# Physically-Realizable Hyperbolic Moment Closures for Predicting Non-Equilibrium Gaseous Flows

James G. McDonald and Clinton P. T. Groth

*University of Toronto Institute for Aerospace Studies, 4925 Dufferin Street, Toronto, Ontario, M3H 5T6, Canada*

Email: *mcdonald@utias.utoronto.ca, groth@utias.utoronto.ca*

## ABSTRACT

Moment closures of gaskinetic theory offer a method for the prediction of non-equilibrium flows which have a wider range of validity than standard continuum methods, such as solution of the Navier-Stokes equations, and can be much more computationally efficient than particle-based techniques, such as Direct Simulation Monte Carlo (DSMC). Moment methods yield systems of first-order partial differential equations in weak-conservation form. Such systems can have computational advantages as they require only the numerical evaluation of first derivatives. One hierarchy of moment closures which seem to have many desirable mathematical properties are those which assume the distribution function is always that which maximizes entropy for a given finite set of velocity moments. These maximum-entropy systems, however, suffer from a major drawback: there exist physically realizable moment values for which a maximum-entropy distribution function does not exist. In these regions the moment equations break down and become ill-posed. This paper demonstrates a correction which can be used to remedy this deficiency in maximum-entropy closures. Several features of the resulting physically-realizable moment closures are described and computational solutions of the proposed moment system are presented for several flow problems for a one-dimensional gas.

## 1 INTRODUCTION

Gas flows existing outside of local thermodynamic equilibrium possess a variety of characteristics which make them difficult to simulate by means of traditional numerical techniques. The regime in which a gas exists can be described by the flow Knudsen numbers (Kn), which is defined as the ratio of the mean free path a gas particle travels between collisions, $\lambda$ to the length scale of the situation. As flow Knudsen numbers increase, traditional fluid-dynamic equation sets based on the continuum assumption are no longer valid.

Particle-simulation techniques, such as the direct-simulation Monte Carlo (DSMC) method [3], have been developed for the prediction of general non-equilibrium gaseous flows. However, for near-continuum through to transitional-regime flows, the computational costs incurred by these techniques are considerable. This is especially true for flows with low Mach numbers and, in these situations, computational expense can prohibit their usage [6, 15].

Alternate approaches for the simulation of non-equilibrium flows include methods based on moment closures [9, 13]. In these techniques, an assumed form for the probability distribution function is chosen such that moments, or macroscopic quantities, whose transport can then be determined by a set of moment equations, can be determined. Moment closures provide an extended set of partial differential equations (PDEs) describing the transport of macroscopic fluid properties. In general, the solution of these PDEs require considerably less effort than that associated with obtaining solutions using particle simulation methods.

Moment closures, unfortunately, are not without their limitations. Although early closure hierarchies, such as those proposed by Grad [9], provide hyperbolic PDEs for the time evolution of non-equilibrium quantities, the equations can suffer from closure breakdown and loss of hyperbolicity for what appear to be relatively benign flows. The Grad closures also do not guarantee moment realizability of solutions (moment realizability refers to the existence of a physically realistic velocity distribution function which corresponds to the given set of predicted velocity moments).

An alternative technique for obtaining moment equations is to chose the moments of interest and assume that the corresponding approximate distribution function be that of maximum entropy subject to the constraint that it be consistent with the given set of velocity moments. Moment closures obtained in this manner appear to have many desirable mathematical properties including hyperbolicity, realizability of moments and an entropy relation [13]. Unfortunately, recent studies have shown that the entropy maximization problem does not always have a solution for the full range of physically realizable moments, and thus the domain for which the resulting maximum-entropy moment equations are well posed can be limited [11, 12]. This problem is particularly devastating as it has been shown that for all moment equations describing moments which correspond to super-quadratic velocity weights, the local equilibrium state lies exactly on the boundary separating the states for which the entropy maximization problem can be solved and those for which it cannot [12].

In the present work, moment methods and the mathematical structure of maximum-entropy moment closures are presented. The problem of moment realizability for these closures is then reviewed and a correction which eliminates this deficiency is proposed and demonstrated. Finally, one-dimensional numerical solutions of a resulting moment system are shown for several flow problems.

