequently with the basis functions (3.7) gives evolution equations for the coefficients of the expansion. The transport term of the kinetic equation requires the use of recursion formulas both for the generalized Laguerre function and the deviator \(v_{i_1 i_2 \cdots i_n}\) in order to simplify the expressions, see [19,23]. The final equations read

\[
\begin{align*}
\partial_t w^{(s)}_{i_1 i_2 \cdots i_n} + \sqrt{\theta_0} \frac{2n}{2n+1} \left( \sqrt{n+s+\frac{1}{2}} \partial_{(i_1} w^{(s)}_{i_2 i_3 \cdots i_n)} - \sqrt{s+1} \partial_{(i_1} w^{(s+1)}_{i_2 i_3 \cdots i_n)} \right) \\
+ \sqrt{\theta_0} \frac{2n+2}{2n+3} \left( \sqrt{n+s+\frac{1}{2}} \partial_k w^{(s)}_{i_1 i_2 \cdots i_k} - \sqrt{s} \partial_k w^{(s-1)}_{i_1 i_2 \cdots i_k} \right) \\
= \begin{cases} 
0, & \text{if } (s,n) \in \{(0,0),(1,0),(0,1)\}, \\
-\frac{1}{\tau} w^{(s)}_{i_1 i_2 \cdots i_n}, & \text{else},
\end{cases}
\end{align*}
\]  

(3.10)
for \( n = 0,1,\cdots,N \), \( s = 0,1,\cdots,M_n \) according to the definition of the theory. For better readability the source term expression is suppressed here, but discussed below. The variables \( w_{i_1i_2\cdots i_n}^{(s)} \) with \( n > N \) or \( s > M_n \) are outside the theory and therefore set to zero. As above the angular brackets denote the deviatoric part of a tensor.

It is easy to check that the first few of these equations indeed correspond to the linearized conservation laws and lower moment equations as shown e.g., in [23].

### 3.3 Moment boundary conditions

For the original regularized 13-moment equations boundary conditions have been derived and discussed in [32]. The conclusion is that relation (2.8) should be projected onto moment components with generators \( \psi(BC)(c) \) selected from the variable set which are odd in \( c \cdot n \). Integration after multiplying with such a polynomial \( \psi(BC)(c) \) gives

\[
\frac{\chi}{2-\chi} \left( \int_0^\infty \psi(BC)(c)f_{wall}(c)dc - \int_0^\infty \psi(BC)(c)f_{N}^{(even)}(c)dc \right)
\]

(3.11)

From this boundary condition for moments of the distribution function are found after inserting the distribution

\[
f_N(x,t,c) = \left( 1 + \varepsilon \sum_{n=0}^N \sum_{s=0}^{M_n} w_{i_1i_2\cdots i_n}^{(s)}(x,t) L_s(\nu) \left( \frac{c^2}{2\theta_0} \right) v_{i_1i_2\cdots i_n} \right) f_0(c)
\]

(3.12)

based on the expansion (3.2). The odd and even part of the distribution are easy to extract by selecting the terms with odd or even tensor components of the coefficients \( w_{i_1i_2\cdots i_n}^{(s)} \) when written in the wall normal frame. The final equations will give relations between the variables \( w_{i_1i_2\cdots i_n}^{(s)} \) of the moment system. We will use \( V_t = v_t - v_t^{(W)} \) for the tangential slip velocity at the wall and \( \Delta \theta = \theta - \theta_W \) for the temperature jump.

### 3.4 Regularized equations

Regularized moment equations [25] are either obtained by an expansion around a pseudo-equilibrium given by a fixed moment description or by the order-of-magnitude method [27]. For details see the text book [23]. In the current linear BGK setting based on the moment equations (3.10) both approaches yield identical results. We will only consider regularization for each ordered theory in the sense of the right-hand-side of Fig. 3. The procedure to construct the regularized equations in the context of a linearized BGK kinetic equation is as follows:

- For a given coefficient set \( W_0 \) of an ordered theory identify the coefficients \( W_1 \not\subset W_0 \) which couple to \( W_0 \). The set \( \{W_0,W_1\} \) will correspond to the ordered theory of the next level.
• According to (3.10) the equations for $W_1$ in general have the form $D(W_0, W_1, W_2) = -\frac{1}{\tau} W_1$ with some differential operator and coupling to some further coefficients $W_2$.

• Instead of setting $W_1$ to zero in the equations for $W_0$ we use the gradient expressions $W_1 = -\tau D(W_0, 0, 0)$ which approximate the equations for $W_1$.

The resulting systems of equations will be labeled R13, R26, R45, etc., according to the ordered theory they are based on. The boundary conditions necessary for a regularized theory correspond to the relations given for the ordered theory on the next level. That is, for example, the R13-equations take the same boundary conditions as the G26-equations.

