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Comparison of Maximum Entropy and Quadrature-Based Moment Closures for Shock Transitions Prediction in One-Dimensional Gaskinetic Theory

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Abstract. The Navier-Stokes-Fourier (NSF) equations are conventionally used to model continuum flow near local thermodynamic equilibrium. In the presence of more rarefied flows, there exists a transitional regime in which the NSF equations no longer hold, and where particle-based methods become too expensive for practical problems. To close this gap, moment closure techniques having the potential of being both valid and computationally tractable for these applications are sought. In this study, a number of five-moment closures for a model one-dimensional kinetic equation are assessed and compared. In particular, four different moment closures are applied to the solution of stationary shocks. The first of these is a Grad-type moment closure, which is known to fail for moderate departures from equilibrium. The second is an interpolative closure based on maximization of thermodynamic entropy which has previously been shown to provide excellent results for 1D gaskinetic theory. Additionally, two quadrature methods of moments (QMOM) are considered. One method is based on the representation of the distribution function in terms of a combination of three Dirac delta functions. The second method, an extended QMOM (EQMOM), extends the quadrature-based approach by assuming a bi-Maxwellian representation of the distribution function. The closing fluxes are analyzed in each case and the region of physical realizability is examined for the closures. Numerical simulations of stationary shock structures as predicted by each moment closure are compared to reference kinetic and the corresponding NSF-like equation solutions. It is shown that the bi-Maxwellian and interpolative maximum-entropy-based moment closures are able to closely reproduce the results of the true maximum-entropy distribution closure for this case very well, whereas the other methods do not. For moderate departures from local thermodynamic equilibrium, the Grad-type and QMOM closures produced unphysical subshocks and were unable to provide converged solutions at high Mach number shocks. Conversely, the bi-Maxwellian and interpolative maximum-entropy-based closures are able to provide smooth solutions with no subshocks that agree extremely well with the kinetic solutions. Moreover, the EQMOM bi-Maxwellian closure would seem to readily allow the extension to fully three-dimensional kinetic descriptions, with the advantage of possessing a closed-form expression for the distribution function, unlike its interpolative counterpart.

INTRODUCTION AND BACKGROUND

In computational fluid dynamics, the Navier-Stokes-Fourier (NSF) equations and direct simulation Monte Carlo (DSMC) [1] are traditionally used to describe continuum and non-equilibrium flows respectively. However, there exists a transitional non-equilibrium regime in which the NSF equations fall short due to assumptions associated with nearness to equilibrium conditions. The transition regime is generally defined by flows where the Knudsen number, Kn, ranges from $0.1 \leq Kn \leq 10 \sim 100$. Examples of transition regime flows include micro-scale flows, such as the ones found in micro-electromechanical systems (MEMS) and high speed flows of gases and plasmas. Though DSMC remains valid in the transition regime, it can become computationally expensive due to the requirement for high numbers of particles. Moment closure methods provide an alternative approach for predicting this class of flow. With respect to the NSF equations, moment closures have the potential of offering a region of validity that extends into the transition regime, while having comparable computational costs. They also yield hyperbolic systems of equations that are well suited for solution by modern upwind finite-volume [2] and Discontinuous Galerkin (DG) [3, 4] schemes.

Moment closure methods can be derived from kinetic theory, in which a fluid particle can be broadly represented by a phase-space distribution function, $\mathcal{F}(x_i, v_i, t)$, which is related to the probability of finding a particle at position x_i

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and time t having a velocity v_i. The evolution of $\mathcal{F}$ is described by the Boltzmann equation. Macroscopic quantities or moments of the distribution function can be defined in terms of the convolution integral of a velocity weight with $\mathcal{F}$ and the transport of the velocity moments is described by Maxwell's equation of change. Theoretically, transporting an infinite set of these moments would replicate results from the Boltzmann equation exactly. This is however practically impossible and certainly not desirable computationally. Instead, a truncated set of moments that can adequately depict the physical phenomena of interest is sought. This introduces the closure problem: at least one higher order moment will be present in the solution flux term of the highest moment and thus the system of moment transport equations becomes unclosed. An expression for the next higher-order moments must be obtained in terms of the known set of moments. This is typically performed by introducing an assumed form of the phase-space distribution function as first considered by Grad [5].

