On the Holway-Weiss Debate: Convergence of the Grad-Moment-Expansion in Kinetic Gas Theory

Zhenning Cai
Department of Mathematics,
National University of Singapore,
10 Lower Kent Ridge Rd, Singapore 119076, Singapore,
matcz@nus.edu.sg

Manuel Torrilhon
Center for Computational Engineering Science,
RWTH Aachen University,
Schinkelstr. 2, 52062 Aachen, Germany,
torrilhon@rwth-aachen.de

(2019)

Abstract
Moment expansions are used as model reduction technique in kinetic gas theory to approximate the Boltzmann equation. Rarefied gas models based on so-called moment equations became increasingly popular recently. However, in a seminal paper by Holway [Phys. Fluids 7/6, (1965)] a fundamental restriction on the existence of the expansion was used to explain sub-shock behavior of shock profile solutions obtained by moment equations. Later, Weiss [Phys. Fluids 8/6, (1996)] argued that this restriction does not exist. We will revisit and discuss their findings and explain that both arguments have a correct and incorrect part. While a general convergence restriction for moment expansions does exist, it cannot be attributed to sub-shock solutions. We will also discuss the implications of the restriction and give some numerical evidence for our considerations.

1 Introduction

Rarefied gas dynamics is encountered in a number of modern technological fields such as high-altitude spacecrafts and microelectromechanical systems, and the modeling of rarefied gases has been of interest for more than one century. It is generally agreed that the Boltzmann equation, the fundamental equation in gas kinetic theory [8], provides an accurate description for rarefied gases in most applications. However, simulations using the Boltzmann equation require to solve a six-dimensional distribution function, which is computationally expensive and often unaffordable. Therefore, researchers have been trying to derive cheaper models from the Boltzmann equation by model reduction. A classical approach is the moment method, which was first introduced to gas kinetic theory by H. Grad in [11]. Grad suggested to expand the distribution function in velocity space using orthogonal polynomials with the local Maxwellian as the weight function, and derived a 13-moment model by a truncation of such expansion.

In the past three decades many successful results in the modeling of rarefied gases could be obtained based on Grad’s approximation. Starting with the close relation to phenomenological extended thermodynamics (ET), Grad’s moment equations were used to compute sound waves, light scattering and shock profiles in the context of ET, see [19]. The regularized theory of [22] allows to formulate consistent boundary conditions [13, 27] based on Grad’s distribution. This leads to the successful application of Grad’s moment equations to a variety of boundary
value problems \cite{25}. Recently, Grad’s distribution has also been used with very high number of moments such that moment equations become a numerical technique to solve the Boltzmann equation efficiently and accurately \cite{5, 26}.

In the early days of Grad’s theory it was far from obvious that the theory was actually useful. In \cite{11} H. Grad reports about artefacts in the shock profile computation obtained with his 13-moment-equations and concludes that the new equations do not show significant improvement over classical theories. The seminal paper of Holway \cite{15} links the shock artefacts to a mathematical statement about the general convergence of moment expansions and concludes that moment equations cannot be used beyond a certain shock strength given by a critical Mach number. However, W. Weiss computed smooth shock profiles beyond the critical Mach number in \cite{28} and subsequently published a paper \cite{29} in which he disproves the statement of Holway about the usefulness of moment equations in shock waves.

In recent years computations of the authors of this paper made it clear that the Holway-Weiss-debate deserves to be revisited, because the current representation in the literature is highly misleading. After introducing the foundations of Grad’s expansion in Sec. 2 we will carefully reframe the argument of Holway in Sec. 3 and discuss in detail in Sec. 3.2 what is right or wrong in both Holway’s statement and Weiss’ rebuttal. In Sec. 4 we discuss the consequences of the argument for nowadays moment models and give some numerical examples.

2 Basic Functional Analysis of the Grad Expansion

Given the density $\rho$, velocity vector $v_i$ and temperature $\theta$ (in energy density units) of the gas the simplest approximation for the underlying distribution function is to assume equilibrium. The Maxwell distribution for the particle velocities $c_i$

\[
    f_{eq}(c) = \frac{\rho/m}{(2\pi \theta)^{3/2}} \exp \left( -\frac{(c_i - v_i)^2}{2\theta} \right)
\]

then gives a distribution that fits the density, velocity and temperature. Here $m$ denotes the mass of a single gas molecule. For more general situations H. Grad proposed in 1949 to use an expansion which in the simplest form reads

\[
    f_{G}(M)(c) = \sum_{|\alpha|=0}^{M} \lambda_{\alpha} c^{\alpha} f_{eq}(c)
\]

and became known as the Grad distribution. The indices $\alpha$ represent multi-indices such that $c^{\alpha}$ are multi-variate monomials up to degree $M$ and the coefficients $\lambda_{\alpha}$ parametrize the distribution. They are computed from the consistency requirement

\[
    u_{\alpha} = \int_{\mathbb{R}^d} c^{\alpha} f_{G}^{(M)}(c) dc \quad |\alpha| = 0, 1, \ldots, M
\]

with given moments $u_{\alpha}$. Using this technique it is possible to reconstruct an approximation to the velocity distribution whenever a set of moments is known. For instance this approximative distribution $f_{G}^{(M)}$ can be used to close the transfer equations of the $u_{\alpha}$ obtained from the Boltzmann equation which gives Grad’s moment equations.

