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On the Application of Maximum-Entropy-Inspired Multi-Gaussian Moment Closure for Multi-Dimensional Non-Equilibrium Gas Kinetics

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Abstract. Maximum-entropy moment closures for describing non-equilibrium rarefied gaseous flows have previously been shown to provide accurate and computationally efficient descriptions of transition-regime flows. Unfortunately, for high-order variants of these closures above second order in velocity space, there are no analytical closures for the systems of hyperbolic partial differential equations (PDEs) which govern the transport of the macroscopic moment quantities and instead approximate closures have been sought. In this study, a bi-Gaussian approximation for the number density function (NDF) is considered both for approximating the NDF and closing moment fluxes of the resulting fourth-order 14-moment maximum-entropy closure associated with fully three-dimensional kinetic theory. Prior investigations of the bi-Gaussian approximation applied to simplified one-dimensional univariate kinetic theory has yielded excellent results when compared to the actual maximum-entropy solutions as well a similar interpolative-based maximum-entropy-based (IBME) closure. In the one-dimensional univariate case, the bi-Gaussian closure is equivalent to the so-called extended quadrature method of moments (EQMOM) with a normal or Gaussian kernel basis function. A potential benefit of the bi-Gaussian approach proposed herein is that an essentially closed-form analytical expression results for the NDF. In this study, the extension of the bi-Gaussian closure to the multi-dimensional case is considered and compared to the equivalent multi-dimensional IBME closure. The approximate form for the NDF and closing fluxes in terms of the relevant moments are derived and the validity and hyperbolicity of the closure for the space of realizable predicted moments are all explored and compared to those of the IBME closure. It is shown that the bi-Gaussian closure in the multi-dimensional case unfortunately suffers from several deficiencies: firstly, the valid region of realizable moment space for the bi-Gaussian closure is a small subset of the full realizable 14-moment space; and secondly, the closure and moment equation eigenstructure for solutions associated with zero heat flux become undefined. The findings herein suggest that the proposed bi-Gaussian closure may not be a good choice for practical multi-dimensional rarefied flow predictions despite the promising results exhibited in the one-dimensional case.

INTRODUCTION AND MOTIVATION

In fluid dynamics, it is typical to use Knudsen number, Kn, to characterize the non-equilibrium behaviour of a flow, where low Knudsen numbers ($\mathrm{Kn} \leq 0.1$) indicate continuum or equilibrium flows which can be treated by the con-ventional Navier-Stokes-Fourier (NSF) equations, and high Knudsen numbers ($\mathrm{Kn} \gtrsim 10$–100) indicate essentially collisionless free-molecular flow conditions which can be readily treated via methods such as direct simulation Monte Carlo (DSMC) [1]. In the transition regime, $0.1 \leq \mathrm{Kn} \leq 10-100$, there exists non-equilibrium behaviour which cannot be captured by the NSF equations and which can be computationally expensive to resolve via DSMC methods due to the requirements for large number of particles [2].

Maximum-entropy moment closures [3, 4, 5] for predicting the behaviour of non-equilibrium rarefied gaseous flows have previously been shown to provide accurate and computationally efficient descriptions of transition-regime flows in which the usual continuum-regime Navier-Stokes-Fourier equations do not hold, and where Monte-Carlo and/or direct-discretization methods can be far too expensive for practical use [2]. Unfortunately, for high-order variants of these closures above second order in velocity space, there are no analytical closed-form expressions for the distribution of molecular velocities nor the closures for the associated systems of hyperbolic partial differential equations (PDEs) which govern the transport of the macroscopic moment quantities. As a consequence, theoretical approximations to these closures have been sought in these cases. In this study, a bi-Gaussian approximation for the number density function (NDF) is considered both for approximating the NDF and closing moment fluxes of the resulting fourth-order 14-moment maximum-entropy closure associated with fully three-dimensional kinetic theory. Prior investigations by

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Laplante and Groth [6] of the bi-Gaussian approximation applied to simplified one-dimensional univariate kinetic theory has demonstrated that this approximation can closely mimic the full maximum-entropy solutions in the one-dimensional case, yielding excellent agreement with the numerically obtained maximum-entropy solutions as well those of a similar interpolative-based maximum-entropy (IBME) closure of McDonald and Torrilhon [7]. In the one-dimensional univariate case, the bi-Gaussian closure is also fully equivalent to the so-called extended quadrature method of moments (EQMOM) with a normal or Gaussian kernel basis function as proposed by Chalons *et al*. [8] and, as such, allows for a closed-form analytical expression for the NDF. An important benefit of the bi-Gaussian approach proposed herein for the multi-dimensional case is that an essentially closed-form analytical expression also results for the NDF. The latter is deemed to be advantageous theoretically for a number of reasons.

The extension of the bi-Gaussian closure to the multi-dimensional case and its ability to mimic the solutions of the equivalent maximum-entropy closure are considered herein and the closure is compared to the corresponding multi-dimensional IBME closure [7, 9, 10]. The objective here is to seek a 14-moment closure based on an analytically integrable multi-Gaussian representation of the NDF that approximates as closely as is possible the corresponding solutions provided by the 14-moment maximum-entropy closure. The approximate form for the NDF and closing fluxes in terms of the relevant macroscopic moments are derived and the validity and hyperbolicity of the closure for the space of realizable predicted moments are all explored and compared to those of the IBME closure. While providing expressions for the closing fluxes, a perceived weakness of the latter is that an explicit analytical expression for the NDF is not provided by the IBME closure. The bi-Gaussian closure is first introduced for the one-dimensional univariate case followed by its extension to the three-dimensional case. Unlike the promising performance previously demonstrated in the one-dimensional case, it is shown that the bi-Gaussian closure in the multi-dimensional case unfortunately suffers from several deficiencies and these flaws make its application to practical multi-dimensional rarefied flow predictions challenging, if not impossible.

