Affordable robust moment closures for CFD based on the maximum-entropy hierarchy

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Abstract
The use of moment closures for the prediction of continuum and moderately non-equilibrium flows offers modelling and numerical advantages over other methods. The maximum-entropy hierarchy of moment closures holds the promise of robustly hyperbolic stable moment equations, however there are two issues that limit their practical implementation. Firstly, for closures that have a treatment for heat transfer, fluxes cannot be written in closed form and a very expensive iterative procedure is required at every flux evaluation. Secondly, for these same closures, there are physically possible moment states for which the entropy-maximization problem has no solution and the entire framework breaks down. This paper demonstrates that affordable closed-form moment closures that are inspired by the maximum-entropy framework can be proposed. It is known that closing fluxes in the maximum-entropy hierarchy approach a singularity as the region of non-solvability is approached. This paper shows that, far from a disadvantage, this singularity allows for smooth and accurate prediction of shock-wave structure, even for high Mach numbers. The presence of unphysical “sub-shocks” within shock-profile predictions of traditional closures has long been regarded as an unfortunate limitation of the entire moment-closure technique. The realization that smooth shock profiles are, in fact, possible for moment methods with a moderate number of moments greatly increases the method’s applicability to high-speed flows. In this paper, a 5-moment system for a simple one-dimensional gas and a 14-moment system for realistic gases are developed and examined. Numerical solution for shock-waves at a variety of incoming flow Mach numbers demonstrate both the robustness and the accuracy of the closures.

1. Introduction

The development of models for moderately rarefied gas-flow prediction has proven difficult. In this transition regime, between the particle-collision-dominated continuum regime and the free-molecular regimes, continuum methods are inaccurate and particle-based methods, such as direct-simulation Monte Carlo (DSMC) [1], become expensive. The expense associated with stochastic particle methods becomes even more extreme for low-speed flows or for time-accurate calculations. Techniques based on the addition of higher-order terms to the Navier–Stokes equations through expansion techniques have failed to provide stable sets of partial differential equations (PDEs) [2]. Moment closures offer the promise of many advantages as compared to traditional methods for both continuum and rarefied gas-flow prediction [3,4]. The resulting first-order balance laws provide a natural stable hyperbolic treatment for effects of local thermal non-equilibrium, such as anisotropic pressures, through their inclusion in an expanded solution vector.

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Moment closures also have the potential for more convenient numerical solution than traditional fluid-dynamic equations, such as the Navier–Stokes equations, which require the evaluation of second derivatives and are of mixed hyperbolic-parabolic type. The requirement to compute only first derivatives means that an extra order of spatial accuracy can potentially be obtained for a given stencil. Also, the requirement for only first derivatives makes numerical solution of systems of moment equations much less sensitive to grid irregularities [5]. Grid irregularities are typical for practical situations in which complex geometries make the generation of high-quality meshes inconvenient. They are also commonly encountered when adaptive mesh refinement or embedded-boundary treatments are used. Recently, moment closures have also been coupled to DSMC techniques in order to reduce the statistical fluctuations of the latter approach [6].

Traditional moment closures do, unfortunately, suffer from their own issues. The original hierarchy proposed by Grad [3] suffers from a restrictive region of hyperbolicity. This is due to the fact that the flux Jacobian can develop complex eigenvalues for moderate departures from equilibrium. Alternatively, the closures of the maximum–entropy hierarchy are globally hyperbolic whenever the underlying constrained entropy-maximization problem can be solved [4,7–9]. Theoretical and practical studies related to maximum–entropy moment closures have been carried out by many authors, including: Brown et al. [10,11], Le Tallec and Perlat [12], McDonald and Groth [13–17], Lam and Groth [18], Suzuki et al. [19,20], Barth [21], Coulombel et al. [22,23], and Carrillo et al. [24]. Unfortunately, the maximum–entropy hierarchy suffers from two apparent problems. Firstly, for closures of sufficiently high order to include a treatment for heat transfer, it is not possible to write the closing fluxes in closed-form. The result is that a very expensive and often ill-conditioned iterative procedure must be used at every flux evaluation. This expense cannot be justified for practical calculations. Also, it has been shown that, again for all closures that include heat transfer, there are physically realistic moment states for which the entropy maximization problem does not have a solution and the whole framework of the closure breaks down [25–27]. If moment closures are to come into practical use, new closures must be developed that are both affordable and robust.

Another issue that is considered a limitation to the usefulness of all hyperbolic moment closures is the presence of artificial discontinuities in flow solutions. These are especially apparent in shock-structure predictions as they cause un-physical “sub-shocks” to form [4]. Many practical applications involving thermal non-equilibrium also involve super-sonic or hypersonic flows and moment closures that predict artificial discontinuities inside shock-wave profiles are obviously unsuitable if the the internal structure of shock waves are of interest [20].

Recently proposed regularized variants of the Grad moment closures allow for the prediction of smooth shock structures through the inclusion of second-order terms [9,28–30]. These closures do not remain first-order or purely hyperbolic due to the parabolic nature the regularizing terms. All numerical advantages associated with a first-order balance-law form are therefore lost. The limited hyperbolicity of the base Grad closure also remains and closure breakdown can still be expected for significant deviations from equilibrium.

1.1. Scope of current study

This paper begins with a review of the theory of moment closures with emphasis on the family of maximum–entropy closures. The two major issues related with this hierarchy, the lack of a closed-form flux and limited moment realizability, are reviewed. Using a simple one-dimensional closure, it is then shown that these issues can be handled in practice through an interpolation technique. It is demonstrated that the nature of the non-realizability of some moment states leads to a singularity in the closing flux that is actually beneficial, as it opens the door to smooth shock profiles for high Mach numbers. Numerical solutions demonstrate the amazing accuracy of the model for shock-structure calculations. This technique is then extended to the fully realistic three-dimensional setting. A closed-form set of moment equations for realistic gases is proposed that has a vastly expanded region of hyperbolicity and is robust enough for the numerical prediction of strong shock waves. Comparisons to Navier–Stokes solutions and direct discretization of the kinetic equation are made.

2. Moment closures

Moment closures follow from the field of gaskinetic theory. In this theory, a monatomic gas is described by a probability density function, $F(x_i, v_i, t)$, that describes the probability of finding a gas particle at a given position, $x_i$, with a velocity, $v_i$, at a time, $t$. This distribution function gives a huge amount of information about the microscopic state of a gas. However, for most practical problems, it is only a small number of macroscopic properties that are of interest. These properties are related to the distribution function through moment relations, taking monomials of the particle velocity as weights, $\phi(v)$. For example,

\[
\begin{align*}
\phi(v_i) = 1 & : \quad \rho = \iint_{\mathbb{R}^3} m F(x, v) \, dv = \langle m F \rangle, \\
\phi(v_i) = v_i & : \quad \rho u_i = \langle m v_i F \rangle, \\
\phi(c_i) = c_i & : \quad P_{ij} = \langle m c_i c_j F \rangle, \\
\phi(c_i) = c_i c_j & : \quad Q_{ijk} = \langle m c_i c_j c_k F \rangle,
\end{align*}
\]

Here, the notation $\langle \cdot \rangle$ denotes integration over all of velocity space, $m$ is the mass of one gas particle, $\rho$ is the mass density, $u_i$ is the bulk velocity, $c_i = v_i - u_i$ is the peculiar component of the gas-particle velocity, $P_{ij}$ is an anisotropic pressure tensor, and $Q_{ijk}$ is the generalized heat-flux tensor. The thermodynamic pressure is found as $p = \frac{1}{3} P_{ii}$ and the traditional heat-flux
vector is given by $h_i = \frac{1}{2} Q_{ii}$. Higher-order moments can be similarly defined, but do not have an obvious macroscopic physical interpretation.

In this paper, third-, fourth-, and fifth-order moments of the peculiar particle velocity are assigned the letters “$Q$”, “$R$”, and “$S$” respectively. All higher-order tensors of the peculiar velocity are given the symbol “$V$” and the order of the moment can be determined by counting the number of indices. For example,

\[
Q_{ii} = \langle mc_i c_j F \rangle, \quad R_{ijk} = \langle mc_i c_j c_k F \rangle, \\
S_{ijk} = \langle mc_i c_j c_k F \rangle, \quad V_{ijklm} = \langle mc_i c_j c_k c_m \ldots c_p F \rangle.
\]

Moments of the full particle velocity are called “full” or “convective” moments and are denoted by the symbol “$U$”, as

\[ U_{gk..n} = \langle mv_i v_j v_k \ldots v_n F \rangle. \tag{1} \]

The Einstein summation convention is always used.

The evolution of a distribution function is governed by the Boltzmann equation,

\[
\frac{\partial F}{\partial t} + \sum_i v_i \frac{\partial F}{\partial x_i} = \frac{\delta F}{\delta t},
\]

shown here in the absence of external acceleration fields. The left-hand side of Eq. (2) describes simple particle streaming while the right-hand side is responsible for the effects of inter-particle collisions on the distribution function. This collision operator is a high-dimensional integral that, in general, cannot be evaluated in closed form. Nevertheless, some information about the behaviour of this operator is readily available. For one thing, it conserves mass, momentum, and energy. It was also shown by Boltzmann that it always increases the entropy monotonically until the distribution function has the form of a Maxwellian (or Maxwell–Boltzmann) distribution,

\[
\mathcal{M} = n \left( \frac{\rho}{2\pi \rho} \right)^\frac{3}{2} \exp \left( \frac{\rho}{2\rho} c_i c_i \right), \tag{3}
\]

where $n$ is the local particle number density ($\rho = nm$). At this point the collision operator has no further effect. Therefore, Eq. (3) is the distribution function with the maximum entropy for a fixed pressure and density.