2.1 Best Approximation

When using orthogonal polynomials instead of monomials the mathematical analysis of the Grad expansion becomes easier. In fact, the Grad distribution represents a best approximation in an appropriate subspace. We recall the following basic theorem, a variant of which could be found, e.g., in \cite{9}.
Theorem (Best Approximation). Consider the weighted space \( V_\omega := L^2(\mathbb{R}^d; \mathbb{R}, \omega \, dc) \) with scalar product

\[
\langle f, g \rangle_\omega = \int_{\mathbb{R}^d} f(c)g(c)\omega(c)dc
\]

for functions on \( \mathbb{R}^d \), and a set of \( \omega \)-orthonormal functions \( U_M = \{ \Psi_\alpha \}_{|\alpha|=0,1,\ldots,M} \subset V_\omega \). For any function \( f \) with \( \| f \|_\omega < \infty \) we find the unique best approximation

\[
f^{(M)} = \sum_{|\alpha|=0}^{M} \langle \Psi_\alpha, f \rangle_\omega \Psi_\alpha = \arg\min_{f^* \in \text{span} \, U_M} \| f - f^* \|_\omega
\]

in the subspace spanned by \( U_M \).

In the Grad expansion the coefficients of \( f^{(M)}_G \) are moments of \( f \) which requires the choice \( \Psi_\alpha(c) = \psi_\alpha(c)\omega(c)^{-1} \) with polynomial functions \( \psi_\alpha(c) \) in order to find

\[
w_\alpha = \langle \Psi_\alpha, f \rangle_\omega = \int_{\mathbb{R}^d} \psi_\alpha(c)f(c)dc \quad \Rightarrow \quad f^{(M)}_G(c) = \sum_{|\alpha|=0}^{M} w_\alpha \psi_\alpha(c)\omega(c)^{-1}
\]

for the expansion. The natural choices for the inverse \( \omega(c)^{-1} \) is a local Maxwellian \( f_{\text{eq}} \) with density \( \rho \), velocity \( v_i \), and temperature \( \theta \) obtained from the respective local distribution \( f \). For more insight into how Grad’s expansion is used in modern gas modeling we refer to the textbook [21]. The polynomial functions \( \psi_\alpha(c) \) satisfy the orthogonality condition

\[
\langle \Psi_\alpha, \Psi_\beta \rangle_\omega = \int_{\mathbb{R}^d} \psi_\alpha(c)\psi_\beta(c)f_{\text{eq}}(c)dc = \begin{cases} 1 & \alpha = \beta \\ 0 & \text{else} \end{cases}
\]

such that they are nothing but Hermite polynomials with the Gaussian of the local equilibrium distribution as weight. The weighted functions \( \Psi_\alpha = \psi_\alpha \omega^{-1} = \psi_\alpha f_{\text{eq}} \) are sometimes called Hermite functions.

The following theorem is the reason for a fundamental condition for the existence of a Grad expansion.

Theorem (Completeness). The infinite set of Hermite functions \( \{ \Psi_\alpha \}_{\alpha \in \mathbb{N}^d} \) form a complete orthogonal basis of the weighted space \( V_\omega \) with \( \omega = f_{\text{eq}}^{-1} \).

This statement means any function \( f \in V_\omega \) with \( \omega = f_{\text{eq}}^{-1} \) can be represented through a Grad expansion and vice versa. Hence, if \( f \) is to be represented as an infinite Grad expansion, necessarily \( \| f \|_\omega < \infty \) must hold.
2.2 Restrictions on the Distribution

The condition $\|f\|_\omega < \infty$ leads to

$$\int_{R^d} \left( f f^{-1/2}_{eq} \right)^2 dc < \infty,$$

hence the decay rate of $f$ must be faster than that of $f^{1/2}_{eq}$. In other words, if we let $\theta^{(\text{tail})}$ be the tail temperature of $f$ such that

$$f(c) \leq R \exp \left( -\frac{c^2}{2\theta^{(\text{tail})}} \right) \quad \text{for} \ |c| > r$$

with some constants $R$ and $r$, then for $\theta$ being the actual temperature of $f_{eq}$ implied by $f$,

$$\theta^{(\text{tail})} < 2\theta$$

must hold. In physical terms this means that the fast particles in the tail of the distribution should not be hotter than twice the average of all particles in the distribution.

2.3 Convergence Failure

However, (10) does not always hold. One typical example of distributions that may violate (10) is the superposition of two Gaussians:

$$f(c) = \frac{\rho_1/m}{(2\pi\theta_1)^{3/2}} \exp \left( -\frac{|c - v_1|^2}{2\theta_1} \right) + \frac{\rho_2/m}{(2\pi\theta_2)^{3/2}} \exp \left( -\frac{|c - v_2|^2}{2\theta_2} \right).$$

The velocity and temperature of such a distribution function can be calculated directly:

$$v = \frac{\rho_1 v_1 + \rho_2 v_2}{\rho_1 + \rho_2}, \quad \theta = \frac{\rho_1 \theta_1 + \rho_2 \theta_2}{\rho_1 + \rho_2} + \frac{\rho_1 \rho_2 |v_1 - v_2|^2}{3(\rho_1 + \rho_2)^2}.$$

Suppose $\theta_1 < \theta_2$. Then the tail of this distribution function is governed by Maxwellian with temperature $\theta_2$. However, by (12), we can see that by decreasing $\rho_2$, the value of $\theta$ can be set to be arbitrarily close to $\theta_1$. This means that when $\theta_2 > 2\theta_1$, for any given $v_1$ and $v_2$, we can always choose $\rho_2 \ll \rho_1$ such that (10) does not hold, leading to the divergence of the Grad expansion.