## 2 Moment Methods

Moment closures arise from the field of gaskinetic theory. This theoretical approach takes into account the particle nature of gases by defining a probability density function, $\mathcal{F}(x_i, v_i, t)$, in six-dimensional phase space which specifies the probability of finding particles at a given location, $x_i$, and time, $t$, having a particular velocity, $v_i$. Macroscopic "observable" properties of the gas are then obtained by taking appropriate velocity moments of $\mathcal{F}$. This is done by integrating the product of the distribution function and an appropriate velocity dependent weight over all velocity space,

$$\langle M(v_i)\mathcal{F}\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} M(v_i)\mathcal{F}(x_i, v_i, t)\, d^3v. \quad (1)$$

For example $\rho = m\langle\mathcal{F}\rangle$, $u_i = m\langle v_i\mathcal{F}\rangle$, and $p_{ij} = m\langle c_i c_j \mathcal{F}\rangle$ Here $m$ is the mass of a particle, $\rho$ is the gas density, $u_i$ is bulk velocity, $c_i = v_i - u_i$ is gas-particle random velocity, and $p_{ij}$ is an anisotropic pressure tensor.

The evolution of the velocity distribution function is prescribed by the Boltzmann equation [5, 4, 8]. This is an integro-differential equation for $\mathcal{F}$ having the form:

$$\frac{\partial \mathcal{F}}{\partial t} + v_i\frac{\partial \mathcal{F}}{\partial x_i} + a_i\frac{\partial \mathcal{F}}{\partial v_i} = \delta\mathcal{F}\,. \quad (2)$$

Here $a_i$ is the acceleration due to external forces. The term on the right hand side of the equation, $\delta\mathcal{F}$, is the Boltzmann collision integral and represents the time rate of change of the distribution function produced by inter-particle collisions.

Transport equations governing the time evolution of macroscopic quantities can be derived by evaluating velocity moments of the Boltzmann equation given above. This leads to Maxwell's equation of change which describes the evolution of the moment $\langle M\mathcal{F}\rangle$ by

$$\frac{\partial}{\partial t}\langle M\mathcal{F}\rangle + \frac{\partial}{\partial x_i}\langle v_i M\mathcal{F}\rangle = \Delta\langle M\mathcal{F}\rangle\,. \quad (3)$$

Here the acceleration field is taken to be zero (as will be the case throughout the present work), $\Delta\langle M\mathcal{F}\rangle = \langle M\delta F\rangle$ is the effect of collisions on the moment quantity, and $M$ is an appropriate velocity dependent weight.

It is at this point that the problem of closure becomes apparent. The time evolution of a given moment $\langle M\mathcal{F}\rangle$ is clearly dependent on the spatial divergence of $\langle v_i M\mathcal{F}\rangle$, a moment of one higher order in terms of the velocity, $v_i$. This pattern is repeated, with the time evolution of every moment being dependent on a moment of one higher order in $v_i$. In general, an infinite number of moment equations is required to fully describe the evolution of a macroscopic flow quantity, and solving this infinite system is equivalent to solving Eq. (2).

One technique used to obtain moment closure is to restrict the distribution function to an assumed form [9]. Restricting the form of the distribution function has the effect of restricting the value of certain higher-order moments to be functions of lower-order moments, thus furnishing a closing relationship in the moment equations. For example, for a monatomic gas if the distribution function is assumed to have the form

$$\mathcal{F}(x_i, v_i, t) = \mathcal{M}(x_i, v_i, t) = n\left(\frac{\beta}{\pi}\right)^{\left(\frac{3}{2}\right)} e^{(-\beta c_i c_i)}\,, \quad (4)$$

where $n$ is the number density, $c_i$ is the random component of the particle velocity and $\beta$ is a function of the local temperature, the method of moments will lead to the well-known compressible Euler equations describing the time evolution of density, momentum, and energy. Equation (4) defines the Maxwell-Boltzmann distribution, $\mathcal{M}$, describing the equilibrium behaviour of a monatomic gas. It can be shown that the collision operator will force all distribution functions towards this form, and, once in this state, the collision operator will produce no further effects. This entropy property of the collision operator is well established by Boltzmann's H theorem. Gases described by this distribution function are said to be in local thermodynamic equilibrium.

## 3 MAXIMUM-ENTROPY MOMENT CLOSURES

Moment methods provide a treatment of non-equilibrium gas behaviour by choosing assumed distributions functions with added degrees of freedom which are then related to lower-order velocity moments. It is generally assumed that the inclusion of more moments in a closure leads to a greater possibility that the resulting system will closely approximate general non-equilibrium behaviour.

