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HYPERBOLIC QUADRATURE METHOD OF MOMENTS FOR THE ONE-DIMENSIONAL KINETIC EQUATION*

RODNEY O. FOX[†] AND FRÉDÉRIQUE LAURENT[‡]

Abstract. A solution is proposed to a longstanding open problem in kinetic theory, namely, given any set of realizable velocity moments up to order $2n$, a closure for the moment of order $2n+1$ is constructed for which the moment system found from the free-transport term in the one-dimensional (1-D) kinetic equation is globally hyperbolic and in conservative form. In prior work, the hyperbolic quadrature method of moments (HyQMOM) was introduced to close this moment system up to fourth order ($n \leq 2$). Here, HyQMOM is reformulated and extended to arbitrary even-order moments. The HyQMOM closure is defined based on the properties of the monic orthogonal polynomials Q_n that are uniquely defined by the velocity moments up to order $2n - 1$. Thus, HyQMOM is strictly a moment closure and does not rely on the reconstruction of a velocity distribution function with the same moments. On the boundary of moment space, n double roots of the characteristic polynomial P_{2n+1} are the roots of Q_n , while in the interior, P_{2n+1} and Q_n share n roots. The remaining $n + 1$ roots of P_{2n+1} bound and separate the roots of Q_n . An efficient algorithm, based on the Chebyshev algorithm, for computing the moment of order $2n + 1$ from the moments up to order $2n$ is developed. The analytical solution to a 1-D Riemann problem is used to demonstrate convergence of the HyQMOM closure with increasing n .

Key words. kinetic equation, quadrature-based moment methods, hyperbolic quadrature method of moments

AMS subject classifications. 82C40, 35L60, 35Q70

1. Introduction. Moment closures in the context of kinetic theory have a long history. The 13-moment closure of Grad [17] and the moment-closure hierarchies of Levermore [26] are two well-known examples. In general, finite-dimensional moment systems derived from a kinetic equation will have unclosed terms, usually involving higher-order moments that are not included in the moment vector. For example, the free-transport term in the Boltzmann equation generates an unclosed spatial flux for the moment of order k that depends on the moment of order $k + 1$. Broadly speaking, the closure of the latter can be accomplished (as proposed by Grad [17]) using a perturbative solution for the velocity distribution function (VDF) valid near the equilibrium distribution, or (as proposed by Levermore [26]) using a non-perturbative reconstruction of the VDF such as entropy maximization [28].

Regardless of the method used to derive it, a well-posed moment closure must ensure that the predicted moments are realizable (i.e., they must be in the interior or on the boundary of the convex moment space [18, 8, 25, 31]) and that the moment system derived from the kinetic equation is globally hyperbolic [26, 20, 9, 10]. Furthermore, the moment closure must be well defined for every set of realizable moments, in particular for every moment vector in the interior of moment space [21, 9], and preferably result in a moment system in conservative form.

One method to ensure realizability of the unknown moments is to reconstruct a non-negative VDF from the known (realizable) moments; however, this is insufficient to ensure that the resulting moment system will be globally hyperbolic. For example,

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a one-dimensional (1-D) kinetic equation can be modeled by a moment system up to an even-order ($2n$) moment, whose flux depends of the unknown moment of order $2n+1$. Since odd-order moments need only be finite to be realizable, any value can be chosen to close the flux (e.g., set the $2n+1$ central moment equal to zero). Moreover, it is always possible to reconstruct a non-negative VDF based on this choice (e.g., a weighted sum of Dirac delta functions [37, 14, 5]), but it is unlikely that such an arbitrary choice will result in a globally hyperbolic moment system [20].

Indeed, there is no need to require that a moment closure corresponds to a *particular* form of the VDF (except on the boundary of moment space where the VDF is unique [31]). In other words, the ability to reconstruct the VDF from its moments is not a necessary condition for global hyperbolicity. Conversely, poor choices for the moment closure can generate unrealizable moments during the time advancement of the moment system, even if the moment system is hyperbolic and in conservative form [36]. Thus, care must be taken to guarantee that moments on the boundary of moment space do not leave it due to the closure for the flux.

For classical applications of the Boltzmann equation [34], it is often acceptable to employ a moment closure that is realizable and conditionally hyperbolic in a subset of moment space [32] (e.g., near the moments of the equilibrium VDF). A recent example of such a closure applied to rarefied gas dynamics can be found in [24]. For the same application, other authors have ‘regularized’ or ‘modified’ the moment system by adding non-conservative terms (see, for example, [1, 2, 23, 9, 11]) to achieve global hyperbolicity. In doing so, the direct connection between the closure and the reconstructed VDF is lost.

As an example, for moment vectors on the boundary of moment space where the VDF is unique [31], it remains to be shown whether or not the eigenvalues of the modified moment system found using the procedure in [23] correspond to the exact values found in [4, 20]. The latter are equal to the roots of the n th-order orthogonal polynomial Q_n , which can be found from the moments using the Chebyshev algorithm [37, 14, 5]. In the context of dilute sprays and particulate flows without collisions [7, 12, 6, 22, 27, 3, 13, 11, 20], moment systems very close to or on the boundary of moment space are regularly encountered. Thus, a robust moment closure must be able to describe accurately the evolution of moment sets near the boundary.

Hereinafter, we consider the velocity moments for a 1-D kinetic equation with only the free-transport term, which suffices for testing whether the proposed moment closure is globally hyperbolic. Further, the moment system consists of the $2n+1$ moments up to order $2n$, so that the spatial flux requires a closure for the moment of order $2n+1$. In prior work [13], the hyperbolic quadrature method of moments (HyQMOM) was developed for $n \leq 2$, and shown to yield a realizable and globally hyperbolic moment system in conservative form. In that work, the motivation for closing the spatial flux was to fix the middle root of the polynomial Q_3 at the mean velocity \bar{u} , which leads to a unique choice for the fifth-order velocity moment and corresponds to a VDF as a weighted sum of Dirac delta functions with one abscissa at \bar{u} . With this choice, it is possible to compute the five eigenvalues of the moment system analytically and prove global hyperbolicity, as well as realizability.

In the present work, we extend HyQMOM to $2 \leq n$ by choosing a closure for the $(2n+1)$ -order moment in conservative form that results in global hyperbolicity. In the process, we again make use of the polynomials Q_n (that are determined from the $2n$ moments up to order $2n-1$) to define a monic polynomial R_{n+1} of order $n+1$ whose roots separate and bound those of Q_n . The Chebyshev algorithm [37, 14, 5] is used to find Q_n from a set of realizable moments. We then demonstrate that

R_{n+1} is defined such that the characteristic polynomial of the 1-D moment system is $P_{2n+1} = Q_n R_{n+1}$. For $n = 2$, this procedure results in the middle root of Q_3 not being equal to \bar{u} , and leads to different locations for the eigenvalues for moment vectors in the interior of moment space than in [13]. Nonetheless, the basic idea for closing the $(2n+1)$ -order moment using the properties of Q_n remains unchanged, and thus we will continue to refer to the proposed extension as HyQMOM.

In the context of moment closures for the kinetic equation, HyQMOM is a *pure* moment closure in the sense that it does not rely on the reconstruction of a VDF to define the closure. In theory, an explicit formulae can be written for the HyQMOM closure that depends on the recurrence formula for the orthogonal polynomials Q_n . However, for large n , this expression is quite complex and must be computed numerically. For this purpose, in section 4, we develop an efficient algorithm for computing the HyQMOM closure based on the Chebyshev algorithm. Before describing the proposed closure, in section 2 we provide background information on the VDF and its moments. In section 3, we introduce the 1-D kinetic equation and prove a theorem that relates the characteristic polynomial of the moment system P_{2n+1} to the functional form of the moment closure for the standardized moment S_{2n+1} . Then, in section 4, we define the HyQMOM closure for arbitrary n by making use of the polynomials Q_n and their recurrence coefficients a_n and b_n .

The remainder of the paper is then devoted to exploring the properties of the proposed closure. In section 5, examples of the HyQMOM closure for $n \leq 5$ are provided to illustrate the behavior of the roots of the characteristic polynomial for selected moment sets. Then, in section 6, a Riemann problem with free transport is solved numerically using the HyQMOM closure and compared to the analytical solution for the moments. For increasing n , we demonstrate numerically that the HyQMOM closure converges uniformly towards the analytical solution. Finally, in section 7, conclusions are drawn and possible future extensions of the HyQMOM closure to multidimensional and bounded domains are briefly discussed.

2. Velocity distribution function and its moments. Consider the 1-D VDF $f(t, x, u)$ defined for $(t, x, u) \in \mathbb{R}^+ \times \mathbb{R} \times \mathbb{R}$. The VDF is non-negative and its moments with respect to the velocity u are finite. For a symmetric VDF about the mean velocity \bar{u} , $f(t, x, u - \bar{u}) = f(t, x, \bar{u} - u)$.

2.1. Moments. The moments of f are defined by

$$(2.1) \quad M_k(t, x) := \int_{\mathbb{R}} f(t, x, u) u^k du \quad \text{for } k \in \{0, 1, \dots, 2n+1\}$$

and $n \in \mathbb{N}$. Let us also denote the moment vector by $\mathbf{M}_{2n} := (M_0, M_1, \dots, M_{2n})^t$. The moment M_{2n+1} is not included in the moment vector, but we wish to specify it as depending on \mathbf{M}_{2n} subject to some constraints. This is the principal challenge faced in moment closures for the kinetic equation.

2.2. Central moments. For $M_0 > 0$, the central moments are defined by

$$(2.2) \quad C_k(t, x) := \frac{1}{M_0} \int_{\mathbb{R}} f(t, x, u) (u - \bar{u})^k du \quad \text{for } k \in \{0, 1, \dots, 2n+1\}$$

where $\bar{u}(t, x) = M_1/M_0$ is the mean velocity. By definition, $C_0 = 1$ and $C_1 = 0$. The next central moment $C_2 \geq 0$ is the velocity variance. Let us remark that the vector $\mathbf{C}_k := (C_0, \dots, C_k)^t = (1, 0, C_2, \dots, C_k)^t$ is the k^{th} -order moment vector corresponding to $v \mapsto \frac{1}{M_0} f(\bar{u} + v)$.

For any $k \geq 2$, the central moment C_k depends uniquely on the moment set $\mathbf{M}_k := (M_0, M_1, \dots, M_k)$ through the relation

$$(2.3) \quad C_k = \sum_{i=0}^k \binom{k}{i} \left(-\frac{M_1}{M_0}\right)^{k-i} \frac{M_i}{M_0}.$$

And inversely, for $k \geq 2$, M_k depends uniquely on the central moment vector $\tilde{\mathbf{C}}_k = (M_0, \bar{u}, C_2, \dots, C_k)^t$ through the relation

$$(2.4) \quad M_k = M_0 \left[\sum_{i=2}^k \binom{k}{i} \bar{u}^{k-i} C_i + \bar{u}^k \right].$$

In particular, the unclosed moment M_{2n+1} can be written in terms of the components of $\tilde{\mathbf{C}}_{2n}$ as

$$(2.5) \quad M_{2n+1} = M_0 \left[\sum_{i=2}^{2n} \binom{2n+1}{i} \bar{u}^{2n+1-i} C_i + \bar{u}^{2n+1} + C_{2n+1} \right]$$

where C_{2n+1} must be specified as an algebraic function of $\tilde{\mathbf{C}}_{2n}$. Thus, in the context of moment closures, specifying C_{2n+1} is equivalent to specifying M_{2n+1} .

2.3. Standardized moments. For $C_2 > 0$, the standardized moments are defined by

$$(2.6) \quad S_k := \frac{C_k}{C_2^{k/2}} \quad \text{for } k \in \{0, 1, \dots, 2n+1\}.$$

By definition, $(S_0, S_1, S_2) = (1, 0, 1)$ and $\mathbf{S}_k := (S_0, \dots, S_k)^t = (1, 0, 1, S_3, \dots, S_k)^t$ is the k^{th} -order moment vector corresponding to $v \mapsto \frac{\sqrt{C_2}}{M_0} f(\bar{u} + \sqrt{C_2}v)$. When $C_2 = 0$, all higher-order central moments are null. Unless stated otherwise, hereinafter we assume that $0 < C_2$ and define the standardized moment vector $\tilde{\mathbf{S}}_k = (M_0, \bar{u}, C_2, S_3, \dots, S_k)^t$, which has a one-to-one relation with \mathbf{M}_k in the interior of moment space. In the context of moment closures, we must specify S_{2n+1} for $2 \leq n$ as an algebraic function of $\tilde{\mathbf{S}}_{2n}$ subject to constraints.