MAXIMUM-ENTROPY-INSPIRED MOMENT CLOSURES IN ONE DIMENSION

Univariate BGK Kinetic Equation

Maximum-entropy-inspired moment closures are first briefly considered here applied to a univariate kinetic equation describing transport of a one-dimensional gas with no external forces where the strictly positive NDF, $\mathscr{F} = \mathscr{F}(x,v,t)$, is dependent on the particle velocity, v, as well as position, x, and time, t, and a simplified relaxation-time or BGK approximation [11] is used for the collision operator, $\delta\mathscr{F}/\delta t$. The NDF is related to the probability of the gaseous particles having velocity v at location and time (x,t) and the corresponding univariate BGK kinetic equation has the form

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

where the equilibrium solution for the NDF, $\mathscr{M}$, (i.e., the equivalent Maxwell-Boltzmann distribution for the univariate case) is given by

$$\mathscr{M}(x,v,t;\rho,u,p) = \frac{\rho}{m\sqrt{2\pi p}} \exp\left[-\frac{\rho(v-u)^2}{2p}\right]. \tag{2}$$

and where m is the particle (molecular) mass, ρ is the gas density, u is the mean velocity of the one-dimensional gaseous particles, and p is the pressure. The NDF provides a statistical based description of the *microscopic* behaviour of the gaseous particles. *Macroscopic* properties of the one-dimensional gas are then associated with velocity moments, $M(x,t)$, defined by

$$M(x,t) = \int_{-\infty}^{\infty} V(v)\mathscr{F}(x,v,t)\,\mathrm{d}v = \int\limits_{\infty} V(v)\mathscr{F}(x,v,t)\,\mathrm{d}v = \langle V(v)\mathscr{F}\rangle_v\,, \tag{3}$$

where $V(v)$ is a velocity-dependent weight which in general is a polynomial (usually a monomial) in v.

Moment Closure Methods

Rather than solving directly the kinetic equation above for the NDF, $\mathscr{F}$, in moment closure techniques as originally proposed by Grad [12], solutions for the moments, M, of the NDF are sought. To exactly replicate the behaviour of non-equilibrium solutions of the underlying kinetic equation, an infinite number of velocity moments must be considered. This is obviously practically impossible. Instead, a truncated set of velocity moments is generally considered whereby only the maximum number of moments necessary to capture essential physical phenomena of practical interest are incorporated in the closure. The solution of the moments of interest are then described by Maxwell's equation of change given by

$$\frac{\partial}{\partial t}(M)+\frac{\partial}{\partial x}\langle v V(v)\mathscr{F}\rangle_v=-\frac{1}{\tau}\left[M-\langle V(v)\mathscr{M}\rangle_v\right], \tag{4}$$

which follows from the evaluation of appropriate velocity moments of the kinetic equation. The use of a truncated set of moments introduces a closure problem: values of one higher order velocity moment, $\langle v V(v)\mathscr{F}\rangle_v$, than the highest velocity moment considered are required to complete the moment description and thereby provide closure. In general, this is achieved by assuming a form for the NDF, parameterized in terms of the known moments, and given this assumed form, the closing flux can then be directly evaluated via integration over velocity space. Theoretically, a wide range of choices are possible for the assumed or approximate NDF when dealing with the closure problem; however, some NDFs provide more accurate representation of the underlying physics than others.

It is well established that a gas in equilibrium has a distribution of molecular velocities given by the Maxwell-Boltzmann distribution, $\mathscr{M}$. In order to describe non-equilibrium behaviour and correctly recover the equilibrium solution, Grad originally considered moment closures in which the NDF is approximated by a truncated Hermite polynomial expansion about the Maxwellian solution. However, Grad's method suffered from several limitations including loss of hyperbolicity of the moment equations for even modest departures from equilibrium and the fact that the approximate NDF is not strictly positive. More recently, Levermore [4] formulated a hierarchy of closed moment systems based on the principle of maximizing the statistical entropy having many desirable mathematical features. The Levermore hierarchy allowed for the treatment of non-equilibrium behaviour while preserving the strict hyperbolicity of the moment equations and having a strictly positive approximate NDF. The approximate NDF also corresponds to the most likely form for the distribution given the finite set of moments.

In Levermore's hierarchy, the maximum-entropy closures above second order are of particular interest, as these moment closures include a treatment for heat flux. In the three-dimensional case, the 14-moment closure is lowest-order super-quadratic maximum-entropy closure [4]. While this 14-moment maximum-entropy closure is potentially able to accurately treat non-equilibrium gaseous flow behaviour, it suffers from two deficiencies: (i) it is not able to represent the entirety of the 14-moment phase space due to singular behaviour within a region of valid (physically realizable) moment space known as the Junk subspace [13]; and (ii) analytical closed-form expressions for the NDF and the associated closing flux is not possible as the NDF is based on an exponential of a fourth-order polynomial. Nevertheless, Groth and McDonald [2], McDonald and Groth [14], and McDonald and Torrilhon [7] have demonstrated that the singularity associated with the Junk subspace was not actually a major deficiency of the 14-moment maximum-entropy closure and, once carefully navigated, allowed shock behaviour to be captured in a fully hyperbolic framework without partially-dispersed features and the occurrence of sub shocks [6, 7, 14]. The lack of an analytical closure for the high-order maximum-entropy closures remains however a detraction. It can introduce expensive numerical integration procedures which add to the computational expense of the closure. This motivates the consideration of the bi-Gaussian closures of interest here.

Fourth-Order Maximum-Entropy Closure

For the one-dimensional univariate kinetic theory considered here, the five-moment, fourth-order, maximum-entropy closure is equivalent to the 14-moment maximum-entropy closure in the three-dimensional case. In the five-moment approximation, the set of velocity moments of interest correspond to $\mathbf{M}=[\rho,\rho u,\rho u^2+p,\rho u^3+3up+q,\rho u^4+6u^2p+4uq+r]$ where q and r represent the heat flux and kurtosis, respectively. The approximate NDF for the maximum-entropy moment closure is then taken to have the form

$$\mathscr{F}(x,v,t)=\exp\left(\alpha_0+\alpha_1 v+\alpha_2 v^2+\alpha_3 v^3+\alpha_4 v^4\right), \tag{5}$$

where the parameters α_i are in effect Lagrange multipliers which can evaluated by solving for the stationary point of the objective function, $\mathbb{F}$, defined by

$$\mathbb{F} = \langle \mathscr{F}(x,v,t) \rangle_v - \alpha^{\mathrm{T}} \mathbf{M}, \tag{6}$$

and where $\mathbf{M}$ is again the vector of known moments and $\alpha = [\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4]$. In general, this will require the use of an iterative numerical solution scheme. The resulting moment equations of this five-moment closure can then be written as

$$\frac{\partial}{\partial t}[\mathbf{M}] + \frac{\partial}{\partial x}[\mathbf{F}] = \mathbf{S}, \tag{7}$$

where the moment vector and source vector are

$$\mathbf{M} = \begin{bmatrix} \rho \\ \rho u \\ \rho u^2 + p \\ \rho u^3 + 3up + q \\ \rho u^4 + 6u^2 p + 4uq + r \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\dfrac{q}{\tau} \\ -\dfrac{1}{\tau}\left(4uq + r - \dfrac{3p^2}{\rho}\right) \end{bmatrix}, \tag{8}$$

the moment flux vector is given by

$$\mathbf{F} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u^3 + 3up + q \\ \rho u^4 + 6u^2 p + 4uq + r \\ \rho u^5 + 10u^3 p + 10u^2 q + 5ur + s \end{bmatrix}, \tag{9}$$

and where the closing high-order (fifth-order) flux is given by

$$s = m \left\langle (v-u)^5 \mathscr{F} \right\rangle_v, \tag{10}$$

thus completing the closure. In general, numerical quadrature is required to evaluate s.