4 Flow and heat test cases

4.1 Shear flow

The most relevant quantity in steady shear flow is the velocity field $v_x(y) = \sqrt{\theta_0} w^{(0)}(y)$. The coupling of the moment equations (3.10) reveals that only the tensorial components with all $y$-indices except one $x$-index are influencing the velocity field. Note, that also other tensor components, for example those with an odd number of $x$-indices larger than one, have non-trivial values triggered by the shear flow, but they do not couple back to velocity and will be ignored. Additionally, the scalar moments like density and temperature do not couple at all to the shear process in the linear case considered, so that we consider $n > 0$. As variable abbreviation we define

$$w^{(s,n)}(y) := w_{xyy \cdots y}^{(s \cdot n)}(s, n-1)$$

with $(s,n)$ according to a given moment theory and the equations for the steady process simplify to

$$\sqrt{\theta_0} \frac{2n}{2n+1} \frac{(n-1)(n+1)}{n(2n-1)} \left( \sqrt{n+s+\frac{1}{2}} \partial_y w^{(s,n-1)} - \sqrt{s+1} \partial_y w^{(s+1,n-1)} \right)$$

$$+ \sqrt{\theta_0} \frac{2n+2}{2n+3} \left( \sqrt{n+s+\frac{3}{2}} \partial_y w^{(s,n+1)} - \sqrt{s} \partial_y w^{(s-1,n+1)} \right)$$

$$= \begin{cases} \frac{a_x}{\sqrt{\theta_0}}, & \text{if } (s,n) = (0,1), \\ -\frac{1}{\tau} \omega^{(s,n)}, & \text{else}, \end{cases}$$

(4.2)

where the tracefree gradient has been simplified according to [23]. As above, all variables that are not part of the variable set will be put to zero in the equations. In the case of an acceleration-driven shear flow like Poiseuille-flow the equation for $w^{(0,1)}$ has a forcing term where $a_x$ is the $x$-component of the acceleration.
If we denote the vector of variables as $U$ the system of moment equations have the form

$$A \partial_y U = PU + S$$

(4.3)

with constant matrices $A$ and $P$ and the source vector $S$ has only one entry that may depend on $y$ in general. The matrix $A$ is symmetric and $P$ is diagonal with zero rows for the conservation laws. In Appendix A.1 we give an explicit example of the resulting system for the case of the full theory with 35 variables up to tensor fourth degree.

The complete solution of the system (4.3) consists of a particular solution to the inhomogeneous system and a homogeneous solution which is a superposition of $\exp(\pm \lambda y)$ with generalized eigenvalues $\lambda$ of the system. The integration constants are computed from symmetry constraints and boundary conditions (3.11). The solutions of this paper have been obtained explicitly with help of computer algebra software. For the boundary conditions the distribution (3.12) can be simplified in the shear flow setting using

$$w^{(s)}_{i_1 i_2 \ldots i_n} v_{i_1 i_2 \ldots i_n} = \sum_{k=0}^{n-1} \frac{(-1)^k n!}{(n-2k-1)! (2k)!} v_{i_1 y \ldots y z \ldots z}$$

(4.4)

which exploits the tracefree character of $w^{(s)}_{i_1 i_2 \ldots i_n}$ and where the components of $v_{i_1 \ldots i_n}$ can be computed with the formula in (3.3). The final distribution function to be inserted in (3.11) is given by

$$f_N(x,t,c) = \left(1 + \varepsilon \sum_{n=0}^{N} \sum_{s=0}^{M_n} w^{(s,n)} L_s^{(n)} \left(\frac{c^2}{2\theta_0} \right) \sum_{k=0}^{n-1} \frac{(-1)^k n!}{(n-2k-1)! (2k)!} v_{i_1 y \ldots y z \ldots z} \right) f_0(c).$$

(4.5)

The odd and even part (in the component normal to the wall) of this function are easily found by constructing $f_N^{(even)}$ based on only coefficients $w^{(s,n)}$ with $n$ odd and $f_N^{(odd)}$ based on only coefficients $w^{(s,n)}$ with $n$ even. Similarly for the generating function of the boundary conditions we use

$$\psi^{(BC)}(c) = \sum_{n=0}^{M_n} \sum_{s=0}^{L_s^{(n)}} \left(\frac{c^2}{2\theta_0} \right) v_{i_1 y \ldots y} \quad (n \text{ even}).$$

(4.6)

The final relations for the coefficients at the wall are computed by symbolic integration of the integrals in (3.11) based on the shear flow distribution (4.5). This is also done by use of computer algebra software. After inserting the explicit expression of the solution – particular plus homogeneous part – the solution of a linear system gives the values of the integration constants.

### 4.2 Heat conduction

The most relevant quantity in heat conduction is the temperature field $\theta(y) = \theta_0 w^{(1)}(y)$. In this case the coupling of the moment equations (3.10) reveals that only the tensorial
components with none or exclusively $y$-indices are influencing the temperature field. As above, also other tensor components are triggered to be non-zero, but do not couple to temperature themselves. These variables are not considered. The shear flow variables as discussed above entirely de-coupled from the heat conduction equations in an analogous way as vice-versa. As variable abbreviation for a heat conduction process we define

$$w^{(s,n)}(y) := w^{(s)}_y \cdot y(y)$$

(4.7)

with $(s,n)$ according to a given moment theory and the equations for the steady heat conduction process simplify to

$$\sqrt{\frac{2}{3} \frac{2n}{2n+1}} \left( \sqrt{n+s+\frac{1}{2}} \partial_y w^{(s,n-1)} - \sqrt{s+1} \partial_y w^{(s+1,n-1)} \right)$$

$$+ \sqrt{\frac{2}{3} \frac{2n+2}{2n+3}} \left( \sqrt{n+s+\frac{3}{2}} \partial_y w^{(s,n+1)} - \sqrt{s} \partial_y w^{(s-1,n+1)} \right)$$

$$= \begin{cases} \sqrt{2/3 \tau / (\rho_0 \theta_0)} / \nu, & \text{if } (s,n) = (1,0), \\ \frac{1}{\tau} w^{(s,n)}, & \text{else}, \end{cases}$$

(4.8)

which use a different simplification for the tracefree gradient than the shear flow equations due to different tensorial components. In the above equations the source term follows the description in Section 2.2. Formally, the heat conduction variables contain the density in form of $w^{(0,0)}$ and the $y$-component of velocity in form of $w^{(0,1)}$. As steady heat conduction happens at rest we set $w^{(0,1)} = 0$ which decouples the density from the rest of the variables. Hence, we may ignore the variable $w^{(0,0)}$ as well. If the field of density is of interest, it can be computed a-posteriori from the normal stress $w^{(0,2)}$ via the momentum balance. A concrete example for an explicit system of equations is given in Appendix A.2.