More recently, reconstruction of the distribution function based on maximization of thermodynamic entropy principles has been proposed [6, 7, 8]. Maximum entropy closures have attractive mathematical and physical properties. For one, the maximum entropy distribution function remains positive for all physically realizable moments. The assumed form also produces the most likely distribution function given a truncated moment set. However, there exists no general closed-form expression for the maximum-entropy distribution when moments of interest contain velocity weights higher than second order. A computationally prohibitive iterative procedure is required to reconstruct the distribution function and thus alternative methods are sought. Notable alternatives have been proposed by McDonald and Groth [9] and McDonald and Torrilhon [10]. In the latter, an interpolative maximum-entropy-based (IMEB) procedure is performed to obtain closed-form expressions of the higher order moments. This procedure has been shown to reproduce closely the maximum-entropy results. The interpolative closure however has the disadvantage of still not having a closed-form expression for the distribution function in terms of the known set of moments. This can be particularly problematic in the implementation of boundary conditions (BCs) or evaluation of realistic collision operators.

The current work will thus focus on various alternative closure approximations and their comparison with the interpolative closure of McDonald and Torrilhon [10]. A bi-Maxwellian closure and more standard methods, such as Grad-type [5] and quadrature-based [11, 12] moment closures, are all compared for a model one-dimensional (1D) kinetic equation applied to shock structure prediction. These three other categories of closures all rely on an assumed form of the distribution that can be recovered analytically from the known set of moments, thus presenting modeling advantages over the original maximum-entropy and IMEB closures. To assess the capabilities of the closures, they will be compared to the direct numerical solution of the underlying kinetic equation. A near-equilibrium Navier-Stokes-like model will also be used as a basis for the comparisons.

FIVE-MOMENT CLOSURES FOR ONE-DIMENSIONAL KINETIC THEORY

For this study, the hyperbolic five-moment system examined previously by McDonald and Groth [9] and Mcdonald and Torrilhon [10] will be reconsidered. A so-called "1D gas" will be examined for which the particle movement is constrained to a single direction. A further simplification is made by considering the relaxation-time or BGK collision operator [13], in which the distribution function relaxes to an equilibrium Maxwellian, $\mathcal{M}$, as dictated by a single characteristic relaxation time, τ. The governing BGK kinetic equation in this case is given by

$$\frac{\partial \mathcal{F}}{\partial t} + v\frac{\partial \mathcal{F}}{\partial x} = \frac{\mathcal{F} - \mathcal{M}}{\tau}, \tag{1}$$

where a constant relaxation time is assumed. The five-moment system corresponding to Eq. (1) can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \tag{2}$$

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

$$\frac{\partial}{\partial t}\left(\rho u^2 + p\right) + \frac{\partial}{\partial x}\left(\rho u^3 + 3up + q\right) = 0, \tag{4}$$

$$\frac{\partial}{\partial t}\left(\rho u^3 + 3up + q\right) + \frac{\partial}{\partial x}\left(\rho u^4 + 6u^2 p + 4uq + r\right) = -\frac{q}{\tau}, \tag{5}$$

$$\frac{\partial}{\partial t}\left(\rho u^4 + 6u^2 p + 4uq + r\right) + \frac{\partial}{\partial x}\left(\rho u^5 + 10u^3 p + 10u^2 q + 5ur + s\right) = -\frac{1}{\tau}\left(4uq + r - 3\frac{p^2}{\rho}\right), \tag{6}$$

where the moments ρ, u, p, q, r and s are defined by

$$\rho = \langle m\mathcal{F}\rangle, \qquad u = \langle mv\mathcal{F}\rangle, \qquad p = \left\langle mc^2\mathcal{F}\right\rangle, \qquad q = \left\langle mc^3\mathcal{F}\right\rangle, \qquad r = \left\langle mc^4\mathcal{F}\right\rangle, \qquad s = \left\langle mc^5\mathcal{F}\right\rangle, \tag{7}$$

and $c = v - u$ is the random velocity. The resulting system is unclosed. A closing expression is required for the fifth random velocity moment, s in terms of the other known moments. The following subsections will distinguish between three categories of closure methods for s, namely: Grad-type, IMEB, and quadrature-based moment closures.