Five-Moment Interpolative-Based Maximum-Entropy (IBME) Closure

In order to avoid the costly numerical procedures associated with the five-moment maximum-entropy closure outlined above, McDonald and Torrilhon [7] proposed an interpolative-based approximation to the maximum-entropy closure which is based on a parabolic interpolation procedure for the closing flux. The latter interpolates between known values of the maximum-entropy closing flux at the edge of realizable moment space and the equilibrium solution to achieve a closing flux which closely approximates that of the maximum-entropy solution while still retaining the singular behaviour of the maximum-entropy closure as the Junk subspace is approached. As the closure is for the closing flux directly, there is no corresponding analytical approximation for the NDF; thus, moments outside the specified set cannot be directly evaluated. However, for the one-dimensional case, the interpolative closure has been shown to provide very accurate results, virtually indistinguishable from the full maximum-entropy closure, and remain hyperbolic for even very large departures from equilibrium conditions.

For the one-dimensional univariate case, the fifth-order closing flux, s, of the IBME closure is defined in terms of the interpolation parameter, $\sigma_{\mathrm{IM}} \in [0,1]$, which itself is defined by

$$r = \frac{1}{\sigma_{\mathrm{IM}}} \frac{q^2}{p} + (3 - 2\sigma_{\mathrm{IM}}) \frac{p^2}{\rho}, \tag{11}$$

and used in the expression for the closing flux given by

$$s = \frac{q^3}{\sigma_{\mathrm{IM}}^2 p^2} + (10 - 8\sigma_{\mathrm{IM}}^{1/2}) \frac{pq}{\rho}. \tag{12}$$

From Equation (12), the singular behaviour associated with the Junk subspace can be seen to be contained in the interpolation parameter and, in particular, the expression for s becomes singular as $\sigma_{\mathrm{IM}} \to 0$. To work around the Junk subspace in actual numerical simulations, typically the value of σ_{IM} is maintained above a small value such that $\sigma_{\mathrm{IM}} \in (\varepsilon, 1)$ for some small tolerance, ε, with $0 < \varepsilon \ll 1$.

Five-Moment Bi-Gaussian Closure

In the one-dimensional case, Chalons *et al*. [8] previously proposed a five-moment EQMOM closure which approximates the NDF in terms of a sum of two Gaussian kernel functions. The form of the bi-Gaussian NDF is given by

$$\mathscr{F} = \frac{\rho_1}{\sqrt{2\pi}a} \exp\left[-\frac{(v-v_1)^2}{2a^2}\right] + \frac{\rho_2}{\sqrt{2\pi}a} \exp\left[-\frac{(v-v_2)^2}{2a^2}\right], \tag{13}$$

where ρ_1 and ρ_2 are the weights of the Gaussian distributions, v_1 and v_2 are the velocity abscissas, and a is a standard deviation which is shared by the two Gaussian distributions. Unlike the original maximum-entropy form for the NDF, the bi-Gaussian NDF above can be analytically integrated to produce expressions for any velocity moments of interest and, for the five-moment closure, expressions for parameters ρ_1, ρ_2, v_1, v_2, and a defining the NDF can be derived in terms of the known velocity moments, $[\rho, u, p, q, r]$. Similar to the IBME closure above, an expression for a bi-Gaussian parameter, $\sigma_{\mathrm{BG}} \in [0,1]$, can obtained by solving

$$r = \frac{1}{\sigma_{\mathrm{BG}}} \frac{q^2}{p} + (3 - 2\sigma_{\mathrm{BG}}^2) \frac{p^2}{\rho}. \tag{14}$$

The preceding equation can be re-expressed as a third-order polynomial in terms of σ_{BG}, the appropriate real root of which provides values for σ_{BG}. The closing flux of the five-moment bi-Gaussian closure is then given by analytical integration of the bi-Gaussian NDF to yield

$$s = \frac{q^3}{\sigma_{\mathrm{BG}}^2 p^2} + (10 - 8\sigma_{\mathrm{BG}}) \frac{pq}{\rho}. \tag{15}$$

It is evident from the expression above that the closing flux of the bi-Gaussian closure has a similar form to that of the IBME closing flux as given in Equation (12), with σ_{BG} playing a similar role to that of σ_{IM}. Figure 1 provides a direct comparison of the values of the closing fluxes for the IBME and bi-Gaussian five-moment closures in realizable moment space defined by the non-dimensional heat flux, Q^*, and kurtosis, R^*. Clearly, the closing flux of the bi-Gaussian closure closely approximates that of the IBME closure. Note additionally that the closing flux of the IBME closure is also virtually identical to that of the maximum-entropy closure on which it is based.

Comparison of Results for One-Dimensional Stationary Shock Structure

Laplante and Groth [6] have previously shown the similarities of the non-equilibrium solutions provided by the IBME and bi-Gaussian, maximum-entropy-inspired, five-moment closures. In particular, properties of the bi-Gaussian were compared to the IBME and BGK solutions for stationary one-dimensional shock structure [6]. The reader is referred to this previous work for detailed information pertaining to the shock structure problems considered and the numerical methods used to obtain the solutions. For the purposes of the present comparisons, it is sufficient to know that the results provided here in Figure 2 represent a relatively strong stationary shock with a shock Mach number of 8. From Figure 2, it can be seen that the predictions of the bi-Gaussian and IBME closures agree quite well to those of the BGK solution for number density. The two closures are seen to produce somewhat different behaviour from the BGK solution in terms of non-dimensional heat transfer, for which the IBME is seen to produce a slightly more accurate heat flux in the upstream portions of the stationary shock wave. The IBME and bi-Gaussian closures agree almost perfectly in the downstream portions of the shock and show strong agreement with the BGK solution also for $x > 0$. This particular non-equilibrium case exaggerates the differences between the IBME and bi-Gaussian closures. As previously shown by Laplante and Groth [6], even better agreement between the two approaches is observed at lower values of the shock Mach number (i.e., for weaker shocks). The additional benefit offered by the bi-Gaussian closure is the resulting explicit analytical expression for the approximate NDF in terms of the known macroscopic moments.