One technique for choosing an assumed form for the distribution function is to chose the function which maximizes entropy while satisfying certain desired moments [13]. It can be shown that this technique will yield distribution functions of the form

$$\mathcal{F} = \exp\left(\boldsymbol{\alpha}\cdot\mathbf{m}\right), \tag{5}$$

where $\mathbf{m}$ is the vector particle-velocity-dependent functions corresponding to the desired moments of the system, i.e. $\mathbf{U} = m\langle\mathbf{m}\mathcal{F}\rangle$, and $\boldsymbol{\alpha}$ is a vector of coefficients related to the macroscopic state of the gas. The vector $\mathbf{m}$ must be selected such that $\mathcal{F} = \exp(\boldsymbol{\alpha}\cdot\mathbf{m})$ can remain finite even as $|v_i| \to \infty$. The familiar Euler equations of fluid dynamics are recovered by selecting $\mathbf{m} = \{1, v_i, v_i v_i\}$ (this is equivalent to the equilibrium moment system described in the previous section).

Levermore [13] has demonstrated the hyperbolicity of these moment equations by defining a density potential $h$ and a flux potential $j_i$ as

$$h(\boldsymbol{\alpha}) = m\langle\mathcal{F}\rangle = m\langle\exp(\boldsymbol{\alpha}\cdot\mathbf{m})\rangle, \tag{6}$$

$$j_i(\boldsymbol{\alpha}) = m\langle v_i\mathcal{F}\rangle = m\langle v_i\exp(\boldsymbol{\alpha}\cdot\mathbf{m})\rangle. \tag{7}$$

The conserved moments and their fluxes can then be expressed as

$$\mathbf{U} = m\langle\mathbf{m}\mathcal{F}\rangle = \frac{\partial h}{\partial\boldsymbol{\alpha}}, \tag{8}$$

$$\mathbf{F_i} = m\langle v_i\mathbf{m}\mathcal{F}\rangle = \frac{\partial j}{\partial\boldsymbol{\alpha}}. \tag{9}$$

Using these relations, the moment equations can be written as

$$\frac{\partial}{\partial t}\frac{\partial h}{\partial\boldsymbol{\alpha}} + \nabla\cdot\frac{\partial j}{\partial\boldsymbol{\alpha}} = \mathbf{S}. \tag{10}$$

The hyperbolicity of this equation becomes evident upon rewriting as

$$\frac{\partial^2 h}{\partial\boldsymbol{\alpha}^2}\frac{\partial\boldsymbol{\alpha}}{\partial t} + \frac{\partial^2 j}{\partial\boldsymbol{\alpha}^2}\nabla\cdot\boldsymbol{\alpha} = \mathbf{S}. \tag{11}$$

The Hessians $\frac{\partial^2 h}{\partial\boldsymbol{\alpha}^2}$ and $\frac{\partial^2 j}{\partial\boldsymbol{\alpha}^2}$ are obviously symmetric. Moreover, $\frac{\partial^2 h}{\partial\boldsymbol{\alpha}^2}$ is positive definite, as

$$\begin{aligned}\mathbf{W}^{\mathrm{T}}\frac{\partial^2 h}{\partial\boldsymbol{\alpha}^2}\mathbf{W} &= \mathbf{W}^{\mathrm{T}} m\left\langle\mathbf{m}\mathbf{m}^{\mathrm{T}}\mathcal{F}\right\rangle\mathbf{W} \\ &= m\left\langle\left(\mathbf{W}^{\mathrm{T}}\mathbf{m}\right)^2\mathcal{F}\right\rangle \geq 0\end{aligned} \tag{12}$$

with equality only if $\mathbf{W} = 0$. Eq. (11) therefore defines a classic Friedrichs-Lax hyperbolic system [7].

### 3.1 Realizability of Maximum-Entropy Distribution Functions

The proof of hyperbolicity given above seems very elegant and establishes a lot of promise for the technique of maximum-entropy moment closure; however, there is a significant problem. All of the desirable mathematical properties that these moment systems appear to have assume that a maximum-entropy distribution function for the selected set of velocity moments always exists; this is not the case. Junk has shown that for any moment system based on moments which correspond to super-quadratic polynomial weight functions there are physically realizable situations for which a maximum entropy distribution function cannot be found [12]. This deficiency is related to the requirement that the restriction placed on the coefficients, $\alpha$. Moreover, the state describing local thermodynamic equilibrium always lies on the boundary of the region where a maximum-entropy distribution function exists. There is therefore always a region with equilibrium on its boundary for which these moment methods will become ill-posed or undefined.

