Three-dimensional conditional hyperbolic quadrature method of moments

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Abstract
The conditional hyperbolic quadrature method of moments (CHyQMOM) was introduced by Fox et al. [19] to reconstruct 1- and 2-D velocity distribution functions (VDF) from a finite set of integer moments. The reconstructed VDF takes the form of a sum of weighted Dirac delta functions in velocity phase space, and provides a hyperbolic closure for the spatial flux term in the corresponding moment equations derived from a kinetic equation for the 3-D VDF. Here, CHyQMOM is extended for 3-D velocity phase space using the modified conditional quadrature method of moments with 16 (or 23) trivariate velocity moments up to fourth order. In order to verify the numerical implementation, it is applied to simulate several canonical particle-laden flows including crossing jets, cluster-induced turbulence (CIT), and vertical channel flow. The numerical results are compared with those from Euler–Lagrange simulations and two other quadrature-based moment methods, namely, anisotropic Gaussian (AG) and 8-node tensor-product (TP) quadrature. The relative advantages and disadvantages of each method are discussed. The crossing-jet problem highlights that CHyQMOM handles particle crossing more accurately than AG. For CIT, the results from all methods are similar, but the computational cost of TP is significantly larger than AG and CHyQMOM, both of which have nearly the same cost.

Keywords
Kinetic equation, Quadrature-based moment methods, Conditional quadrature method of moments, Hyperbolic moment closures

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Three-dimensional conditional hyperbolic quadrature method of moments

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\section*{ABSTRACT}

The conditional hyperbolic quadrature method of moments (CHyQMOM) was introduced by Fox et al.\([19]\) to reconstruct 1- and 2-D velocity distribution functions (VDF) from a finite set of integer moments. The reconstructed VDF takes the form of a sum of weighted Dirac delta functions in velocity phase space, and provides a hyperbolic closure for the spatial flux term in the corresponding moment equations derived from a kinetic equation for the 3-D VDF. Here, CHyQMOM is extended for 3-D velocity phase space using the modified conditional quadrature method of moments with 16 (or 23) trivariate velocity moments up to fourth order. In order to verify the numerical implementation, it is applied to simulate several canonical particle-laden flows including crossing jets, cluster-induced turbulence (CIT), and vertical channel flow. The numerical results are compared with those from Euler–Lagrange simulations and two other quadrature-based moment methods, namely, anisotropic Gaussian (AG) and 8-node tensor-product (TP) quadrature. The relative advantages and disadvantages of each method are discussed. The crossing-jet problem highlights that CHyQMOM handles particle crossing more accurately than AG. For CIT, the results from all methods are similar, but the computational cost of TP is significantly larger than AG and CHyQMOM, both of which have nearly the same cost.

\section*{1. Introduction}

The physics of inertial particles can be described by a velocity density function (VDF) satisfying a kinetic equation. Solving such an equation relies on either a sample of discrete numerical parcels through a Lagrangian Monte-Carlo approach or on a moment approach resulting in a Eulerian system of conservation laws on velocity moments. For the latter, the main difficulty for particles with high Knudsen numbers wherever the VDF can be very far from equilibrium, is the closure of the free-stream transport term in the kinetic equation. One way to proceed is to use quadrature-based moment methods (QBMM) where the higher-order moments required for closure are evaluated from the lower-order transported moments using multi-dimensional quadrature \([13,16,17]\). In previous work, Fox and coworker have developed the conditional quadrature method of moments (CQMOM) \([32]\), leading to a well-behaved kinetic numerical scheme \([1]\). CQMOM has been shown to capture particle trajectory crossing (PTC) where the distribution in the exact kinetic equation remains at all times in the form of a sum of Dirac delta functions \([10,31,32]\). The moment system found with the CQMOM flux closure is weakly hyperbolic.

\footnotesize
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leading to delta shocks when multiple PTC occur at the same spatial location. To achieve hyperbolicity, a multi-Gaussian QBMM closure was proposed [9]. However, this closure cannot access all of moment space [21,23,24] due to the form of Gaussian distribution (e.g. the two-node closure cannot represent fourth-order velocity moments larger than a Gaussian distribution). Moreover, working with a continuous representation of the VDF loses the discrete velocity representation of CQMOM. The parameters of the kernels used for the continuous representation must be found iteratively. Source terms are also more difficult to evaluate using the continuous representation [33].