2.4. Realizability. In this work, we will not attempt to reconstruct the VDF from its moments. Instead, we approximate the moment of order $2n+1$ given lower-order moments, i.e., we seek a particular solution to the truncated Hamburger moment problem [18]. Nonetheless, given the data $(M_0, \bar{u}, C_2, S_3, \dots, S_{2n}, S_{2n+1})$ with $M_0 > 0$, $C_2 > 0$, a reconstructed VDF consisting of a sum of weighted Dirac delta functions can be found when the moment set is realizable. The latter is verified using the Hankel determinants [31]:

$$(2.7) \quad H_{2k} = \begin{vmatrix} 1 & 0 & 1 & S_3 & \cdots & S_k \\ 0 & 1 & S_3 & S_4 & & \\ 1 & S_3 & S_4 & S_5 & & \\ S_3 & S_4 & S_5 & S_6 & & \\ \vdots & & & & \ddots & \\ S_k & & & & & S_{2k} \end{vmatrix}, \quad k \in \{2, \dots, n\}.$$

If $H_{2k} > 0$ for $k \in \{2, \dots, n\}$, then the moment set is realizable and lies in the interior of moment space. It is then said to be strictly realizable. If $H_{2k} < 0$ for any $k \in \{2, \dots, n\}$ then the moment set is unrealizable. Otherwise, the moment set is realizable if and only if there exists $k \in \{2, \dots, n\}$ such that $H_4 > 0, \dots, H_{2k-2} > 0, H_{2k} = \dots = H_{2n} = 0$ and the vector $(S_{n+1}, \dots, S_{2n+1})$ is in the span of $(S_j, S_{j+1}, \dots, S_{j+n}), j = 0, \dots, n$. In this last case, the moment set then lies on the boundary of moment space and the VDF is exactly a weighted sum of k Dirac delta functions.

Note that $0 = H_{2n}$ defines the lower bound for S_{2n} (i.e., the even-order moments). In contrast, for the Hamburger moment problem, if $H_{2k} > 0$ for $k \in \{2, \dots, n\}$, the odd-order moment S_{2n+1} can take on any finite real value. In the context of moment closures, we require that the algebraic function defining S_{2n+1} be valid for any vector of realizable moments \mathbf{M}_{2n} .

2.5. Linear functional associated with a moment vector. For a moment vector \mathbf{M}_N , one can define the linear functional $\langle \cdot \rangle_{\mathbf{M}_N}$ on the space $\mathbb{R}[X]_N$ of the real polynomial function of degree smaller than N by

$$(2.8) \quad \langle X^k \rangle_{\mathbf{M}_N} = M_k, \quad \text{for } k \in \{0, 1, \dots, N\}.$$

Let us remark that if \mathbf{M}_N is associated with a VDF f , then

$$(2.9) \quad \forall P \in \mathbb{R}[X]_N \quad \langle P \rangle_{\mathbf{M}_N} = \int_{\mathbb{R}} P(u) f(u) du.$$

Let us consider the linear functionals $\langle \cdot \rangle_{\mathbf{S}_N}$ associated with the standardized moments defined in [subsection 2.3](#). It is linked to the one associated with \mathbf{M}_N by

$$(2.10) \quad \forall P \in \mathbb{R}[X]_N \quad \langle P(X) \rangle_{\mathbf{M}_N} = M_0 \left\langle P \left(\bar{u} + \sqrt{C_2} X \right) \right\rangle_{\mathbf{S}_N}.$$

In the following, the notation $\langle \cdot \rangle$ is used for simplicity and corresponds to $\langle \cdot \rangle_{\mathbf{S}_{2n}}$. Indeed, it is easier to work with $\tilde{\mathbf{S}}_{2n}$ than directly with \mathbf{M}_{2n} , and it is equivalent as soon as $M_0 > 0$ and $C_2 > 0$. Moreover, as soon as \mathbf{M}_{2n} (or equivalently \mathbf{S}_{2n}) is strictly realizable, the application $(p, q) \mapsto \langle pq \rangle$ defines a scalar product on $\mathbb{R}[X]_n$.

3. Kinetic equation and its moment system. The 1-D kinetic equation for the VDF including only free transport is

$$(3.1) \quad \partial_t f + u \partial_x f = 0,$$

with initial condition $f(0, x, u) = f_0(x, u)$. The exact solution is given by $f(t, x, u) = f_0(x - ut, u) = f_0(x - ut, u)$. In this work, we seek to approximate the moments of the VDF found from (3.1) by formulating a finite-dimensional moment system.

3.1. Moment system. The unclosed governing equations for the moment vector are

$$(3.2) \quad \begin{aligned} \partial_t M_0 + \partial_x M_1 &= 0, \\ \partial_t M_1 + \partial_x M_2 &= 0, \\ &\vdots \\ \partial_t M_N + \partial_x M_{N+1} &= 0; \end{aligned}$$

or, in vector form,

$$(3.3) \quad \partial_t \mathbf{M}_N + \partial_x \mathbf{F}(\mathbf{M}_N) = \mathbf{0}$$

where the unclosed flux vector is $\mathbf{F}(\mathbf{M}_N) = (M_1, M_2, \dots, M_N, M_{N+1})^t$. A viable moment closure provides an algebraic function $M_{N+1}(\mathbf{M}_N)$ that is well defined for any realizable moment vector \mathbf{M}_N . It then must be demonstrated that such a closure is globally hyperbolic. In this work, the characteristic polynomial derived from (3.3) will be used for this purpose. The system (3.3) with the closed flux vector will then have a conservative hyperbolic form.

3.2. Characteristic polynomial. The Jacobian matrix of system (3.3) is given by

$$(3.4) \quad \frac{D\mathbf{F}}{D\mathbf{M}} = \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 \\ \frac{\partial M_{N+1}}{\partial M_0} & \frac{\partial M_{N+1}}{\partial M_1} & \frac{\partial M_{N+1}}{\partial M_2} & \dots & \frac{\partial M_{N+1}}{\partial M_N} \end{pmatrix}.$$

Equivalently, as soon as $M_0 > 0$, the variable set $\tilde{\mathbf{C}}_N = (M_0, \bar{u}, C_2, \dots, C_N)^t$ can be used, as well as $\tilde{\mathbf{S}}_N = (M_0, \bar{u}, C_2, S_3, \dots, S_N)^t$ if in addition $M_2 M_0 > M_1^2$, where the central moments C_k and the standardized moments S_k are defined by (2.3) and (2.6), respectively. The closure is then given by the algebraic function $C_{N+1}(\tilde{\mathbf{C}}_N)$ or $S_{N+1}(\tilde{\mathbf{S}}_N)$, and (2.5).

In terms of the central moments, as soon as the variables are regular enough, the system can be rewritten:

$$(3.5) \quad \partial_t \tilde{\mathbf{C}}_N + \mathbf{J} \partial_x \tilde{\mathbf{C}}_N = \mathbf{0}$$

with

$$(3.6) \quad \mathbf{J} := \frac{D\mathbf{M}^{-1}}{D\tilde{\mathbf{C}}} \frac{D\mathbf{F}}{D\mathbf{M}} \frac{D\mathbf{M}}{D\tilde{\mathbf{C}}}.$$

Of course, the characteristic polynomial of $\frac{D\mathbf{F}}{D\mathbf{M}}$ is the same as the one of \mathbf{J} and is denoted $\bar{P}_{N+1}(X) := |\mathbf{J} - X\mathbf{I}|$. The following proposition can then be shown.

PROPOSITION 3.1. *Let $\mathbf{M}_N = (M_0, M_1, M_2, \dots, M_N)^t$ be a realizable moment vector such that $M_0 > 0$ and $M_2 M_0 > M_1^2$, and let $\tilde{\mathbf{S}}_N = (M_0, \bar{u}, C_2, S_3, \dots, S_N)^t$ be the corresponding standardized moment vector. Let us assume that the function S_{N+1} does not depend on (M_0, \bar{u}, C_2) , i.e., $S_{N+1}(S_3, \dots, S_N)$. Then, the following polynomial*

$$(3.7) \quad P_{N+1}(X) := \bar{P}_{N+1} \left(\bar{u} + C_2^{1/2} X \right) C_2^{-(N+1)/2} \\ = \left| \mathbf{J} - \left(\bar{u} + C_2^{1/2} X \right) \mathbf{I} \right| C_2^{-(N+1)/2},$$

where \mathbf{J} is defined by (3.6), only depends on (S_3, \dots, S_N) .

Proof. The equations for M_0 and \bar{u} are

$$(3.8) \quad \begin{aligned} \partial_t M_0 + \bar{u} \partial_x M_0 + M_0 \partial_x \bar{u} &= 0, \\ \partial_t \bar{u} + \frac{C_2}{M_0} \partial_x M_0 + \bar{u} \partial_x \bar{u} + \partial_x C_2 &= 0. \end{aligned}$$

Since the moment vector $\mathbf{M}_{N+1}(t, x)$ is realizable for each (t, x) , it can be associated with a VDF $f(t, x, u)$. Setting $u = v + \bar{u}(t, x)$, the function $\tilde{f}(t, x, v) := f(t, x, v + \bar{u}(t, x))$ is then such that

$$(3.9) \quad \partial_t f + u \partial_x f = \partial_t \tilde{f} + v \partial_x \tilde{f} + \bar{u} \partial_x \tilde{f} - (\partial_t \bar{u} + \bar{u} \partial_x \bar{u} + v \partial_x \bar{u}) \partial_v \tilde{f}.$$

The central moments are such that $M_0 C_k = \int_{\mathbb{R}} v \tilde{f}(t, x, v) dv$ for $k = 2, \dots, N$. Since $\int_{\mathbb{R}} u^k (\partial_t f + u \partial_x f)(t, x, u) du = 0$, for $k = 2, \dots, N$, then, thanks to (3.9):

$$(3.10) \quad \begin{aligned} \partial_t (M_0 C_k) + \partial_x (M_0 C_{k+1}) + \bar{u} \partial_x (M_0 C_k) + (\partial_t \bar{u} + \bar{u} \partial_x \bar{u}) k M_0 C_{k-1} \\ + (\partial_x \bar{u}) (k+1) M_0 C_k = 0. \end{aligned}$$

This equation can be rewritten, using (3.8):

$$(3.11) \quad \partial_t C_k + \frac{C_{k+1} - k C_2 C_{k-1}}{M_0} \partial_x M_0 + k C_k \partial_x \bar{u} - k C_{k-1} \partial_x C_2 + \bar{u} \partial_x C_k + \partial_x C_{k+1} = 0.$$

This result, along with (3.8), allows to write the matrix \mathbf{J} . Then, $\left| \mathbf{J} - \left(\bar{u} + C_2^{1/2} X \right) \mathbf{I} \right|$ can be written as

$$\begin{vmatrix} -X\sqrt{C_2} & M_0 & 0 & & & & & & & & \\ \frac{C_2}{M_0} & -X\sqrt{C_2} & 1 & & & & & & & & \\ \frac{C_3}{M_0} & 2C_2 & -X\sqrt{C_2} & & & & & & & & \\ \frac{C_4-3C_2C_2}{M_0} & 3C_3 & -3C_2 & & & & & & & & \\ \vdots & \vdots & \vdots & & & & & & & & \\ \frac{C_{N-1}-(N-2)C_2C_{N-3}}{M_0} & (N-2)C_{N-2} & -(N-2)C_{N-3} & & & & & & & & \\ \frac{C_N-(N-1)C_2C_{N-2}}{M_0} & (N-1)C_{N-1} & -(N-1)C_{N-2} & & & & & & & & \\ \frac{C_{N+1}-NC_2C_{N-1}}{M_0} & NC_N & -NC_{N-1} + \frac{\partial C_{N+1}}{\partial C_2} & & & & & & & & \\ & & 0 & \dots & 0 & & & & 0 & & \\ & & 0 & \dots & 0 & & & & 0 & & \\ & & 1 & \dots & 0 & & & & 0 & & \\ & & -X\sqrt{C_2} & \ddots & 0 & & & & 0 & & \\ & & & \ddots & & & & & \vdots & & \\ & & & & & & & & 0 & & \\ & & & & & & & & 1 & & \\ & & & & & & & & -X\sqrt{C_2} & & \\ & & & & & & & & \frac{\partial C_{N+1}}{\partial C_3} & \dots & \frac{\partial C_{N+1}}{\partial C_{N-1}} & \frac{\partial C_{N+1}}{\partial C_N} - X\sqrt{C_2} & \end{vmatrix}.$$

Let us remark that, thanks to the assumption on S_{N+1} , $C_{N+1}(C_2, \dots, C_N)$. Factoring $C_2^{1/2}/M_0$ to the first row, $C_2^{i/2}$ to each row $i > 1$ and M_0 to the first column and