Such an example is of interest since it comes from the Mott-Smith bimodal theory for the steady shock structure problem \[18\]. In such a theory, one considers a plane shock wave with...
Mach number $Ma$, and it is assumed that the distribution function takes the form (11) everywhere, with the following dimensionless parameters:

$$\rho_1 = 1 - \kappa,$$  
$$\mathbf{v}_1 = \left(\sqrt{5/3}Ma, 0, 0\right)^T,$$  
$$\theta_1 = 1,$$  
$$\rho_2 = \kappa \frac{4Ma^2}{Ma^2 + 3},$$  
$$\mathbf{v}_2 = \left(\sqrt{\frac{5}{3}} \frac{Ma^2 + 3}{4Ma}, 0, 0\right)^T,$$  
$$\theta_2 = \frac{(5Ma^2 - 1)(Ma^2 + 3)}{16Ma^2},$$

where $\kappa \in [0, 1]$ varies with spatial location. To illustrate the divergence, we present in Fig. 1 the magnitude of the expansion coefficients for different $\kappa$ and $Ma$, from which one can observe that the coefficient $|w_\alpha|$ does increase when $Ma$ is large and $\kappa$ is small. In Fig. 2, we provide the comparison between the distribution function and the truncated Grad’s expansion. For $Ma = 3$ and $\kappa = 0.15$, Grad’s expansion converges, and the figure shows that the truncation at $M = 10$ gives better approximation than $M = 3$. For $Ma = 4$ and $\kappa = 0.1$, Grad’s expansion diverges. Although the truncation at $M = 3$ still seems to be approximating the original distribution function, the result given by $M = 10$ clearly shows the failure of convergence.

3 A General Variant of Holway’s Argument

We will generalize the original argument of Holway to the case of a multi-dimensional domain $\Omega$ in which we consider two arbitrary points $x_0, x_1 \in \Omega$ connected by a straight line of length $L$ and direction unit vector $\mathbf{n}$ as shown in Fig. 3. While Holway constructed his statement for the full Boltzmann collision operator, assuming some estimates for the gain part, we will directly use the BGK approximation to simplify the presentation. The extension to the Boltzmann operator is of purely technical nature and is not relevant for our discussion.

3.1 Derivation

The steady BGK equation is written with constant collision frequency for a particle velocity $\mathbf{c} = \mathbf{c} \mathbf{n}$ pointing from $x_0$ to $x_1$

$$\mathbf{c} \mathbf{n} \cdot \nabla f(x, \mathbf{c} \mathbf{n}) = -\nu f(x, \mathbf{c} \mathbf{n}) + \nu f_{eq}(x, \mathbf{c} \mathbf{n})$$

which can be transformed into

$$\mathbf{n} \cdot \nabla \left(f(x, \mathbf{c} \mathbf{n}) \exp\left(\frac{\nu}{c} \|x - x_0\|\right)\right) = \frac{\nu}{c} \exp\left(\frac{\nu}{c} \|x - x_0\|\right) f_{eq}(x, \mathbf{c} \mathbf{n})$$

after multiplying with $\frac{1}{L} \exp\left(\frac{\nu}{c} \|x - x_0\|\right)$. If we replace $x$ by the parametrization of the line $x(s) = x_0 + s \|x_1 - x_0\| \mathbf{n}$, we can integrate from $x(0) = x_0$ to $x(1) = x_1$, which gives

$$\int_0^1 \mathbf{n} \cdot \nabla \left(f(x(s), \mathbf{c} \mathbf{n}) \exp\left(\frac{\nu}{c} \|x(s) - x_0\|\right)\right) \|x'(s)\| \, ds =$$

$$\frac{\nu}{c} \int_0^1 \exp\left(\frac{\nu}{c} \|x(s) - x_0\|\right) f_{eq}(x(s), \mathbf{c} \mathbf{n}) \|x'(s)\| \, ds.$$

Replacing $\|x'(s)\| = \|x_1 - x_0\| = L$ and $\mathbf{n} \cdot \nabla \to \partial_s$ we can compute the integral on the left hand side explicitly and find

$$f(x_1, \mathbf{c} \mathbf{n}) = f(x_0, \mathbf{c} \mathbf{n}) \exp\left(-\frac{\nu L}{c}\right) + \frac{\nu L}{c} \int_0^1 \exp\left(-\frac{\nu L}{c}(1 - s)\right) f_{eq}(x(s), \mathbf{c} \mathbf{n}) \, ds$$

after multiplication with $\exp\left(-\frac{\nu L}{c}\right)$. Note that all terms in this equation are positive. Holway
then integrates from $x_0$ to $x_\sigma = x(1 - \sigma)$ with $0 < \sigma < 1$ and writes

$$f(x_1, c n) \geq \frac{\nu L}{c} \int_0^{1-\sigma} \exp \left( -\frac{\nu L}{c} (1-s) \right) f_{\text{eq}}(x(s), c n) \, ds$$