For the purposes of analysis, it is convenient to define a shift in velocity space such that $u = 0$ and then work with a non-dimensional set of moments defined by

$$\rho_\star = 1, \qquad u_\star = 0, \qquad p_\star = 1, \qquad q_\star = \frac{1}{\rho}\left(\frac{\rho}{p}\right)^{\frac{3}{2}} q, \qquad r_\star = \frac{1}{\rho}\left(\frac{\rho}{p}\right)^{2} r, \qquad s_\star = \frac{1}{\rho}\left(\frac{\rho}{p}\right)^{\frac{5}{2}} s. \tag{8}$$

These definitions will allow the study of the properties of the moment closures by considering only the dimensionless values of the heat flux, $q_\star$, and kurtosis, $r_\star$.

Grad-Type Moment Closure

In the original moment closure of Grad [5], the distribution function is represented as a polynomial expansion about the equilibrium Maxwellian, which for the univariate kinetic equation above can be expressed as

$$\mathcal{F}_{\text{Grad}} = \mathcal{M}\left[1 + \alpha_0 + \alpha_1\left(\frac{c}{a}\right) + \alpha_2\left(\frac{c}{a}\right)^2 + \alpha_3\left(\frac{c}{a}\right)^3 + \alpha_4\left(\frac{c}{a}\right)^4\right], \tag{9}$$

where the coefficients, α_i, are determined by ensuring $\mathcal{F}_{\text{Grad}}$ satisfies the lower order moments. Unfortunately, the distribution above has a limited range in the space of realizable moments for which it is strictly positive. In fact, the usual Grad third-order closures are almost everywhere non-positive. More importantly, it has also been shown that for modest deviations from equilibrium, the hyperbolicity of the associated moment equations is lost and the closure breaks down [14]. The consequences of this breakdown will be illustrated in the results to follow.

For the studied five-moment system, the closure resulting from Grad's polynomial expansion has been derived previously by McDonald *et al.* [10] and yields the simple closing relation:

$$s_\star = 10q_\star. \tag{10}$$

Interpolative Maximum-Entropy-Based (IMEB) Moment Closure

Dreyer [6], Müller and Ruggeri [7] and Levermore [8] provided the initial framework for maximum entropy closures as pertains to kinetic theory. This approach assumes a phase-space distribution function that maximizes the thermodynamic entropy of the system, thus producing the most likely distribution while remaining consistent with a set of given moments. For the 1D kinetic equation given above, the form of the maximum-entropy distribution function is

$$\mathcal{F}_{\text{MaxEnt}} = \exp\left(\alpha_0 + \alpha_1 c + \alpha_2 c^2 + \alpha_3 c^3 + \alpha_4 c^4\right) \tag{11}$$

and the coefficients, α_i, are determined via the maximization of the Boltzmann entropy $m\langle\mathcal{F}\ln\mathcal{F}\rangle$. Maximum entropy closures have many desirable mathematical properties including global hyperbolicity and a definable entropy [8]. A significant drawback is that, as in the present case, a numerical approach is generally required to determine α_i in terms of the moments ρ, u, p, q and r.