$1/C_2^{(j-1)/2}$ to each column $j > 1$, we obtain

$$C_2^{(N+1)/2} \left| \begin{array}{ccc} -X & 1 & 0 \\ 1 & -X & 1 \\ S_3 & 2 & -X \\ S_4 - 3S_2 & 3S_3 & -3 \\ \vdots & \vdots & \vdots \\ S_{N-1} - (N-2)S_{N-3} & (N-2)S_{N-2} & -(N-2)S_{N-3} \\ S_N - (N-1)S_{N-2} & (N-1)S_{N-1} & -(N-1)S_{N-2} \\ S_{N+1} - NS_{N-1} & NS_N & -NS_{N-1} + \frac{N+1}{2}S_{N+1} \\ 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & 0 \\ 1 & \cdots & 0 & 0 \\ -X & \ddots & 0 & 0 \\ & \ddots & & \vdots \\ 0 & & 1 & 0 \\ 0 & & -X & 1 \\ \frac{\partial S_{N+1}}{\partial S_3} & \cdots & \frac{\partial S_{N+1}}{\partial S_{N-1}} & \frac{\partial S_{N+1}}{\partial S_N} - X \end{array} \right|.$$

This result shows that $P_{N+1}(X)$ only depends on (S_3, \dots, S_N) , thus concluding the proof. \square

The eigenvalues of (3.3) are then written $\lambda_k = \bar{u} + C_2^{1/2} \mu_k$, where μ_k is a root of P_{N+1} that only depends on (S_3, \dots, S_N) . It is then easy to calculate the coefficients of the characteristic polynomial:

THEOREM 3.2. *With the same assumptions as in Proposition 3.1, the scaled characteristic polynomial defined by (3.7) has the form*

$$(3.12) \quad P_{N+1}(X) = \sum_{m=0}^{N+1} c_m X^m$$

with coefficients defined by

$$(3.13) \quad \begin{aligned} c_{N+1} &= 1, \quad c_N = -\frac{\partial S_{N+1}}{\partial S_N}, \quad c_{N-1} = -\frac{\partial S_{N+1}}{\partial S_{N-1}}, \quad \dots, \quad c_3 = -\frac{\partial S_{N+1}}{\partial S_3}, \\ c_2 &= -\frac{1}{2} \sum_{m=3}^{N+1} m S_m c_m, \quad c_1 = -\sum_{m=3}^{N+1} m S_{m-1} c_m, \\ c_0 &= \frac{1}{2} \sum_{m=3}^{N+1} (m-2) S_m c_m = -c_2 - \sum_{m=3}^{N+1} S_m c_m. \end{aligned}$$

Proof. We denoted $\mathbf{S}_N := (1, 0, 1, S_3, \dots, S_N)^t$. From Proposition 3.1, it is known that P_{N+1} does not depend on (M_0, \bar{u}, C_2) , so that we can choose $(M_0, \bar{u}, C_2) = (1, 0, 1)$ in such a way that $\tilde{\mathbf{S}}_N = \mathbf{S}_N$. This implies that the corresponding moment vector is $\mathbf{M}_N = \mathbf{S}_N$, as well as for the central moment vector: $\tilde{\mathbf{C}}_N = \mathbf{S}_N$. Then P_{N+1} is equal to the characteristic polynomial of $\frac{D\mathbf{F}}{D\mathbf{M}}$ for $\mathbf{M}_N = \mathbf{S}_N$. Thus, from (3.4), the

coefficients of this polynomial can be written:

$$\begin{aligned} c_{N+1} = 1, \quad (c_0, c_1, \dots, c_N) &= - \frac{DM_{N+1}}{DM} \Big|_{\mathbf{M}_N = \mathbf{S}_N} \\ &= - \frac{DM_{N+1}}{D\tilde{\mathbf{S}}} \Big|_{\mathbf{M}_N = \mathbf{S}_N} \left(\frac{DM}{D\tilde{\mathbf{S}}} \Big|_{\mathbf{M}_N = \mathbf{S}_N} \right)^{-1}. \end{aligned}$$

Moreover, from (2.4), we can write

$$\frac{DM}{D\tilde{\mathbf{S}}} \Big|_{\mathbf{M}_N = \mathbf{S}_N} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ S_3 & 3S_2 & \frac{3}{2}S_3 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \ddots & \\ S_N & NS_{N-1} & \frac{N}{2}S_N & 0 & \cdots & 1 \end{pmatrix},$$

and then

$$\left(\frac{DM}{D\tilde{\mathbf{S}}} \Big|_{\mathbf{M}_N = \mathbf{S}_N} \right)^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 1 & 0 & \cdots & 0 \\ (\frac{3}{2} - 1)S_3 & -3S_2 & -\frac{3}{2}S_3 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \ddots & \\ (\frac{N}{2} - 1)S_N & -NS_{N-1} & -\frac{N}{2}S_N & 0 & \cdots & 1 \end{pmatrix}.$$

Furthermore, from (2.5), we can write

$$\frac{DM_{N+1}}{D\tilde{\mathbf{S}}} \Big|_{\mathbf{M}_N = \mathbf{S}_N} = \left(S_{N+1}, (N+1)S_N, \frac{N+1}{2}S_{N+1}, \frac{\partial S_{N+1}}{\partial S_3}, \dots, \frac{\partial S_{N+1}}{\partial S_N} \right).$$

Multiplying this row by the previous matrix concludes the proof. \square

3.3. Properties of the characteristic polynomial. From the definition in subsection 2.5 of the linear functional $\langle \cdot \rangle$ associated with the moment vector \mathbf{S}_N , one has

$$(3.14) \quad \langle P_{N+1} \rangle = c_{N+1}S_{N+1} + c_N S_N + \cdots + c_3 S_3 + c_2 + c_0.$$

If we define the polynomial $P'_{N+1}(X)$ by

$$(3.15) \quad P'_{N+1}(X) = \sum_{m=1}^{N+1} m c_m X^{m-1},$$

then the properties (3.13) of the coefficients of the scaled characteristic polynomial provide directly the following three constraints:

COROLLARY 3.3. *The scaled characteristic polynomial P_{N+1} defined by (3.7) is such that*

$$(3.16) \quad \langle P_{N+1} \rangle = 0, \quad \langle P'_{N+1} \rangle = 0, \quad \langle X P'_{N+1} \rangle = 0.$$

As shown in subsection 4.3, these constraints are used to define the HyQMOM closure.

4. Quadrature-based moment closure for S_{2n+1} . In general, QBMM provide a closure for higher-order moments in terms of the known lower-order moments. For example, M_{2n} given \mathbf{M}_{2n-1} , or M_{2n+1} given \mathbf{M}_{2n} . Without loss of generality, we describe QBMM using the standardized moments. Before defining the moment closure for S_{2n+1} used in HyQMOM, we first review the quadrature method of moments (QMOM), which provides a closure for S_{2n} in such a way that \mathbf{S}_{2n} is on the boundary of moment space.

4.1. QMOM closure for S_{2n} and orthogonal polynomials. QMOM considers moments up to S_{2n-1} with the closure for S_{2n} found from $H_{2n} = 0$, i.e., on the boundary of moment space. In this case, the unique VDF has the form of a sum of weighted Dirac delta functions located at the roots of the polynomial Q_n defined just below. Indeed, to compute the quadrature points, it is interesting to introduce the family of monic orthogonal polynomials Q_n , $\deg(Q_n) = n$, for the scalar product defined in [subsection 2.5](#), i.e., $\langle Q_m Q_n \rangle = \langle Q_n^2 \rangle \delta_{mn}$. Moreover, $\langle Q_n^2 \rangle = H_{2n}/H_{2n-2}$. This family satisfies the following recurrence relation

$$(4.1) \quad Q_{n+1}(X) = (X - a_n)Q_n(X) - b_n Q_{n-1}(X)$$

with $Q_{-1} = 0$ and $Q_0 = 1$. The recurrence coefficients a_n and b_n can be found from the standardized moments using the Chebyshev algorithm [\[37, 14, 5\]](#), which is given in [Appendix A](#). They are related to the orthogonal polynomials by

$$(4.2) \quad a_n = \frac{\langle X Q_n^2 \rangle}{\langle Q_n^2 \rangle}, \quad b_n = \frac{\langle Q_n^2 \rangle}{\langle Q_{n-1}^2 \rangle} = \frac{H_{2n} H_{2n-4}}{H_{2n-2}^2}.$$

The first few are $a_0 = 0$, $a_1 = S_3$, $a_2 = \frac{S_5 - S_3(2 + S_3^2 + 2H_4)}{H_4}$, $b_0 = 1$, $b_1 = 1$, $b_2 = H_4$, and $b_3 = H_6/H_4^2$. For QMOM with a given n , starting from the standardized moments up to S_{2n-1} , the Chebyshev algorithm computes the recurrence coefficients up to a_{n-1} and b_{n-1} to define Q_n . Note that a_n depends on standardized moments up to S_{2n+1} , with the highest-order moment having a linear dependence; and b_n depends on standardized moments up to S_{2n} . The b_n are positive except at the boundary of moment space where they can be zero.

Remark 4.1. For Gaussian moments, Q_n is the monic Hermite polynomial He_n .

Remark 4.2. The relation [\(2.10\)](#) between $\langle \cdot \rangle$ and $\langle \cdot \rangle_{\mathbf{M}_{2n}}$ induces that the orthogonal monic polynomials \bar{Q}_k related to the scalar product $(p, q) \mapsto \langle pq \rangle_{\mathbf{M}_{2n}}$ on $\mathbb{R}[X]_{2n}$ are such that

$$(4.3) \quad \bar{Q}_k(X) = C_2^{k/2} Q_k \left(\frac{X - \bar{u}}{\sqrt{C_2}} \right),$$

and the corresponding coefficients \bar{a}_n and \bar{b}_n are

$$(4.4) \quad \bar{a}_n = \frac{\langle X \bar{Q}_n^2 \rangle_{\mathbf{M}_{2n}}}{\langle \bar{Q}_n^2 \rangle_{\mathbf{M}_{2n}}} = \frac{\langle \bar{u} + \sqrt{C_2} X Q_n^2 \rangle}{\langle Q_n^2 \rangle} = \bar{u} + \sqrt{C_2} a_n,$$

$$(4.5) \quad \bar{b}_n = \frac{\langle \bar{Q}_n^2 \rangle_{\mathbf{M}_{2n}}}{\langle \bar{Q}_{n-1}^2 \rangle_{\mathbf{M}_{2n}}} = C_2 \frac{\langle Q_n^2 \rangle}{\langle Q_{n-1}^2 \rangle} = C_2 b_n.$$

In general, if the standardized moments correspond to a strictly realizable moment set, then there exists a one-to-one relationship between the moment vector \mathbf{S}_{2n-1} and

the recurrence coefficients $(a_1, \dots, a_{n-1}, b_2, \dots, b_{n-1})$. Thus, the quadrature-based moment closure can be expressed equivalently in terms of the standardized moments or the recurrence coefficients. We will use this fact when defining the HyQMOM closure in [subsection 4.3](#). Moreover, for all $n = 1, 2, \dots$; S_{2n} and S_{2n+1} expressed in terms of $\mathbf{Y} = (a_1, b_2, a_2, \dots, a_{n-1}, b_n, a_n)$ are multivariate polynomials (see [Appendix A](#)), as are the components of the vectors of partial derivatives $\frac{DS_{2n}}{D\mathbf{Y}}$ and $\frac{DS_{2n+1}}{D\mathbf{Y}}$.

Finally, the QMOM closure for S_{2n} corresponds to setting $b_n = 0$ to find S_{2n} . The form of the characteristic polynomial P_{2n} for the corresponding system were given in [\[4, 20\]](#).

THEOREM 4.3. *The QMOM closure $b_n = 0$ induces the following characteristic polynomial $P_{2n} = Q_n^2$ and the system is only weakly hyperbolic.*

4.2. Preliminary results. Before defining the HyQMOM closure, we will first need the following relations for the monic orthogonal polynomials Q_n :

LEMMA 4.4. *For all $n = 0, 1, \dots$;*

$$(4.6) \quad \frac{\langle XQ'_{n+1}Q_n \rangle}{\langle Q_n^2 \rangle} = \sum_{k=0}^n a_k, \quad \frac{\langle X^2Q'_nQ_n \rangle}{\langle Q_n^2 \rangle} = na_n + \sum_{k=0}^{n-1} a_k.$$

Proof. First, let us remark that $XQ_n = Q_{n+1} + a_nQ_n + b_nQ_{n-1}$, so that

$$\langle XQ'_{n+1}Q_n \rangle = (n+1)a_n\langle Q_n^2 \rangle + b_n\langle Q'_{n+1}Q_{n-1} \rangle,$$

since each Q_k is monic and orthogonal to any polynomial of degree at most $k-1$. Moreover, since $Q'_{n+1} = Q_n + (X - a_n)Q'_n - b_nQ'_{n-1}$, one can deduce:

$$\langle Q'_{n+1}Q_{n-1} \rangle = \langle XQ'_nQ_{n-1} \rangle - na_n\langle Q_{n-1}^2 \rangle.$$

Then, using $b_n = \frac{\langle Q_n^2 \rangle}{\langle Q_{n-1}^2 \rangle}$:

$$\frac{\langle XQ'_{n+1}Q_n \rangle}{\langle Q_n^2 \rangle} = (n+1)a_n + \frac{\langle XQ'_nQ_{n-1} \rangle - na_n\langle Q_{n-1}^2 \rangle}{\langle Q_{n-1}^2 \rangle} = a_n + \frac{\langle XQ'_nQ_{n-1} \rangle}{\langle Q_{n-1}^2 \rangle},$$

which allows to prove the first equality.