For the boundary conditions of the heat conduction problem the distribution (3.12) can be simplified using

$$w^{(s)}_{i_1i_2\ldots i_n} v_{i_1i_2\ldots i_n} = w^{(s,n)} \sum_{k=0}^{\frac{n}{2}} \frac{(-1)^k n!}{(n-2k)! (2k)!} v^{(s)}_y \cdot y^{(n-2k)} \cdot \cdots \cdot y^{(2k)}$$

(4.9)

which yields a distribution function analogous to (4.5). This time however, the odd and even part (in the component normal to the wall) of the distribution function are constructed such that $f^{(\text{even})}_n$ is based on only coefficients $w^{(s,n)}$ with $n$ even and $f^{(\text{odd})}_n$ is based on only coefficients $w^{(s,n)}$ with $n$ odd. Consequently, for the generating function of the boundary conditions we use

$$\psi^{(\text{BC})} (c) = L^{(n)}_a \left( \frac{c^2}{2\theta_0} \right) v_\cdot y \cdot y \cdot \cdots \cdot y (n \text{ odd}).$$

(4.10)
As above the final relations for the coefficients at the wall are computed by symbolic integration of the integrals through computer algebra software.

### 4.3 Reference solutions

Below, all four processes – Couette flow, Poiseuille flow, heat conduction between walls and Poiseuille heat conduction – will be used to study the approximation quality of moment equations. In this study the solutions are compared to reference solutions which are obtained by direct velocity space discretization.

The specialization of the linear BGK equation (2.1) with (2.4) to the channel geometry can be dimensionally reduced by projection in the \(x-z\)-velocity-plane. The result are equations for three distribution functions that only depend on \(c_y\) and partly decouple. This allows to set up a direct discretization of the linear steady BGK kinetic equation which uses only one dimensions for the velocity (\(y\)-direction) and one dimension in space. The discretization is based on second order finite differences and the final linear system of equations have been solved by a direct linear solver after assembling the matrix in sparse format. The reference solutions shown below have been computed with a 400 grid for velocity and 400 spatial grid points. A grid refinement study showed that the numerical result can be considered converged for the purposes of this paper.

### 4.4 Exemplary fields for \(Kn = 0.3\)

Before we study the convergence behavior of the moment theories based on precise error measures we present some plots of the fields to give an impression on the considered processes and considered moment theories. All simulation cases considered in this paper are dominated by Knudsen layers [23]. That is, the exponential layers that describe the relaxation of the boundary discontinuity of the distribution function towards a smoother bulk distribution are not squeezed into the wall but instead cover a significant part of the channel.

As boundary conditions and source terms we use

\[
\begin{align*}
\text{Couette:} & \quad \frac{v^{(W)}}{\sqrt{\theta_0}} = 1; \quad \text{heat conduction between walls:} \quad \frac{\theta_W}{\theta_0} = 1; \\
\text{Poiseuille:} & \quad \frac{a_x L}{\theta_0} = 1; \quad \text{Poiseuille heat conduction:} \quad \frac{\tau L}{\rho_0 \theta_0^{3/2}} = \left(\frac{y}{L}\right)^2.
\end{align*}
\]

(4.11)

We scale the \(y\)-coordinate by \(L\) such that the channel dimensions are \([-1/2,1/2]\) and use \(\rho_0\) and appropriate powers of \(\theta_0\) to scale the physical variables, like heat flux, etc. The remaining parameter in the equations is the Knudsen number \(Kn = \tau / (L \sqrt{\theta_0})\).

The top row in Fig. 4 shows the result for the velocity field \(v_x(y)\) and parallel heat flux \(q_x(y)\) in Couette flow at \(Kn = 0.3\). Only the right hand side of the channel is displayed. The velocity field is shown as difference \(\Delta v_x = v_x - v_x^{(NSF)}\) where \(v_x^{(NSF)} = C y\) is the solution of
Figure 4: Results for Couette flow (top) and heat conduction between walls (bottom) obtained from different regularized moment theories at $Kn=0.3$. The left plots show the difference of the velocity and temperature field with respect to the classical gas dynamic theory (Navier-Stokes-Fourier). The right plots show non-standard variables triggered by the rarefied setting.

classical gas dynamics with Navier-Stokes law and first order slip boundary conditions. The slope is given by $C \approx 0.57078 \cdots$. The parallel heat flux transports heat along the channel even though there is not temperature difference. This is a known rarefaction effect in channel flows, see e.g., [29, 32]. The results of regularized moment equations presented in the figure refer to the theories indicated on the right hand side of Fig. 3. The plots reveal a rather irregular and oscillatory convergence behavior.

The bottom row of Fig. 4 shows analogous results for the temperature field $\theta(y)$ and normal stress $\sigma_{yy}(y)$ in the heat conduction experiment between the channel walls at $Kn=0.3$. Again we plot the difference $\Delta \theta = \theta - \theta^{(NSF)}$ to the classical solution $\theta^{(NSF)}(y) = Cy$ based on Fourier’s law and temperature jump boundary conditions. We have $C \approx 1.03094 \cdots$. The results of the different theories show similar pattern as in the Couette case.