## 4 PHYSICALLY-REALIZABLE MOMENT CLOSURES

One possible technique to avoid issues with non-realizability is to slightly modify the assumed form for the distribution function. This can easily be done by adding an additional term to the exponential in Eq. (5),

$$\mathcal{F} = \exp\left(\boldsymbol{\alpha}\cdot\mathbf{m} + \sigma\right). \tag{13}$$

The velocity-dependent term, $\sigma$, must be chosen such that it approaches negative infinity more quickly than the polynomial, $\boldsymbol{\alpha}\cdot\mathbf{m}$, can approach positive infinity as $v_i$ increases in magnitude. It is interesting to note that if the term, $\sigma$, is not a function of the closure coefficients the proof of hyperbolicity, as given by Levermore, remains valid.

A simple example where this is true is to take $\sigma = -bv^n$ where $b$ is a positive number and $n$ is an even integer larger than the highest power of the velocity in $m$. For this case $\frac{\partial\sigma}{\partial\boldsymbol{\alpha}} = 0$ and the above proof of hyperbolicity remains valid. Unfortunately, this choice of term will not lead to moment equations which are Galilean invariant. This modification to the maximum-entropy moment system seems to have been first proposed by Au [1]. A similar modification which leads to Galilean-invariant closures is $\sigma = -bc^n$ where $c$ is the random component of the particle velocity. This however is problematic as $\frac{\partial c}{\partial\boldsymbol{\alpha}} \neq 0$ and hyperbolicity is no longer assured via Levermore's proof.

The addition of $\sigma$ in Eq. (13) can be seen as equivalent to multiplying the distribution by a "window function" which attenuates the distribution for large velocities. It is desirable to have the coefficient $b$ be dependent on the unmodified distribution function in order to match the standard deviation in some way and provide and appropriate windowing. This renders strict proof of hyperbolicity even more elusive, however it will be shown through numerical results that the equations are well behaved and remain hyperbolic for a very wide range of flow conditions.

For the current work, the modification to the maximum-entropy distribution is given by

$$\sigma = -b\left(\frac{\rho}{p}\right)^{\frac{L+2}{2}} c^{L+2}, \tag{14}$$

where $L$ is the highest velocity exponent in the moment system and $b$ is some specified positive number.

## 5 Investigation of One-Dimensional System

In order to explore the behaviour of this new family of closures, a simple five-moment one-dimensional system is examined. This closure is one-dimensional in both physical and velocity space (i.e. gas particles can have velocities in only one direction). The moment system describing the evolution of the five lowest-order moments is given by

$$\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \tag{15}$$

$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = 0 \tag{16}$$

$$\frac{\partial}{\partial t}\left(\rho u^2 + p\right) + \frac{\partial}{\partial x}\left(\rho u^3 + 3up + q\right) = 0 \tag{17}$$

$$\frac{\partial}{\partial t}\left(\rho u^3 + 3up + q\right) + \frac{\partial}{\partial x}\left(\rho u^4 + 6u^2 p + 4uq + r\right) = C_3 \tag{18}$$

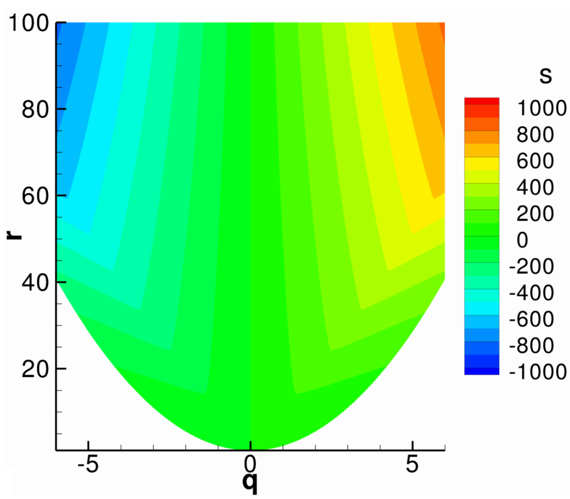
$$\frac{\partial}{\partial t}\left(\rho u^4 + 6u^2 p + 4uq + r\right) + \frac{\partial}{\partial x}\left(\rho u^5 + 10u^3 p + 10u^2 q + 5ur + s\right) = C_4\,, \tag{19}$$

where $C_n$ is the effect of the collision operator on the $n$th conserved moment. Here $q = m\left\langle c^3\mathcal{F}\right\rangle$ is the heat flux, $r = m\left\langle c^4\mathcal{F}\right\rangle$ is the fourth-order random-velocity moment, and $s = m\left\langle c^5\mathcal{F}\right\rangle$ is the fifth-order random-velocity moment. It is this fifth-order moment which must be determined through the integration of the assumed form of the distribution function to close the system.