For the second one, we still use $XQ_n = Q_{n+1} + a_nQ_n + b_nQ_{n-1}$ to find

$$\langle X^2Q'_nQ_n \rangle = na_n\langle Q_n^2 \rangle + b_n\langle XQ'_nQ_{n-1} \rangle = \left(na_n + \frac{\langle XQ'_nQ_{n-1} \rangle}{\langle Q_{n-1}^2 \rangle} \right) \langle Q_n^2 \rangle.$$

Thanks to the first equality, this concludes the proof. \square

Finally, the following result is needed to relate a generalized recurrence relation involving Q_n to the constraints in [\(3.16\)](#):

THEOREM 4.5. *For all $n = 1, 2, \dots$; let the monic polynomial P_{2n+1} be given by*

$$(4.7) \quad P_{2n+1} = Q_n [(X - \alpha_n)Q_n - \beta_nQ_{n-1}]$$

where α_n and β_n are some real numbers. Then, the following statements are equivalent:

$$(i) \quad \langle P_{2n+1} \rangle = 0, \quad \langle P'_{2n+1} \rangle = 0 \quad \text{and} \quad \langle XP'_{2n+1} \rangle = 0.$$

$$(ii) \quad \alpha_n = a_n = \frac{1}{n} \sum_{k=0}^{n-1} a_k \quad \text{and} \quad \beta_n = \frac{2n+1}{n} b_n.$$

Proof. It is easy to see that

$$(4.8) \quad \langle P_{2n+1} \rangle = \langle XQ_n^2 \rangle - \alpha_n \langle Q_n^2 \rangle = (a_n - \alpha_n) \langle Q_n^2 \rangle.$$

Moreover, since $P'_{2n+1} = 2(X - \alpha_n)Q'_n Q_n + Q_n^2 - \beta_n(Q'_n Q_{n-1} + Q_n Q'_{n-1})$,

$$(4.9) \quad \langle P'_{2n+1} \rangle = 2n \langle Q_n^2 \rangle + \langle Q_n^2 \rangle - n\beta_n \langle Q_{n-1}^2 \rangle = [(2n+1)b_n - n\beta_n] \langle Q_{n-1}^2 \rangle.$$

And finally

$$\langle XP'_{2n+1} \rangle = 2 \langle X^2 Q'_n Q_n \rangle - 2n\alpha_n \langle Q_n^2 \rangle + \langle XQ_n^2 \rangle - \beta_n \langle XQ'_n Q_{n-1} \rangle.$$

Using (4.2) and Lemma 4.4, this leads to

$$(4.10) \quad \langle XP'_{2n+1} \rangle = \left[(2n+1)a_n + 2 \sum_{k=0}^{n-1} a_k - 2n\alpha_n - \frac{\beta_n}{b_n} \sum_{k=0}^{n-1} a_k \right] \langle Q_n^2 \rangle.$$

Equations (4.8), (4.9) and (4.10) allow to conclude the proof. \square

4.3. HyQMOM closure for S_{2n+1} . With HyQMOM, the moments up to S_{2n} are known, and a closure for S_{2n+1} is sought that makes the moment system globally hyperbolic. The choice is not unique (see Appendix B for a discussion of the case with $n = 2$), so we favor closures that are relatively simple to compute for arbitrary n , and for which global hyperbolicity can be demonstrated explicitly for $n \leq 9$ and is postulated for larger values of n .

THEOREM 4.6 (HyQMOM closure for S_{2n+1}). *Let Q_n be the monic orthogonal polynomial defined by (4.1), with $Q_{-1} = 0$, $Q_0 = 1$, and R_{n+1} be the monic polynomial defined by*

$$(4.11) \quad R_{n+1}(X) = (X - \alpha_n)Q_n(X) - \beta_n Q_{n-1}(X).$$

For all $n = 1, 2, \dots, 9$; the scaled characteristic polynomial in Theorem 3.2 can be written as

$$(4.12) \quad P_{2n+1}(X) = Q_n(X)R_{n+1}(X)$$

if and only if the closure on S_{2n+1} , defined through the coefficient a_n , and the coefficients α_n and β_n in (4.11) are related to the recurrence coefficients a_k and b_k by

$$(4.13) \quad a_n = \alpha_n = \frac{1}{n} \sum_{k=0}^{n-1} a_k, \quad \beta_n = \frac{2n+1}{n} b_n.$$

Proof. First, if the scaled characteristic polynomial P_{2n+1} is given by (4.12), then equations (4.13) follow directly from Theorem 4.5 and the properties (3.16) of the characteristic polynomial.

Conversely, using the closure $a_n = \alpha_n$, we just need to prove the relation (4.12). For that, it is easier to use the vector $\mathbf{Y} = (a_1, b_2, \dots, a_{n-1}, b_n)$, which is uniquely

Algorithm 1: Verification of Theorem 4.6

Data: $(a_k)_{k=1,\dots,n-1}, (b_k)_{k=2,\dots,n}$

Result: $P_{2n+1} - Q_n R_{n+1}$

$(a_0, b_0, b_1) \leftarrow (0, 1, 1);$

$a_n \leftarrow \frac{1}{n} \sum_{k=0}^{n-1} a_k$ // Set the closure;

$(S_0, S_1, S_2) \leftarrow (1, 0, 1);$

Initialize each scalar $Z_{k,p}$ to zero for $k \in \{-1, \dots, n\}, p \in \{0, \dots, 2n+1\};$

$Z_{0,0} \leftarrow 1$ // Reverse Chebyshev algorithm;

$Z_{0,1} \leftarrow 0;$

for $k \leftarrow 1$ **to** n **do**

$Z_{k,0} \leftarrow b_k Z_{k-1,0};$

$Z_{k,1} \leftarrow Z_{k,0} \left(a_k + \frac{Z_{k-1,1}}{Z_{k-1,0}} \right);$

for $p \leftarrow 1$ **to** $2n$ **do**

for $k \leftarrow 0$ **to** $\lfloor n + 1 - \frac{p}{2} \rfloor$ **do**

$Z_{k,p+1} \leftarrow Z_{k+1,p-1} + a_k Z_{k,p} + b_k Z_{k-1,p+1};$

$S_{p+1} \leftarrow Z_{0,p+1};$

$\mathbf{Y} \leftarrow (a_1, b_2, a_2, \dots, a_{n-1}, b_n)$ // Computation of the $c_k;$

$(c_3, \dots, c_{2n}) \leftarrow -\frac{DS_{2n+1}}{DY} \left(\frac{D(S_3, \dots, S_{2n})}{DY} \right)^{-1};$

$(c_0, c_1, c_2) \leftarrow \left(\frac{1}{2} \sum_{m=3}^{2n+1} (m-2) S_m c_m, -\sum_{m=3}^{2n+1} m S_{m-1} c_m, -\frac{1}{2} \sum_{m=3}^{2n+1} m S_m c_m \right);$

$P_{2n+1} \leftarrow X^{2n+1} + \sum_{k=0}^{2n} c_k X^k;$

$Q_{-1} \leftarrow 0$ // Computation of the polynomials $Q_k;$

$Q_0 \leftarrow 1;$

for $k \leftarrow 0$ **to** $n-1$ **do**

$Q_{k+1} \leftarrow (X - a_k) Q_k - b_k Q_{k-1};$

$R_{n+1} \leftarrow (X - a_n) Q_n - \frac{2n+1}{n} b_n Q_{n-1};$

return $P_{2n+1} - Q_n R_{n+1}$ // Final verification;

defined from (S_3, \dots, S_{2n}) . We can then use the following relation to compute the coefficients of the characteristic polynomial P_{2n+1} :

$$(4.14) \quad (c_3, \dots, c_{2n}) = -\frac{DS_{2n+1}}{DY} \left(\frac{D(S_3, \dots, S_{2n})}{DY} \right)^{-1}.$$

Then, such computations are done using Matlab symbolic to check (4.12) for $n = 2, 3, \dots, 9$. Algorithm 1 gives the details of these computations and the Matlab source code can be found in Appendix C. For $n = 1$ the result is obvious from the closure (see subsection 5.1). \square

Remark 4.7. For realizable moments, $\beta_n \geq 0$ in (4.11).

The main result concerning global hyperbolicity is as follows.

THEOREM 4.8. *When $\beta_n > 0$, the $n + 1$ roots of R_{n+1} in (4.11) are real-valued and bound and separate the n roots of Q_n .*

Proof. When $\beta_n > 0$ (and thus $b_n > 0$), the confluent form of the Christoffel–Darboux formula yields

$$\sum_{k=0}^n \frac{Q_k^2(X)}{\langle Q_k^2 \rangle} = \frac{Q_n(X)R'_{n+1}(X) - R_{n+1}(X)Q'_n(X)}{\langle Q_n^2 \rangle} > 0,$$

and thus

$$(4.15) \quad Q_n(X)R'_{n+1}(X) - R_{n+1}(X)Q'_n(X) > 0.$$

The n roots of Q_n are real and distinct [14] and denoted by $x_1 < x_2 < \dots < x_n$. For any two consecutive roots x_k and x_{k+1} , (4.15) implies that

$$R_{n+1}(x_k)R_{n+1}(x_{k+1}) < 0.$$

Then the polynomial R_{n+1} has at least one root between x_k and x_{k+1} , for each $k = 1, \dots, n-1$. Moreover, $Q'_n(x_n) > 0$, because of the behavior of Q_n at $+\infty$. Then $R_{n+1}(x_n) < 0$ and R_{n+1} has a root larger than x_n . In the same way, it has also a root smaller than x_1 . This concludes the proof. \square

Remark 4.9. When $\beta_n = 0$, n roots of R_{n+1} are shared with Q_n and the root α_n has multiplicity of either 1 or 3. The latter occurs when $Q_n(\alpha_n) = 0$, e.g., due to symmetry.

In summary, the HyQMOM closure in [Theorem 4.6](#) is globally hyperbolic for the moment system associated with the 1-D kinetic equation, and is well defined for any realizable moment vector \mathbf{M}_{2n} .

4.4. Computation of M_{2n+1} and the eigenvalues. Formulas for the closure $S_{2n+1}(S_3, \dots, S_{2n})$ could be given analytically. This is done in the next section for $n = 1$ and $n = 2$, but these formulas becomes increasing more complicated due to the number of moments involved. In the general case, the Chebyshev and reverse Chebyshev algorithms (see [Appendix A](#)) can be used to compute S_{2n+1} . But the transformation into standardized moment is not necessary, thanks to [Remark 4.2](#), as well as [Proposition 3.1](#). Indeed, the characteristic polynomial \bar{P}_{2n+1} of the system of moments \mathbf{M}_{2n} is linked to P_{2n+1} by (3.7), the monic orthogonal polynomials \bar{Q}_k corresponding to \mathbf{M}_{2n} are linked to the Q_k by (4.3). One can therefore define $\bar{\alpha}_n = \bar{u} + \sqrt{C_2}\alpha_n$, $\bar{\beta}_n = \sqrt{C_2}\beta_n$ and $\bar{R}_{n+1}(X) = C_2^{(n+1)/2}R_{n+1}\left(\frac{X-\bar{u}}{\sqrt{C_2}}\right)$ in such a way that in [Theorem 4.6](#), the relations (4.13) are equivalent to

$$(4.16) \quad \bar{\alpha}_n = \frac{1}{n} \sum_{k=0}^{n-1} \bar{a}_k, \quad \bar{\beta}_n = \frac{2n+1}{n} \bar{b}_n,$$

(4.11) is equivalent to

$$(4.17) \quad \bar{R}_{n+1}(X) = (X - \bar{\alpha}_n)\bar{Q}_n(X) - \bar{\beta}_n\bar{Q}_{n-1}(X),$$

and (4.12) is equivalent to

$$(4.18) \quad \bar{P}_{2n+1}(X) = \bar{Q}_n(X)\bar{R}_{n+1}(X).$$

Then, M_{2n+1} can be found from \mathbf{M}_{2n} by Algorithm 2: the \bar{a}_k and \bar{b}_k are first computed from the moments by the Chebyshev algorithm, the value of \bar{a}_n is given by the closure $\bar{a}_n = \bar{\alpha}_n$, and the reverse Chebyshev algorithm then allows to compute M_{2n+1} .