Equations governing the evolution of macroscopic moments can be found by taking moments of Eq. (2). This leads to Maxwell’s equation of change,

\[
\langle m_i \frac{\partial F}{\partial t} \rangle + \langle m_i \phi \frac{\partial F}{\partial x_i} \rangle = \frac{\partial}{\partial t} \langle m_i \phi F \rangle + \frac{\partial}{\partial x_i} \langle m_i \phi \frac{\partial F}{\partial x_i} \rangle = \langle m_i \frac{\partial F}{\partial t} \rangle. \tag{4}
\]

Usually one is interested in a set of macroscopic moments, thus is it convenient to define a vector of generating weights, \( \Phi(v_i) = [\phi_1(v_i), \phi_2(v_i), \ldots, \phi_n(v_i)]^T \). This vector can then be used in Eq. (4),

\[
\frac{\partial}{\partial t} \langle m_i \Phi F \rangle + \frac{\partial}{\partial x_i} \langle m_i \Phi \frac{\partial F}{\partial x_i} \rangle = \frac{\partial U}{\partial t} + \frac{\partial F_i}{\partial x_i} = C, \tag{5}
\]

where $U = \langle m_i \Phi F \rangle$ is the solution vector containing the full moments of interest, $F_i = \langle m_i \Phi \frac{\partial F}{\partial x_i} \rangle$ is the corresponding flux dyad, and $C = \langle m_i \Phi \frac{\partial F}{\partial x_i} \rangle$ is the source vector representing the effect of the collision operator on the moments contained in $U$. These equations are of first-order balance-law form. Unfortunately, this system of equations is not closed. There are always moments present in the flux dyad that are of higher order than any moment in the solution vector. The effect of the collision operator on the moments is also not known in general.

### 2.1. The BGK collision operator

As mentioned above, the collision operator in Eq. (2) is very difficult to use in practice. As the goal of the current research is in the development of effective moment closures for the modelling of the left-hand side of the Boltzmann equation, the simple BGK relaxation-time collision operator is used [31].

\[
\frac{\delta F}{\delta t} = - \frac{F - \mathcal{M}}{\tau}. \tag{6}
\]

In this model, any non-equilibrium distribution, $F$, simply relaxes to the equilibrium Maxwellian, $\mathcal{M}$, that has the same density, momentum, and energy. Once the distribution function is a Maxwellian, the operator has no more effect. Though the model has limited physical accuracy, this simple collision operator is convenient for the evaluation of moment equations as it allows an easy automatic closure for the right-hand side of Eq. (4).

### 2.2. Moment closure

In order to obtain a useful model, the system of equations resulting from Eq. (5) must be closed. One way to do this is to restrict the distribution function, $F$, to some assumed form. This form must have the same number of free parameters,
\( \mathbf{z} = [x_1, x_2, \ldots, x_i]^T \), as there are entries in \( \mathbf{U} \). The value of these free parameters is chosen so that the moment relations, given in Eq. (1), are satisfied. This ensures that all entries in both the flux dyad, \( \mathbf{F}_i \), and the source vector, \( \mathbf{C} \), are functions of the known moments of the solution vector. Thus, the system is closed.

The earliest moment closures were those proposed by Grad [3], in which the distribution function was assumed to be a polynomial expansion around the equilibrium Maxwellian, Eq. (3), with the same density, momentum, and energy.

\[
\mathcal{F}_{\text{Grad}} = \mathcal{M} \mathbf{z}^\intercal \Phi.
\]

Unfortunately, moment closures based on such an assumed form suffer from several problems. Firstly, the distribution function is not always positive, as the polynomial, \( \mathbf{z}^\intercal \Phi \), can be negative, and is thus not a properly defined probability density function. More devastatingly, for modest departures from equilibrium, the hyperbolicity of the resulting system of equations can break down [32–34]. This is caused by the fact that the flux Jacobian can develop complex eigenvalues. As a result, the system of moment equations may not be well posed for initial-value problems.

3. Maximum-entropy moment closures

A more mathematically elegant hierarchy of closures can be obtained by assuming the distribution function is that which maximizes the entropy while remaining consistent with the moments in the solution vector [4,7–9]. For classical gases, for which the entropy density is known to be \( \ln \mathcal{F} / C_0 \), this assumption leads to distribution functions of the form

\[
\mathcal{F}_{\text{MaxEnt}} = e^{\mathbf{z}^\intercal \phi}.
\]

This distribution function is positive valued, and, through careful selection of the generating velocity weights in \( \Phi \), it can be assured that the distribution remains finite [8].

Aside from the mathematical beauty of the maximum-entropy theory, there are strong physical arguments as to why it should provide accurate predictions. Not only does the collision operator always acts to increase entropy, as was stated in Section 2, but the maximum-entropy distribution is also statistically the most likely distribution that is consistent with the known moments [9,35,36]. It is therefore, in some sense, the best possible choice given the limited information in the solution vector.

3.1. Properties of maximum-entropy moment closures

In this section, useful mathematical properties of the maximum-entropy hierarchy are reviewed. Following Levermore, [8], this study begins by defining density and flux potentials,

\[
h(\mathbf{z}) = \langle m e^{\mathbf{z}^\intercal \phi} \rangle, \quad f_i(\mathbf{z}) = \langle m v_i e^{\mathbf{z}^\intercal \phi} \rangle.
\]

It is clear that the conserved moments and fluxes of the system can be expressed as

\[
\frac{\partial h}{\partial \mathbf{z}} = h_{\mathbf{z}} = \langle m \Phi e^{\mathbf{z}^\intercal \phi} \rangle = \mathbf{U}, \quad \frac{\partial f_i}{\partial \mathbf{z}} = f_{i,\mathbf{z}} = \langle m v_i \Phi e^{\mathbf{z}^\intercal \phi} \rangle = \mathbf{F}_i.
\]

Eq. (5) can therefore be written as

\[
\frac{\partial}{\partial t} h_{\mathbf{z}} + \frac{\partial}{\partial \mathbf{x}_i} f_{i,\mathbf{z}} = \mathbf{C}.
\]

The terms \( h_{\mathbf{z}} \) and \( f_{i,\mathbf{z}} \) can be differentiated again to give

\[
\frac{\partial}{\partial \mathbf{U}} h_{\mathbf{z}} = h_{\mathbf{z},\mathbf{U}} = \langle m \Phi \Phi^\intercal e^{\mathbf{z}^\intercal \phi} \rangle, \quad \frac{\partial}{\partial \mathbf{U}} f_{i,\mathbf{z}} = f_{i,\mathbf{z},\mathbf{U}} = \langle m v_i \Phi \Phi^\intercal e^{\mathbf{z}^\intercal \phi} \rangle.
\]

The flux Jacobian is therefore

\[
\frac{\partial \mathbf{F}_i}{\partial \mathbf{U}} = \frac{\partial \mathbf{F}_i}{\partial \mathbf{z}} \left( \frac{\partial \mathbf{U}}{\partial \mathbf{z}} \right)^{-1} = f_{i,\mathbf{z},\mathbf{U}}(h_{\mathbf{z},\mathbf{U}})^{-1}.
\]

In fact, the global hyperbolicity of the system of moment equations can be demonstrated by re-expressing Eq. (11) as

\[
\frac{\partial}{\partial t} h_{\mathbf{z},\mathbf{U}} + f_{i,\mathbf{z},\mathbf{U}} \frac{\partial}{\partial \mathbf{x}_i} \mathbf{U} = \mathbf{C}.
\]

This relation describes the time evolution of the closure coefficients for a maximum-entropy distribution. Hyperbolicity of this system is assured by the symmetry of \( f_{i,\mathbf{z},\mathbf{U}} \) and symmetric positive definiteness of \( h_{\mathbf{z},\mathbf{U}} \). The positive-definiteness of \( h_{\mathbf{z},\mathbf{U}} \) is known because for any vector \( \mathbf{w} \),

\[
\mathbf{w}^\intercal h_{\mathbf{z},\mathbf{U}} \mathbf{w} = \langle m \mathbf{w}^\intercal \Phi \Phi^\intercal e^{\mathbf{z}^\intercal \phi} \rangle = \langle m (\mathbf{w}^\intercal \Phi)^2 e^{\mathbf{z}^\intercal \phi} \rangle \geq 0.
\]

and hence \( h_{\mathbf{z},\mathbf{U}} \) is both symmetric and positive definite.
3.2. Issues related to the maximum-entropy hierarchy

The two lowest-order member of the maximum-entropy family are 5-moment and 10-moment closures. The 5-moment closure leads to the familiar Euler equations, while the 10-moment system is known as the Gaussian closure. The Gaussian closure gives a hyperbolic treatment for viscous gas flows, but does not have a treatment for heat flux. Numerical Computations have demonstrated that this model can be very successful for continuum and transition-regime flows for which heat-transfer is not important [10,11,15,19,21].

Given the mathematical elegance and physical arguments presented above, it may initially seem surprising that the maximum-entropy hierarchy has not gained more popularity. This is due to several issues related to the higher-order members of this family.