The test case of Poiseuille flow and Poiseuille heat conduction are more involved because the driving forces act as a local source and also varies in space for Poiseuille heat conduction. Fig. 5 shows the results for these two settings. Again we show velocity and heat flux for the shear flow and temperature and normal stress for the heat conduction. Velocity and temperature field are depicted as a whole. To gain insight into the behavior of different families of moment theories, the top row shows the results of ordered theories (right of Fig. 3) while the bottom row shows full theories (left of Fig. 3). It is interesting to
Figure 5: Results for Poiseuille flow (top) and Poiseuille heat conduction (bottom) obtained from different moment theories at \(Kn = 0.3\). The left plots show the velocity and temperature field. The right plots show non-standard variables triggered by the rarefied setting.

Note, that some moment theories give rather bad approximations even though they use a significant number of variables.

5 Approximation quality

As stated in the introduction the important question of moment approximations is, to know what moment theory gives the best result. For a fair comparison of theories with different choices of variables in the form of the tuple (3.6) we need to take into account the total number of fields or unknown coefficients. The quality of a result can only be judged in relation to the number of numerical unknowns which are available to approximate the distribution and consequently the process.

For the shear flow setting the scalar variables are irrelevant and the tuple (3.6) that defines a moment theory reduces to \((M_1, M_2, \cdots, M_N)\) with \(M_1 \geq \cdots \geq M_N\). The total number of unknowns used to generate a result for, e.g., the velocity field, is \(\sum_{j=1}^{N} M_j\) because we only use one component of each tensorial variable due to the geometry of the channel. For the heat conduction problems we use the tuple (3.6) to characterize a theory, but again only use one component per tensor. Additionally, density and normal velocity decouple from the resulting moment system and are not considered. Hence, the total number of unknowns in a theory for normal heat conduction is \(\sum_{j=0}^{N} M_j - 2\).
5.1 Empirical best approximation

If we fix the number of unknowns there remains a set of tuples \((M_0, M_1, \ldots, M_N)\) which all result in the same number of total unknowns. Essentially, this means that different coefficients in the multiple sum in (3.2) are used to represent the distribution. The question of best approximations seeks the theory with the highest accuracy given a fixed number of unknowns. While this best approximation is very hard to select a-priori in the case of moment approximations for kinetic equations, it can be checked a-posteriori or in a brute-force approach. We may select all theories yielding a given number of unknowns and compute the accuracy of the result. Obviously, this is not a practical way to find the best theory but it gives insight into the fundamental capability of moment approximations.

In the context of this paper we investigate this brute-force approach in order to gain insight into the approximation quality of moment equations. As an exemplary case Fig. 6 presents the errors of various moment theories for Couette flow at \(Kn = 0.1\) ordered by total number of unknowns between 6 and 8. The left plot shows the relative maximum error of the velocity field, on the right hand side the relative maximum error of the parallel heat flux is displayed. Each dot represents the error in the respective field produced by a specific theory and each dot is labeled with a tag of the form \((M_1, \ldots, M_N)\) characterizing the moment theory used. The blue dot marks the full theory corresponding to G35, while the green dot gives the errors of the order theory G45. Note, that the first entry \(M_0\) is dropped from the tuples as scalar variables are not considered in Couette flow.

The figure implies that the approximation quality depends strongly on the choice of moments. Furthermore, a moment theory that gives high accuracy for velocity may not be very accurate in heat flux. Unfortunately, there is apparently no pattern arising after which the best theory could be constructed empirically. However, this brute force approach gives in principle the best error that is achievable for velocity and heat flux when choosing from any moment theory with a certain number of unknowns. This best approximation error is computed for all processes considered in this paper and will be an important threshold for the investigation of different families of theories below.

![Figure 6: Error distribution for different moment approximations at fixed total number of unknowns for the Couette flow setting at \(Kn = 0.1\).](image-url)
5.2 Convergence behaviour

We will now restrict our attention to the errors of the families of full, ordered and regularized theories separately for Couette flow, heat conduction between walls, Poiseuille flow and Poiseuille heat conduction.

An overview of the moment theories considered is given in Fig. 7. We will consider only relatively small theories, hence focuses on the quality of coarse approximations. The first two tables show the two families of full and ordered theories under their name $G_{xy}$ where $xy$ is the number of three-dimensional fields. For the shear flow and heat conduction processes this number reduces to a smaller number of unknowns listed in the respective columns of the table. The regularized theories of Section 3.4 in the right table can further be reduced to equations using only those number of unknowns as indicated in the brackets. As a result a regularized theory $R_{xy}$ contains more variables as the corresponding ordered theory $G_{xy}$, but the equations are less complex than those of the next higher ordered theory. For instance, $R_{13}$ is obtained from the $G_{26}$ theory using 5 equations, but the resulting system can be reduced to a smaller system with only 3 equations, which however is more complex than the $G_{13}$ system. In order to allow a comparison with full and ordered theories we define the total number of unknowns of a regularized theory as the average of the number of unknowns of the two encapsulating ordered theories, that is, the average of the two numbers in the entries of the right table in Fig. 7.

![Figure 7: The table shows the effective number of equations of the various theories when specialized to shear flow or heat conduction processes.](image)

All errors will be relative maximum errors which have been scaled with respect to the maximum norm of the respective field of the reference solution.