Due to the absence of a closed-form expression for this distribution, IMEB moment closures for have been proposed by McDonald and Torrilhon and subsequently studied by Tensuda *et al.* [10, 15]. For the 5-moment model, the interpolative approximation to the true maximum-entropy closure yields an analytical expression for the random fifth moment, $s_\star$, which closely matches the values of the actual maximum-entropy closure and can be expressed as

$$s_\star = \frac{q_\star^3}{\sigma_{\text{M}}^2} + \left(10 - 8\sigma_{\text{M}}^{\frac{1}{2}}\right)q_\star, \tag{12}$$

where the parameter σ_M is the result of a parabolic mapping in the $q_\star - r_\star$ plane and is given by

$$\sigma_\mathrm{M} = \frac{3 - r_\star + \sqrt{(3 - r_\star)^2 + 8q_\star^2}}{4}. \tag{13}$$

Although the IMEB closure presents many modeling and implementation advantages, including strict hyperbolicity of the 5-moment set for virtually all realizable moments [10], it still does not provide a closed-form expression for the distribution function. Arbitrary higher-order moments can therefore not be integrated analytically and this can be viewed as a significant drawback.

Quadrature-Based Moment (QMOM) Closure

Quadrature methods of moments (QMOMs) were first described by McGraw in the context of aerosol dynamics [11]. Many variants of the QMOM have since been developed [12], but they have mainly been applied to the prediction of multiphase flows. A simple variant of the QMOM approach is evaluated here. The representation of the distribution function is based on the summation of three weighted with velocity weights, w_k, and abscissas, c_k. In order to produce a five-moment closure, the first abscissa is set to $c_1 = 0$ here. This choice is made since the second random velocity moment is always null and results in a five-equation system for the parameters of $\mathcal{F}_\delta$ given by

$$\sum_{k=1}^{3} w_k c_k^\alpha = M_\alpha^\star, \tag{14}$$

where $M_\alpha^\star$ is a dimensionless moment of order $\alpha = \{0, 4\}$. The solution to Eq. (14) yields an analytic expression for the weights and abscissas. The random fifth moment can then be written as

$$s_\star = \sum_{k=1}^{3} w_k c_k^5 = \left(1 - a^4\right)\left(1 + a\right)^2 \left(\frac{q_\star}{1 - a^2}\right)^3, \tag{15}$$

where the weight ratio, $a = w_2/w_3$, is a root of the fourth-order polynomial

$$\left(q_\star^2 - r_\star\right) a^4 + \left(q_\star^2\right) a^3 + (2r_\star)\, a^2 + \left(q_\star^2\right) a + \left(q_\star^2 - r_\star\right) = 0. \tag{16}$$

While this quadrature approach can be shown to have a strictly positive distribution function for all realizable moments and is expected to be quite flexible in producing solutions for the full range of moment values, it is also expected to have similar issues with non-hyperbolic behaviour and breakdown as the Grad-type closure, due to the finite extent of the Dirac basis function and hence finite wave propagation velocities represented by the closure.

EQMOM Bi-Maxwellian Moment Closure

Multi-Gaussian or multi-Maxwellian closures were previously considered by Chalons *et al.* [16]. The concept essentially extends the idea of the QMOM closure by replacing the basis function at each quadrature point by a Maxwellian distribution shifted in velocity space, with the influence of the new basis functions now extending over the full range of velocities. Such an approach is also referred to as an extended quadrature method of moments (EQMOM) [12, 17]. It is noted that Fan and Li [18] have also recently evaluated bi-Gaussian closures for application to gas kinetic theory and compared features of the closure to that of maximum-entropy closures.

For the 5-moment system, two Maxwellians sharing the same standard deviation, σ, are used as an ansatz for representing the phase-space distribution function. The bi-Maxwellian form for the distribution function is written as

$$\mathcal{F}_\mathrm{bM} = \frac{w_1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(c - c_1)^2}{2\sigma^2}\right) + \frac{w_2}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(c - c_2)^2}{2\sigma^2}\right). \tag{17}$$

An analytical solution to the system of equations for w_k, c_k and σ was previously derived by Chalons *et al.* [16]. It can be shown that the resulting closing expression for the random fifth moment is

$$s_\star = \frac{q_\star^3}{\sigma_\mathrm{Q}^2} + (10 - 8\sigma_\mathrm{Q})\, q_\star, \tag{18}$$