Firstly, if the vector of generating weights, \( \Phi \), contains super-quadratic terms, moments of the distribution function cannot be given in closed form. That is, the relationship

\[
U(\alpha) = \langle m \Phi \mathcal{F}(\alpha) \rangle
\]

cannot be evaluated for general \( \alpha \). The inversion of this expression, giving the coefficients as a function of the known moments, \( \alpha(U) \), is also impossible. The system’s fluxes, \( F_i(U) \), therefore cannot be expressed as functions of the known moments, \( F_i(U) \). Practically, this means that, when the closure coefficients are needed for flux evaluation during the numerical solution of the moment equations, they must be found iteratively. This iterative process requires the accurate integration of the distribution function over all velocity space be evaluated numerically many times [8,12]. This expense cannot be justified for practical computations. As the heat flux is a third-order moment, any closure with a treatment for heat flux will suffer from this problem.

In what has been regarded as a more devastating issue related to the maximum-entropy hierarchy, Junk has shown that, again for all maximum-entropy distributions with super-quadratic terms in \( \Phi \), there are physically realistic states for which closure coefficients cannot be found [25]. In these regions, the entropy-maximization problem on which the theory is founded does not have a solution, the arguments of Section 3.1 do not hold, and the entire theory of maximum-entropy moment closures breaks down. In the following, approximations to maximum-entropy closures are presented that maintain the attractive features of the true maximum-entropy hierarchy while addressing these two deficiencies.

4. Closed-form approximation to a one-dimensional moment closure

The two issues relating to maximum-entropy moment closures may seem devastating at first. However, a recent study has found that both issues can be handled in practice for a simple one-dimensional system [17]. The procedure has now been refined and is shown here. A new simpler and superior moment system is the result.

4.1. Moment closures for one-dimensional physics

For one space dimension and one velocity dimension, the velocity-distribution function reduces to \( \mathcal{F}(x, v, t) \), where position and velocity are now scalars. The Boltzmann equation with the BGK collision operator shown in Section 2.1 becomes

\[
\frac{\partial \mathcal{F}}{\partial t} + v \frac{\partial \mathcal{F}}{\partial x} = -\mathcal{F} + \frac{\mathcal{M}}{\tau}.
\]  

Here, the equilibrium state given by the one-dimensional Maxwell–Boltzmann distribution is

\[
\mathcal{M} = n \sqrt{\frac{\rho}{2\pi \rho^2}} \exp \left( -\frac{\rho - \rho_0}{2\rho_0} \right).
\]

The simplest member of the one-dimensional maximum entropy hierarchy with super-quadratic generating weights is a five moment system. It has a distribution function given by

\[
\mathcal{F}_5 = \exp (\alpha_0 + \alpha_1 v + \alpha_2 v^2 + \alpha_3 v^3 + \alpha_4 v^4).
\]

The corresponding system of moment equations is

\[
\frac{\partial \rho}{\partial t} + \frac{\partial }{\partial x} (\rho u) = 0,
\]

\[
\frac{\partial }{\partial t} (\rho u) + \frac{\partial }{\partial x} (\rho u^2 + p) = 0,
\]

\[
\frac{\partial }{\partial t} (\rho u^2 + p) + \frac{\partial }{\partial x} (\rho u^3 + 3\rho p + q) = 0.
\]
\[ \frac{\partial}{\partial t} (pu^3 + 3up + q) + \frac{\partial}{\partial x} (pu^4 + 6u^2p + 4uq + r) = -\frac{q}{\tau}. \]  
\[ \frac{\partial}{\partial t} (pu^4 + 6u^2p + 4uq + r) + \frac{\partial}{\partial x} (pu^5 + 10u^3p + 10u^2q + 5ur + s) = -\frac{1}{\tau} \left( 4uq + r - \frac{3}{5} \frac{p^2}{\rho} \right). \]

The moments present in the system are
\[ \rho = \langle m^4 \mathcal{F}_s \rangle, \quad \rho u = \langle m^3 v \mathcal{F}_s \rangle, \]
\[ p = \langle m^3 \mathcal{F}_s \rangle, \quad q = \langle m^2 \mathcal{F}_s \rangle, \]
\[ r = \langle m^4 \mathcal{F}_s \rangle, \quad s = \langle m^5 \mathcal{F}_s \rangle. \]

Lower-case symbols are used to denote one-dimensional physics. It is the fifth-order moment, \( s \), which is present in the flux, but not the solution vector, that must be found through the assumed form of the distribution to close the system. As stated earlier, a closed-form expression for this moment as a function of the lower-order moments in not possible for the maximum-entropy hierarchy. Nevertheless, an investigation into the behaviour of this moment reveals that closed-form approximations which maintain many of the attractive features of the true maximum-entropy flux can be found.

### 4.2. Non-dimensionalization of the five-moment closure

In order to investigate the properties of the resulting system, it is convenient to apply a shift of the probability density function in velocity space such that \( u = 0 \), followed by a non-dimensionalization such that \( \rho = 1 \) and \( p = 1 \). This leads to non-dimensionalized third, fourth, and fifth moments given by
\[ q_* = \frac{1}{\rho} \left( \frac{\rho}{\rho} \right)^{\frac{1}{2}} q, \quad r_* = \frac{1}{\rho} \left( \frac{\rho}{\rho} \right)^{\frac{1}{2}} r, \quad s_* = \frac{1}{\rho} \left( \frac{\rho}{\rho} \right)^{\frac{1}{2}} s. \]

### 4.3. Realizability of a five-moment closure

When analyzing the realizability of moment closures, there are two types of realizability that must be considered. First, there is the question of physical realizability, which asks which moment states can be reached by an arbitrary positive distribution function. Second, one must consider which moment states can be reached by distribution functions of the assumed form used to close the system.

Physical realizability can be calculated through the solution of the Hamburger moment problem [39,40]. This is done by first defining a vector of velocity weights, \( \mathbf{M} = \left[ 1, v, v^2, \ldots, v^n \right]^T \). This is then used to define a matrix
\[ \mathbf{Y} = \left\langle m \mathbf{M}^T \mathcal{F} \right\rangle. \]

For a positive distribution, \( \mathcal{F} \), it is obviously necessary that this matrix be be positive definite, as
\[ \mathbf{W}^T \mathbf{Y} \mathbf{W} = \mathbf{W}^T \left\langle m \mathbf{M}^T \mathcal{F} \mathcal{X} \right\rangle \mathbf{W} = \left\langle m \mathbf{W}^T \mathbf{M}^T \mathcal{F} \mathcal{X} \mathbf{W} \right\rangle = \left\langle m \mathbf{W}^T \mathbf{M}^T \mathcal{F} \mathcal{X} \mathbf{W} \right\rangle > 0, \]
for any vector \( \mathbf{W} \). For one-dimensional distribution functions it can also be shown that this is a sufficient condition for physical realizability [41].

For the one-dimensional five-moment closure, one should take \( \mathbf{M} = \left[ 1, v, v^2 \right]^T \). This leads to the realizability condition
\[ r_* \geq q_*^2 + 1. \]

One must now consider which physically possible states can be realized by a distribution of the form given in Eq. (19). Junk has shown, [25], that this distribution function cannot realize states on the line
\[ q_* = 0 \quad \text{and} \quad r_* > 3. \]

In other words, if there is no heat flux, the distribution function cannot have a fourth moment that is higher than it is for an equilibrium Maxwellian, \( r_* = 3 \). Fig. 1 shows the region of realizability for this 5-moment system.

### 4.4. Parabolic mapping of phase space

In order to make interpolation of the closing flux more convenient, a parabolic mapping is employed. This is done by defining a new variable, \( \sigma \), that replaces \( r_* \), through the relation
\[ r_* = \frac{1}{\sigma} q_*^2 + 3 - 2\sigma \quad \text{for} \quad 0 \leq \sigma \leq 1. \]
On the physical-realizability boundary, $\sigma = 1$. As $\sigma$ decreases, lines of constant sigma are parabolas of increasing curvature and increasing $y$ intercept. At $\sigma = 0$, the parabola collapses to a line coinciding with the Junk subspace of non-realizability for this maximum-entropy distribution function. The expression for $\sigma$ as a function of $q_*$ and $r_*$ can easily be found to be

$$\sigma(q_*, r_*) = \frac{3 - r_* + \sqrt{(3 - r_*)^2 + 8q_*^2}}{4}. \quad (32)$$

In this new mapped description, both realizability limits described in Section 4.3 represent domain boundaries. This makes a closed-form interpolation of the closing flux more convenient to propose.

### 4.5. Exact flux expressions on boundaries

If the goal is the development of closed-form approximations to the closing flux, one sensible strategy is to find the exact value wherever possible and interpolate. An investigation into the behaviour of the closing moment, $s_*$, is therefore of interest. The non-dimensional closing flux for the five-moment maximum-entropy system is shown in Fig. 2. It can readily be seen that, as the Junk subspace is approached, the flux becomes singular.
Numerical investigation has also revealed that, on the physical-realizability boundary, the non-dimensionalized distribution function degenerates into two delta functions. This investigation simply involved numerically solving the entropy-maximization problem for many states that are very close to the boundary and examination of the resulting distribution functions. The weights and positions of the deltas can be found by ensuring agreement with the zeroth through third moment (the fourth moment agrees automatically). The distribution function on this boundary is found to be

$$F_H(v) = \frac{2}{q^2_H + 4 + q_H \sqrt{q^2_H + 4}} \delta \left( v - \frac{q_H - \sqrt{q^2_H + 4}}{2} \right) \frac{2}{q^2_H + 4 + q_H \sqrt{q^2_H + 4}} \delta \left( v + \frac{q_H + \sqrt{q^2_H + 4}}{2} \right).$$

(33)

This can be integrated analytically to give a closing flux on the boundary of

$$s_H = q_H^3 + 2q_H^5.$$  

(34)

Using Eq. (13), it is also possible to find partial derivative of this moment with respect to the other non-dimensionalized moments at the equilibrium state. The moments in the Hessians of the density and flux potentials can be taken analytically at equilibrium and the derivatives can then be found as

$$\frac{\partial s_H}{\partial q_H} \bigg|_{(q_H=0,r_H=0)} = 10, \quad \frac{\partial s_H}{\partial r_H} \bigg|_{(q_H=0,r_H=0)} = 0.$$  

(35)

It must be remembered that there is a singularity intersecting this state and derivatives are therefore not properly defined in all directions. Nevertheless, these values, computed here using the theories of Section 3.1, are used for the following derivations.