The eigenvalues of the corresponding system, i.e., the roots of \bar{Q}_n and \bar{R}_{n+1} , are then the eigenvalues of the following Jacobi matrices:

$$(4.19) \quad \mathbf{J}_n = \begin{pmatrix} \bar{a}_0 & \sqrt{\bar{b}_1} & & & \\ \sqrt{\bar{b}_1} & \bar{a}_1 & \sqrt{\bar{b}_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\bar{b}_{n-2}} & \bar{a}_{n-2} & \sqrt{\bar{b}_{n-1}} \\ & & & \sqrt{\bar{b}_{n-1}} & \bar{a}_{n-1} \end{pmatrix}$$

and

$$(4.20) \quad \mathbf{K}_{n+1} = \begin{pmatrix} \bar{a}_0 & \sqrt{\bar{b}_1} & & & \\ \sqrt{\bar{b}_1} & \bar{a}_1 & \sqrt{\bar{b}_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\bar{b}_{n-1}} & \bar{a}_{n-1} & \sqrt{\bar{\beta}_n} \\ & & & \sqrt{\bar{\beta}_n} & \bar{\alpha}_n \end{pmatrix}.$$

5. Examples of the HyQMOM closure for $n \leq 5$. In this section, we apply the HyQMOM closure for S_{2n+1} from Theorem 4.6 with Theorem 3.2 to find the characteristic polynomial P_{2n+1} for $n \leq 5$. Example plots are shown to illustrate the behavior of the roots of these polynomials as a function of H_{2n} (i.e., distance from the boundary of moment space). For completeness, we begin with the trivial case $n = 1$.

5.1. $n = 1$. As first shown in [13], here $S_3 = 0$ and the characteristic polynomial is

$$(5.1) \quad P_3 = X(X^2 - 3) = Q_1 R_2 \quad \implies \quad R_2 = X^2 - 3 = XQ_1 - \beta_1 Q_0.$$

Thus, for $n = 1$, there are three real-valued roots ($0, \pm\sqrt{3}$), which correspond to the root of Q_1 and the two roots of R_2 . As is well known in the literature, the moment system (i.e., the 1-D Euler equations) with (M_0, M_1, M_2) is globally hyperbolic.

5.2. $n = 2$. Here $\alpha_2 = \frac{1}{2}S_3$ yields $S_5 = \frac{1}{2}S_3(5S_4 - 3S_3^2 - 1)$. The coefficients of the characteristic polynomial P_5 are

$$(5.2) \quad c_5 = 1, \quad c_4 = -\frac{5}{2}S_3, \quad c_3 = \frac{1}{2}(-4 + 4S_3^2 - 5H_4), \quad c_2 = \frac{1}{2}S_3(6 - S_3^2 + 5H_4), \\ c_1 = \frac{1}{2}(2 - 2S_3^2 + 5H_4), \quad c_0 = -\frac{1}{2}S_3.$$

When $H_4 = 0$, the middle root is located at α_2 . Otherwise, there are two real-valued roots at $\frac{1}{2}[S_3 \pm (4 + S_3^2)^{1/2}]$ (i.e., the roots of Q_2), and three distinct real-valued roots from

$$(5.3) \quad R_3 = X^3 - \frac{3}{2}S_3 X^2 + \frac{1}{2}(-2 + S_3^2 - 5H_4)X + \frac{1}{2}S_3.$$

Figure 1 illustrates the behavior of the roots for $S_3 = -1$ with varying H_4 . The roots of Q_2 are independent of H_4 and the two roots of R_3 join those of Q_2 when H_4 tends

Algorithm 2: Computation of M_{2n+1} **Data:** M_{2n} strictly realizable**Result:** M_{2n+1} Initialize each scalar $\sigma_{k,p}$ to zero for $k \in \{-1, \dots, n\}, p \in \{0, \dots, 2n+1\}$;**for** $p \leftarrow 0$ **to** $2n$ **do** // Chebyshev algorithm└ $\sigma_{0,p} \leftarrow M_p$; $\bar{a}_0 \leftarrow \frac{M_1}{M_0}$; $\bar{b}_0 \leftarrow 0$;**for** $k \leftarrow 1$ **to** $n-1$ **do**└ **for** $p \leftarrow k$ **to** $2n-k$ **do**└└ $\sigma_{k,p} \leftarrow \sigma_{k-1,p+1} - \bar{a}_{k-1}\sigma_{k-1,p} - \bar{b}_{k-1}\sigma_{k-2,p}$; $\bar{a}_k \leftarrow \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}$; $\bar{b}_k \leftarrow \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}$; $\sigma_{n,n} \leftarrow \sigma_{n-1,n+1} - \bar{a}_{n-1}\sigma_{n-1,n} - \bar{b}_{n-1}\sigma_{n-2,n}$; $\bar{b}_n \leftarrow \frac{\sigma_{n,n}}{\sigma_{n-1,n-1}}$; $\bar{a}_n \leftarrow \frac{1}{n} \sum_{k=0}^{n-1} \bar{a}_k$ // Set the closure; $\sigma_{n,n+1} \leftarrow \sigma_{n,n} \left(\bar{a}_n + \frac{\sigma_{n-1,n}}{\sigma_{n-1,n-1}} \right)$ // Reverse Chebyshev algorithm;**for** $k \leftarrow n-1$ **to** 0 **do**└ $\sigma_{k,2n-k+1} \leftarrow \sigma_{k+1,2n-k} + \bar{a}_k\sigma_{k,2n-k} + \bar{b}_k\sigma_{k-1,2n-k}$; $M_{2n+1} \leftarrow \sigma_{0,2n+1}$;

to zero. Moreover, we can also see how the absolute value of the extremal roots of R_3 increase with H_4 . We can also remark that with Gaussian moments, Q_2 is the Hermite polynomial He_2 and $R_3 = X^3 - 6X$.

5.3. $n > 3$. For $n = 3, 4, 5$, the characteristic polynomial P_{2n+1} is found from $\alpha_n = a_n$. In the same way as for $n = 2$, Figure 1 illustrates the behavior of its roots with fixed values of (S_3, \dots, S_{2n-1}) and varying S_{2n} , or equivalently H_{2n} . For $n = 3$, we took $(S_3, S_4, S_5) = (-1, 5, -8)$; for $n = 4$, $(S_3, S_4, S_5, S_6, S_7) = (-1, 5, -8, 67.3, -100)$; and for $n = 5$,

$$(S_3, S_4, S_5, S_6, S_7, S_8, S_9) = (-1, 5, -8, 67.3, -100, 3000, 0).$$

The same type of behavior as for the case $n = 2$ is observed. Notwithstanding, for large n , the roots of Q_n depend on all the standardized moments up to S_{2n-1} . Thus, the roots can be very different depending, for example, on how close the moment vector is to the boundary of moment space (which determines the lower bound on the even-order standardized moments).

Let us also remark that for $n = 3$, with Gaussian moments, Q_3 is the Hermite polynomial He_3 and $R_4 = X^4 - 10X^2 + 9$. In the case $n = 4$, with nine roots depending on six parameters, the root locations can vary greatly for different values of the central moments, and will be very different from the roots of the Hermite

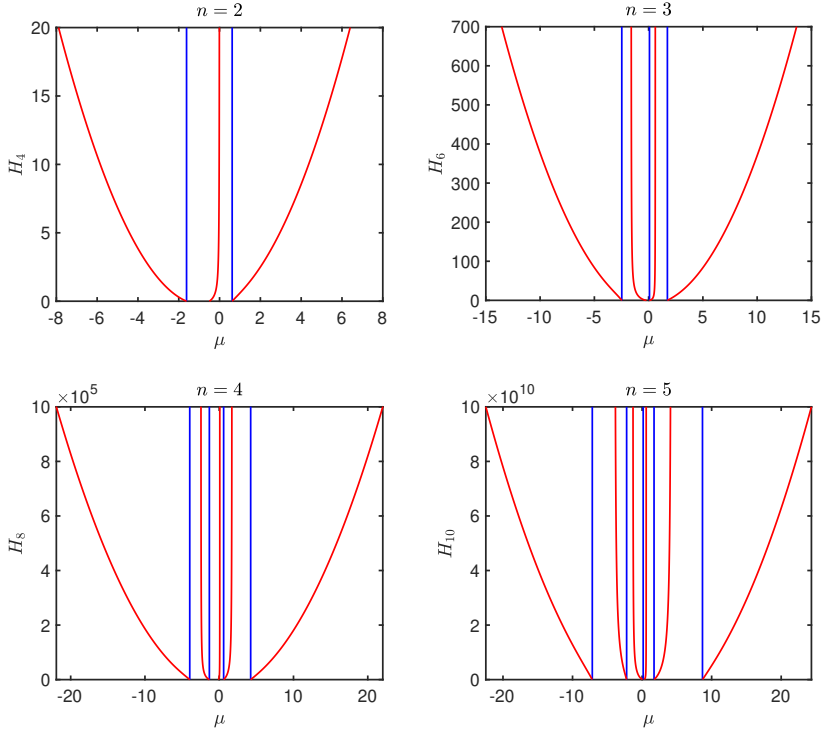


Fig. 1: Roots μ of Q_n (blue lines) and R_{n+1} (red lines) and thus of $P_{2n+1} = Q_n R_{n+1}$ as functions of H_{2n} for $n = 2$ and $S_3 = -1$ (top left), $n = 3$ and $(S_3, S_4, S_5) = (-1, 5, -8)$ (top right), $n = 4$ and $(S_3, S_4, S_5, S_6, S_7) = (-1, 5, -8, 67.3, -100)$ (bottom left) and $n = 5$ for $(S_3, S_4, S_5, S_6, S_7, S_8, S_9) = (-1, 5, -8, 67.3, -100, 3000, 0)$ (bottom right). For clarity, the lower-order standardized moments are held constant, but would likely also vary in real applications.

polynomial He_9 used in Grad's moment closure [17]. For $n = 5$, Q_5 is the Hermite polynomial He_5 . For nearly Gaussian, asymmetric moment sets, the roots of Q_n will be slightly displaced from those of the Hermite polynomial.

For the example in section 6, calculations are done for n up to 20 with no particular difficulties. In practice, the only foreseeable difficulty with using the HyQMOM closure for even larger n is that associated with the accuracy of using the Chebyshev algorithm to find the recurrence coefficients from a realizable moment vector [14].

6. Numerical example for the 1-D kinetic equation. In order to illustrate the predictions of the HyQMOM closure, we consider the 1-D Riemann problem from [3, 13], for which the analytical solution for the VDF can be used to find reference solutions for the moments [3]. The initial condition for the mean velocity has a step at $x = 0$:

$$\bar{u} = \begin{cases} +1 & \text{if } x < 0, \\ -1 & \text{if } x \geq 0. \end{cases}$$

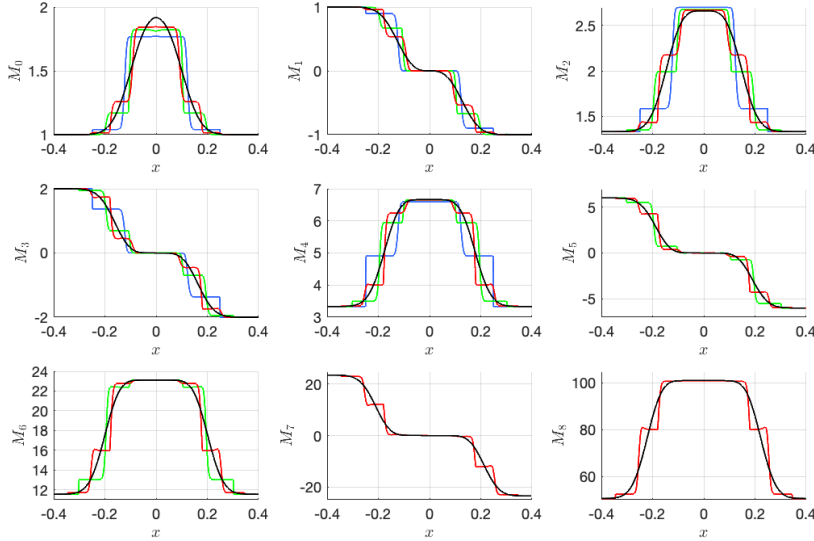


Fig. 2: Numerical solution at $t = 0.1$ of 1-D Riemann problem for the moments. Black, analytical solution. Blue, $n = 2$. Green, $n = 3$. Red, $n = 4$.

Otherwise, for all x , the initial moments correspond to a Maxwellian distribution function (i.e., $S_{2k+1} = 0$ and $S_{2k+2} = (2k + 1)S_{2k}$ for $k \geq 1$) with $M_0 = 1$ and $C_2 = \frac{1}{3}$. Due to the discontinuous mean velocity, for $t > 0$ and starting near $x = 0$, the VDF quickly becomes far from Maxwellian. The analytical solution is given in [3], and reported in Figures 2 and 3 at $t = 0.1$.