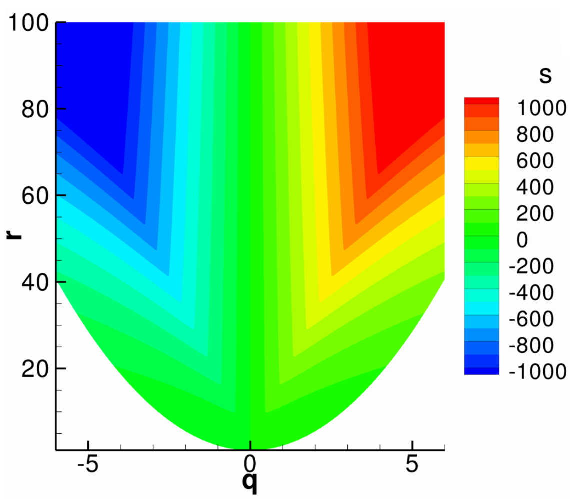
The collision operator in Eq. (2), which has given rise to the $C_n$ terms in Eq. (15), is a complex integral relationship. For the purpose of assessing the accuracy of the moment closure, it is sufficient to use a simplified collision term. For this study, the relaxation collision operator of Bhatnager, Gross, and Krook [2] is used. When this simple collision operator is used in Eq. (2) it becomes the so-called BGK equation.

Without loss of generality, the distribution function used in this closure can be normalized such that it describes a gas with a density of one, a bulk velocity of zero and a pressure of one. The relationship of the fifth-order moment $s$ can then be examined as a function of the normalized heat flux $q$ and fourth-order moment $r$. It can be shown [11] that, for this normalized situation, $r > 1 + q^2$ for the specified moments to be physically realizable. Figure 1 shows the numerical computation of $s$ as predicted by the new closure for a wide range of physically realizable situations with $b = 1\times10^{-4}$ and $b = 1\times10^{-5}$. It is interesting to note that $s$ does not appear to be a smooth function of $q$ and $r$.

A main motivating reason for considering moment closures is that they hold the promise of a hyperbolic treatment of non-equilibrium gas behaviour. The modification to the maximum-entropy distribution function has lead to a moment closure which covers the whole realizable moment space, however, the proof of global hyperbolicity must been abandoned. In order to investigate the hyperbolicity of the new closure, flux Jacobians are computed numerically using centered differences. Eigenvalues, $\Lambda$, are then computed numerically. The system of moment equations is deemed hyperbolic whenever the eigenvalues are real. Figure 2 shows the largest imaginary part of the computed eigenvalues as a function of $q$ and $r$ for the normalized distribution function. It can be seen that the computed eigenvalues do not remain real, and hence, the system is not globally hyperbolic. Fortunately, as $b$ decreases, the region of hyperbolicity expands greatly. The orbits of



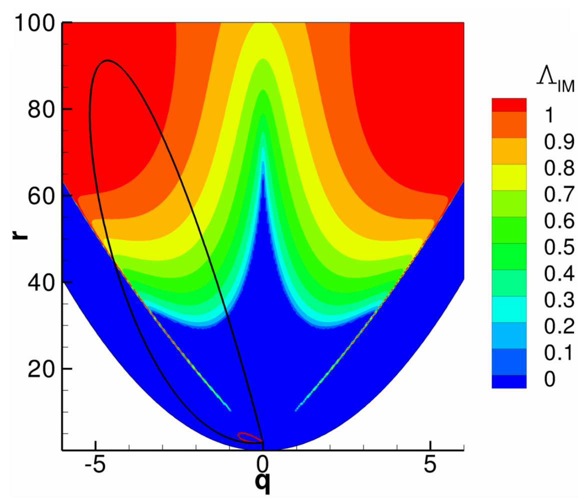

(a)