4.6. Postulated interpolated closure

It now comes time to propose a form for the closing flux. The goal, of course, is a postulated flux that correctly agrees with all the information that could be analytically determined about the maximum-entropy closing flux and transitions in close agreement with the true flux.

It has been found that a simple interpolation function that preserves the singularity is a very accurate approximation to the true maximum-entropy closing flux. This function is given by

$$s_* = \frac{q_*^2}{\sigma^2} + 2\sigma^2 q_* + 10(1 - \sigma^2) q_* = \frac{q_*^3}{\sigma^2} + \left(10 - 8\sigma^2\right) q_*.$$  

(36)

The exponents 2 and $\frac{1}{3}$ were determined through numerical experimentation in an attempt to closely match the maximum-entropy closure with the simplest possible expression. This was done by numerically solving the entropy-maximization problem for many moment states and searching for the exponents which allowed the simple expression in Eq. (36) to most closely match the resulting closing flux. Special attention was payed to the area near the physical-realizability boundary, on
which the maximum-entropy closure itself loses hyperbolicity, as eigenvalues and corresponding eigenvectors of the flux Jacobian become equal on this boundary.\footnote{In a previous study, \cite{17}, fitting software was used to find an approximation to the closing flux in Eq. (24). The resulting function is a complicated expression that does not preserve the singularity present in the maximum-entropy system. At the time it was thought that the presence of this singularity is undesirable and therefore a function that transitioned smoothly across this line was sought. The expression given in Eq. (36) is much simpler, produces superior results, and is recommended.}

Plots of $s_*$ as a function of $q_*$ and $r_*$ are shown in Fig. 3. Comparison with Fig. 2 shows that this simple expression agrees very well with the true maximum-entropy closing flux throughout realizable moment space. Fig. 3(b) shows a zoom-in of the area surrounding local equilibrium ($q_* = 0, r_* = 3$). It can clearly be seen that the singularity touches equilibrium from above.

### 4.7. Hyperbolicity of closed-form one-dimensional closure

One goal of this research is moment closures with hyperbolicity that is expanded as compared to traditional moment closures. The original, and still the most popular, family of moment closures is that proposed by Grad \cite{3}, shown above in Section 2.2. It is well known that this family suffers from a restrictive region of hyperbolicity \cite{32–34}. This is caused by the flux Jacobian developing complex eigenvalues.

The five-moment one-dimensional Grad moment closure gives the simple closing relation

$$s_* = 10q_*.$$  \hspace{1cm} (37)

The small region of hyperbolicity of this closure is contained within a circle around local equilibrium with a radius of approximately three in the $q_* - r_*$ plane. By contrast, the new closure given in Eq. (36) has a vastly expanded region of hyperbolicity. Numerical investigation suggests that this new closure is hyperbolic for $0.001 < \sigma < 0.999$ and for $r_*$ all the way up to a value of 50,000—truly extreme non-equilibrium.

### 4.8. Numerical results

In order to investigate the behaviour of the new moment equations, a numerical investigation of the internal structure of stationary shock waves is shown. Comparisons are made between the five-moment model, shown above; the numerical solution of the BGK equation, using the discrete-velocity method of Mieussens \cite{42}; and the Navier–Stokes-like equations that result from a Chapman–Enskog expansion of Eq. (17) \cite{17}. The system resulting from this expansion is

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0,$$  \hspace{1cm} (38)

$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0,$$  \hspace{1cm} (39)

$$\frac{\partial (\rho u^2 + p)}{\partial t} + \frac{\partial (\rho u^3)}{\partial x} - \frac{\partial \left(3 \tau \frac{\partial (\rho u)}{\partial x}\right)}{\partial x} = 0,$$  \hspace{1cm} (40)

and can be regarded as the continuum (Navier–Stokes) model for one-dimensional physics.

An upwind Godunov-type finite-volume scheme with piece-wise limited-linear reconstruction \cite{43} and HLL flux function \cite{44} is used for the numerical solution of the moment equations. Wave speeds are determined by numerically computing the eigenvalues of the analytic flux Jacobian. A second-order-accurate time-marching scheme is used that treats the hyperbolic left-hand side of the moment equations explicitly while employing a point-implicit treatment for the stiff, but local, right-hand side \cite{17}. It is given by

$$\hat{U}_i^{n+1} = \hat{U}_i^n + \frac{\Delta t}{\Delta x} \left( \hat{F}_{i+\frac{1}{2}}^n - \hat{F}_{i-\frac{1}{2}}^n \right) + \Delta t \hat{C}_i^n,$$  \hspace{1cm} (41)

$$\tilde{U}_i^{n+1} = \tilde{U}_i^n + \frac{\Delta t}{2\Delta x} \left( \tilde{F}_{i+\frac{1}{2}}^n - \tilde{F}_{i-\frac{1}{2}}^n + \tilde{F}_{i+\frac{3}{2}}^n - \tilde{F}_{i-\frac{3}{2}}^n \right) + \frac{\Delta t}{2} \left( \tilde{C}_i^n + \tilde{C}_{i+1}^{n+1} \right).$$  \hspace{1cm} (42)

Here, the subscript denotes the cell index and the superscript denotes the time-step index, with a “$p$” denoting the predictor-step value. An overbar denotes the cell-average value and $\hat{F}_{i+\frac{1}{2}}$ denoted the numerical flux between cell $i-1$ and cell $i$ evaluated at the $n$th time step. A spatial discretization of five thousand equal-sized volumes is used. As Eq. (36) approaches a singularity and the Junk line is approached, special care must be taken during numerical calculations. For this study, the value of $\sigma$ used in the flux calculation is simply assigned a lower limit of $\hat{\sigma} = 2.0 \times 10^{-4}$, if $\sigma$ is less than this value, $\hat{\sigma}$ is used in Eq. (36). This is obviously a crude fix, but it is sufficient for the current purposes.

The relaxation time for the BGK collision operator is held fixed at a value of $\tau = 10^{-7}$ s for all computations. The computed results are therefore not physically accurate, however they do allow an evaluation of the behaviour of the closure for...
non-equilibrium flows. The upstream values of pressure and density are taken to be standard atmospheric values, 101,325 Pa and 1.225 kg/m³, respectively. The mean free path, $\lambda$, is taken to be

$$\lambda = \frac{16\tau}{5} \sqrt{\frac{p}{2\pi\rho}} = 3.67 \times 10^{-5} \text{ m.}$$

This follows from the expression for hard-sphere collisional processes given by Bird [1],

$$\lambda = \frac{16\mu}{5\sqrt{2\pi\rho}} ,$$

and the relationship between the relaxation time and fluid viscosity for the BGK collision operator,

$$\mu = \frac{\rho}{C_s} .$$

This approximation for the mean free path is not perfectly correct for this one-dimensional situation, however, as this relation is only used to non-dimensionlize the $x$ axis in the results that follow, it provides an acceptable approximation.

Fig. 4 shows the numerical solutions of the 5-moment system as compared to the solution to the one-dimensional Navier–Stokes-like equation and the direct numerical solution of the BGK equation with the BGK collision operator using the conservative discrete-velocity method of Mieussens [42]. For the solution of the BGK equation, velocity space is discretized using 500 velocities spanning –5000 m/s to 5000 m/s for the cases with an upstream Mach number of 2 and 4. For the case with an upstream Mach number of 8, 1000 velocities spanning –10,000 m/s to 10,000 m/s is needed. Comparison is made to the BGK equation rather than the Boltzmann equation with the true collision operator so as more accurately make a comparison to the moment closure. Since both solutions have the same collision operator, the only source of deviation is the moment approximation, which is the interest of this study.

It can be seen that the moment solutions are in far better agreement with direct solution of the kinetic equation than the Navier–Stokes is for all Mach numbers. It can also be observed that, as Mach number increases and non-equilibrium effects become more strong, the Navier–Stokes solutions become worse and worse, whereas the moment solutions maintain a good agreement with the BGK-equation solutions. Another striking observation is that the hyperbolic moment closure solutions are smooth—even at high Mach numbers.

4.9. Remarks regarding the smooth shock-structure predictions

For hyperbolic balance laws, it is well known that information travels at finite velocities that are described by the eigenvalues of the flux Jacobian. For shock-structure predictions, if the incoming flow velocity is larger than the fastest equilibrium wavespeed in the system, then all characteristics will point in the downstream direction and there is no possibility of upstream information propagation. The only way the flow can transition to the downstream state is through an initial discontinuity, or “sub-shock”. All previous hyperbolic closures have suffered from this mathematical artifact [4,45].