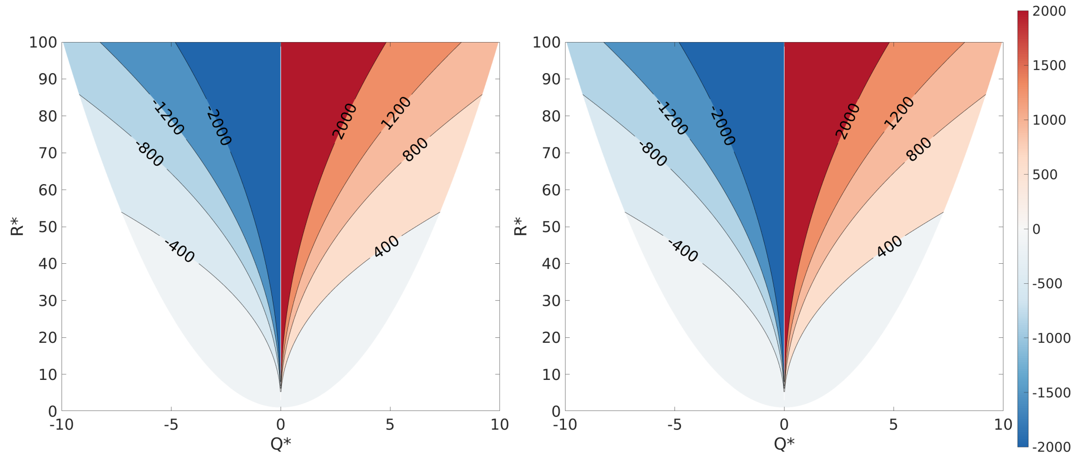

FIGURE 1. Comparison of contour plots of closing fifth-order flux for the five-moment closures showing (left) the closing flux for the IBME closure and (right) the closing flux for the bi-Gaussian closure in realizable moment space defined by the non-dimensional heat flux, Q^*, and kurtosis, R^*.

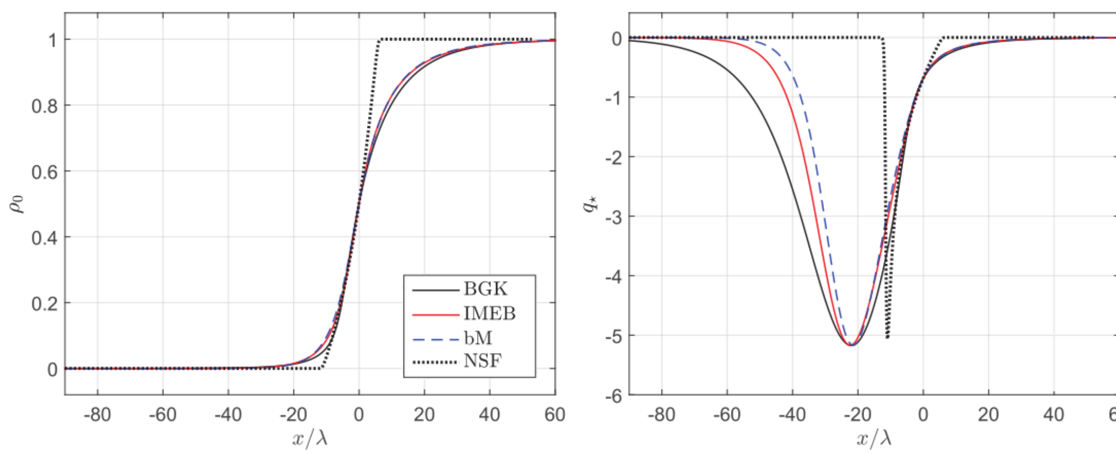

FIGURE 2. Profiles of the normalized density (left) and dimensionless heat transfer (right) for a Mach number 8 stationary shock wave (results taken from Laplante and Groth [6]).

MAXIMUM-ENTROPY-INSPIRED CLOSURES IN MULTI-DIMENSIONS

Boltzmann Kinetic Equation

A microscopic statistical description of three-dimensional non-equilibrium flows is offered by the Boltzmann kinetic equation which, neglecting external forces, is given by

$$\frac{\partial \mathscr{F}}{\partial t} + v_i \frac{\partial \mathscr{F}}{\partial x_i} = \frac{\delta \mathscr{F}}{\delta t}\,, \tag{16}$$

and where the NDF, $\mathscr{F} = \mathscr{F}(x_i, v_i, t)$, is now a function of the particle position and velocity vectors, x_i and v_i, and time, t, and $\delta\mathscr{F}/\delta t$ is the Boltzmann collision integral [15]. Macroscopic moments now involve weighted integration over three-dimensional velocity space and are given by

$$M(x_i,t) = \iiint\limits_{\infty} V(v_i)\mathscr{F}(x_i,v_i,t)\,\mathrm{d}^3 v = \langle V(v_i)\mathscr{F}\rangle_v\,. \tag{17}$$

14-Moment Interpolative-Based Maximum-Entropy (IBME) Closure

As in the 14-moment closure of the Levermore hierarchy in three-dimensional space, the 14-moment IBME closure of McDonald and Torrilhon [7] considers a moment set that includes the density, ρ, the mean velocity, u_i, the second-order pressure tensor, P_{ij}, the third-order heat flux vector, $q_i = Q_{ijj}/2$, and the scalar kurtosis, $r = R_{iijj}$. The resulting moment equations of the 14-moment maximum-entropy closure can then be summarized as

$$\frac{\partial}{\partial t}(\mathbf{M}) + \frac{\partial}{\partial x_k}(\mathbf{F}_k) = \mathbf{S}, \tag{18}$$

where the moment and moment flux vectors are given by

$$\mathbf{M} = \begin{bmatrix} \rho \\ \rho u_i \\ \rho u_i u_j + P_{ij} \\ \rho u_i u_j u_j + u_i P_{jj} + 2u_j P_{ij} + Q_{ijj} \\ \rho u_i u_i u_j u_j + 2u_i u_i P_{jj} + 4u_i u_j P_{ij} \\ +4u_i Q_{ijj} + R_{iijj} \end{bmatrix}, \tag{19}$$

$$\mathbf{F}_k = \begin{bmatrix} \rho u_i \\ \rho u_i u_j + P_{ij} \\ \rho u_i u_j u_k + u_i P_{jk} + u_j P_{ik} + u_k P_{ij} + Q_{ijk} \\ \rho u_i u_k u_j u_j + u_i u_k P_{jj} + 2u_i u_j P_{jk} + 2u_j u_k P_{ij} + u_j u_j P_{ik} \\ +u_i Q_{kjj} + u_k Q_{ijj} + 2u_j Q_{ijk} + R_{ikjj} \\ \rho u_k u_i u_i u_j u_j + 2u_k u_i u_i P_{jj} + 4u_i u_i u_j P_{jk} + 4u_i u_j u_k P_{ij} \\ +2u_i u_i Q_{kjj} + 4u_i u_k Q_{ijj} + 4u_i u_j + Q_{ijk} + 4u_i R_{ikjj} + u_k R_{iijj} + S_{kiijj} \end{bmatrix}, \tag{20}$$

and the source vector, $\mathbf{S}$, represents the time rate of change of the moments produced by inter-particle collision processes. Closure of this 14-moment set of hyperbolic equations requires the specification of the third-order heat flux tensor, Q_{ijk}, second-order kurtosis tensor, R_{ikjj}, and the fifth-order moment vector, S_{kiijj}, which all appear the the moment flux vector, $\mathbf{F}_k$.