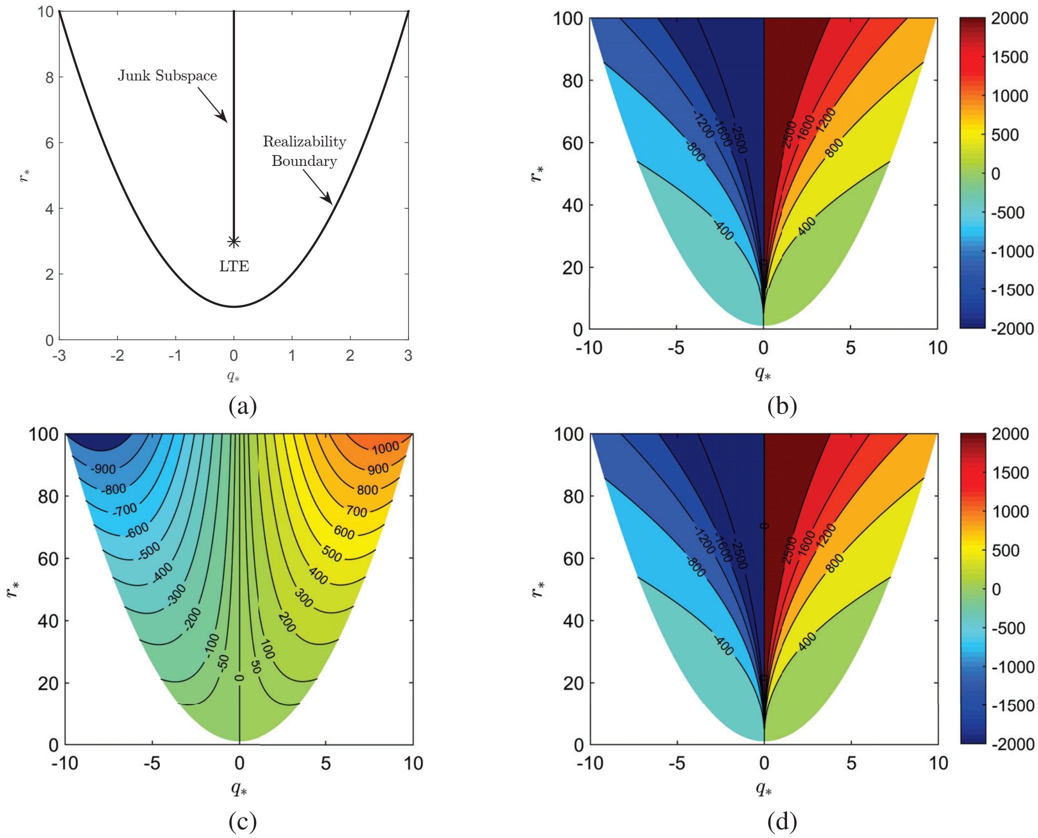

FIGURE 1: Domain of physical realizability for the five-moment system: (a) realizability boundaries [19] and contours of (b) IMEB, (c) QMOM and (d) bi-Maxwellian closing values for $s_\star$.

where $\sigma_\mathrm{Q} = 1 - \sigma^2$ and the variance, σ^2, is the real root of a third order polynomial and can be written as [12]

$$\sigma^2 = 1 - C_2 + \frac{C_1}{C_3}, \tag{19}$$

where the values of C_1, C_2 and C_3 are given by

$$C_1 = \frac{1}{6}(r_\star - 3), \qquad C_2 = \frac{q_\star^2}{4}, \qquad C_3 = \left(\sqrt{C_1^3 + C_2^2} + C_2\right)^{\frac{1}{3}}. \tag{20}$$

A similar result was also found by Fan and Li [18]. The form of $\mathcal{F}_\mathrm{bM}$ is such that it will remain positive valued for all realizable moments. An interesting comparison can also be made between the closures of Eqs. (12) and (18). Both expressions lead to singular behaviour within a portion of realizability space and fixed values of the parameters σ_M and σ_Q both define parabolas in the $q_\star - r_\star$ plane ranging from the outer physical realizability boundary to the singular region. The strict hyperbolicity of the bi-Maxwellian closure can also be shown [18].