If the theory of Section 3.1 is followed, the maximum wave speed for a gas at rest and local equilibrium predicted by a five-moment maximum-entropy closure appears to be less than Mach 2. Therefore, why is there no discontinuity in any of the results? It is because of the singularity in the closing flux. As the Junk subspace is approached and the closing flux becomes singular, the maximum wavespeeds also become arbitrarily large. Because this singularity touches equilibrium, there are states arbitrarily close to equilibrium where the wavespeeds are arbitrarily large. If the solution leaves equilibrium with a trajectory that takes it into a region of very high wavespeeds, discontinuities can travel upstream at very high velocity.

For the shock-structure predictions presented in this paper, the gas always leaves a state of equilibrium with a trajectory in moment space that takes it into a region where the wavespeeds are high enough that discontinuities generated by the breakup of the initial conditions always travel upstream and out of the computational domain. Due to the singular nature of the closing flux, the details regarding the behaviour of the moment system near equilibrium are difficult to assess and much of the theory for hyperbolic systems is not applicable. This is the subject of ongoing research and will be more deeply examined in future work.

5. Closed-form approximation to a three-dimensional moment closure

The above analysis demonstrates the potential for closed-form robustly hyperbolic moment closures to provide affordable and highly-accurate predictions for both equilibrium and non-equilibrium flow predictions. The resulting system, with a singularity touching local equilibrium, is also a very interesting from a mathematical standpoint. Nevertheless, to be useful for practical applications, an extension to realistic, three-dimensional gases is required. The technique used to find the above five-moment system followed three steps:

1. First, the region of realizability was determined and a suitable remapping of moment space was employed.
2. Next, information about the behaviour of the closing flux at equilibrium and on the realizability boundaries was determined.
3. Finally, a form for the closing flux that transitions between the known boundary states was postulated.

This analysis has been extended to the physically realistic three-dimensional case and is shown here.
Fig. 4. Predicted normalized density and non-dimensionalized heat-transfer through a stationary shock wave for a one-dimensional gas as determined using the 5-moment closure, direct numerical solution of the BGK kinetic equation, and Navier–Stokes-like equations: (a)–(b) $Ma = 2$, (c)–(d) $Ma = 4$, and (e)–(f) $Ma = 8$. 

(a) Normalized density, $Ma = 2$.  
(b) Non-dimensionalized heat flux, $Ma = 2$.  

(c) Normalized density, $Ma = 4$.  
(d) Non-dimensionalized heat flux, $Ma = 4$.  

(e) Normalized density, $Ma = 8$.  
(f) Non-dimensionalized heat flux, $Ma = 8$. 
5.1. Fourteen-moment closure

The simplest member of the maximum-entropy hierarchy which has a treatment for heat-transfer for a physically realistic gas is a 14-moment closure. This is the closure that will be investigated. The vector of generating weights is \( \Phi = [1, v_1, v_2, v_3, v_4, v_5, v_6] \), This leads to a solution vector containing the following moments: \( \rho = \langle mF \rangle \), \( u_i = \langle m_{c_i}F \rangle \), \( P_y = \langle m_{c_y}F \rangle \), \( Q_{ijkl} = \langle m_{c_{ijkl}}F \rangle \), and \( R_{ijkl} = \langle m_{c_{ijkl}}F \rangle \). The resulting system of moment equations is

\[
\begin{align*}
\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial x_i} \left[ \rho u_i \right] &= 0, \\
\frac{\partial}{\partial t} [\rho u_i] + \frac{\partial}{\partial x_j} \left[ \rho u_i u_j + P_{ij} \right] &= 0, \\
\frac{\partial}{\partial t} \left[ \rho u_i u_j + u_i P_{jj} \right] + \frac{\partial}{\partial x_k} \left[ \rho u_i u_k u_j + u_i P_{jk} + u_k P_{ij} + Q_{ijk} \right] &= C_{ij}, \\
\frac{\partial}{\partial t} \left[ \rho u_i u_j u_k + u_i u_j P_{jk} + 2u_k P_{ij} + Q_{ijk} \right] + \frac{\partial}{\partial x_k} \left[ \rho u_i u_j u_k u_l + u_i u_j u_k P_{lj} + 2u_k u_l P_{ij} + u_l u_k P_{ij} + u_k Q_{ijkl} + u_l Q_{ijlk} + 2u_l Q_{jikl} + R_{ijkl} \right] &= C_{ijkl}. 
\end{align*}
\]

In order to close the system, expressions for the following moments, which appear only in the flux dyad, are needed: \( Q_{ijk} = \langle m_{c_{ijkl}}F \rangle \), \( R_{ijkl} = \langle m_{c_{ijkl}}F \rangle \), and \( S_{ijkl} = \langle m_{c_{ijkl}}F \rangle \).

5.2. Realizability of a fourteen-moment three-dimensional closure

In order to determine the region of physical realizability for the moment in the solution vector of the 14-moment closure, an analysis similar to that of Section 4.3 can be undertaken. For this case, the vector, \( M \), is taken as \( M = [1, v_1, v_2, v_3, v_4] \), Choosing the bulk velocity to be zero, this leads to a matrix

\[
Y = \langle mMM^TF \rangle = \begin{bmatrix}
\rho & 0 & 0 & 0 & P_{ii} \\
0 & P_{xx} & P_{xy} & P_{xz} & Q_{xii} \\
0 & P_{xy} & P_{yy} & P_{yz} & Q_{yii} \\
0 & P_{xz} & P_{yz} & P_{zz} & Q_{zii} \\
P_{ii} & Q_{xii} & Q_{yii} & Q_{zii} & R_{ijkl}
\end{bmatrix}
\]

This matrix is positive definite whenever

\[
R_{ijkl} \geq Q_{xii} P_{ii} + P_{jj}^2. \tag{52}
\]

The theory of physical realizability for one-dimensional distribution functions in Section 4.3 gives a sufficient condition on realizability, however, for the multi-dimensional case, it provides only a necessary condition. Nevertheless, for the choice of fourteen moments considered here, experience and experimentation involving the numerical solution of many entropy-maximization problems suggests that Eq. (52) does, in fact, describe all physically realizable states.

For this 14-moment closure, the junk subspace of physically realizable states that cannot be realized by a maximum-entropy distribution function is given by

\[
Q_{ijkl} = 0 \quad R_{ijkl} > \frac{2P_{ii}P_{jj} + P_{jj}^2}{\rho}. \tag{53}
\]

This is very similar to the one-dimensional case. If there is any heat flux, there is no problem and if the heat flux is zero, there is some maximum value of the fourth moment. For the one-dimensional case, this value was that of local equilibrium. Here, when there is no heat flux, the maximum value of \( R_{ijkl} \) is the value this moment takes when the distribution function is a Gaussian, 10-moment distribution [8,45].
5.3. Parabolic mapping of phase space

The similarity of the realizable region for the three-dimensional gas to that of the one-dimensional gas makes a similar parabolic mapping possible. The following expression is used to define the variable, \( r \), which transitions from the Junk subspace for \( r = 0 \) to the physical-realizability boundary for \( r = 1 \),

\[
R_{ijj} = \frac{1}{\sigma} Q_{kii} (P^{-1})_{kl} Q_{ljj} + \frac{2P_{ji}P_{ji} + P_{ij}P_{ij} - \sigma}{\rho} 2P_{ji}P_{ij} = \frac{1}{\sigma} Q_{kii} (P^{-1})_{kl} Q_{ljj} + \frac{2(1 - \sigma)P_{ij}P_{ij} + P_{ii}P_{jj}}{\rho}. \tag{54}
\]

Given a state, one can therefore compute sigma as

\[
\sigma = \frac{[2P_{ji}P_{ij} + P_{ij}P_{ij} - \rho R_{ijj}] + \sqrt{[2P_{ji}P_{ij} + P_{ij}P_{ij} - \rho R_{ijj}]^2 + 8\rho P_{mn}P_{mn}Q_{kii} (P^{-1})_{kl} Q_{ljj}}}{4P_{ij}P_{ij}}. \tag{55}
\]

5.4. Exact flux expressions on boundaries

A numerical investigation into the maximum-entropy distribution functions corresponding to moment states on the physical-realizability boundary reveals that, on this boundary, all particles exist on a sphere in velocity space. Fig. 5 shows four such distribution functions (non-dimensionalized axi-symmetric cases, with \( v^2 = v_x^2 + v_y^2 \), are chosen for ease of illustration).

The fact that the distribution function is non-zero only on a sphere is advantageous. To realize this advantage, one must first define a shifted particle velocity, such that

\[
v_i = \hat{v}_i + \bar{v}_i, \tag{56}
\]

![Fig. 5](image-url) Non-dimensionalized axi-symmetric probability-density function corresponding to several moment states on the physical realizability boundary.
where $\tilde{v}_i$ is the shift and $\tilde{v}_i$ is the particle velocity in the new frame of reference. This is obviously a simple Galilean transformation. As the form of the distribution function is invariant under Galilean transformation [8,26], the effect is simply to look at the same distribution function from a different inertial frame of reference. Moments of the peculiar component of particle velocity are obviously unaffected by this translation. The only effect on macroscopic moments is a shift of the apparent bulk velocity,

$$u_i = \tilde{u}_i + \tilde{v}_i.$$  \hfill (57)

It is obvious that one such shift results in the sphere of particles being centred on the origin of the new $\tilde{v}_i$ space. For the remainder of this work, $\tilde{v}_i$ is taken to be the particular shift that accomplished this centring for a given moment state. Therefore, $\tilde{u}_i$ is the apparent bulk velocity in the frame of reference that centres the sphere for the state of interest.