McDonald and Torrilhon [7] arrived at an interpolative-based closure that approximates the 14-moment maximum-entropy closure guided by the results for the five-moment closure in the one-dimensional univariate case described above. Nevertheless, the interpolative closure presents some challenges when considering the fully multi-dimensional case and the reader is referred to the original paper [7] for the full derivation. McDonald and Torrilhon [7] suggest closing the heat flux tensor, Q_{ijk}, by using the derivatives of the heat flux tensor when the distribution function is a Gaussian. Thus, an approximation for the closing heat flux tensor is given by

$$Q_{ijk} = \left[\frac{\partial Q_{ijk}}{\partial Q_{mnn}}\right]_{\text{Gaussian}} Q_{mnn}. \tag{21}$$

However, it should be noted that this representation becomes more inaccurate as the solution moves away from the equilibrium solution in moment space. The closing kurtosis tensor, R_{ijkk}, can be evaluated analytically at equilibrium and solved on the realizability boundary allowing for the definition of an interpolant between these two limits. Again introducing an interpolation parameter, $\sigma_{\text{IM}} \in (0,1]$, as in the one-dimensional case, the closing kurtosis is specified as [7]

$$R_{ijkk} = \frac{1}{\sigma_{\text{IM}}} Q_{ijl}\left(P^{-1}\right)_{lm} Q_{mkk} + 2(1-\sigma_{\text{IM}})\frac{P_{ik}P_{kj}}{\rho} + \frac{P_{ij}P_{kk}}{\rho}. \tag{22}$$

The closing fifth-order velocity moment is proposed as a function of the derivative of S_{ijjkk} at a Gaussian solution and the derived expression on the realizability boundary. As with the closing heat flux, the resulting form is not a direct interpolation using σ_{IM} but instead is defined such that the derived expression is recovered on the realizability boundary; the form of the expression is made to match that of the one-dimensional case such that a contraction of the fifth-order tensor should produce a similar formula to the one dimensional case. The closing fifth-order flux is [7]

$$S_{ijjkk} = \frac{1}{\sigma_{\text{IM}}^2} P_{kn}^{-1} P_{lm}^{-1} Q_{npp} Q_{mjj} Q_{ikl} + 2\sigma_{\text{IM}}^{3/5}\frac{P_{jj}Q_{ikk}}{\rho} + (1-\sigma_{\text{IM}}^{3/5})\left[\frac{\partial S_{ijjkk}}{\partial Q_{mnn}}\right]_{\text{Gaussian}} Q_{mnn}. \tag{23}$$

The interpolation parameter in the three-dimensional case, σ_{IM}, is defined again such that $\sigma_{\mathrm{IM}} = 0$ on the Junk space and $\sigma_{\mathrm{IM}} = 1$ on the realizability boundary. The value of σ_{IM} is defined by the equation [7]

$$R_{iijj} = \frac{1}{\sigma_{\mathrm{IM}}} Q_{kii}(P^{-1})_{kl} Q_{ljj} + \frac{2(1-\sigma_{\mathrm{IM}}) P_{ji}P_{ij} + P_{ii}P_{jj}}{\rho} . \tag{24}$$

While the IBME closure of McDonald and Torrilhon does not mimic the maximum-entropy closure in the three-dimensional case as the closely as it does in the simplified one-dimensional case, it has been shown to produce quite reasonable and accurate results for a range of non-equilibrium in multi-dimensional flows [7, 9, 10], including stationary shock structure and rarefied flows past circular cylinders.

14-Moment Bi-Gaussian Closure

In three dimensional space, the bi-Gaussian NDF that forms the basis for the approximation of the 14-moment maximum-entropy closure is given as a sum of two Gaussian distributions with different weights, velocity abscissas, and a shared standard second-order variance tensor, Θ_{ij}. The NDF of the bi-Gaussian closure can thus be written as

$$\mathscr{F}_{(}x_i, c_i, t) = \sum_{k=1}^{2} \frac{\rho_k}{m(2\pi)^{3/2}\sqrt{\det \Theta_{ij}}} \exp\left(-\frac{1}{2} \Theta_{ij}^{-1} (v_i - v_{ki})(v_j - v_{kj}) \right) , \tag{25}$$

where ρ_k, v_{ki}, and Θ_{ij} are the 14 parameters defining the approximate form for the NDF. Expressions for these parameters can be found in terms of the known set of 14 moments $[\rho, u_i, P_{ij}, Q_{ijj}, R_{iijj}]$. In the original study by Chalons *et al.* [8] with the bi-Gaussian closure for multidimensional flows, the one-dimensional bi-Gaussian kernel functions are used in conjunction with the conditional quadrature method of moments (CQMOM) and this results in a 16-moment closure, which can be computationally quite expensive. The 14-moment bi-Gaussian closure considered here seeks to mimic the 14-moment maximum-entropy closure as closely as possible in an analogous fashion to the one-dimensional case and is based on fully three-dimensional Gaussian kernel functions. Unfortunately, the derivation of the full set of expressions for the closure is too long for inclusion in this paper; the full derivation can however be found in the recent thesis by Brooks [16].