(18)

to be used as lower bound of $f$ at $x_1$. Using the mean value theorem with an $s^* \in (0, 1-\sigma)$, and $x(s^*) = x^*$ we find

$$f(x_1, c n) \geq f_{\text{eq}}(x^*, c n) \left( \exp \left( -\frac{\nu L}{c} \sigma \right) - \exp \left( -\frac{\nu L}{c} \right) \right)$$

(19)

(20)

hence obtain

$$K_\sigma \left( \frac{\nu L}{c} \right) f_{\text{eq}}(x^*, c n) \leq f(x_1, c n)$$

(21)

with some positive constant $K_\sigma \leq 1$, independent of $x^*$ and $x_1$ for fixed $\sigma$. For $x_\sigma$ close to either $x_0$ or $x_1$ the value of $K_\sigma$ is very small and $K_\sigma = \mathcal{O}(\frac{\nu L}{c})$ for $c \to \infty$ at fixed collision frequency and length. If we assume an asymptotic decay of $f_1(c) := f(x_1, c n)$ in the form

$$f_1(c) \leq R_1 \exp \left( -\frac{c^2}{\theta_1^{(\text{tail})}} \right) \quad \text{for all } c > r,$$

(22)

the precise condition of Holway reads

$$K_\sigma \left( \frac{\nu L}{c} \right) \frac{\rho^*/m}{(2\pi \theta^*)^{3/2}} \exp \left( -\frac{(c - \nu^*)^2}{2\theta^*} \right) \leq R_1 \exp \left( -\frac{c^2}{2\theta_1^{(\text{tail})}} \right) \quad \text{for all } c > r,$$

(23)

which implies the bound $\theta^* \leq \theta_1^{(\text{tail})}$ with the temperature $\theta^*$ at the position $x^*$. This is because no matter how small $K_\sigma$ becomes for large velocities, the exponentials are dominating and the inequality is only satisfied for all $c$, if the exponential decays are behaving accordingly. Combining this with the decay restriction (10) of the Grad expansion at $x_1$ gives

$$\theta^* < 2\theta_1,$$

(24)

a condition involving the actual temperatures of the gas at two separated positions.
3.2 Holway’s Original Conclusions and Weiss’ Objection

In the original presentation of the argument in [15], Holway considered the one-dimensional situation of a normal shock wave. Translated to our Fig. 3 he assumed a shock transition between $x_1$ and $x_2$. He is using the coordinates $x_1 \approx x_{1,\text{eq}}$ and $x_2 \approx x_{2,\text{eq}}$ and considers particles moving in negative direction such that $x_1 < x_2$. His coordinate $x_{\infty} > x_2 > x_1$ maybe identified with our position $x_0$. Holway assumes that the shock is so thin that asymptotic shock conditions can be found already at $x_1$ and $x_2$. Hence, the distributions at these points are given by the Maxwellians

$$
\lim_{x \to x_1} f(x, c) = f_{\text{eq}}^{(1)}(c) := \frac{\rho_1}{(2\pi\theta_1)^{3/2}} \exp\left(-\frac{|c - v_1|^2}{2\theta_1}\right),
$$

$$
\lim_{x \to x_2} f(x, c) = f_{\text{eq}}^{(2)}(c) := \frac{\rho_2}{(2\pi\theta_2)^{3/2}} \exp\left(-\frac{|c - v_2|^2}{2\theta_2}\right),
$$

where the parameters $\rho_1, \theta_1$ and $\rho_2, \theta_2$ are defined in (13). Considering our setup in Fig. 3 this means that we find the equilibrium $f_{\text{eq}}^{(2)}$ essentially in all positions $x_{\sigma,\text{eq}}$, $x^*$ and $x_0$, and $f_{\text{eq}}^{(1)}$ at position $x_1$. In particular Holway identified for the temperature $\theta^* = \theta_2$ and concluded from (24) that $2\theta_1 > \theta_2$ must hold in the boundary conditions for the applicability of Grad’s moment expansion.

The temperatures before and after the shock are connected by Rankine-Hugoniot conditions depending on the shock’s Mach number. Assuming that $\theta_2$ belongs to the downstream or hot part after the shock and $\theta_1$ to the upstream or cold part before the shock, Holway computed a critical Mach number

$$
Ma^{(\text{crit})} < \sqrt{\frac{9}{5} + \frac{4\sqrt{6}}{5}} \approx 1.939
$$

(27)

beyond which the temperatures before and after the shock would fail to satisfy condition (24). Actually, Holway [15] solved the equation incorrectly and got the limiting Mach number 1.851, as has been pointed out by Weiss in [29].

With this result Holway conjectured that when Grad’s moment expansion is truncated, the range of Mach numbers in which shock solutions exist is the interval $(1, M)$, with $M$ being a number less than 1.851. Holway’s original phrasing was “When the expansion is truncated after a few terms, the region of convergence may be expected to be smaller than given by [the condition]”, where the condition refers to “$M \leq 1.851$” (as mentioned, that number is the result of a minor miscalculation). Although Holway did not explicitly explain what he meant by “the region of convergence”, he did provide a table showing “the ranges of convergence”, and the caption of the table is “range of Mach numbers for which continuous shock solutions exist”. Hence, he connected the convergence limit to the sub-shock artefacts of shock waves as reported by Grad [12].