The fact that, on the realizability boundary, particles exist only on a sphere can now be used to relate some higher-order moments to known lower-order moments. This is because the magnitude of the particle velocity is constant on the sphere and any $\tilde{v}^2$ terms in higher-order contracted moment relation can then be taken out of the integral of the moment definition. For example,

$$\bar{U}_i = \langle m\tilde{v}^2 F \rangle = \tilde{v}^2 (m F) = \tilde{v}^2 \rho.$$  \hfill (58)

The radius of this spherical distribution function is therefore

$$\gamma = \sqrt{\frac{\bar{U}_i}{\rho}} = \sqrt{\frac{p_{ii} + \rho \tilde{u}_i \tilde{u}_i}{\rho}}.$$  \hfill (59)

The bulk velocity of the gas, as viewed from the frame of reference that centres the spherical distribution function on the origin, can also easily be found, as

$$\langle m \tilde{v} \tilde{v} F \rangle = \gamma^2 \langle m \tilde{v} F \rangle,$$

$$\rho \tilde{u}_i \tilde{u}_j + \tilde{u}_i P_{ij} + 2 \tilde{u}_j P_{ij} + Q_{ij} = \left( \tilde{u}_i \tilde{u}_j + \frac{P_{ij}}{\rho} \right) (\rho \tilde{u}_i),$$

$$\rho \tilde{u}_i \tilde{u}_j + \tilde{u}_i P_{ij} + \tilde{u}_j P_{ij} + 2 \tilde{u}_j P_{ij} + Q_{ij} = \rho \tilde{u}_i \tilde{u}_j + \tilde{u}_i P_{ij} + \tilde{u}_j P_{ij}.$$  \hfill (60)

This leads to a bulk velocity of

$$\tilde{u}_j = -\frac{1}{2} (P^{-1})_{ij} Q_{kk}.$$  \hfill (61)

This technique can also be used to find expressions for $R_{ijk}$ and $S_{ijk}$ on this boundary. These longer calculations are shown in Appendices B and C.

5.5. Postulated interpolated closure

The task now comes to postulating closing relations for the tree tensors mentioned in Section 5.1. These tensors are investigated individually in the following subsections. Long calculations are contained in the appendix to this paper.

5.5.1. Postulated $Q_{ijk}$

As $Q_{ijk}$ is not a contracted tensor, the knowledge of the shape of the distribution function on the realizability boundary is of no use. It is possible to determine the derivatives of this moment when the distribution function is a Gaussian. This derivation is shown in Appendix A, the result is

$$\frac{\partial Q_{ijk}}{\partial Q_{mmn}} = \left[ 2P_{il}(P^2)_{jk} + 2P_{il}(P^2)_{lj} + 2P_{il}(P^2)_{il} \right]^{-1} = K_{ijkm},$$  \hfill (61)

with

$$B_{lm} = 2P_{lm}(P^2)_{xx} + 4(P^3)_{lm}.$$  \hfill (62)

Given the small amount of information available about this tensor, the assumed expression for $Q_{ijk}$ is taken to be

$$Q_{ijk} = K_{ijkm} Q_{mn},$$  \hfill (63)

with $k_{ijk}$ defined in Eq. (61).
5.5.2. Postulated $R_{ijk}$

Next an expression for $R_{ijk}$ is developed. At a Gaussian distribution, this can be integrated analytically and has the value

$$
R_{ijk} = \frac{1}{\rho} (p_i p_k + 2p_ip_j).
$$

(64)

On the realizability boundary, this moment can be determined by expanding the moments in the equation $U_{ijk} = (m^i v_i v_j F_i v_j F_i) = \frac{m}{\rho} J_i$ and solving for $R_{ijk}$. On this boundary it has the expression

$$
R_{ijk} = Q_{ijl} (p-1)_{lm} Q_{mkk} + \frac{p_j p_k}{\rho}.
$$

(65)

The derivation of this is shown in Appendix B.

Remembering the definition of $\sigma$ in Eq. (54), the interpolation that seems most appropriate is

$$
R_{ijk} = \frac{1}{\sigma} Q_{ijl} (p-1)_{lm} Q_{mkk} + \frac{2(1-\sigma) p_i p_j + p_j p_k}{\rho}.
$$

(66)

5.5.3. Postulated $S_{ijk}$

Finally, an expression for $S_{ijk}$ is sought. When the distribution function is Gaussian, the following derivative can be found

$$
\frac{\partial S_{ijk}}{\partial Q_{mn}} = \frac{1}{\rho} \left[ 2p_i (p_x x)_x + 12p_i (p^3)_{xx} + 14(p^2)_{x2} (p^2)_2 + 20p^3 (p^2)_3 + 20(p^3)_{32} - 2(p^2)_{x3} p_i p_j - 6(p^3)^2 (p^2)_2 \right] B_{mn}^1
$$

$$
= W_{ij}.
$$

(67)

This derivation is also shown in Appendix A.

On the physical realizability boundary, one can use $\bar{U}_{ijk} = \langle m^i v_i v_j F_i v_j F_i \rangle = \bar{Y}^2 (m^i v_i F_i) = \left( \frac{\bar{U}}{\rho} \right) ^2 U_j$ to find $S_{ijk}$ on this boundary. This derivation is shown in Appendix C and leads to the expression

$$
S_{ijk} = p_i p_j p_k Q_{mnp} Q_{nij} Q_{blk} + 2 \frac{p_i Q_{jkl}}{\rho}.
$$

(68)

Using this knowledge, the following expression for $S_{ijk}$ is proposed

$$
S_{ijk} = \frac{1}{\sigma} p_i p_j p_k Q_{mnp} Q_{nij} Q_{blk} + 2 \frac{p_i Q_{jkl}}{\rho} + (1 - \sigma^2) W_{ij} Q_{mn}.
$$

(69)

The exponents 2 and $\frac{2}{3}$ are chosen for consistency with the one-dimensional study above.

5.6. Numerical results

With the aim of assessing the behaviour of this closure for one-dimensional flows, stationary shock-structure solutions are again investigated, now for a realistic three-dimensional gas. When restricted to only spatial variations in the $x$ direction, the distribution function remains axi-symmetric about the $v_x$ axis. Therefore, the radial particle velocities can be defined as $v_x = v_x^2 + v_x^3$ and $v_r = v_r + v_r^2$. This leads to moment relations: $u_y = u_z = 0$, $P_{rr} = P_{yy} + P_{zz}$, $P_{yy} = P_{xz} = P_{yz} = 0$, and $Q_{xx} = Q_{xx} = 0$. The fourteen-moment equations with BGK collision operator then reduce to six moment equations,

$$
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} [pu_x] = 0,
$$

(70)

$$
\frac{\partial}{\partial t} [pu_x] + \frac{\partial}{\partial x} [\rho u_x^2 + P_{xx}] = 0,
$$

(71)

$$
\frac{\partial}{\partial t} [\rho u_x^2 + P_{xx}] + \frac{\partial}{\partial x} [\rho u_x^2 + 3 u_x P_{xx} + Q_{xxx}] = \frac{P_{rr} - 2P_{xx}}{3\tau},
$$

(72)

$$
\frac{\partial}{\partial t} [P_{rr}] + \frac{\partial}{\partial x} [u_x P_{rr} + Q_{xxx}] = \frac{2P_{xx} - P_{rr}}{3\tau},
$$

(73)

$$
\frac{\partial}{\partial t} [\rho u_x^2 + u_x (3P_{xx} + P_{rr}) + Q_{xxx}] + \frac{\partial}{\partial x} [\rho u_x^4 + u_x^2 (6P_{xx} + P_{rr}) + 2u_x (Q_{xxx} + Q_{xxx}) + R_{xxx}] = \frac{2u_x (P_{rr} - 2P_{xx}) - 3Q_{xx}}{3\tau},
$$

(74)
\[
\frac{\partial}{\partial t} \left( \rho u^a_i + u^a_i (6P_{xx} + 2P_{rr}) + 4u_s Q_{xii} + R_{xii} \right) \\
+ \frac{\partial}{\partial x} \left[ \rho u^a_i + u^a_i (10P_{xx} + 2P_{rr}) + u^a_s (6Q_{xii} + 4Q_{xxx}) + u_s (R_{xii} + 4R_{xii}) + S_{xii} \right] \\
= \frac{1}{3} \tau \left[ 4u^2_s (P_{rr} - 2P_{xx}) - 12u_s Q_{xii} + 5 \left( \frac{P_{xx} + P_{rr}}{\rho} \right)^2 - 3R_{xii} \right].
\]
(75)

The closing relations postulated above reduce to
\[
Q_{xii} = A Q_{xii}, \quad Q_{xii} = (1 - A) Q_{xii},
\]
(76)
\[
R_{xii} = \frac{A Q_{xii}^2}{\sigma} \frac{2(1 - \sigma)P_{xx}^2 + (P_{xx} + P_{rr})P_{xx}}{P_{xx}},
\]
(77)
\[
S_{xii} = \frac{A Q_{xii}^3}{\sigma^2 P_{xx}^2} + \frac{2}{\rho} \left( P_{xx} + P_{rr} + \left( 1 - \sigma^2 \right) \frac{P_{rr}^3 + 2P_{xx}P_{rr}^2 + 24P_{xx}^3}{P_{xx}^2 + 6P_{xx}^2} \right) Q_{xii},
\]
(78)
with
\[
A = \frac{6P_{xx}^2}{P_{rr}^2 + 6P_{xx}^2},
\]
(79)
and
\[
\sigma = \frac{(2P_{xx}^2 + P_{rr}^2) + (P_{xx} + P_{rr})^2 - \rho R_{xii} \sqrt{\left( 2P_{xx}^2 + P_{rr}^2 \right) + (P_{xx} + P_{rr})^2 - \rho R_{xii}}} {2(2P_{xx}^2 + P_{rr}^2)}
\]
(80)