Closing Moment and Region of Moment Realizability

Following the realizability analysis for the five-moment system of interest by McDonald and Groth [9], the physical realizability limit can be defined by the parabola $r_\star = 1 + q_\star^2$. Any combination of $q_\star$ and $r_\star$ lying above this parabola is said to correspond to a physically realizable solution. Furthermore, Junk [19, 20] has shown that maximum entropy solutions do not exist within this region on the line $q_\star = 0$, above $r_\star = 3$ (i.e., for $r_\star > 3$). The maximum-entropy distribution function does not remain finite along this line and therefore solutions cannot be found. While strict hyperbolicity and a well-behaved closure is assured everywhere else, the resulting moment equations are also singular on the Junk line. These properties are particularly inconvenient, since ($q_\star = 0, r_\star = 3$) corresponds to local thermodynamic equilibrium (LTE). The realizability region and so-called Junk subspace corresponding to the invalid region of the maximum entropy closure are depicted in Figure 1a.

For this theoretical 1D gas, the IMEB closure of McDonald and Torrilhon [10] has been shown to exhibit excellent agreement with the true maximum-entropy closure. It matches the true maximum-entropy distribution exactly at the parabola of the realizability boundary, where $\mathcal{F}_{\mathrm{MaxEnt}}$ reduces to two Dirac deltas. Furthermore, its singular behavior (as evidenced by undefined discontinuous values for $s_\star$) at the Junk subspace is also reproduced as can be clearly seen in Figure 1b. The exact representation of the distribution at the lower realizability boundary is also captured by $\mathcal{F}_\delta$ and $\mathcal{F}_{\mathrm{bM}}$, where the values of $s_\star$ obtained using these two closures exactly replicate the $\mathcal{F}_{\mathrm{MaxEnt}}$ results. Refer to Figures 1c and 1d. Interestingly, the bi-Maxwellian closure has very similar behavior to that of the true maximum entropy solution over the entire realizability region and exhibits the characteristic singular behaviour along the Junk subspace. In contrast, the QMOM closure does not replicate the maximum-entropy behavior within the realizability region away from the boundary. Additionally, while a global solution for $s_\star$ is obtained, the QMOM closing flux remains finite and non-singular for all possible moments. Although originally a perceived drawback of maximum-entropy-based closures, the singular behaviour along the Junk space is a property that can be coped with numerically and is key to accurate predictions of non-equilibrium shock structures as will be shown in the results that now follow.

NUMERICAL RESULTS FOR STATIONARY SHOCK STRUCTURES

To evaluate the capabilities of each closure for different degrees of departure from equilibrium, stationary shock structures are studied for upstream Mach numbers of $M = \{1.25, 2, 4, 8\}$, with increasing Mach number representing a larger departure from LTE. The five-moment system of differential equations for each closure was solved using a second-order Godunov-type upwind finite-volume scheme [2] with piece-wise linear reconstruction. An HLL approximate Riemann solver [21] is used along with Venkatakrishnan slope limiting [22]. As a reference non-equilibrium solution, Eq. (1) was solved directly using the discrete velocity method of Mieussens [23]. Additionally, the solution of a three-moment system resulting from a Chapman-Enskog expansion applied to the kinetic equation of Eq. (1) is also used as a reference solution. The latter is the equivalent Navier-Stokes equations for a 1D gas [9].

Figure 2 shows shock structure results for the IMEB, Grad-type, QMOM and bi-Maxwellian closures as compared to the reference solutions. The $M = 1.25$ case represents a rather modest departure from equilibrium, and it can be seen that all closure approximations along with the NSF model are in good agreement with the full solution of the kinetic equation. However, the shortcomings of the Grad-type and QMOM can immediately be seen in Figures 2c and 2d for a $M = 2$ shock, where undesirable and unphysical subshocks are present in both solutions. It is important to note that the Grad-type closure formally becomes non-hyperbolic at this relatively low Mach number; however the approximate numerical flux functions and associated numerical viscosity allowed the computation of solutions for this case. For further departures from LTE, only first-order solutions of the Grad-type and QMOM moment equations could be obtained and those required an unreasonable number of grid points for grid-independent solutions. Results are therefore not shown for Mach numbers above $M = 2$ for these two closures.