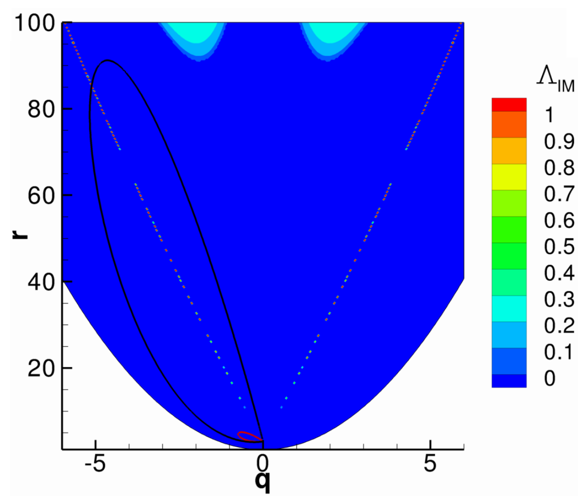

(b)

Figure 1: *Fifth-order random-velocity moment, s, as a function of q and r for five-moment one-dimensional realizable moment closure with (a)* $b = 1 \times 10^{-}4$*, (b)* $b = 1 \times 10^{-}5$.

moments describing the structure of shockwaves with Mach numbers of 2 and 8 as predicted by a high-resolution numerical solution of the kinetic equation (Eq. 2) with the BGK collision operator are shown on both Figures 2(a) and 2(b) in red and black respectively (the orbit corresponding to a shock with an upstream Mach number of 2 is very small as compared to that of the stronger shock). It can be seen that if $b$ is taken to be $10^{-5}$, even for the case of the relatively strong Mach-8 shock the moment closure remains in the hyperbolic region. The appearance of complex eigenvalues along the line across which $s$ seems to be a non-smooth function of $q$ and $r$ may be due to the unsuit-




(a)




(b)

Figure 2: *Largest imaginary part of computed eigenvalues of flux Jacobian for five-moment one-dimensional realizable moment closure with (a)* $b = 10^{-}4$*, (b)* $b = 10^{-}5$*. The orbits of moments describing the structure of Mach-*2 *and Mach-*8 *shock structures are shown in red and black respectively.*

ability of finite differences across this line. The hyperbolic nature of the closure and its moment equations is difficult to evaluate on this line.

## 6 Finite-Volume Flow Solver

As a preliminary investigation into the predictive capability offered by the proposed higher-order realizable hyperbolic moment equations, a one-dimensional flow solver for the one-dimensional moment system described above has been constructed. This system is solved using a Godunov-type finite-volume scheme with the HLL [10] approximate Riemann solver used to evaluate inter-cellular fluxes. Higher-order accuracy is achieved through piecewise limited linear reconstruction. A point-implicit time-integration scheme is used to advance the solution [14].

For maximum-entropy moment closures with velocity basis functions of order higher than two, there is no explicit conversion from conserved moments $\mathbf{U}$ to the closure coefficients $\boldsymbol{\alpha}$. The evaluation of the highest-order flux requires that the coefficients be known, therefore, these coefficients must be determined after each time step. This can be done by finding $\boldsymbol{\alpha}$ that minimizes

$$J = \langle m\mathcal{F}\rangle - \boldsymbol{\alpha}^{\mathrm{T}}\mathbf{U}. \tag{20}$$

This function can be shown to be convex, as the Hessian of Eq. (20) is equal to the positive-definite Hessian of Levermore's density potential described above, $\frac{\partial^2 J}{\partial \boldsymbol{\alpha}^2} = \frac{\partial^2 h}{\partial \boldsymbol{\alpha}^2}$. This matrix contains only moments of the distribution function, which must be computed through numerical quadrature. The minimization problem can be solved using an approximate Newton's method. In some cases, it is possible for the computed update from Newton's method to move the vector $\boldsymbol{\alpha}$ to a location where numerical integration of the moments is not possible due to numerical issues. When this happens, a back-tracking technique is used to step back into a computable configuration. The convexity of Eq. 20 assures that there is only a single minimum when

$$\frac{\partial J}{\partial \boldsymbol{\alpha}} = \langle m\mathbf{m}\mathcal{F}\rangle - \mathbf{U} = 0 \tag{21}$$

which is the requirement for consistency between the coefficients, $\boldsymbol{\alpha}$, and the conserved moments, $\mathbf{U}$.