In [28], Weiss found that the 21-moment theory of extended thermodynamics [19] predicts smooth shock structures for any Mach number less than 1.887, which is in agreement with the theory of hyperbolic partial differential equations presented in [20]. However, this is beyond Holway’s proposed limit. This inspired Weiss to revisit Holway’s proof. Besides finding the calculational error, he also proposed another objection on Holway’s derivation. He claimed that Holway’s argument does not fix the direction of the shock wave and continues to derive the statement $\theta_1 \geq \theta^*$ from the relation (21). Weiss concludes that this shows that one should set the boundary condition in the opposite way: $x_1$ should point to the hot fluid behind the shock, while $x_2 \approx x^*$ should point to the cold fluid before the shock. In that case condition (24) is naturally satisfied, because $\theta_1 > \theta_2$ in such a shock and the restriction on the Mach number is removed. In particular, Weiss concluded that Holway’s argument does not affect the existence of sub-shock artefacts in shock solutions of moment equations.
4 Further Discussion

4.1 What Holway and Weiss got right and what wrong

According to our derivation in Sec. 3.1, there is no restriction how to place a normal shock wave along the line from $x_0$ to $x_1$. Weiss was right to point out that the shock direction could have been chosen differently from Holway. However, our multi-dimensional derivation also shows that the temperature condition (24) actually holds between the temperatures of any two position in any process.

Furthermore, in our view, one cannot conclude from (21) that $\theta_1 \geq \theta^*$. Note that the “constant” $K_\sigma$ appearing in that statement actually depends on $\sigma$, that is, the scaled distance between $x_1$ and $x^*$, with $\sigma = 1$ corresponding to $x^* = x_0$ the furthest away from $x_1$. In fact, in the shock scenario of Holway we find

$$\lim_{x^* \to x_0} f(x^*, c) = f_{eq}^{(2)}(c), \quad \text{and} \quad \lim_{x^* \to x_0} K_\sigma = 0,$$

hence, no contradiction to (21). In this sense, we support Holway’s argument on the convergence of Grad’s method, and in view of Sec. 3.1, we also conclude that Grad’s expansion might not converge in a process in which temperature ratios of more than a factor of 2 are present between any two points.

However, it remains unclear how this relates to the existence of smooth shock structure. Despite Holway’s conjecture, there is no clear evidence in his argument showing that a smooth shock structure does not exist for a Mach number larger than 1.939, especially for a low-moment theory. Holway’s convergence argument can only explain the limiting diverging behavior of Grad’s theory, while it can be seen from Fig. 2 that sometimes an early truncation of Grad’s series can generate modest approximations of the distribution function. Although Weiss’ work [28] still focused only on Mach numbers less than 1.887, he has extended the same result to the 35-moment theory, for which smooth shock structures exist for Mach number less than 2.2. The results are reported in [19, Chapter 12, Section 5]. In this sense, we support Weiss’ argument that the sub-shock problem cannot be related to the convergence restriction. Indeed, we tend to believe that low-moment theories may still provide decent predictions for moderately rarefied gases, despite the possible divergence of Grad’s expansion in the limit of infinitely many moments.

Note, that the occurrence of subshocks in shock solutions of moment equations is extensively explained, for example, in theoretical terms in the book [19] and on the basis of a model problem in [23]. The reason lies in the characteristics of the hyperbolic waves generated by the equation and their interaction with the relaxational part of the moment system. The highest characteristic velocity of the system gives the maximal speed with which infinitesimal disturbances can propagate. An inflow velocity exceeding this speed can only be sustained in a steady shock solution by introducing a discontinuous sub-shock, which due to its nonlinearity may move faster than the characteristic limit.

4.2 Consequences for Moment Equations

Nowadays, a lot more numerical experiments have been done for Grad’s method with a large number of moments. To obtain results in strong non-equilibrium, another issue of Grad’s equations is the loss of hyperbolicity [19], that has to be fixed. Such an issue has been addressed systematically in [2, 3], which provides hyperbolic versions of Grad’s equations for any number of moments. However, such hyperbolicity fix does not change Grad’s ansatz, and therefore the convergence issue remains.

Based on the hyperbolic moment equations, several numerical experiments have been carried out in [6, 4, 7]. All the three works used a large number of moments in the simulation. However, after examining all the numerical tests in these three works, we find that for most cases, the maximum temperature ratio in the numerical solution is less than 2. There are only three exceptions, all found in [6]:
• Shock tube problem with Knudsen number 0.0251 computed using 20/84 moments. See [6, Fig. 2].

• Fourier flow with Knudsen number 0.0298 computed using 56 moments. See [6, Fig. 10(a)].

• Fourier flow with Knudsen number 0.0658 computed using 56 moments. See [6, Fig. 10(b)].

In all the three cases, the Knudsen number is relatively small, so that the distribution function is close to the local equilibrium. Meanwhile, note that the numbers of moments presented in the above list correspond to the three-dimensional case, meaning that an early truncation of Grad’s series is used equivalent to \( M \approx 4 - 6 \), and by our observation in Sec. 2.3, it can still be expected that one can get reasonable approximations of the distribution functions. Additionally, in all the above cases, the maximum temperature ratio does not exceed 3, so that the problem may still be manageable for a small number of moments. As a summary, existing numerical experiments support our conclusion that moderate non-equilibrium flow can still be well captured by Grad’s method with a moderate number of moments.