**Couette Flow:** Fig. 8 shows the relative maximum errors of the three families of moment theories obtained in the case of Couette flow at $Kn = 0.1$ and $Kn = 0.5$. We present the errors of velocity and parallel heat flux separately in the left and right column of the
Figure 8: **Couette Flow.** Convergence behavior for different theories for velocity (left) and heat flux (right) at $Kn = 0.1$ (top) and $Kn = 0.5$ (bottom) for various number of unknowns (x-axis). The black line indicates the best errors achievable by any moment theory for the respective field and given number of unknowns.

The ordered theory with three unknowns corresponds to G13 which considers the velocity, shear stress and parallel heat flux as variables. The solution is equivalent to the solution of classical gas dynamics with the law of Navier-Stokes. The smallest full theory is G20 using four unknowns and includes besides velocity, shear and heat flux also the traceless part of the third moment tensor (related to $w_{ijk}^{(0)}$). R13 is the first regularized theory at four unknowns, which considers velocity, shear, heat flux and simplified equations for both the traceless part of the third moment and of the first trace of the fourth moment (related to $w_{ij}^{(1)}$).

Each plot of Fig. 8 also shows a black line which gives the error of the respective best approximation obtained by a brute-force approach. For a given number of unknowns all shear flow moment theories given by variable tuples $(M_1,\ldots,M_N)$ satisfying $M_1 \geq \cdots \geq M_N$ with the same number of total unknowns are searched for the result with the smallest error for the considered Knudsen number and field. Note, that the theory producing an optimal result at a given number of unknowns may vary between the plots of Fig. 8.
Figure 9: Heat conduction between walls. Convergence behavior for different theories for temperature (left) and normal stress (right) in at $Kn = 0.1$ (top) and $Kn = 0.5$ (bottom) for various number of unknowns ($x$-axis). The black line indicates the best errors achievable by any moment theory for the respective field and given number of unknowns.

Heat Conduction Between Walls: Fig. 9 presents the relative maximum errors of the moment theories for the case of heat conduction between channel walls kept at different temperatures. As above the top row shows the results at $Kn = 0.1$, the bottom row results at $Kn = 0.5$ and use the families from the table in Fig. 7. For the heat conduction problem we show the errors of the temperature field on the left and the normal stress component on the right of the figure.

In the case of heat conduction the smallest ordered theory G13 with three unknowns considers the fields of temperature, normal heat flux and normal stress. The result of G13 is equivalent to the classical gas dynamics case with Fourier’s law. The smallest full theory is G20 which uses the four variables temperature, normal heat flux, normal stress and tracefree third moment tensor. The first regularized theory R13 is located between G13 and G26 using temperature, normal heat flux, normal stress as well as a simplified equation for the tracefree part of the third moment tensor and of the first trace of the fourth moment as above.

The black line for the best approximation error has been obtained based on the heat conduction moment equations and a brute-force search. As above what theory gives the best result depends on the Knudsen number and field quantity considered.
Figure 10: Poiseuille flow. Convergence behavior for different theories for velocity (left) and heat flux (right) in at $Kn = 0.1$ (top) and $Kn = 0.5$ (bottom) for various number of unknowns (x-axis). The black line indicates the best errors achievable by any moment theory for the respective field and given number of unknowns.

Poiseuille Flow: Fig. 10 shows result of the shear flow moment system but this time for the Poiseuille flow setting. The general layout for the figure is identical to Fig. 8 with results for $Kn = 0.1$ and $Kn = 0.5$ showing velocity and heat flux errors for the theories of Fig. 7. The best approximation errors are re-computed for the Poiseuille setting.

Note, that the errors computed for the regularized theories tend to drop slightly below the optimal line in some of the plots of Fig. 10. This is due to the fact that these theories are hybrid constructions between two ordered theories and the number of unknowns is arbitrarily computed as the average of the two order theories. When computing the best approximation only moment theories that fit in the standard frame are considered. Hence, regularized theories may show slightly smaller errors.

Poiseuille Heat Conduction: The last convergence investigation is presented in Fig. 11 and considers heat conduction based on a quadratic local source. This problem corresponds to the heat conduction due to dissipation from a Poiseuille channel flow. The plots in the figure correspond to those shown in Fig. 9 with Knudsen numbers and fields remaining the same.

Due to the local variation of the source this process poses the strongest difficulties to moment approximations. This results also in strong differences in the results of different
Figure 11: Poiseuille heat conduction. Convergence behavior for different theories for temperature (left) and normal stress (right) in at $Kn = 0.1$ (top) and $Kn = 0.5$ (bottom) for various number of unknowns ($x$-axis). The black line indicates the best errors achievable by any moment theory for the respective field and given number of unknowns.

moment theories. Consequently, plot ranges for the errors especially for the rarefaction variable in Fig. 11 is larger than in the previous plots.

5.3 Discussion

All error plots in the figures above show a similar irregular or oscillatory convergence behavior for all considered families of moment theories. However, despite the oscillatory errors there is a clear tendency to be observed in all cases, which indicates that all moment theories considered converge eventually if only enough variables are included. Studies involving larger moment systems (not shown in this paper) confirm that the oscillatory convergence is persistent, but the error decreases with higher numbers of variables. In other words, moment approximation are capable to describe processes which are entirely dominated by Knudsen layers. The remaining challenge is to obtain an accurate result with as few moment variables as possible. For this, the irregularities in the errors are a major obstacle which need to be studied in detail.