This technique to synchronize $\boldsymbol{\alpha}$ and $\mathbf{U}$ involves many numerical integrations of the velocity distribution function and is very computationally expensive compared to the other elements of the flow solver. A technique to reduce the number of resynchronizations required is therefore very desirable. One possibility is to again make use of the Hessian of the density potential, $\frac{\partial^2 h}{\partial \boldsymbol{\alpha}^2} = \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\alpha}}$ to update the closure coefficients after each time step through the relationship

$$\Delta\boldsymbol{\alpha} = \left(\frac{\partial \mathbf{U}}{\partial \boldsymbol{\alpha}}\right)^{-1} \Delta\mathbf{U}. \tag{22}$$

If this coefficient update is sufficiently accurate, the resynchronization of $\boldsymbol{\alpha}$ to $\mathbf{U}$ may not be required, thus greatly reducing the cost of the scheme. However, determining the effectiveness of this simplified update and deciding when a full resynchronization is required can be difficult. One possibility is to apply the simple update and integrate one velocity moment and compare it to the target value; a large deviation can be used as a trigger for a resynchronization using the above technique.

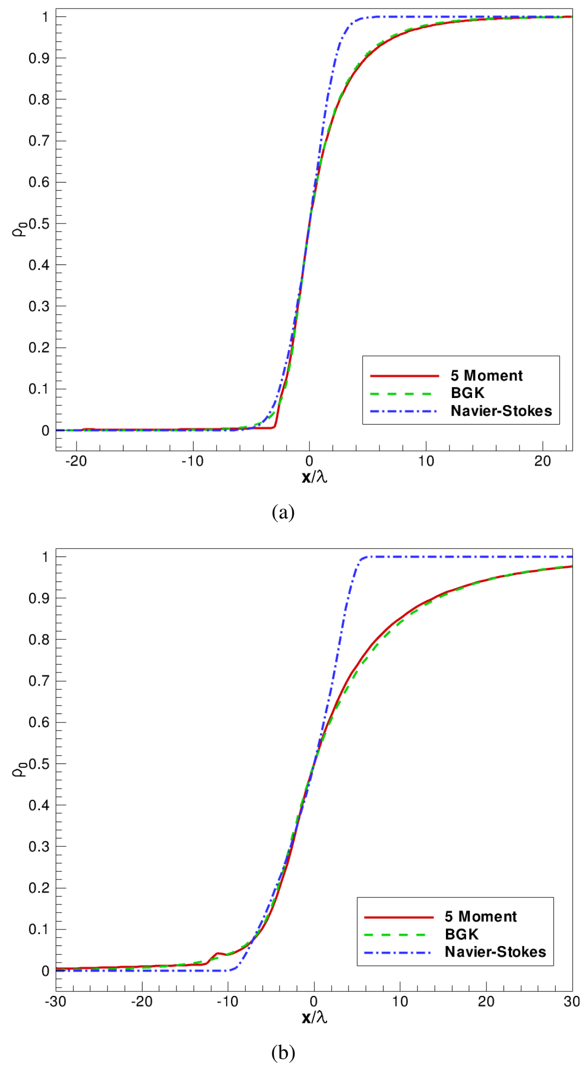



Figure 3: *Shock-structure calculations for one-dimensional gas computed using modified maximum-entropy five moment system as compared to direct numerical solution of kinetic equation and Navier-Stokes equations: (a) Mach = 2, (b) Mach = 8.*

## 7 PRELIMINARY NUMERICAL RESULTS

Predictions of the structure of stationary shocks for the one-dimensional gas obtained by solving the five-moment version of the physically-realizable moment equations are shown in Figure 3 and compared with numerical solutions to the equivalent "Navier-Stokes" equations and high-resolution numerical solutions of the one-dimensional BGK equation for this one-dimensional gas. It can be seen that even at high Mach numbers, where the Navier-Stokes equations do a poor job of predicting shock structure, the hyperbolic five-moment system agrees surprisingly well with the numerical solutions of the full kinetic equation.

In order to explore the behaviour of the moment system across a range of Knudsen numbers, a shock-tube problem is considered. The case considered consists of a two-state initial condition with a pressure ratio of 2.5 and a density ratio of 2. Three different situations were considered corresponding to Knudsen numbers of $2.3 \times 10^{-5}$, $2.3 \times 10^{-2}$, and 23, thus spanning the continuum, transition and free-molecular flow regimes. The resulting solutions are shown in Figure 4. Here the five-moment system is compared to the three-moment system (which is equivalent to the Euler equations for a one-dimensional gas), high-resolution numerical solution of the BGK equation and numerical solution of the Navier-Stokes equations.