The moment system (3.3) is solved numerically on the 1-D computational domain $-0.5 < x < 0.5$ discretized into 4000 finite volumes using a first-order HLL scheme [33]. The CFL number is set to 0.5. The maximum/minimum eigenvalues over the domain needed to define the HLL fluxes are computed at each time step. They are the maximum/minimum roots of \bar{R}_{n+1} and these roots are computed from the coefficients \bar{a}_k and \bar{b}_k by computing the eigenvalues of the corresponding Jacobi matrix given by (4.20). For comparison, the results found using the Gaussian, the Gaussian-EQMOM, and the entropy maximization closures are given in Fig. 2 of [3]. Results with $n = 2$ for the previous definition of HyQMOM (i.e., with $a_2 = 0$) and QMOM are given in Figs. 1 and 2 of [13].

Qualitatively, the HyQMOM results for $n = 2$ with $a_2 = \frac{1}{2}S_3$ are better than with $a_2 = 0$. This is likely due to the fact that the three eigenvalues are different due to their dependence on a_2 . For example, when $S_3 < 0$ (i.e., $x < 0$), the most negative eigenvalue with $a_2 = \frac{1}{2}S_3$ has larger magnitude than with $a_2 = 0$. Thus, information propagates faster towards the left, giving, for example, a better approximation of the moments when compared to the analytical solution. This is clearly seen for S_3 where the location of the minimum (maximum) is better predicted with $a_2 = \frac{1}{2}S_3$, as is the maximum of S_4 . With $a_2 = 0$, the latter is significantly under-predicted (by a factor of two). In summary, for $n = 2$ using the HyQMOM closure from this work yields more accurate predictions for the eigenvalues and thus for the moments. Notwithstanding,

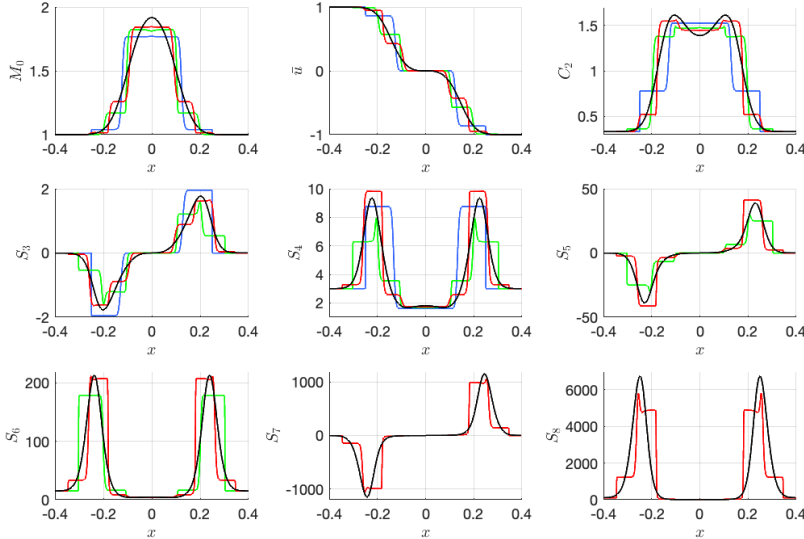


Fig. 3: Numerical solution at $t = 0.1$ of 1-D Riemann problem for the standardized moments. Black, analytical solution. Blue, $n = 2$. Green, $n = 3$. Red, $n = 4$.

both definitions lead to globally hyperbolic moment systems, indicating that even within the family of hyperbolic closures improvements are possible by modifying the eigenvalues.

As can be seen from [Figures 2 and 3](#), the HyQMOM prediction improves with increasing n . As expected for a hyperbolic system with $2n + 1$ degrees of freedom, the different speeds associated with the eigenvalues result in sub-shocks that are not present in the infinite-dimensional analytical solution. Remarkably, as n increases, the speeds adapt to better capture the shapes of the moment profiles. We should remind the reader that these speeds are not known in advance (i.e., unlike with Hermite expansions), but adapt to the changing moments in a highly nonlinear manner. Although this non-linearity makes the analysis of the moment system challenging, it is a significant strength of QBMM because it allows the characteristic speeds to reflect very accurately the underlying moments. For example, with Gaussian moments a subset of the speeds correspond to the roots of a Hermite polynomial, while on the boundary of moment space they reduce to QMOM as required by the known form of the VDF.

To examine convergence, the simulations were done without any trouble up to $n = 20$, showing the robustness of the method. Moreover, for the final solution, the maximal eigenvalue in absolute value is about 3.34 for $n = 2$, 5.32 for $n = 10$, and 6.5 for $n = 20$; so they do not increase drastically. The L_2 norm of the error for each moment is then computed for each simulation and normalized by the L_2 norm of the analytical solution. These results are plotted on [Figure 4](#) as functions of n , varying from 2 to 20. Each line corresponds to a moment, from M_0 to M_{20} , with a gradation of the color from red to blue and then from blue to green. The group of curves at the bottom corresponds to even-order moments, whereas the top group

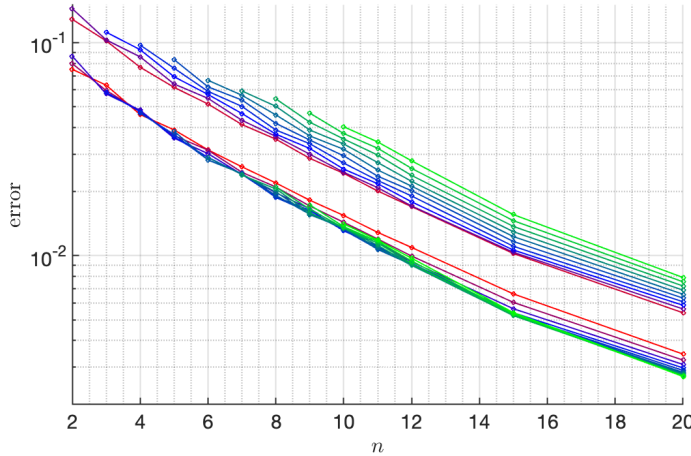


Fig. 4: Error on the moments for the numerical solution at $t = 0.1$ of the 1-D Riemann problem depending on n . Color gradation from red (for M_0) to blue (for M_5) and from blue (for M_5) to green (M_{20}).

corresponds to odd-order moments, with (for fixed n) an error that increases with the order. Example results for the moments with $n = 10$ are given in [Appendix D](#). With $n = 20$ the curves nearly overlap and cannot be distinguished with the scaling used for the plots. Based on these results and [Figure 4](#), the HyQMOM closure appears to converge with increasing n . As a measure of the computation cost, the case with $n = 20$ required 22 mins using Matlab on a laptop computer.

7. Discussion and conclusions. Despite its apparently simple form, the path from the original HyQMOM closure for $n = 2$ to the general HyQMOM closure in [Theorem 4.6](#) was not straightforward. In [\[13\]](#), the 1-D HyQMOM closure for $n = 2$ was discovered by forcing an abscissa of a representing VDF to be located at the mean velocity (this induces $a_2 = 0$). We therefore first sought to extend this condition to $2 < n$, but were unsuccessful at finding a globally hyperbolic closure. By relaxing this condition, we were able to find closures with $\alpha_n \neq 0$ that are hyperbolic in restricted regions of moment space. However, the first real breakthrough came from the realization that as $H_{2n} \rightarrow 0$, we must have $P_{2n+1}(X) \rightarrow (X - \alpha_n)Q_n^2(X)$. When combined with the condition $\langle P_{2n+1} \rangle = 0$, this implies that on the boundary of moment space we must have $a_n = \alpha_n$, which provides a closure for S_{2n+1} . Thus, using the results from [Proposition 3.1](#) and [Theorem 3.2](#), we next sought functional forms for a_n depending only on the standardized moments.

This approach turned out to be relatively fruitful, enabling us to find closures up to $n = 5$ that, at least numerically, appeared to be globally hyperbolic. Nevertheless, it was impossible to prove global hyperbolicity as the expressions were too complicated to advance analytically. However, we did observe that all such closures were *nearly* of the form $P_{2n+1} = Q_n R_{n+1} + \text{remainder}$, where the remainder term went to zero as $H_{2n} \rightarrow 0$. As discussed in [Appendix B](#) for $n = 2$, the family of closures with $P_{2n+1} = Q_n R_{n+1}$ is not unique, nor is it usually possible to prove global hyperbolicity for larger n . But searching only for candidate polynomials R_{n+1} greatly narrowed the

field of possible closures. The decisive final breakthrough was [Theorem 4.5](#), which led us directly to [Theorem 4.6](#). The classical proof of the relationship between the roots of Q_n and R_{n+1} in [Theorem 4.8](#) followed immediately, and established global hyperbolicity at least for $n \leq 9$.

From a computational standpoint, [Algorithm 2](#) for computing M_{2n+1} (and its extension in [Appendix E](#)) is extremely efficient, especially when compared to the other candidate closures discussed above for which the cost of computing M_{2n+1} becomes intractable for $5 \leq n$. Likewise, the Jacobi matrices in [\(4.19\)](#) and [\(4.20\)](#) provide the eigenvalues of the free-transport term at very little additional cost. As demonstrated in [section 6](#), this efficiency allowed us to test the convergence of the HyQMOM closure for $n = 20$ (i.e., up to M_{41}). Nonetheless, it should be possible to go to even larger n using [Algorithm 2](#) if needed.

Because it was developed to control the eigenvalues of the free-transport term in the 1-D kinetic equation, one can ask whether the HyQMOM closure will be useful for closing other terms such as collisions or drag exchange with a second phase [\[27\]](#). In any case, a VDF as a weighted sum of $n + 1$ Dirac delta functions found from \mathbf{J}_{n+1} defined in [\(4.19\)](#) can be uniquely associated with the HyQMOM closure. The pragmatic response is that HyQMOM will be at least as good as QMOM with $n + 1$ weights and abscissas for evaluating unclosed integrals with respect to the unknown velocity VDF.

For population balance equations defined on semi-infinite or finite domains, it is not obvious that HyQMOM will provide any advantage relative to QMOM. Given that HyQMOM uses the even-order moment M_{2n} while QMOM uses the odd-order moment M_{2n+1} , it will be necessary to prove that the HyQMOM closure for M_{2n+1} is realizable for semi-infinite and finite domains. If this is the case, then the HyQMOM closure presented in this work can be used to investigate convergence with increasing n . Besides the kinetic equation and population balances, other potential applications of the HyQMOM closure include radiation transport [\[35, 9, 10\]](#) and multiphase-flow models derived from a kinetic equation [\[27\]](#).

Our current research is focused on the extension of 1-D HyQMOM to multiple dimensions (e.g., 2-D and 3-D) and infinite domains. In prior work with $n = 2$ [\[13, 29\]](#), this was accomplished using the conditional QMOM [\[38\]](#) and a reconstructed VDF based on the weights and abscissas corresponding to Q_3 . For our extension of 1-D HyQMOM, we eschew that approach, and instead seek to close the multi-dimensional moments appearing in the free-transport flux vector using ideas developed in the present work. Our initial results in this direction are promising from both an analytical and computational perspective.

Appendix A. Chebyshev and reverse Chebyshev algorithms.

Let us consider a strictly realizable moment vector \mathbf{M}_N and the associated linear functional $\langle \cdot \rangle_{\mathbf{M}_N}$ on $\mathbb{R}[X]_N$ defined by [\(2.8\)](#). Let us also define the sequence $(Q_k)_{k=0, \dots, n}$ of monic orthogonal polynomials for the scalar product $(p, q) \mapsto \langle pq \rangle_{\mathbf{M}_N}$ of $\mathbb{R}[X]_n$, with $n = \lfloor \frac{N}{2} \rfloor$. The coefficients $(a_k)_{k=0, \dots, \lfloor \frac{N-1}{2} \rfloor}$ and $(b_k)_{k=0, \dots, \lfloor \frac{N}{2} \rfloor}$ of the recurrence relation for the monic orthogonal polynomials ($Q_{k+1} = (X - a_k)Q_k - b_k Q_{k-1}$ with $Q_0 = 1, Q_{-1} = 0$) can be computed from the moments thanks to several algorithms: Rutishauser's QD algorithm [\[30, 19\]](#), Gordon's PD algorithm [\[15, 16\]](#), and a variation of an algorithm attributed to Chebyshev and given by Wheeler in [\[37\]](#). However, except for the last one (referred to as the Chebyshev algorithm here), these algorithms first compute the variables $(\zeta_k)_{k=1, \dots, N}$ such that $b_k = \zeta_{2k-1} \zeta_{2k}$ and $a_k = \zeta_{2k} + \zeta_{2k+1}$. They can then fail as a result of symmetries in a VDF corresponding

Algorithm 3: Computation of the coefficients of the recurrence relation from the moments

Data: \mathbf{M}_N strictly realizable

Result: $(a_k)_{k=0,\dots,\lfloor \frac{N-1}{2} \rfloor}$ and $(b_k)_{k=0,\dots,\lfloor \frac{N}{2} \rfloor}$

$n \leftarrow \lfloor \frac{N}{2} \rfloor$;

Initialize each scalar $\sigma_{k,p}$ to zero for $k \in \{-1, \dots, n\}, p \in \{0, \dots, N\}$;

for $p \leftarrow 0$ **to** N **do**

$\sigma_{0,p} \leftarrow M_p$;

$b_0 \leftarrow M_0$;

$a_0 \leftarrow \frac{M_1}{M_0}$;

for $k \leftarrow 1$ **to** n **do**

for $p \leftarrow k$ **to** $N - k$ **do**

$\sigma_{k,p} \leftarrow \sigma_{k-1,p+1} - a_{k-1}\sigma_{k-1,p} - b_{k-1}\sigma_{k-2,p}$;

$b_k \leftarrow \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}$;

if $k < n$ **or** N **is odd** **then**

$a_k \leftarrow \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}$;

to \mathbf{M}_N : the values ζ_k are indeed well defined and positive when the support of the VDF is included on $(0, +\infty)$, whereas some of them cannot be defined in some cases, like when the VDF corresponding to the moments is symmetric. That is why we use only the Chebyshev algorithm.