The oscillations in the convergence are most pronounced in the heat flux of Couette flow where very accurate and rather poor results interchange in all moment theories. The behavior is slightly less pronounced in the heat conduction cases except for the full
theories (blue triangles) in the Poiseuille heat conduction of Fig. 11. Note, however, that there is no persisting rule which theory gives the more accurate result. While in the Poiseuille heat conduction G20 performs much better than G35 it is the other way around in Couette flow in Fig. 8. The reason for the oscillation is hidden in the mathematical structure of the moment equations, but difficult to pin-point. Further research is needed to investigate this behavior.

Another obvious implication of the results presented in Figs. 8 through 11 is that the fluid dynamic quantities like velocity or temperature show much smaller relative error than the non-standard variables like parallel heat flux and normal stress. However, this is mainly due to the relatively large values of temperature and velocity in the reference solutions in the order $O(1)$, while both parallel heat flux and normal stress are $O(Kn^2)$ in the above processes. Still, the errors show that, for example, for a Couette flow at $Kn=0.5$ very few moment variables are able to provide a relative error of 10% for the velocity profile, which means halfening the error of the classical gas dynamic result. Still, the rarefaction effects are important features especially in relevant quantities like heat flux and stress tensor and they can be accurately reproduced as well. It is the small reference value that leads to large relative values of the error. Note, that qualitative aspects of the rarefaction effects are easily covered as visible in the field plots of Figs. 4 and 5.

Interestingly, the errors of the best approximation in each process show a rather monotone behavior and provide very good accuracy already at very low numbers of unknowns. As discussed above the best approximation depends strongly on the process and the field to be approximated. Hence, it is impressive to see that some moment families like full or ordered theories achieve nearly optimal errors. For example, the R13 theory gives almost optimal results for Couette flow, heat conduction between walls and Poiseuille flow. That is, there seems to exist no moment theory with equally few number of unknowns that give better errors. The accuracy may be considered low for some realistic applications, but given the extremely low number of just four or five variables to approximate a two or three dimensional distribution function, the accuracy can be considered a remarkable achievement. Only for the Poiseuille heat conduction case the R13 theory gives a rather weak performance. This must be attributed to the spatially varying source term which leads to an inhomogeneous solution that couples to rather high moment variables due to the hierarchical structure of the equations. Hence, more variables are needed to approximate accurately.

The Figs. 8-11 also show that at larger numbers of unknowns the regularized theories exhibit an approximation behavior similar to the ordered theories which served to derive them. While at low number of unknowns it seems beneficial to extend the ordered theory for example from G13 to R13, the improvement becomes less significant at higher levels. The similarities between ordered and regularized theories are most prominent in the case of Poiseuille heat conduction where the full theories follow a totally different approximation behavior. In particular, the G20 theory with only four unknowns performs very well. However, such a performance of this theory is absent in the other processes considered.
6 Conclusion

The paper presented an empirical convergence study for one-dimensional boundary value problems for the Boltzmann-BGK equation based on moment approximations. In particular, we considered channel flow of Couette and Poiseuille type as well as heat conduction between heated walls and heat conduction due to a locally varying source. It was shown that moment equations are able to compute these Knudsen-layer dominated processes accurately provided a sufficient number of moments are considered in the approximation.

When considering relatively low order approximations the results of the paper show a very irregular convergence pattern, for example, for the classical families of moment equations which consider only full moment tensors. At coarse approximation levels the choice of moment variables strongly influences the accuracy of the solution. At the same time a best approximation which gives the smallest error at a given number of variables can be found by 'brute force'. This best approximation indeed shows a rather fast and almost monotonic convergence for a particular set of moment equations. Based on these lower bounds for the error the results show that some cases of classical moment families are able to give nearly optimal results in the sense that a smaller error can not be achieved with the same number of variables.

A challenging future task is to find an empirical rule or mathematical theory how to select the best set of moment variables a-priori for a given process.

A Example: 35 moment case

In order to clarify the structure of the moments systems used in the paper we discuss the specific case using 35 fields (G35). This theory uses at most a tensor degree of 4 and is characterized by

\[(M_0, M_1, M_2, M_3, M_4) = (3, 2, 2, 1, 1)\]

(A.1)

given by Section 3.1. The moment generating functions are given by

\[
\begin{align*}
L_0 & = (v_i, L_1^{(0)} (2) (2 \theta_0 v_i), L_1^{(1)} (2) (2 \theta_0 v_i) \nu_{ij}, L_1^{(2)} (2) (2 \theta_0 v_i) \nu_{ijk}, L_1^{(0)} (2) (2 \theta_0 v_i) \nu_{ijkl}) \\
& = \left(1, \frac{3 \theta_0 - c^2}{\sqrt{6} \theta_0}, \frac{c^4 - 10 c^2 \theta_0 + 15 \theta_0^2}{\sqrt{12} \theta_0^2}, \frac{c_i}{\sqrt{\theta_0}}, \frac{5 \theta_0 - c^2}{\sqrt{10} \theta_0^{3/2}}, \frac{c_{ij}}{\sqrt{2} \theta_0}, \frac{\nu_{ij}}{\theta_0}, \frac{c_{ijk}}{\sqrt{6} \theta_0^{7/2}}, \frac{c_{ijkl}}{\sqrt{24} \theta_0^2}\right)
\end{align*}
\]

(A.2)
following the definition (3.7), which yields the 35 variables
\[
\left( w^{(0)}, w^{(1)}, w^{(2)}, w^{(0)}_x, w^{(1)}_x, w^{(1)}_y, w^{(0)}_{ij}, w^{(0)}_{ijkl} \right). \tag{A.3}
\]

Note that all higher degree tensors are symmetric and tracefree which gives 5, 7, and 9 entries for a tensor of degree 2, 3, and 4, respectively. We give the equations for this theory in case of the two specific cases of shear flow and heat conduction.