It is worth mentioning that the situation may change once Grad’s equations are linearized [24]. In the Grad expansion, the nonlinearity comes completely from the involvement of velocity and temperature in the distribution function. Therefore, the linearization of Grad’s equations changes the ansatz of the distribution function by replacing the local equilibrium by a global equilibrium:

\[
\begin{align*}
\tilde{f}_{LG}^{(M)}(\mathbf{c}) &= \sum_{|\alpha|=0}^{M} \lambda_{\alpha} \mathbf{c}^\alpha f_{\text{global}}(\mathbf{c}), \\
\end{align*}
\]

where

\[
\begin{align*}
f_{\text{global}}(\mathbf{c}) &= \frac{1}{m(2\pi\theta(0))^{3/2}} \exp \left( -\frac{(c_i - v_i^{(0)})^2}{2\theta(0)} \right),
\end{align*}
\]

with \( v_i^{(0)} \) and \( \theta(0) \) being constants. Similar to (10), the convergence of the above expansion as \( M \rightarrow \infty \) requires that \( 2\theta(0) > \theta^{(\text{tail})} \). For linearized Grad’s equations, this parameter is manually chosen by setting the global equilibrium about which the linearization is performed. Therefore, if \( \theta(0) \) is chosen sufficiently large such that \( 2\theta(0) > \theta^{(\text{tail})} \) throughout the computational domain, then the convergence can again be achieved regardless of whether the original Grad’s method converges. Such numerical results have appeared in a recent work [16] and [16, Figure 5.7] shows the result of the Fourier flow with Knudsen number 0.1 and up to 5456 moments, where the temperature ratio is larger than 2.5. No divergence is observed since the value of \( \theta(0) \) is chosen to be even larger than the highest temperature in the numerical result. Nevertheless, such a method discards the consideration that the distribution functions are close to local equilibrium for dense gases, and therefore may lose efficiency of Grad’s method in the near-continuum regime. In fact, any equilibrium distribution with temperature different from \( \theta(0) \) will require a non-trivial expansion (29).

In his dissertation [14] Holway suggests a non-linear alternative to Grad’s expansion specifically for the computation of normal shock profiles. He modifies the Mott-Smith-ansatz [18] of a bimodal distribution by replacing the Maxwellian with the lower temperature with a Grad expansion. Due to the superposition with the hotter Maxwellian a hot tail can be approximated at any point in the shock profile and convergence is recovered. Unfortunately, this approach hardly generalizes to other multi-dimensional processes in which the highest temperature is a-priori not known.

Full non-linear expansions like the maximum-entropy distribution [10, 17] do not rely on the form (2). Hence, the arguments of this paper do not apply. However, convergence of the maximum-entropy distribution in the limit of many moments remains an open problem in itself.
4.3 Numerical Evidence

Since existing results do not explicitly show the failure of Grad’s method, we are going to support our argument by showing some results for a one-dimensional problem \((d=1)\) with boundary conditions. We assume that the fluid is located between two parallel diffusive walls with temperature \(\theta_l\) and \(\theta_r\), and we want to solve for steady state. By approximating the collisions using the BGK operator, the governing equation can be written as

\[
c \cdot \partial_x f(x,c) = \frac{1}{Kn} [f_{eq}(x,c) - f(x,c)], \quad \forall x \in (-1/2, 1/2), \quad \forall c \in \mathbb{R},
\]

with boundary conditions

\[
f(-1/2,c) = \frac{\rho_l/m}{\sqrt{2\pi\theta_l}} \exp\left(-\frac{c^2}{2\theta_l}\right), \quad \forall c > 0,
\]

\[
f(1/2,c) = \frac{\rho_r/m}{\sqrt{2\pi\theta_r}} \exp\left(-\frac{c^2}{2\theta_r}\right), \quad \forall c < 0,
\]

where \(Kn\) is the Knudsen number, and in the boundary conditions, \(\rho_l\) and \(\rho_r\) are chosen such that

\[
\int_{\mathbb{R}} c f(-1/2,c) \, dc = \int_{\mathbb{R}} c f(1/2,c) \, dc = 0,
\]

which ensures the mass conservation. Furthermore, we assume that the total mass equals 1:

\[
m \int_{-1/2}^{1/2} \int_{\mathbb{R}} f(x,c) \, dc \, dx = 1.
\]

For this problem, we can find the exact solution in the limits \(Kn \to +\infty\) and \(Kn \to 0\). When \(Kn \to +\infty\), the BGK equation shows that \(f(x,c)\) is independent of \(x\). Thus by the boundary condition, we see that

\[
f(x,c) = \begin{cases} f(-1/2,c), & \text{if } c > 0, \\ f(1/2,c), & \text{if } c < 0. \end{cases}
\]

The values of \(\rho_l\) and \(\rho_r\) can be solved from (35) and (34), and the result is

\[
\rho_l = \frac{2\sqrt{\theta_r}}{\sqrt{\theta_l} + \sqrt{\theta_r}}, \quad \rho_r = \frac{2\sqrt{\theta_l}}{\sqrt{\theta_l} + \sqrt{\theta_r}}.
\]