As explained for example in [37, 14, 5], the Chebyshev algorithm introduces the quantities $\sigma_{k,p} = \langle Q_k X^p \rangle_{\mathbf{M}_N}$ and uses the formulas

$$(A.1) \quad b_k = \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}} \quad a_k = \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}$$

$$(A.2) \quad \sigma_{k+1,p} = \sigma_{k,p+1} - a_k \sigma_{k,p} - b_k \sigma_{k-1,p} \quad p \geq k + 1.$$

This is given in Algorithm 3.

Conversely, from the coefficients $(a_k)_{k=0,\dots,n}$ and $(b_k)_{k=0,\dots,n}$, one can compute the moment vector \mathbf{M}_{2n+1} through the reverse Chebyshev Algorithm 4, using $Z_{k,p} = \sigma_{k,k+p}$. Let us remark that it induces

$$(A.3) \quad Z_{k,0} = \prod_{j=0}^k b_j, \quad Z_{k,1} = Z_{k,0} \sum_{j=0}^k a_j, \quad Z_{k,p+1} = Z_{k+1,p-1} + a_k Z_{k,p} + b_k Z_{k-1,p+1},$$

which imply that each $Z_{k,p}$, and then also M_p , is a multivariate polynomial function of the a_j and b_j .

Appendix B. Hyperbolic closures for $n = 2$.

Let us consider the case with five moments. The closure $S_5(S_3, S_4)$ allows to compute the characteristic polynomial of the system:

$$(B.1) \quad P_5(X) = c_0 + c_1 X + c_2 X^2 + c_3 X^3 + c_4 X^4 + X^5$$

Algorithm 4: Computation of the moments from the coefficients of the recurrence relation

Data: $(a_k)_{k=0,\dots,n}$ and $(b_k)_{k=0,\dots,n}$

Result: \mathbf{M}_{2n+1}

Initialize each scalar $Z_{k,p}$ to zero for $k \in \{-1, \dots, n\}, p \in \{0, \dots, 2n\}$;

$Z_{0,0} \leftarrow b_0$;

$Z_{0,1} \leftarrow b_0 a_0$;

for $k \leftarrow 1$ **to** n **do**

$Z_{k,0} \leftarrow b_k Z_{k-1,0}$;
 $Z_{k,1} \leftarrow Z_{k,0} \left(a_k + \frac{Z_{k-1,1}}{Z_{k-1,0}} \right)$;

for $p \leftarrow 1$ **to** $2n$ **do**

for $k \leftarrow 0$ **to** $\lfloor n - \frac{p}{2} \rfloor$ **do**
 $Z_{k,p+1} \leftarrow Z_{k+1,p-1} + a_k Z_{k,p} + b_k Z_{k-1,p+1}$;

for $p \leftarrow 0$ **to** $2n + 1$ **do**

$M_p \leftarrow Z_{0,p}$;

with

$$(B.2) \quad \begin{aligned} c_4 &= -\frac{\partial S_5}{\partial S_4}, & c_3 &= -\frac{\partial S_5}{\partial S_3}, & c_2 &= -\frac{1}{2}(3S_3c_3 + 4S_4c_4 + S_5), \\ c_1 &= -(3c_3 + 4S_3c_4 + 5S_5), & c_0 &= \frac{1}{2}(S_3c_3 + 2S_4c_4 + 3S_5). \end{aligned}$$

Also recall that $Q_2(X) = X^2 - S_3X - 1$. The following theorem addresses the existence of hyperbolic closures for which P_5 is divisible by Q_2 .

THEOREM B.1 (Hyperbolic closure for $n = 2$). *The polynomial P_5 is divisible by Q_2 , i.e., $P_5 = Q_2R_3$ with R_3 a real monic polynomial of degree 3, if and only if there exists a real number γ such that*

$$(B.3) \quad S_5(S_3, S_4) = S_3 \left(2 + S_3^2 + \frac{5}{2}H_4 \right) + \gamma H_4 \sqrt{4 + S_3^2}.$$

Moreover, R_3 has three real roots, which separate those of Q_2 , if and only if $\gamma \in]-\frac{5}{2}, \frac{5}{2}[$.

Proof. Identifying the coefficients, $P_5 = Q_2R_3$ with $R_3 = X^3 + aX^2 + bX + c$ is equivalent to

$$\begin{pmatrix} 1 & 0 & 0 & 0 & -1 \\ -S_3 & 1 & 0 & -1 & 0 \\ -1 & -S_3 & 1 & \frac{3}{2}S_3 & 2S_4 \\ 0 & 1 & S_3 & -3 & -4S_4 \\ 0 & 0 & 1 & \frac{1}{2}S_3 & S_4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} S_3 \\ 1 \\ -\frac{5}{2}S_5 \\ 5S_4 \\ -\frac{3}{2}S_5 \end{pmatrix}.$$

This system gives c_3 and c_4 , and, with the change of variable $S_4 = H_4 + S_3^2 + 1$,

$$\frac{\partial S_5}{\partial H_4} \Big|_{S_3} = \frac{S_5 - S_3^2 - 2S_3}{H_4}, \quad \frac{\partial S_5}{\partial S_3} \Big|_{H_4} = \frac{S_3S_5 + 2S_3^4 + 12S_3^2 + 10H_4 + 8}{4 + S_3^2}.$$

Let us define $Y(S_3, S_4)$ such that $S_5(S_3, S_4) = S_3(2 + S_3^2 + \frac{5}{2}H_4 + YH_4)$. Then

$$\left. \frac{\partial Y}{\partial H_4} \right|_{S_3} = 0, \quad S_3(4 + S_3^2) \left. \frac{\partial Y}{\partial S_3} \right|_{H_4} = -4Y.$$

This leads to $Y = \gamma \frac{\sqrt{4+S_3^2}}{S_3}$, so that we obtain (B.3).

Moreover, let $r_{\pm} = \frac{S_3}{2} \pm \frac{\sqrt{4+S_3^2}}{2}$ denote the roots of Q_2 . The values of R_3 at these points are

$$R_3(r_+) = -\frac{H_4}{2}(2\gamma + 5)r_+, \quad R_3(r_-) = \frac{H_4}{2}(5 - 2\gamma)(-r_-).$$

Since $r_+ > 0$ and $r_- < 0$, it is easy to see that $R_3(r_+) < 0$ and $R_3(r_-) > 0$ if and only if $\gamma \in]-\frac{5}{2}, \frac{5}{2}[$, thus concluding the proof. \square

The five-moment system with the closure (B.3) is globally hyperbolic for any $\gamma \in]-\frac{5}{2}, \frac{5}{2}[$. Let us remark that (B.3) is equivalent to

$$a_2 = \frac{S_3}{2} + \gamma \sqrt{4 + S_3^2} \left(= \frac{(1 + 2\gamma)r_+ + (1 - 2\gamma)r_-}{2} \right).$$

So, for $\gamma = 0$, one have $a_2 = (a_0 + a_1)/2$, which is the HyQMOM closure from [Theorem 4.6](#). Furthermore, the globally hyperbolic closure introduced in [\[13\]](#) corresponds to $Y = -\frac{1}{2}$ (and $a_2 = 0$). However, since Y is constant, [Theorem B.1](#) does not apply and P_5 found with this closure is not divisible by Q_2 .

Appendix C. Matlab program for the proof of [Theorem 4.6](#). A Matlab symbolic code can be used to verify the result of [Theorem 4.6](#). For example, with $n = 9$ the code is as follows:

```
clear all
close all

N = 9
Nmom = 2*N+1;

a = sym('a',[1,N+1],'real');
b = sym('b',[1,N+1],'real');
a(1) = 0;
b(1) = 1;
b(2) = 1;
% closure: a(N+1)
a(N+1) = sum(a(1:N))/N;
% reverse Chebyshev algorithm
sig = sym('sig',[N+2,2*N+3],'real');
sig = sym(zeros(N+2,2*N+3));
S = sym('S',[1 2*N+1],'real');
S(1) = 0;
S(2) = 1;
sig(2,2) = 1;
sig(2,3) = a(1);
for k = 2:N+1
```

```

    sig(k+1,2) = sig(k,2)*b(k);
    sig(k+1,3) = sig(k+1,2)*(a(k)+sig(k,3)/sig(k,2));
end
for p = 3:2*N+2
    for k = 2:floor(N+3-p/2)
        sig(k,p+1) = sig(k+1,p-1)+a(k-1)*sig(k,p)+b(k-1)*sig(k-1,p+1);
    end
    S(p-1) = sig(2,p+1);
end

Y = [a(2) reshape([b(3:N+1);a(3:N+1)], [2*N-2 1])'];
J=simplify(jacobian(S(3:2*N),Y(1:2*N-2)));

Sc = S(2*N+1);

DSc = sym('DSc',[1 2*N],'real');
DScDab = jacobian(Sc,Y(1:2*N-2));
DSc(3:2*N) = (J'\ DScDab(1:2*N-2)')';
clear sig DScDab Y

% characteristic polynomial
P = sym(zeros(1,Nmom+1));
P(1) = 1;
P(2:Nmom-2) = -DSc(Nmom-1:-1:3);
P(Nmom-1)=sum((3:Nmom-1).*S(3:Nmom-1).*DSc(3:Nmom-1))/2-Nmom*Sc/2;
P(Nmom)=sum((3:Nmom-1).*S(2:Nmom-2).*DSc(3:Nmom-1))-Nmom*S(Nmom-1);
P(Nmom+1)=-sum((1:Nmom-3).*S(3:Nmom-1).*DSc(3:Nmom-1))/2 ...
    +(Nmom-2)*Sc/2;
clear J DSc S Sc

% calc Q
Q = sym('Q',[N+1,N+1],'real');
Q = sym(zeros(N+1,N+1));
% Q0
Q(1,1) = 1;
% Q1
Q(2,1) = 1;
% Qk
for k = 3:N+1
    Q(k,1:k) = Q(k-1,1:k)-a(k-1)*[0,Q(k-1,1:k-1)] ...
        -b(k-1)*[0,0,Q(k-2,1:k-2)];
end

syms x
PP = poly2sym(P,x);
QN = poly2sym(Q(N+1,1:N+1),x);
QNm = poly2sym(Q(N,1:N),x);
clear Q P
RR = simplify(expand(PP-QN*((x-a(N+1))*QN-(2*N+1)/N*b(N+1)*QNm)))

```

Appendix D. Results for 1-D Riemann problem with $n = 10$.