It can be seen in Figure 4(a) that in the continuum regime all the equations agree with the equivalent "Euler" equations for this one-dimensional gas. On this scale any areas in the flow which are not in local thermodynamic equilibrium are to small to be resolved.

Figure 4(b) shows a flow situation in the transition regime between continuum and free-molecular flow. In this regime the three-moment model, which can only correctly account for flows in thermodynamic equilibrium, gives an identical solution to that in the continuum regime. The five-moment model, Navier-Stokes equations and BGK equation all give similar results. The apparent discontinuities in the continuum situation are now close enough together and diffuse enough that they interact to create a smooth transition between the two constant initial states.

The free-molecular case is considered in Figure 4(c). Again in this case the three-moment model gives the same continuum solution. Now the collision operator in the five-moment model has become so insignificant that the moment equations behave as a purely hyperbolic system five separate waves separating constant states. For this highly rarefied case, the time-step restriction for the explicit time marching used for the Navier-Stokes equations which is caused by the elliptic terms makes numerical simulations difficult.

## 8 CONCLUSIONS

A hierarchy of moment systems based on assumed distribution functions which are slight modifications to the maximum-entropy distribution function have been shown. This hierarchy is based on a small modification to the maximum-entropy moment method. Though the resulting equations are not globally hyperbolic, they do have a very large area of hyperbolicity which should make them useful for many practical flow situations.

Numerical solutions of the resulting system were presented for shock-structure and shock-tube flow problems. It was demonstrated that the moment equations lead to enhanced accuracy in non-equilibrium flow situations when compared to classical continuum fluid-dynamic equations, such as the Euler and Navier-Stokes equations.

## ACKNOWLEDGMENTS

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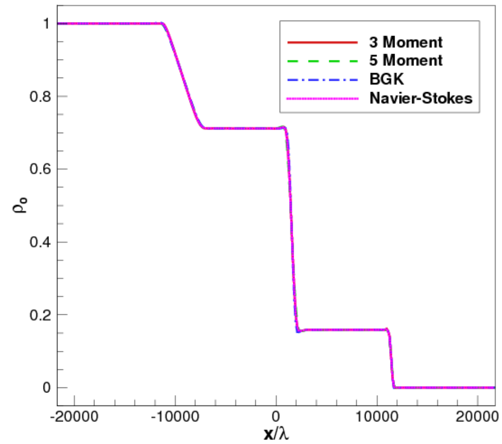
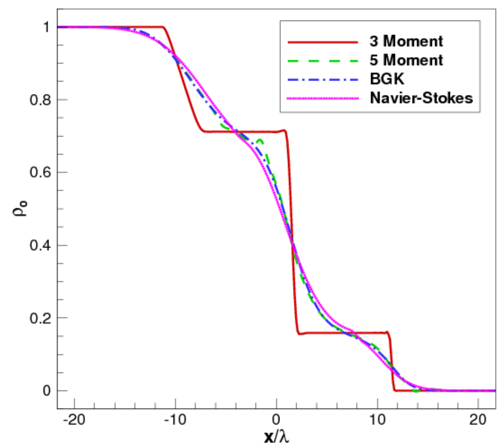



(a)

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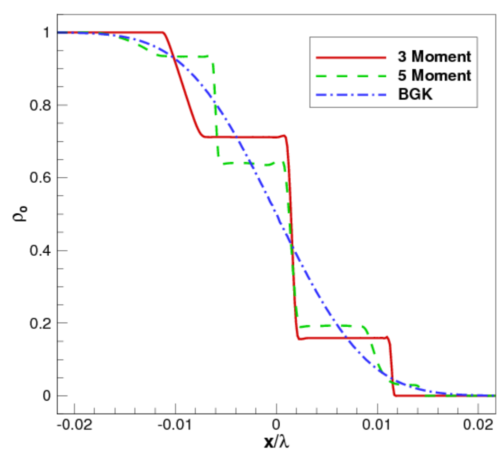


(c)

Figure 4: *Shock-tube calculations for one-dimensional gas computed using modified maximum-entropy five moment system as compared to the equilibrium three-moment system, direct solution of kinetic equation, and Navier-Stokes equations: (a)* $Kn = 2.3 \times 10^{-5}$*, (b)* $Kn = 2.3 \times 10^{-2}$*, (c)* $Kn = 23$.