The corresponding temperature is \(\theta(x) \equiv \sqrt{\theta_l \theta_r}\). Consider the distribution function on the boundaries. We see that a necessary condition for the convergence of the Grad expansion is \(\sqrt{\theta_l \theta_r} > \theta_l/2\) and \(\sqrt{\theta_l \theta_r} > \theta_r/2\). This shows that if \(\theta_l > 4\theta_r\) or \(\theta_r > 4\theta_l\), the convergence of the Grad expansion fails if \(Kn\) is sufficiently large.
To study the limit of the solution as $\text{Kn} \to 0$, we integrate the BGK equation with respect to $c$, which gives us $v'(x) = 0$. By the boundary condition, we see that $v(x) = 0$. Similarly, by multiplying the equation by $c$ and integrating with respect to $c$, we know that $\rho(x)\theta(x)$ is a constant. Now we use Chapman-Enskog expansion and assume

$$f(x, c) = f_{eq}(x, c) + \text{Kn} f^{(1)}(x, c) + \text{Kn}^2 f^{(2)}(x, c) + \cdots .$$  

By matching the $O(1)$ terms, we get $f^{(1)}(x, c) = c \cdot \partial_c f_{eq}(x, c)$. We integrate the BGK equation against $c^2$ and approximate $f$ by $f_{eq} + \text{Kn} f^{(1)}$, and the resulting equation, which is actually the Fourier equation, is

$$\theta''(x) = 0.$$  

Therefore $\theta(x)$ is approximately a linear function. When $\text{Kn} \to 0$, the distribution function $f(x, c)$ tends to the local Maxwellian. Therefore by the boundary condition,

$$\lim_{\text{Kn} \to 0} \theta(-1/2) = \theta_l, \quad \lim_{\text{Kn} \to 0} \theta(1/2) = \theta_r.$$  

Consequently,

$$\lim_{\text{Kn} \to 0} \theta(x) = \left( \frac{1}{2} - x \right) \theta_l + \left( \frac{1}{2} + x \right) \theta_r.$$  

This shows that if $\theta_l > 2\theta_r$ or $\theta_r > 2\theta_l$, we can find a sufficiently small $\text{Kn}$ such that the Grad expansion fails to converge.

To validate our argument that the Grad expansion may still work for small values of $M$, in the numerical test, we choose the Knudsen number $\text{Kn} = 0.2$ and $\text{Kn} = 5$, and we set the wall temperatures to be $\theta_l = 1$ and $\theta_r = 5$, so that the Grad expansion will diverge for both small and large Knudsen numbers. In order to ensure that the number of boundary conditions matches the number of characteristics pointing inside the domain (which is necessary for the existence of the solution), we adopt the variation of Grad’s equations with global hyperbolicity [1], and we always choose an odd $M$ since the equations for even $M$ may have multiple exact solutions. For this one-dimensional problem, the moment equations are solved with the shooting method with a quasi-Newton method used for the iteration. The solutions for the temperature field are shown in Fig. 4 together with the result of the discrete velocity model (DVM) as reference solution.

From the DVM results, we see that for $\text{Kn} = 0.2$, the temperature on the right boundary exceeds twice the temperature on the left boundary. Therefore the Grad expansion is expected to be divergent. When $\text{Kn} = 5$, the temperature on the right boundary is less than $\theta_r/2$, so that the Grad expansion also diverges. However, when we solve the moment equations, the quasi-Newton iteration does not converge for some $M$. For $\text{Kn} = 0.2$, the iteration converges only for $M = 5$ and $M = 7$, while for $\text{Kn} = 5$, the iteration diverges for $M = 5, 9, 13$, but we can find solution for $M = 7, 11, 15$. For large $M$, we cannot find solution for both Knudsen numbers.

From Fig. 4, one can also see that all the results are qualitatively correct. For smaller Knudsen number $\text{Kn} = 0.2$, in general, the result of $M = 7$ gives better approximation. However, near the left boundary, where the Grad expansion is expected to be divergent, $M = 7$ gives even larger error than $M = 5$. This can be observed more clearly from the approximation of the distribution functions, which are plotted in Fig. 5. It is shown that on the left boundary, the result of $M = 5$ is closer to the DVM result, whereas on the right boundary, the result of $M = 7$ is slightly better.

Similar plots for $\text{Kn} = 5$ are provided in Fig. 6. In this example, due to the large discontinuity in the exact solution, it is harder for the moment method to get a good approximation. Nevertheless, when $M$ is not too large, the moment method still describes the general profile of the distribution functions.
On the Holway-Weiss-Debate

Z. Cai and M. Torrilhon

Figure 5: Distribution functions at (a) the left boundary, and (b) the right boundary, for Knudsen number 0.2

Figure 6: Distribution functions at (a) the left boundary, and (b) the right boundary, for Knudsen number 5.0

5 Conclusion

We revisited a debate between L. H. Holway and W. Weiss on the convergence of moment approximations which keeps generating confusion in the community. In our view Holway was correct to show that there is a limit on the applicability of Grad’s moment expansion and in fact we generalized his argument to general multi-dimensional steady processes. However, Holway’s attempt to attribute the sub-shock behavior of moment equations when computing shock profiles to this convergence restriction is wrong. This misconception has been correctly pointed out by Weiss, whose smooth shock profile solutions based on moments remain valid. However, Weiss’ more substantial criticism of Holway’s argument turned out to be unfounded in our study.