The more interesting comparisons can be made between the IMEB and bi-Maxwellian closures, which provide smooth solutions, with no subshocks, for all Mach numbers. In fact, the singularity in the closing flux, which presents a slight numerical difficulty, is extremely beneficial in this case since it allows very large wavespeeds which provide upstream influence that prevents the appearance of subshocks in the predicted solutions. Both closures show excellent agreement with the discrete velocity methods for the normalized density in all cases. They however show some increasing discrepancies with the upstream heat transfer profile with the IMEB closure always performing slightly better than the bi-Maxwellian model.

Comparing the moment closure results to the NSF-like model demonstrates their advantage in modeling non-equilibrium phenomena. The near-equilibrium model is clearly unable to accurately capture the density profile for shocks above $M = 2$, and completely breaks down in terms of density and heat transfer predictions at $M = 4$ and 8.

It is also of interest to observe the distribution function predicted by the bi-Maxwellian model using the moments of the BGK solution. As equilibrium is departed upstream of the shock, the moment state nears the singular Junk subspace. A second Maxwellian with an infinitesimal weight and theoretically infinite velocity then appears in the representative distribution. This is depicted in Figure 3 for a $M = 8$ shock, where it is shown that the infinitesimally weighted Maxwellian's magnitude increases and approaches $c = 0$ at more downstream positions. This peak finally merges with the first Maxwellian to recover downstream equilibrium conditions. This behaviour of the bi-Maxwellian distribution is analogous to that of the true maximum entropy distribution for moment states found in shock transitions.