Comparisons will again be made to the Navier–Stokes equations that result from a Chapman–Enskog expansion of the BGK kinetic equation [46]. For a realistic three-dimensional monatomic gas, this results in the following equations for one-dimensional flows,
\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} [\rho u_s] = 0,
\]
(81)
\[
\frac{\partial}{\partial t} [\rho u_s] + \frac{\partial}{\partial x} [\rho u_s^2 + p] - \frac{\partial}{\partial x} \left[ \frac{4}{3} \tau p \frac{\partial u_s}{\partial x} \right] = 0,
\]
(82)
\[
\frac{\partial}{\partial t} \left[ \frac{1}{2} \rho u_s^2 + \frac{3}{2} p \right] + \frac{\partial}{\partial x} \left[ \frac{1}{2} \rho u_s^2 + \frac{5}{2} u_s p \right] - \frac{\partial}{\partial x} \left[ \frac{4}{3} \tau p \frac{\partial u_s}{\partial x} + \frac{5}{2} \tau p \frac{\partial}{\partial x} \left( \frac{p}{\rho} \right) \right] = 0.
\]
(83)

These are the classical one-dimensional Navier–Stokes equations with viscosity, \( \nu = \tau p \), and thermal conductivity, \( \kappa = 5k \tau p / (2m) \) (here, \( k \) is Boltzmann’s constant).

The same numerical scheme presented in Section 4.8 is used with the upstream density and pressure given by standard atmospheric values and a relaxation time of \( \tau = 10^{-3} \) s. The spatial domain is now discretized into one thousand cells. Once again, upstream Mach numbers of 2, 4, and 8 are considered. The speed of sound for a monatomic gas at these conditions is
\[
v_{\text{sound}} = \sqrt{\frac{5}{3} \text{1.225 kPa/m}^2} \approx 371 \text{ m/s}.
\]
(84)

**Table 1**

Discretization of velocity space for three-dimensional conservative BGK numerical solutions.

<table>
<thead>
<tr>
<th>Mach</th>
<th>Mach 2</th>
<th>Mach 4</th>
<th>Mach 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum ( \nu_s )</td>
<td>-2000 m/s</td>
<td>-3000 m/s</td>
<td>-5000 m/s</td>
</tr>
<tr>
<td>Maximum ( \nu_s )</td>
<td>3000 m/s</td>
<td>4000 m/s</td>
<td>7000 m/s</td>
</tr>
<tr>
<td>Maximum ( \nu_l )</td>
<td>2000 m/s</td>
<td>3000 m/s</td>
<td>5000 m/s</td>
</tr>
<tr>
<td>( n_x )</td>
<td>250</td>
<td>350</td>
<td>600</td>
</tr>
<tr>
<td>( n_x )</td>
<td>100</td>
<td>150</td>
<td>250</td>
</tr>
<tr>
<td>Total number of discrete velocities</td>
<td>25,000</td>
<td>52,000</td>
<td>150,000</td>
</tr>
<tr>
<td>( \Delta \nu_s )</td>
<td>20 m/s</td>
<td>20 m/s</td>
<td>20 m/s</td>
</tr>
<tr>
<td>( \Delta \nu_s )</td>
<td>20 m/s</td>
<td>20 m/s</td>
<td>20 m/s</td>
</tr>
</tbody>
</table>
Fig. 6. Predicted normalized density, pressure, and temperature profiles as well as non-dimensionalized heat-transfer through a stationary shock wave with an inflow Mach number of 2 for a realistic three-dimensional gas as predicted by the closed-form 14-moment equations, Navier–Stokes equations, and BGK kinetic equation. Symbol spacing is not representative of grid resolution.
Fig. 7. Predicted normalized density, pressure, and temperature profiles as well as non-dimensionalized heat-transfer through a stationary shock wave with an inflow Mach number of 4 for a realistic three-dimensional gas as predicted by the closed-form 14-moment equations, Navier–Stokes equations, and BGK kinetic equation. Symbol spacing is not representative of grid resolution.
Fig. 8. Predicted normalized density, pressure, and temperature profiles as well as non-dimensionalized heat-transfer through a stationary shock wave with an inflow Mach number of 8 for a realistic three-dimensional gas as predicted by the closed-form 14-moment equations, Navier–Stokes equations, and BGK kinetic equation. Symbol spacing is not representative of grid resolution.
For the BGK computations, the velocity distribution function will remain axi-symmetric and a two-dimensional discretization of velocity space is sufficient. Table 1 shows the maximum and minimum velocities; number of discrete velocities, \(n_x\) and \(n_r\); and the spacing of discrete velocities, \(\Delta v_x\) and \(\Delta v_r\), used for the three cases considered.

Results of this study are shown in Fig. 6–8. Again, the moment-closure solutions are smooth and are in much better agreement with those of the kinetic equation than the Navier–Stokes solutions. The predicted non-dimensionalized heat flux is in far better agreement, especially at higher Mach numbers. The moment-closure solution also predicts pressure and temperature anisotropies that are not possible within the Navier–Stokes treatment. The overshoot of the temperature normal to the shock wave is in amazing agreement with the solution to the kinetic equation at all Mach numbers. This overshoot is expected in shock waves, as energy is added more quickly to this mode and is then later redistributed by inter-particle collisions as local equilibrium is recovered.

5.7. Hyperbolicity of three-dimensional closure

Though the closure for a one dimensional gas shown in Section 4 is thought to be globally hyperbolic for all physically realizable states. This closure for a three-dimensional gas is not. For the numerical results shown above, the eigenvalues of the analytic flux Jacobian in each cell were computed at each time step for use in the HLL flux function and CFL time-step restriction. During the computation of the shock profiles for flows with Mach numbers of 2 and 4, these eigenvalues were always real and the system deemed hyperbolic. For the case with a flow Mach number of 8, some complex eigenvalues with small imaginary components were observed. The region of hyperbolicity does, however, seem to be large enough for the reliable computation of flow solutions involving large deviation from local thermal equilibrium. It is hoped that further refinement of this model will bring true global hyperbolicity and may lead to even better solution agreement with the kinetic equation.

6. Conclusions

It has been demonstrated that affordable closed-form moment closures can be postulated if one takes the maximum-entropy hierarchy as a guide. The widespread adoption of moment-closure-based techniques has always been hampered by the lack of such affordable and robustly hyperbolic closures. For the one-dimensional gas examined in Section 4, a simple system with an extremely, possibly global, region of hyperbolicity is demonstrated. Though the closed-form closure for a realistic gas developed in Section 5 is not globally hyperbolic, it does appear to have a region of hyperbolicity that is large enough to allow the reliable prediction of flows with much larger non-equilibrium effects than traditional closures have allowed.

The presence of the Junk subspace of non-realizability for the maximum-entropy framework has been considered a somewhat devastating characteristic of these closures. This paper shows that, for the closures considered, the nature of this region and the behaviour of the closing fluxes as it is approached actually gives the possibility of smooth shock profiles, even for flows with very high Mach numbers. The undesirable “sub-shocks”, present in other moment-closure solutions, have long been considered an inevitable characteristic of all hyperbolic moment closures. This works shows that this is not the case. Smooth shock profiles are possible in a hyperbolic setting.

Acknowledgement

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Appendix A. Determination of \(\frac{\partial Q_{ijk}}{\partial U_{mn}}\) and \(\frac{\partial S_{ijkk}}{\partial U_{mn}}\) at a Gaussian distribution

As stated in Section 3.1, the flux Jacobian in the \(\xi\) direction for a maximum-entropy moment closure can be computed using Eq. (13). When the distribution function is a Gaussian \([8,45]\) with zero bulk velocity, all odd moments are zero. By symmetry, the derivatives of all even moments with respect to odd moments as well as the derivatives of odd moments with respect to even moments must be zero. This causes Eq. (13) to decompose into two separate systems. One of these systems is given by

\[
\frac{\partial F_{i}}{\partial U} = (f_{x}^{(x)}(h_{xx})^{-1}. \tag{A.1}
\]

Using the fact that, with zero bulk velocity, \(\frac{\partial U_{ij}}{\partial U_{mn}} = \frac{\partial U_{ij}}{\partial U_{mn}}\) and \(\frac{\partial U_{ij}}{\partial U_{mn}} = \frac{\partial U_{ij}}{\partial U_{mn}}\), these matrices are given by the following expressions:
These higher-order moments can be integrated exactly when the distribution function is a Gaussian and have the values

\[
R_{ijkl} = \left( P_{ik} P_{jk} + P_{ik} P_{jl} + P_{il} P_{jk} \right) \rho, \\
R_{ijkk} = \frac{P_{ik} P_{kk} + 2P^2(i)}{\rho}, \\
V_{ijklmm} = \frac{P_{mm} \left[ P_{ik} P_{jk} + P_{ik} P_{jl} + P_{il} P_{jk} \right]}{\rho^2} + 2 \frac{P_{ij} (P^2)_{ij} + P_{ik} (P^2)_{jl} + P_{il} (P^2)_{jk} + P_{ik} (P^2)_{ij} + P_{ik} (P^2)_{jl} + P_{il} (P^2)_{jk}}{\rho^2},
\]

with

\[
A = \left( P_{ij} - R_{ijkl} (V^{-1})_{kmnnoo} R_{mnpq} \right)^{-1}, \\
B = - (P^{-1})_{kmn} R_{mnpq} \left( V_{ijkl} - R_{ijkl} (P^{-1})_{km} R_{mjj} \right)^{-1}, \\
C = \left( V_{ijkl} - R_{ijkl} (P^{-1})_{km} R_{mjj} \right)^{-1}.
\]