Roughly speaking, Holway’s argument means that whenever there is a hot spot in a process, fast particles originating from that spot can be found anywhere in the domain, generating hot distribution tails that make Grad’s expansion diverge. While this behavior is real and can be observed in specific computations, its implications for gas models based on a relatively small number of moments is probably negligible. We also discussed that even in simulations with many moments, convergence issues often remain undetected due to stabilizing effects like dissipation at moderate Knudsen numbers.

References

[1] Z. Cai, Y. Fan, and R. Li, Globally hyperbolic regularization of Grad’s moment system in one-dimensional space, Comm. Math. Sci., 11 (2013), pp. 547–571.
[2] ———, Globally hyperbolic regularization of Grad’s moment system, Comm. Pure Appl. Math., 67 (2014), pp. 464–518.
[3] ———, A framework on moment model reduction for kinetic equation, SIAM J. Appl. Math., 75 (2015), pp. 2001–2023.
[4] Z. Cai, Y. Fan, R. Li, and Z. Qiao, Dimension-reduced hyperbolic moment method for the Boltzmann equation with BGK-type collision, Comm. Comput. Phys., 15 (2014), pp. 1368–1406.
[5] Z. Cai and R. Li, Numerical regularized moment method of arbitrary order for Boltzmann-BGK equation, SIAM J. Sci. Comput., 32 (2010), pp. 2875–2907.
[6] Z. Cai, R. Li, and Z. Qiao, Globally hyperbolic regularized moment method with applications to microflow simulation, Comput. Fluids, 81 (2013), pp. 95–109.
[7] Z. Cai and M. Torrilhon, Numerical simulation of microflows using moment methods with linearized collision operator, J. Sci. Comput., 74 (2018), pp. 336–374.
[8] C. Cercignani, The Boltzmann Equation and its Applications, Applied Mathematical Sciences, Springer, New York, 1988.
[9] E. W. Cheney, Introduction to Approximation Theory, Chelsea, New York, 1982.
[10] W. Dreyer, Maximisation of the entropy in non-equilibrium, J. Phys. A, 20 (1987), pp. 6505–6517.
[11] H. Grad, On the kinetic theory of rarefied gases, Comm. Pure Appl. Math., 2 (1949), pp. 331–407.
[12] ———, The profile of a steady plane shock wave, Comm. Pure Appl. Math., 5 (1952), pp. 257–300.
[13] X.-J. Gu and D. Emerson, A computational strategy for the regularized 13 moment equations with enhanced wall-boundary conditions, J. Comput. Phys., 225 (2007), pp. 263–283.
[14] L. H. Holway, Approximation Procedures for Kinetic Theory, PhD Thesis, Harvard University, 1963.
[15] ———, Existence of kinetic theory solutions to the shock structure problem, Phys. Fluids, 7 (1965), pp. 911–913.
[16] Z. Hu, Z. Cai, and Y. Wang, Numerical simulation of microflows using Hermite spectral methods, 2019. arXiv:1807.06236.
[17] C. Levermore, Moment closure hierarchies for kinetic theories, J. Stat. Phys., 83 (1996), pp. 1021–1065.
[18] H. M. Mott-Smith, The solution of the boltzmann equation for a shock wave, Phys. Rev., 82 (1951), pp. 885–892.
[19] I. Müller and T. Ruggeri, Rational Extended Thermodynamics, Second Edition, Springer, 1998.
[20] T. Ruggeri, Breakdown of shock wave structure solutions, Phys. Rev. E, 47 (1993).
[21] H. Struchtrup, Macroscopic Transport Equations for Rarefied Gas Flows, Interaction of Mechanics and Mathematics, Springer, New York, 2005.
[22] H. Struchtrup and M. Torrilhon, Regularization of Grad’s 13 moment equations: Derivation and linear analysis, Phys. Fluids, 15 (2003), pp. 2668–2680.
[23] M. Torrilhon, Characteristic waves and dissipation in the 13-moment-case, Cont. Mech. Thermodyn., 12 (2000), p. 289.
[24] ———, Convergence study of moment approximations for boundary value problems of the Boltzmann-BGK equation, Commun. Comput. Phys., 18 (2015), pp. 529–557.
[25] M. Torrilhon, Modeling nonequilibrium gas flow based on moment equations, Ann. Rev. Fluid Mech., 48 (2016), pp. 429–458.
[26] M. Torrilhon and N. Sarna, Hierarchical boltzmann simulations and model error estimation, J. Comput. Phys., 342 (2017), pp. 66–84.
[27] M. Torrilhon and H. Struchtrup, Boundary conditions for regularized 13-moment-
equations for micro-channel-flows, J. Comput. Phys., 227 (2008), pp. 1982–2011.

[28] W. Weiss, Continuous shock structure in extended thermodynamics, Phys. Rev. E, 52 (1995), pp. R5760–R5763.

[29] ——, Comments on “Existence of kinetic theory solutions to the shock structure problem” [Phys. Fluids 7, 911 (1964)], Phys. Fluids, 8 (1996), pp. 1689–1690.