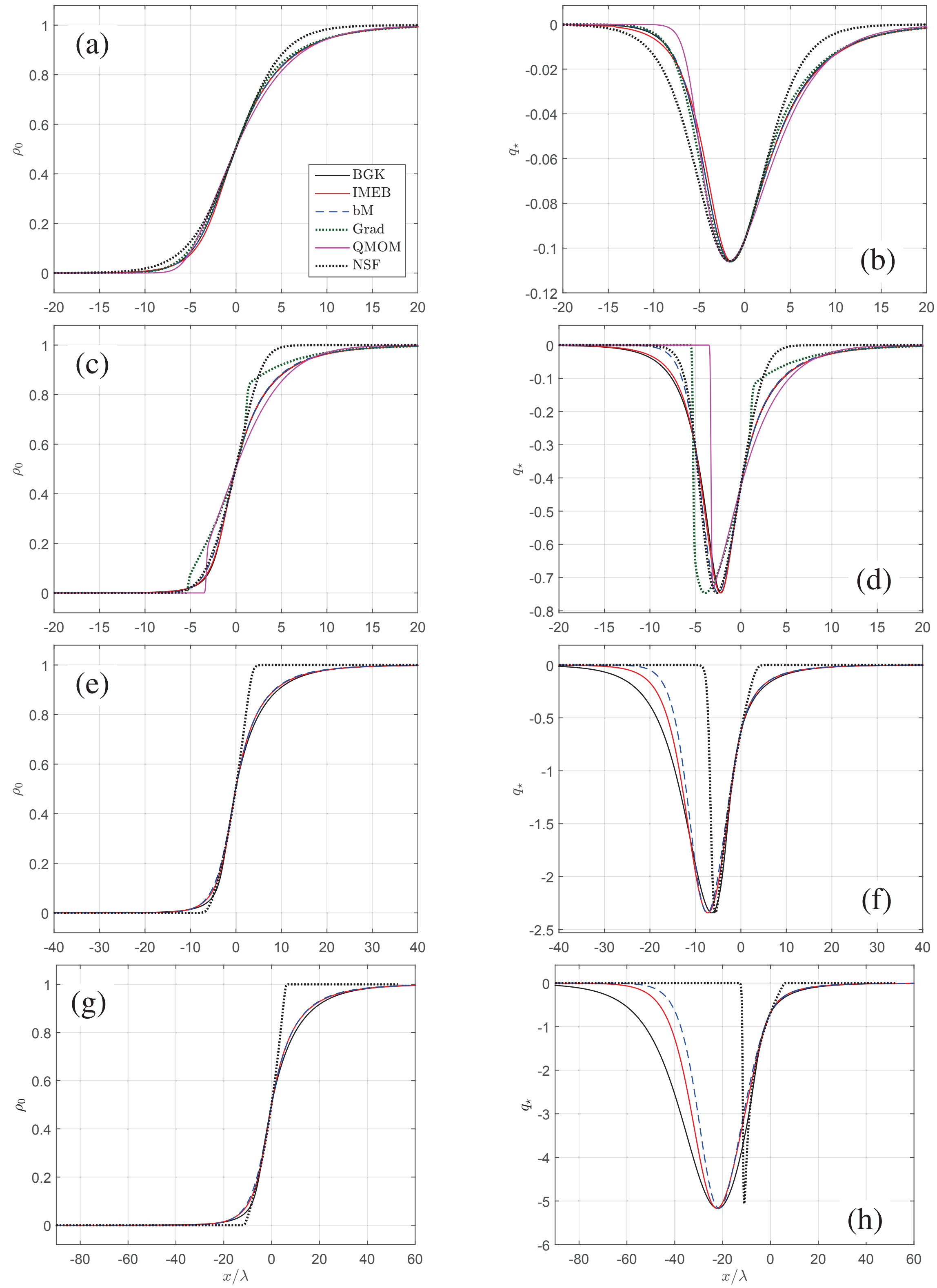

FIGURE 2: Predicted normalized density and dimensionless heat transfer through a stationary shock wave for a one-dimensional gas as determined by the IMEB, bi-Maxwellian (bM), Grad and Dirac3 closures: (a)–(b) $M = 1.25$, (c)–(d) $M = 2$, (e)–(f) $M = 4$, and (g)-(h) $M = 8$.

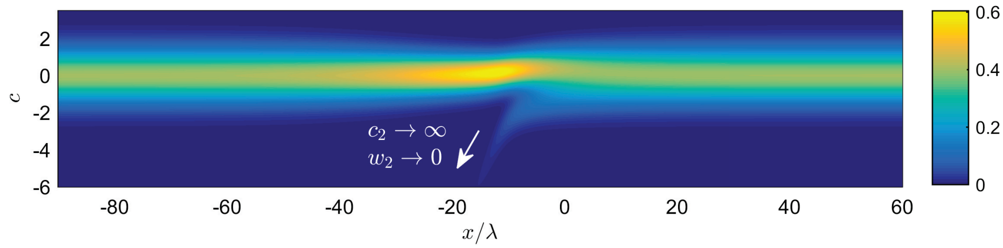

FIGURE 3: Variation of computed bi-Maxwellian distribution, $\mathcal{F}_{\mathrm{bM}}$, within a $M = 8$ shock as predicted by the moments of the solution of the BGK equation.

CONCLUSIONS

It has been demonstrated that the moment closures able to mimic the results of true maximum-entropy closures by far outperform other QMOM and Grad-type moment closures in terms of their ability to predict non-equilibrium phenomena associated with stationary shocks. Due to their singular behaviour, they provide smooth shock transitions where the more standard closures produce subshocks, and are able to capture additional physics, as represented by higher order moments, with considerably more precision than the NSF equations for a 1D gas. Though the IMEB closure always performs slightly better than the bi-Maxwellian, the fact that the latter provides an analytic expression of the distribution function suggests it as an alternative to both IMEB and true maximum-entropy closures. This could be particularly relevant when considering more realistic collision operators and/or boundary conditions in three-dimensional kinetic descriptions. An additional advantage of multi-Gaussian-type closures is that they can be extended to higher moment systems containing additional non-equilibrium physics by adding more quadrature points (Gaussians) or considering less restrictive ansatzes (e.g., allowing multiple values for σ). Ongoing and future research will consider multi-Gaussian closures applied to fully three-dimensional kinetic theory.

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