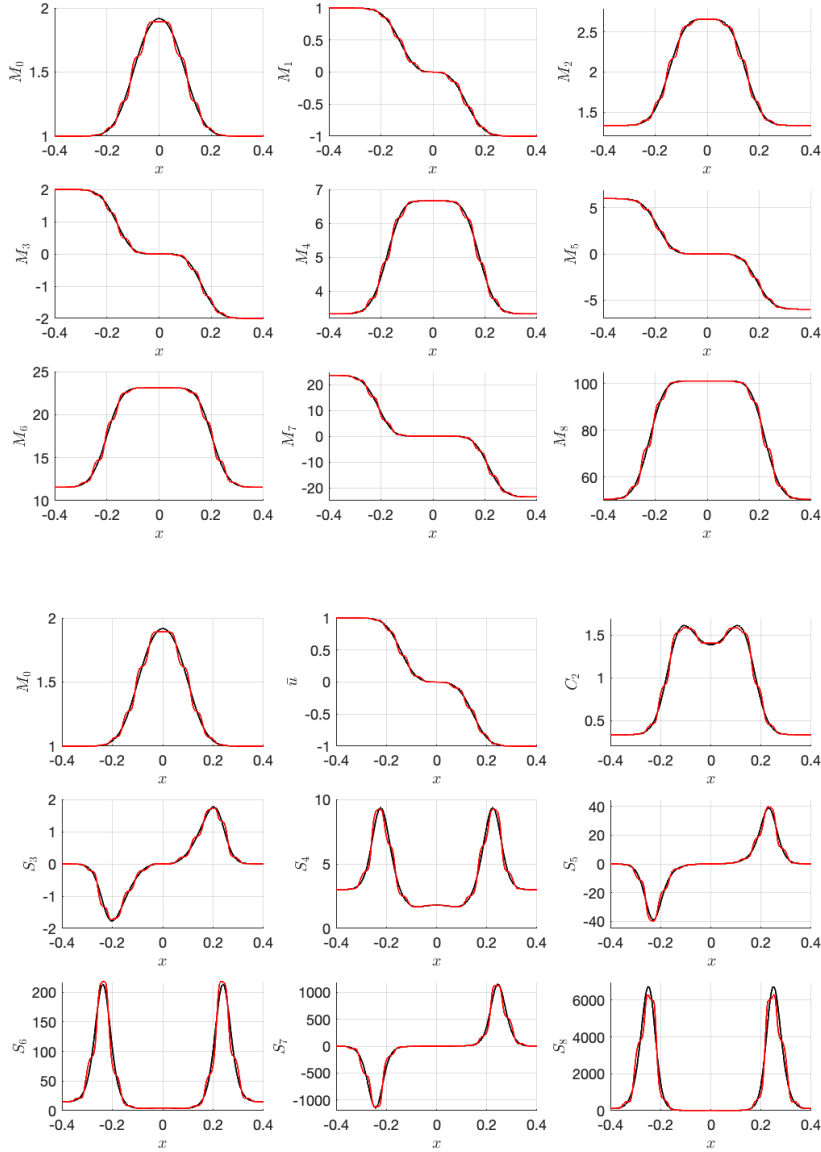


Fig. 5: Numerical solution at $t = 0.1$ of 1-D Riemann problem for the moments (top) and standardized moments (bottom). Black, analytical solution. Red, $n = 10$.

Appendix E. Algorithm for the computation of M_{2n+1} for any realizable moment vector.

Algorithm 2 was restricted to a strictly realizable moment vector. It can be generalized to any realizable moment vector, i.e., possibly on the boundary of moment space. This includes the case $M_0 = 0$, where the VDF is zero and the case $C_2 = 0$

where the VDF is a Dirac delta function at $u = M_1/M_0$. This also includes the case where \mathbf{M}_{2n} is a sum of k Dirac delta functions, with $k < n$, i.e., in such a case that $b_k = 0$. In this last case, the abscissas x_p and weights w_p for $p = 1, \dots, k$ are computed from the Jacobi matrix \mathbf{J}_k defined by (4.19). The abscissas are the eigenvalues of this matrix and the weights are computed from the eigenvectors [14].

Algorithm 5: Computation of M_{2n+1}

Data: \mathbf{M}_{2n} realizable

Result: M_{2n+1}

if $M_0 = 0$ **then**

$M_{2n+1} \leftarrow 0$

else if $M_2 M_0 - M_1^2 = 0$ **then**

$M_{2n+1} \leftarrow \frac{M_1^{2n+1}}{M_0^{2n}}$;

else

 Initialize each scalar $\sigma_{k,p}$ to zero for $k \in \{-1, \dots, n\}, p \in \{0, \dots, 2n+1\}$;

for $p \leftarrow 0$ **to** $2n$ **do**

$\sigma_{0,p} \leftarrow M_p$;

$\bar{a}_0 \leftarrow \frac{M_1}{M_0}$;

$\bar{b}_0 \leftarrow M_0$;

$k \leftarrow 0$;

while $k \leq n-2$ **and** $\bar{b}_k > 0$ **do**

$k \leftarrow k+1$;

for $p \leftarrow k$ **to** $2n-k$ **do**

$\sigma_{k,p} \leftarrow \sigma_{k-1,p+1} - \bar{a}_{k-1}\sigma_{k-1,p} - \bar{b}_{k-1}\sigma_{k-2,p}$;

$\bar{a}_k \leftarrow \frac{\sigma_{k,k+1}}{\sigma_{k,k}} - \frac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}$;

$\bar{b}_k \leftarrow \frac{\sigma_{k,k}}{\sigma_{k-1,k-1}}$;

if $k = n-1$ **then**

$\sigma_{n,n} \leftarrow \sigma_{n-1,n+1} - \bar{a}_{n-1}\sigma_{n-1,n} - \bar{b}_{n-1}\sigma_{n-2,n}$;

$\bar{b}_n \leftarrow \frac{\sigma_{n,n}}{\sigma_{n-1,n-1}}$;

$\bar{a}_n \leftarrow \frac{1}{n} \sum_{k=0}^{n-1} \bar{a}_k$;

$\sigma_{n,n+1} \leftarrow \sigma_{n,n} \left(\bar{a}_n + \frac{\sigma_{n-1,n}}{\sigma_{n-1,n-1}} \right)$;

for $k \leftarrow n-1$ **to** 0 **do**

$\sigma_{k,2n-k+1} \leftarrow \sigma_{k+1,2n-k} + \bar{a}_k\sigma_{k,2n-k} + \bar{b}_k\sigma_{k-1,2n-k}$;

$M_{2n+1} \leftarrow \sigma_{0,2n+1}$;

else

 compute the abscissas and weights $(x_p, w_p)_{p=1}^k$ from $(\bar{a}_p, \bar{b}_p)_{p=0}^{k-1}$;

$M_{2n+1} \leftarrow \sum_{p=1}^k w_p x_p^{2n+1}$;

REFERENCES

- [1] Z. CAI, Y. FAN, AND R. LI, *Globally hyperbolic regularization of Grad's moment system in one-dimensional space*, Commun. Math. Sci., 11 (2013), pp. 547–571.
- [2] Z. CAI, Y. FAN, AND R. LI, *A framework on moment model reduction for kinetic equation*, SIAM J. Appl. Math., 75 (2015), pp. 2001–2023.
- [3] C. CHALONS, R. O. FOX, F. LAURENT, M. MASSOT, AND A. VIÉ, *Multivariate Gaussian extended quadrature method of moments for turbulent disperse multiphase flow*, Multiscale Model. Simul., 15 (2017), pp. 1553–1583.
- [4] C. CHALONS, D. KAH, AND M. MASSOT, *Beyond pressureless gas dynamics: quadrature-based velocity moment models*, Commun. Math. Sci., 10 (2012), pp. 1241–1272.
- [5] P. L. CHEBYSHEV, *Sur l'interpolation par la méthode des moindres carrés*, Mém. Acad. Impér. Sci. St. Petersburg, 1 (1859), pp. 1–24. Also in œuvres I pp. 473–498.
- [6] S. DE CHAISEMARTIN, L. FRÉRET, D. KAH, F. LAURENT, R. O. FOX, J. REVEILLON, AND M. MASSOT, *Eulerian models for turbulent spray combustion with polydispersity and droplet crossing*, Comptes Rendus Mécanique, 337 (2009), pp. 438–448.
- [7] O. DESJARDINS, R. O. FOX, AND P. VILLEDIEU, *A quadrature-based moment method for dilute fluid-particle flows*, J. Comput. Phys., 227 (2008), pp. 2514–2539.
- [8] H. DETTE AND W. J. STUDDEN, *The Theory of Canonical Moments with Applications in Statistics, Probability, and Analysis*, Wiley Series in Probability and Statistics: Applied Probability and Statistics, John Wiley & Sons Inc., New York, 1997.
- [9] Y. FAN, R. LI, AND L. ZHENG, *A nonlinear hyperbolic model for radiative transfer equation in slab geometry*, SIAM J. Appl. Math., 80 (2020), pp. 2388–2419.
- [10] Y. FAN, R. LI, AND L. ZHENG, *A nonlinear moment model for radiative transfer equation in slab geometry*, J. Comput. Phys., 404 (2020), p. 109128.
- [11] F. FORGUES AND J. McDONALD, *Higher-order moment models for laminar multiphase flows with accurate particle-stream crossing*, International Journal of Multiphase Flow, 114 (2019), pp. 28–38.
- [12] R. O. FOX, *Higher-order quadrature-based moment methods for kinetic equations*, J. Comput. Phys., 228 (2009), pp. 7771–7791.
- [13] R. O. FOX, F. LAURENT, AND A. VIÉ, *Conditional hyperbolic quadrature method of moments for kinetic equations*, J. Comput. Phys., 365 (2018), pp. 269–293.
- [14] W. GAUTSCHI, *Orthogonal Polynomials: Computation and Approximation*, Oxford University Press, Oxford, UK, 2004.
- [15] R. G. GORDON, *Error bounds in equilibrium statistical mechanics*, Journal of Mathematical Physics, 9 (1968), pp. 655–663.
- [16] R. G. GORDON, *Error bounds in spectroscopy and nonequilibrium statistical mechanics*, Journal of Mathematical Physics, 9 (1968), pp. 1087–1092.
- [17] H. GRAD, *On the kinetic theory of rarefied gases*, Commun. Pure Appl. Math., 2 (1949), pp. 331–407.
- [18] H. L. HAMBURGER, *Hermitian transformations of deficiency-index (1,1), Jacobian matrices, and undetermined moment problems*, Amer. J. Math., 66 (1944), pp. 489–552.
- [19] P. HENRICI, *The quotient-difference algorithm*, Nat. Bur. Standards Appl. Math. Ser. no., (1958), pp. 23–46.
- [20] Q. HUANG, S. LI, AND W.-A. YONG, *Stability analysis of quadrature-based moment methods for kinetic equations*, SIAM J. Appl. Math., 80 (2020), pp. 206–231.
- [21] M. JUNK, *Domain of definition of Levermore's five-moment system*, J. Stat. Phys., 93 (1998), pp. 1143–1167.
- [22] D. KAH, A. VIÉ, C. CHALONS, AND M. MASSOT, *Second-order scheme for quadrature-based velocity high order moment methods for disperse two-phase flows*, Annu. Res. Briefs CTR, (2011), pp. 321–334.
- [23] J. KOELLERMEIER AND Y. FAN, *Diagram notation for the derivation of hyperbolic moment systems*, Commun. Math. Sci., 18 (2020), pp. 1149–1177.
- [24] J. KOELLERMEIER AND U. SCHOLZ, *Spline moment models for the one-dimensional Boltzmann-Bhatnagar-Gross-Krook equation*, Physics of Fluids, 32 (2020), p. 102009.
- [25] J. B. LASSERRE, *Moments, positive polynomials and their applications*, vol. 1 of Imperial College Press Optimization Series, Imperial College Press, London, 2010.
- [26] C. D. LEVERMORE, *Moment closure hierarchies for kinetic theories*, J. Stat. Phys., 83 (1996), pp. 1021–1065.
- [27] D. L. MARCHISIO AND R. O. FOX, *Computational Models for Polydisperse Particulate and Multiphase Systems*, Cambridge University Press, Cambridge, UK, 2013.
- [28] J. McDONALD AND M. TORRILHON, *Affordable robust moment closures for CFD based on the*

- maximum-entropy hierarchy*, J. Comput. Phys., 251 (2013), pp. 500–523.
- [29] R. G. PATEL, O. DESJARDINS, AND R. O. FOX, *Three-dimensional conditional hyperbolic quadrature method of moments*, J. Comput. Phys. X, 1 (2019), p. 100006.
 - [30] H. RUTISHAUSER, *Der Quotienten-Differenzen-Algorithmus*, Z. Angew. Math. Physik, 5 (1954), pp. 233–251.
 - [31] K. SCHMÜDGEN, *The Moment Problem*, vol. 277 of Graduate Texts in Mathematics, Springer, Cham, 2017.
 - [32] H. STRUCHTRUP, *Macroscopic Transport Equations for Rarefied Gas Flows*, Interaction of Mechanics and Mathematics, Springer, Berlin, Germany, 2005. Approximation methods in kinetic theory.
 - [33] E. F. TORO, *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction*, Springer, New York, 1999.
 - [34] M. TORRILHON, *Modeling nonequilibrium gas flow based on moment equations*, Annu. Rev. Fluid Mech., 48 (2016), pp. 429–458.
 - [35] V. VIKAS, C. D. HAUCK, Z. J. WANG, AND R. O. FOX, *Radiation transport modeling using extended quadrature method of moments*, J. Comput. Phys., 246 (2013), pp. 221–241.
 - [36] V. VIKAS, Z. J. WANG, A. PASSALACQUA, AND R. O. FOX, *Realizable high-order finite-volume schemes for quadrature-based moment methods*, J. Comput. Phys., 230 (2011), pp. 5328–5352.
 - [37] J. C. WHEELER, *Modified moments and Gaussian quadratures*, Rocky Mt. J. Math., 4 (1974), pp. 287–296.
 - [38] C. YUAN AND R. O. FOX, *Conditional quadrature method of moments for kinetic equations*, J. Comput. Phys., 230 (2011), pp. 8216–8246.