### A.1 Shear flow

As explained in Section (4.1) the scalar fields \( w^{(0)}, w^{(1)} \) are not relevant to compute the velocity field in channel shear flow. Hence, the theory can be characterized by the tuple \( (2,2,1,1) \) dropping the entry for the scalar variables. This notation is used in Fig. 6. The 35 fields reduce to six variables
\[
\left( w^{(0)}, w^{(1)}, w^{(2)}, w^{(3)}, w^{(4)} \right) = \left( w^{(0)}_x, w^{(1)}_x, w^{(1)}_y, w^{(0)}_{xy}, w^{(0)}_{xxy}, w^{(0)}_{xxyy} \right) \tag{A.4}
\]

which follow from the components of the basis functions
\[
\begin{pmatrix}
    c_x \sqrt{\frac{1}{\theta_0}}, & c_x \frac{5(\theta_0 - c^2)}{\sqrt{10\theta_0^{3/2}}}, & c_x c_y \frac{5(\theta_0 - c^2)}{\sqrt{2\theta_0}}, & c_x \frac{7(\frac{c^2}{2} - c^2)}{\sqrt{28\theta_0}}, & c_x c_y \frac{7(\frac{c^2}{2} - 3c^2)}{5\sqrt{6\theta_0^{3/2}}}, & c_x c_y \frac{7(\frac{c^2}{2} - 3c^2)}{7\sqrt{24\theta_0^{3/2}}}
\end{pmatrix}. \tag{A.5}
\]

They satisfy the moment equations
\[
\sqrt{\frac{14}{5}} \theta_0 \partial_y w^{(0)}, w^{(1)} - \sqrt{\frac{14}{5}} \theta_0 \partial_y w^{(0),2} = -\frac{1}{\tau} w^{(1),1}, \tag{A.6}
\]
\[
\sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} - \sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} = -\frac{1}{\tau} w^{(0),2}, \tag{A.7}
\]
\[
\sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} - \sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} = -\frac{1}{\tau} w^{(0),2}, \tag{A.8}
\]
\[
\sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} - \sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} = -\frac{1}{\tau} w^{(0),2}, \tag{A.9}
\]
\[
\sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} - \sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} = -\frac{1}{\tau} w^{(0),2}, \tag{A.10}
\]
\[
\sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} - \sqrt{\frac{14}{5}} \partial_0 \partial_y w^{(0),1} = -\frac{1}{\tau} w^{(0),2}, \tag{A.11}
\]
as given in (4.2). The first equation corresponds to the \( x \)-component of the conservation law of momentum. The coefficient matrix has the form
\[
A = \sqrt{\theta_0} \begin{pmatrix}
0 & 0 & 1.41 & 0 & 0 & 0 \\
0 & 0 & -0.89 & 1.67 & 0 & 0 \\
0.71 & -0.45 & 0 & 0 & 1.73 & 0 \\
0 & 0.84 & 0 & 0 & -0.93 & 0 \\
0 & 0 & 0.92 & -0.49 & 0 & 2 \\
0 & 0 & 0 & 0 & 1.07 & 0
\end{pmatrix}. \tag{A.12}
\]
which is structurally symmetric and the upper triangular part is roughly twice the lower triangular part. This structure is also present for all larger moment systems for shear flow. The matrix $P$ of the system (4.3) is a matrix with $-1/\tau$ on the diagonal except of the first row which is zero. The source vector $S$ contains only the force $\sqrt{\theta_0 a_x}$ in the first entry.

The distribution function based on these six variables has the form

$$f_N(y, c) = \left( 1 + \frac{c_x}{\sqrt{\theta_0}} w^{(0,1)} + \frac{5\theta_0 - c^2}{\sqrt{10\theta_0^{3/2}}} c_x w^{(1,1)} + \sqrt{2} \frac{c_x c_y}{\theta_0} w^{(0,2)} + \frac{7\theta_0 - c^2}{\sqrt{7\theta_0^2}} c_x c_y w^{(1,2)} + \sqrt{\frac{3}{2}} \left( c_y^2 - c_z^2 \right) \frac{c_x}{\theta_0^{3/2}} w^{(0,3)} + \sqrt{\frac{7}{3}} \left( c_y^2 - 3c_z^2 \right) \frac{c_x c_y}{\theta_0} w^{(0,4)} \right) f_0(c)$$

which follows from (4.5). To obtain boundary conditions for the theory the part of this distribution even in the velocity normal to the wall $c_y$, that is, without the terms with $w^{(0,2)}, w^{(1,2)}$ and $w^{(0,4)}$ needs to be inserted into (3.11) and the integration is conducted using the basis function odd in $c_y$, that is,

$$\psi_{BC}(c) = \left\{ \frac{c_x c_y}{\sqrt{2\theta_0}}, \frac{c_x c_y \left( 7\theta_0 - c^2 \right)}{\sqrt{28\theta_0^2}}, \frac{c_x c_y \left( 7c_y^2 - 3c^2 \right)}{7\sqrt{24\theta_0^2}} \right\}$$

resulting in three boundary conditions for each wall.