Multiplication of these matrices reveals the following expressions:

\[
\frac{\partial Q_{qtr}}{\partial Q_{tli}} = \left[ V_{qtrpp} - R_{qtr} (P^{-1})_{lm} R_{mnpq} \right] \left[ V_{ijkl} - R_{ijkl} (P^{-1})_{km} R_{mjj} \right]^{-1},
\]

and

\[
\frac{\partial Q_{qtr}}{\partial Q_{tli}} = \left[ V_{qtrpp} - V_{qtr} \right] \left[ V_{ijkl} - R_{ijkl} (P^{-1})_{km} R_{mjj} \right]^{-1}.
\]

These higher-order moments can be integrated exactly when the distribution function is a Gaussian and have the values

\[
R_{ijkl} = \frac{P_{ik} P_{jk} + P_{ik} P_{jl} + P_{il} P_{jk}}{\rho}, \\
R_{ijkk} = \frac{P_{ik} P_{kk} + 2P^2(i)}{\rho}, \\
V_{ijklmm} = \frac{P_{mm} \left[ P_{ik} P_{jk} + P_{ik} P_{jl} + P_{il} P_{jk} \right]}{\rho^2} + 2 \frac{P_{ij} (P^2)_{ij} + P_{ik} (P^2)_{jl} + P_{il} (P^2)_{jk} + P_{ik} (P^2)_{ij} + P_{ik} (P^2)_{jl} + P_{il} (P^2)_{jk}}{\rho^2},
\]
\[ V_{ijk} = \frac{(P_{kk})^2 P_{ij} + 4P_{kk}(P_{ij})_y + 2(P_{ij})_y^2 + 8(P_{ij})^3}{P_{ij}^2}, \]  

\[ V_{ijk\text{lim}} = \frac{3(P_{kk})^3 P_{ij} + 12(P_{kk})^2 P_{ij} + 18(P_{kk})P_{ij} + 36P_{kk}(P_{ij})_y + 36(P_{ij})^3}{P_{ij}^4}. \]  

Substituting these expressions into Eq. (A.8) and (A.9) yields

\[ \frac{\partial Q_{ij}}{\partial Q_{kl}} = \left[ 2P_{ij}(P_{kl})_r + 2P_{ij}(P_{kl})_o + 2P_{ij}(P_{kl})_a \right] \frac{1}{2P_{ij}(P_{kl})_a + 4(P_{ij})_o}^{-1}, \]  

and

\[ \frac{\partial S_{ij}}{\partial Q_{kl}} = \left[ 2P_{ij}(P_{kl})_a + 12P_{ij}(P_{kl})_o + 14(P_{ij})_a + 20P_{ij}(P_{kl})_o + 20(P_{ij})_a - 2(P_{ij})_a P_{ij} - 6(P_{ij})^2(P_{ij})_a \right] \frac{1}{2P_{ij}(P_{kl})_a + 4(P_{ij})_o}^{-1}. \]  

**Appendix B. Determination of \( R_{ijk} \) on physical-realizability boundary**

Following the technique shown in Section 5.4 the moment \( R_{ijk} \) on the physical-realizability boundary can be found using the relation,

\[ \bar{U}_{ijk} = \langle \hat{m}_{ij} \hat{n}_{j} \hat{v}_{k} \hat{F} \rangle = \frac{\hat{U}_{kk}}{\hat{P}_{ij}} \bar{U}_{ij}. \]  

This is expanded, then simplified using Eq. (60) as follows,

\[ \bar{U}_{ijk} = \frac{\hat{U}_{kk}}{\hat{P}} \bar{U}_{ij}, \]

\[ \rho \hat{u}_i \hat{u}_j \hat{u}_k + \hat{u}_i \hat{v}_j \hat{P}_{ij} + 2 \hat{u}_j \hat{u}_k \hat{P}_{ik} + 2 \hat{u}_j \hat{u}_k \hat{P}_{ik} + \hat{u}_i \hat{u}_j \hat{P}_{ij} + \hat{u}_i \hat{Q}_{ijk} + \hat{u}_i \hat{Q}_{ijk} + 2 \hat{u}_j \hat{Q}_{ijk} + R_{ijk} = \left( \frac{\hat{u}_i \hat{u}_j + \hat{P}_{ij}}{\rho} \right) \left( \rho \hat{u}_i \hat{P}_y \right), \]

\[ = \rho \hat{u}_i \hat{u}_j \hat{P}_{ij} \hat{u}_k + \hat{u}_i \hat{u}_j \hat{P}_{ij} \hat{u}_k + \hat{u}_i \hat{u}_j \hat{P}_{ij} \hat{u}_k + \hat{u}_i \hat{Q}_{ijk} + \hat{u}_i \hat{Q}_{ijk} + 2 \hat{u}_j \hat{Q}_{ijk} + R_{ijk}, \]

\[ 2 \hat{u}_i \hat{u}_k \hat{P}_{ik} + 2 \hat{u}_i \hat{u}_k \hat{P}_{ik} + \hat{u}_i \hat{Q}_{ijk} + \hat{u}_i \hat{Q}_{ijk} + 2 \hat{u}_i \hat{Q}_{ijk} + R_{ijk} = \frac{P_{ij} P_{ik}}{\rho}, \]

\[ Q_{ijk} = -2 \hat{u}_i P_{ik}, \]

\[ Q_{ijk} = -2 \hat{u}_i P_{ik}, \]

\[ 2 \hat{u}_i \hat{u}_k \hat{P}_{jk} + 2 \hat{u}_i \hat{u}_k \hat{P}_{ik} - 2 \hat{u}_i \hat{u}_k \hat{P}_{jk} - 2 \hat{u}_i \hat{u}_k \hat{P}_{jk} + 2 \hat{u}_i \hat{Q}_{ijk} + R_{ijk} = \frac{P_{ij} P_{ik}}{\rho}, \]

\[ R_{ijk} = \frac{-2 \hat{u}_i \hat{Q}_{ijk} + P_{ij} P_{ik}}{\rho}, \]

\[ R_{ijk} = Q_{ij} \left( P^{-1} \right)_{ijm} \frac{P_{ij} P_{ik}}{\rho}. \]  

**Appendix C. Determination of \( S_{ij} \) on physical-realizability boundary**

The derivation of \( S_{ij} \) on the realizability boundary is similar to that for \( R_{ijk} \) given in Appendix B. It begins with the relation

\[ \bar{U}_{ij} = \langle \hat{m}_{ij} \hat{n}_{j} \hat{v}_{k} \hat{F} \rangle = \frac{\hat{U}_{ij} \hat{U}_{kk} \bar{U}_{ij}}{\rho}, \]  

Again, this is expanded and reduced, making repeated use of Eq. (60), as follows
\[ \hat{U}_{ijk} = \frac{U_{ij} U_{ik}}{\rho} \hat{U}_i, \]

\[ \rho \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 2 \hat{u}_i \hat{u}_j \hat{u}_i \hat{u}_j \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k = \left( \frac{\rho u_i u_j + P_{jk}}{\rho} \right) \left( \frac{\rho u_i u_k + P_{kk}}{\rho} \right) \rho u_i, \]

\[ + \hat{u}_j R_{i j k} + S_{ijk} \]

\[ \frac{\rho \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 2 \hat{u}_i \hat{u}_j \hat{u}_j \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 2 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + \hat{u}_j R_{i j k} + S_{ijk} \]

\[ = \rho \hat{u}_i \hat{u}_j \hat{u}_j \hat{u}_k \hat{u}_k + 2 \hat{u}_i \hat{u}_j \hat{u}_j \hat{u}_k + \frac{\hat{u}_i P_{jk}}{\rho}, \]

\[ 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + \hat{u}_j R_{i j k} + S_{ijk} = \frac{\hat{u}_i P_{jk}}{\rho}. \]

\[ 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + \hat{u}_i \left( Q_{ij}(P^{-1})_{nm} Q_m k_k + \frac{P_{jk}}{P_{kk}} \right) + \frac{P_{jk}}{P_{kk}}, \]

\[ = \frac{R_{ijk}}{S_{ijk}} \]

\[ \frac{Q_{ij} (P^{-1})_{nm} Q_m k_k + \frac{P_{jk}}{P_{kk}}}{S_{ijk}} = 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + \hat{u}_j \left( Q_{ij}(P^{-1})_{nm} Q_m k_k + \frac{P_{jk}}{P_{kk}} \right) + \frac{P_{jk}}{P_{kk}}. \]

\[ 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + \hat{u}_j \left( Q_{ij}(P^{-1})_{nm} Q_m k_k + \frac{P_{jk}}{P_{kk}} \right) + \frac{P_{jk}}{P_{kk}} + S_{ijk} = 4 \hat{u}_i \hat{u}_j \hat{u}_k \hat{u}_k + \hat{u}_j \left( Q_{ij}(P^{-1})_{nm} Q_m k_k + \frac{P_{jk}}{P_{kk}} \right) + \frac{P_{jk}}{P_{kk}}. \]

\[ S_{ijk} = -4 \hat{u}_j \left( R_{i j k} + \hat{u}_k Q_{ij k} \right), \]

\[ \hat{u}_k = -\frac{1}{2} (P^{-1})_{kl} Q_{lm m}. \]

References