Following Brooks [16], the closing heat flux tensor, Q_{ijk}, for the multi-dimensional bi-Gaussian closure can be expressed in terms of the heat flux vector, Q_{ijj}, and given by

$$Q_{ijk} = \frac{Q_{imm} Q_{jmm} Q_{kmm}}{Q_{nmm} Q_{nmm}} . \tag{26}$$

The closing kurtosis tensor, R_{ijkk}, is given as

$$R_{ijkk} = \frac{1}{\sigma_{\mathrm{BG}}} Q_{imm}(P_{kk})^{-1} Q_{jmm} + 2\frac{P_{ik}P_{jk}}{\rho} - 2\frac{Q_{imm}Q_{jmm}}{Q_{nmm}Q_{nmm}} \frac{P_{kk}P_{kk}\sigma_{\mathrm{BG}}^2}{\rho} + \frac{P_{ij}P_{kk}}{\rho} , \tag{27}$$

and the closing fifth-order tensor, S_{ijjkk}, is evaluated as

$$S_{ijjkk} = \frac{1}{\sigma_{\mathrm{BG}}^2} (P_{kk})^{-1}(P_{kk})^{-1} Q_{imm}Q_{jmm}Q_{jmm} + 4\left(\frac{P_{jk}Q_{imm}Q_{jmm}Q_{kmm}}{\rho Q_{nmm}Q_{nmm}} + \frac{P_{ij}Q_{jkk}}{\rho} \right) + 2(1-4\sigma_{\mathrm{BG}})\frac{P_{kk}Q_{ijj}}{\rho} . \tag{28}$$

The bi-Gaussian parameter, σ_{BG}, appearing in the preceding expressions for the closing fluxes is determined via the solution to the equation

$$\sigma_{\mathrm{BG}}^3 + \frac{\rho^2}{2(P_{ii})^2}\left[\frac{R_{iijj}}{\rho} - \left(\frac{P_{ii}}{\rho}\right)^2 - 2\left(\frac{P_{ij}P_{ij}}{\rho^2}\right) \right] \sigma_{\mathrm{BG}} - \frac{Q_{mnn}Q_{mnn}\rho}{2(P_{ii})^3} = 0 . \tag{29}$$

It is worth noting that, as in the one-dimensional case, the equations for the closing fluxes of the bi-Gaussian closure bear some resemblance to those of the IBME closure, with σ_{BG} again playing a similar role to that of σ_{IM} in the IBME three-dimensional closure. However, from equations above, it would seem that the expression for Q_{ijk} is undefined when the contracted heat flux vector, Q_{ijj}, vanishes. Similar issues apply to the expressions for R_{ijkk} and S_{ijjkk}. This is particularly devastating for R_{ijkk} since the kurtosis need not be zero when heat flux becomes zero and any attempts to approximate the offending $Q_{imm}Q_{jmm}/Q_{nmm}Q_{nmm}$ term can produce very different results depending on the direction in three dimensional space assumed for this term.

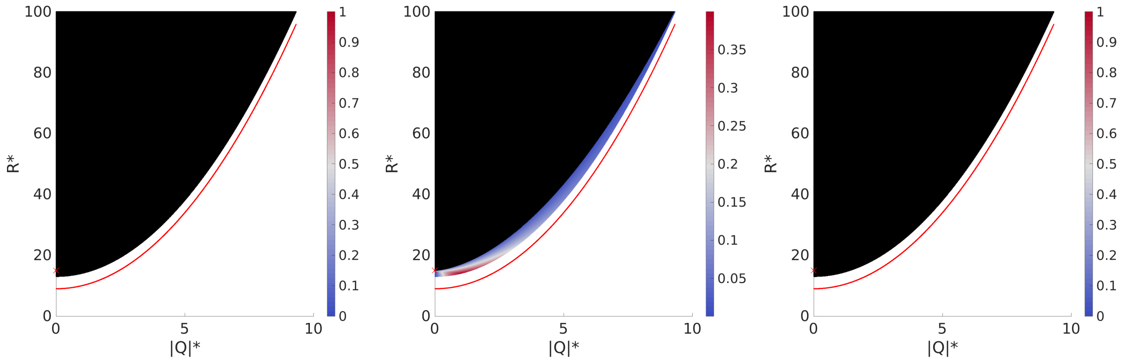

FIGURE 3. Normalized complex component of eigenvalue for $\rho = 1$, $u_i = [0,0]$, $P_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, and directions of heat flux Q_{ijj} are (left) $[0,1]$, (middle) $[1,1]$, and (right) $[1,0]$. Principle stress axes are aligned with the coordinate x and y axes. Local thermodynamic equilibrium is marked by a red 'x' and the realizability limit of the 14-moment space is plotted as a red curve.

Limits of Realizability and Hyperbolicity

One essential feature of the bi-Gaussian closure is the requirement that the standard deviation tensor, Θ_{ij}, be positive definite. This tensor defines the spread of the Gaussian kernel functions in each direction and cannot be negative since a negative tensor would imply that the value of the NDF is complex. The σ_{BG} term is defined in such a way as to require the limits of the parameter to be always between 0 and 1 in 14-moment space, however the standard deviation tensor applies an additional constraint on the value of σ_{BG} such that

$$\sigma_{\mathrm{BG}} \leq \frac{Q_{nmm} Q_{nmm}}{P_{mm} Q_{imm} Q_{jmm} (P_{ij})^{-1}} \,. \tag{30}$$

This expression suggests that σ_{BG} will almost never be equal to 1 and therefore the multidimensional bi-Gaussian is not realizable for the entire range of phase space defined by the set of 14 macroscopic moments.

The hyperbolicity of the moment equations of the bi-Gaussian closure is also of interest. The latter is a requirement for the well-posedness of initial boundary-value problems. Unfortunately, it is not possible to present a full analysis of hyperbolicity as it would necessitate a plot in at least four dimensional space. Instead, a few slices of that four dimensional space is presented to give the reader an idea of the hyperbolicity of the bi-Gaussian closure. A plot of the maximum normalized complex component of the eigenvalues of the bi-Gaussian flux Jacobian is given in Figure 3 in which non-dimensional kurtosis is shown as a function of the magnitude of the heat flux vector for several two-dimensional macroscopic flow situations. In each case, the heat flux vector is directed in a different direction in two dimensional space to demonstrate the differences as the direction of heat flux is changed. Figure 4 shows the same information; however, demonstrates the difficulties introduced by a non-zero fluid stress.

Interestingly, when heat flux is aligned with the $[1,1]$ direction, as shown Figure 4, the bi-Gaussian closure remains realizable for a wider range of 14-moment space than when the heat flux is not aligned with this axes. This behaviour is best explained by considering a case with a highly non-equilibrium pressure. Figure 5 shows the bi-Gaussian for a strong non-equilibrium flow whereby the x-axis is a principle stress axis. The results in this case demonstrate the ability of the bi-Gaussian closure to remain hyperbolic in a region where the macroscopic flow is largely one-dimensional. Figure 5 shows clearly that, in situations for which Q_{ijj} is aligned with the principle stress axis (the x direction axis), the bi-Gaussian closure is able to provide good coverage of the full 14-moment space. In situations for which Q_{ijj} is orthogonal to (i.e., not aligned with) the principle stress axis, the bi-Gaussian closure's coverage of realizability space is significant reduced in the region below local thermodynamic equilibrium. These findings suggests that the bi-Gaussian closure is best able to treat macroscopic moment sets corresponding to nearly one-dimensional flow in which the heat flux vector is more or less aligned with the principal stress axis.