### A.2 Heat conduction

Following Section 4.2 the G35 moment theory for heat conduction uses the seven variables

$$\left( w^{(1,0)}, w^{(2,0)}, w^{(1,1)}, w^{(0,2)}, w^{(1,2)}, w^{(0,3)}, w^{(0,4)} \right) = \left( w^{(1)}, w^{(2)}, w^{(y)}, w^{(y)}, w^{(yy)}, w^{(yy)}, w^{(yyy)} \right),$$

where density and velocity have been dropped. The corresponding components of the basis functions are given by

$$\left( \frac{3\theta_0 - c^2}{\sqrt{6\theta_0}}, \frac{c^4 - 10c^2\theta_0 + 15\theta_0^2}{\sqrt{120\theta_0^3}}, \frac{5\theta_0 - c^2}{\sqrt{10\theta_0^{3/2}}} c_y, \frac{3c_y^2 - c^2}{3\sqrt{2\theta_0}}, \frac{7\theta_0 - c^2 (3c_y^2 - c^2)}{3\sqrt{28\theta_0^2}}, \frac{5(c_y^2 - 3c_z^2)}{5\sqrt{6\theta_0^{3/2}}} c_y, \frac{35c_y^4 - 30c_y^2c^2 + 3c^4}{35\sqrt{24\theta_0^2}} \right)$$
and the equations read
\[
\sqrt{\frac{5}{3}} \theta_0 \partial_y w^{(1,1)} = -\sqrt{\frac{2}{3}} \frac{\rho_0}{\theta_0} \tau(y),
\] (A.14)
\[
- \sqrt{\frac{4}{5}} \theta_0 \partial_y w^{(1,1)} = -\frac{1}{\tau} w^{(2,0)},
\] (A.15)
\[
- \frac{4}{5} \sum \theta_0 \partial_y w^{(0,2)} + \sqrt{\frac{5}{3}} \sum \theta_0 \partial_y w^{(1,0)} + \sqrt{\frac{14}{5}} \sum \theta_0 \partial_y w^{(1,2)} + \sqrt{\frac{4}{3}} \sum \theta_0 \partial_y w^{(2,0)} = -\frac{1}{\tau} w^{(1,1)},
\] (A.16)
\[
\sqrt{3} \sum \theta_0 \partial_y w^{(0,3)} - \sqrt{\frac{16}{45}} \sum \theta_0 \partial_y w^{(1,1)} = -\frac{1}{\tau} w^{(0,2)},
\] (A.17)
\[
- \frac{6}{7} \sum \theta_0 \partial_y w^{(0,3)} + \sqrt{\frac{56}{45}} \sum \theta_0 \partial_y w^{(1,1)} = -\frac{1}{\tau} w^{(1,2)},
\] (A.18)
\[
\sqrt{\frac{27}{25}} \sum \theta_0 \partial_y w^{(0,2)} + 2 \sqrt{\frac{17}{5}} \sum \theta_0 \partial_y w^{(0,4)} - \sqrt{\frac{54}{175}} \sum \theta_0 \partial_y w^{(1,2)} = -\frac{1}{\tau} w^{(0,3)},
\] (A.19)
\[
\frac{8}{7} \sqrt{\frac{1}{\theta_0}} \partial_y w^{(0,3)} = -\frac{1}{\tau} w^{(0,4)},
\] (A.20)

based on the coefficient matrix

\[
A = \sqrt{\theta_0} \begin{pmatrix}
0 & 0 & 1.29 & 0 & 0 & 0 & 0 \\
0 & 0 & -1.15 & 0 & 0 & 0 & 0 \\
1.29 & -1.15 & 0 & -0.89 & 1.67 & 0 & 0 \\
0 & 0 & -0.59 & 0 & 0 & 1.73 & 0 \\
0 & 0 & 1.12 & 0 & 0 & -0.93 & 0 \\
0 & 0 & 0 & 1.04 & -0.56 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 & 1.14 & 0 \\
\end{pmatrix}
\] (A.21)

which shares similar properties as the matrix in the shear case. Based on (4.9) the distribution function for heat conduction reads

\[
f_N (y, c) = \left(1 + \frac{c^2 - 3 \theta_0}{\sqrt{6 \theta_0}} w^{(1,0)} + \frac{c^4 - 10 c^2 \theta_0 + 15 \theta_0^2}{\sqrt{120 \theta_0^2}} w^{(2,0)} + \frac{5 \theta_0 - c^2}{\sqrt{10 \theta_0^{3/2}}} c_y w^{(1,1)} + \frac{c^2 - c_y^2}{\theta_0 \sqrt{2}} w^{(0,2)} \right)
\]
\[
+ \frac{7 \theta_0 - c^2}{2 \sqrt{\theta_0^2}} (c_y^2 - c_z^2) w^{(1,2)} + \frac{c_y^2 - 3 c_z^2}{\sqrt{6 \theta_0^{3/2}}} c_y w^{(0,3)} + \frac{c_y^4 - 6 c_y^2 c_z^2 + c_z^4}{\sqrt{24 \theta_0^2}} w^{(0,4)} \right) f_0 (c)
\]

of which the even part containing the terms with \(w^{(1,0)}\), \(w^{(2,0)}\), \(w^{(0,2)}\), \(w^{(0,4)}\), and \(w^{(0,4)}\) is used for the boundary conditions. In this case the odd basis functions for integration are given by

\[
\psi_{BC} (c) = \left\{ \begin{array}{c}
\frac{5 \theta_0 - c^2}{\sqrt{10 \theta_0^{3/2}}} c_y \left( 5 c_y^2 - 3 c_z^2 \right) \\
\frac{5 \theta_0 - c^2}{\sqrt{10 \theta_0^{3/2}}} c_y \left( 5 c_y^2 - 3 c_z^2 \right) \\
\end{array} \right\}
\] (A.22)

which implies only two boundary conditions on each wall. In fact, the coefficient matrix has three zero eigenvalues and more boundary conditions are not required.
References