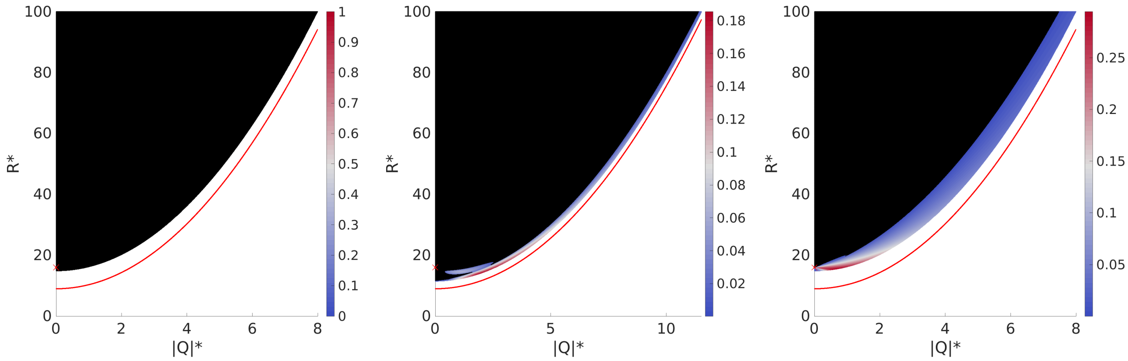

FIGURE 4. Normalized complex component of eigenvalue for $\rho = 1$, $u_i = [0,0]$, $P_{ij} = \begin{bmatrix} 1 & 0.5 & 0 \\ 0.5 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$, and directions of heat flux Q_{ijj} are (left) $[0,1]$, (middle) $[1,1]$, and (right) $[1,0]$. Local thermodynamic equilibrium is marked by a red 'x' and the realizability limit of the 14-moment space is plotted as a red curve.

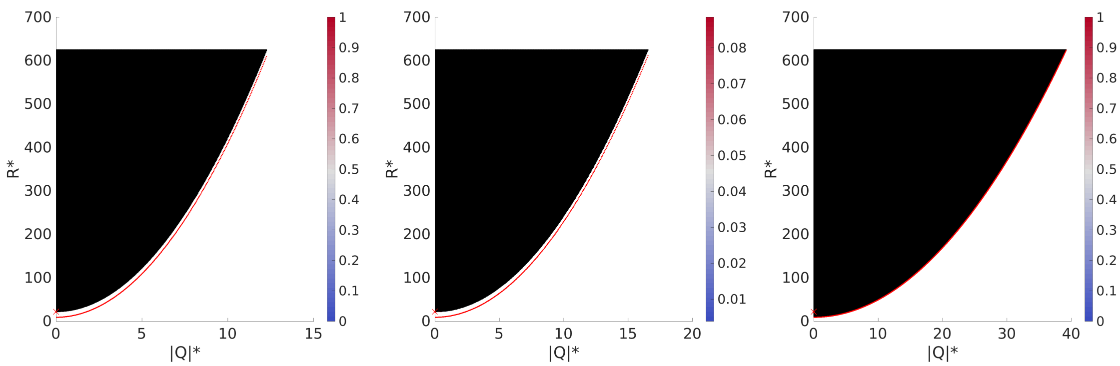

FIGURE 5. Normalized complex component of eigenvalue for $\rho = 1$, $u_i = [0,0]$, $P_{ij} = \begin{bmatrix} 1 & 0.0 & 0 \\ 0.0 & 0.1 & 0 \\ 0 & 0 & 0.1 \end{bmatrix}$, and directions of heat flux Q_{ijj} are (left) $[0,1]$, (middle) $[1,1]$, and (right) $[1,0]$. Local thermodynamic equilibrium is marked by a red 'x' and the realizability limit of the 14-moment space is plotted as a red curve.

Limits of Vanishing Heat Transfer

As eluded to in prior sections, the bi-Gaussian derivation leaves a considerable amount of uncertainty relating to the handling of a vanishing heat flux vector. A comparison of the bi-Gaussian NDF to the true maximum-entropy NDF for some cases where $Q_{ijj} = 0$ for all directions i provides insight into why it is difficult to specify the behaviour in this regime using a sum of positively weighted Gaussian kernel functions. Here, this analysis is again conducted for a two dimensional space of the macroscopic flow. It is worth noting that at thermodynamic equilibrium, both the maximum-entropy and bi-Gaussian closures produce identical results as both reduce to that of a simple Gaussian distribution.

One case to be considered is where the two-dimensional primitive macroscopic moments are given by

$$\rho = 1, \quad u_i = [0,0,0], \quad P_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad Q_{ijj} = [\varepsilon, 0, 0], \quad R_{iijj} = 14.5\,, \tag{31}$$

where ε is a small value which is almost equal to zero. Selecting a non-zero value for ε allows the bi-Gaussian closure to be defined; if the closure is well posed, the selection of ε in any direction for heat flux should not affect the resulting NDF significantly. Figure 6 presents a comparison of the maximum-entropy and bi-Gaussian NDFs for

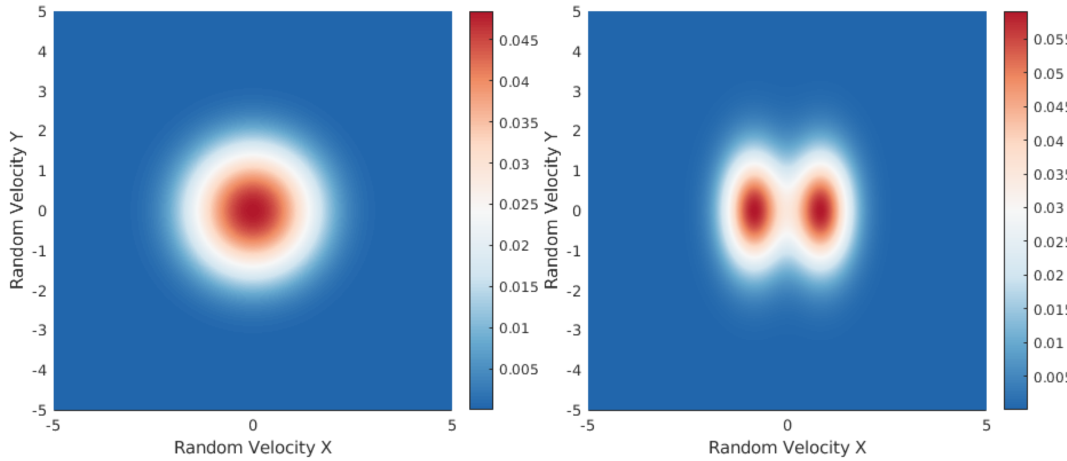

FIGURE 6. NDFs for primitive moments given in text for (left) maximum-entropy closure, and (right) bi-Gaussian closure for $c_z = 0$ plane of random velocity space.

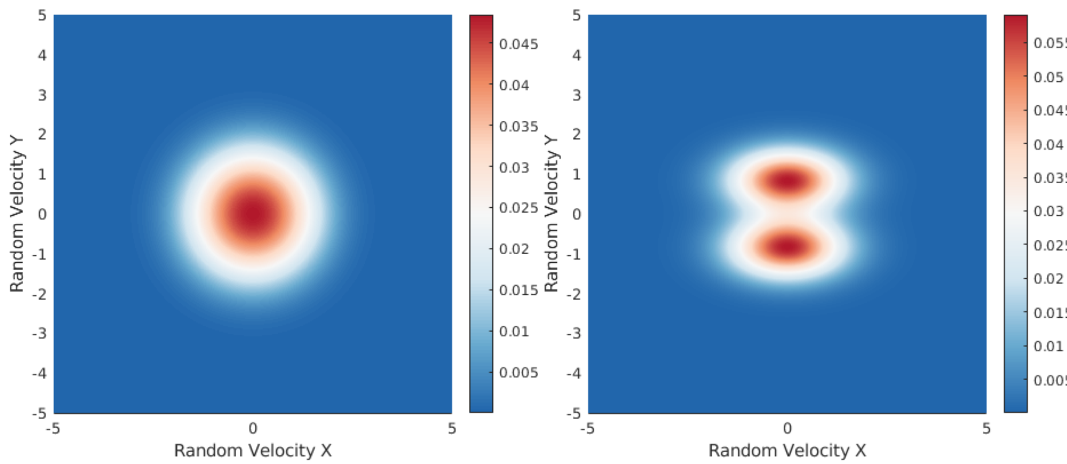

FIGURE 7. NDFs for primitive moments given in text for (left) maximum-entropy closure, and (right) bi-Gaussian closure for $c_z = 0$ plane of random velocity space.

the given parameters in a plane of random velocity space with $c_z = 0$. Immediately it is apparent that the bi-Gaussian distribution does not closely resemble the maximum-entropy NDF and produces two peaks instead of the expected single peak. If the heat flux vector is instead defined as $Q_{ijj} = [0, \varepsilon, 0]$, the results of Figure 7 are returned whereby the maximum-entropy NDF is essentially identical to that of the original case, whereas the bi-Gaussian NDF is entirely different, with the two peaks being oriented in a different direction entirely.

The fact that the form of bi-Gaussian NDF can be completely different depending on the direction of the heat flux vector as the magnitude of heat flux approaches zero can present significant problems for numerical solution methods. For example, taking a Frechét derivative in this region will yield eigenvalues of the Jacobian matrices that approach infinity as heat flux approaches zero. Numerical analysis of the closure confirms this result, with the bi-Gaussian closure producing infinite eigenvalues anywhere the heat flux reaches zero. By comparison, in the same regions that the bi-Gaussian becomes infinite, the IBME closure produces eigenvalues that are well bounded between 1 and 2. To further illustrate this issue, a comparison of the eigenvalues of the IBME closure to those of the bi-Gaussian approach is depicted in Figure 8 for a two-dimensional macroscopic flow case with

$$\rho = 1, \quad u_i = [0,0,0], \quad P_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad Q_{ijj} = [x, 0, 0], \quad \sigma_{\mathrm{IM}} = 0.1\,. \tag{32}$$

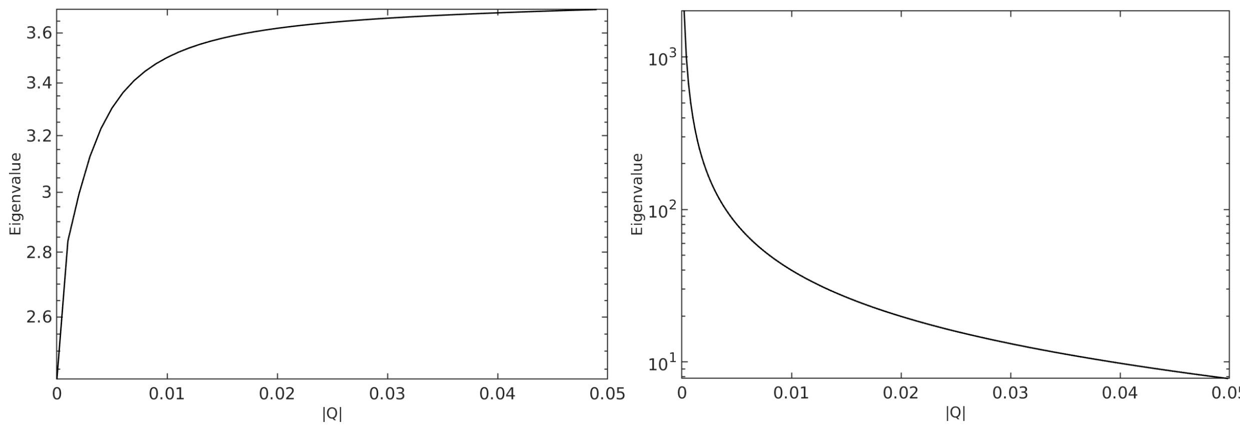

FIGURE 8. Largest eigenvalue component for (left) IBME closure and (right) bi-Gaussian closure for conditions given by Equation (32).

CONCLUSIONS

While the bi-Gaussian closure has previously been shown to provide very promising results in applications to one-dimensional univariate kinetic theory that closely approximate the solutions of the corresponding maximum-entropy closure [6], it would seem that its application does not extend easily to multi-dimensional descriptions. While a CQMOM approach can be adopted in the multi-dimensional case based on a Gaussian kernel function [8], the present study has shown that improving computational efficiency by analytically inverting a bi-Gaussian closure based on fully multi-dimensional kernel functions, while providing an analytical expression for the NDF, does not appear to yield a useful closure for practical non-equilibrium flow problems. Issues arise in the multi-dimensional case associated with the validity and hyperbolicity of the bi-Gaussian approximation to the maximum-entropy closure for significant portions of realizable moment space.

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