More recently, a hyperbolic moment closure was introduced that retains the properties of QMOM [19]. Because $N$-node QMOM requires the moment set $\{M_0, M_1, ..., M_{2N-1}\}$, the basic idea is to solve for moments $\{M_0, M_1, ..., M_{2N-2}\}$ and to fix $M_{2N-1}$ such that the moment system is hyperbolic. In 1-D phase space, this closure is referred to as $N$-node hyperbolic QMOM or HyQ MOM. In previous work [19], its favorable mathematical and computational properties have been investigated for $N = 2$ and 3 [19]. Furthermore, using ideas from CQMOM, the extension of HyQ MOM (referred to here as CHyQ MOM) to a 2-D phase space has been proposed and used to solve 2-D moment systems [19]. In particular, it has been demonstrated that HyQ MOM and CHyQ MOM can accurately capture particle trajectory crossing (PTC) without exhibiting unphysical behavior such as delta shocks. The purpose of the work reported here is to extend the 3-node hyperbolic reconstruction of the VDF (HyQ MOM 1-D and CHyQ MOM 2-D phase space) to a 3-D velocity phase space (i.e., CHyQ MOM 27). In 1-D phase space, the moment set controlled by HyQ MOM is integer moments up to $M_4$. Here we use velocity moments up to order 4 in all three directions, and apply CHyQ MOM 27 to solve a variety of 3-D kinetic equations relevant to particle-laden flows. The proposed extension now makes it possible to solve numerically a wide range of non-equilibrium problems in 3-D spatial domains such as gas–particle flows and rarefied gases.

The remainder of the work is organized as follows. In Sec. 2, HyQ MOM is briefly reviewed, including its application to 1-D kinetic equations. In Sec. 3, we review CHyQ MOM and its application to 2-D kinetic equations. In Sec. 4, we derive CHyQ MOM 27 for a 3-D phase space, and apply it to 3-D kinetic equations without acceleration terms. Our numerical implementation for coupling CHyQ MOM 27 for the particle phase with a Navier–Stokes solver for the fluid phase is described in Sec. 5. Applications of the coupled solver to moderately dilute gas–particle flows are provided in Sec. 6. Finally, conclusions are drawn in Sec. 7.

2. HyQ MOM 3 for 1-D kinetic equations

As in [19], consider a VDF $f(u)$ defined for $u \in \mathbb{R}$. Let us assume that the moments of $f$ defined by

$$M_k := \int_{\mathbb{R}} f(u)u^k \, du \quad \text{for } k = 0, 1, \ldots, \infty$$

are finite and $M_0 > 0$. Let us define the central moments by

$$C_k := \frac{1}{M_0} \int_{\mathbb{R}} f(u)(u - \bar{u})^k \, dv \quad \text{for } k = 0, 1, \ldots, \infty$$

where $\bar{u} = M_1/M_0$. By definition, $C_0 = 1$ and $C_1 = 0$. The next central moment $C_2 \geq 0$ is the velocity variance. The central moment $C_k$ depends uniquely on the moments $\{M_0, M_1, \ldots, M_k\}$ [19]. Furthermore, when $0 < C_2$ we define the scaled moments by

$$S_k := \frac{C_k}{C_2^{k/2}} \quad \text{for } k = 2, 3, \ldots, \infty.$$  

For non-negative $f(u)$, the moments are said to be realizable. The realizability of a finite set of moments can be checked using Hankel matrix determinants [14]. For HyQ MOM 3, realizability requires that $M_0 \geq 0$, $C_2 \geq 0$ and $S_4 \geq S_2^2 + 1$, while the odd-order moments $\bar{u}$ and $S_3$ can take any real values. Hereinafter we will assume that the moment set under consideration is realizable.

2.1. Definition of HyQ MOM 3

HyQ MOM 3 provides a discrete approximation $f^a$ defined such that [19]

$$C_k = C_k^a := \frac{1}{M_0} \int_{\mathbb{R}} f^a(u)(u - \bar{u})^k \, du \quad \text{for } k = 0, 1, 2, 3, 4,$$

and the scaled moment $S_5 = S_3(2S_4 - S_2^2)$. More precisely, $f^a$ has the form:

$$f^a(u) = M_0 \sum_{\alpha=1}^3 \rho_\alpha \delta_{u_\alpha + \bar{u}}(u)$$
where \( \delta_{u_\alpha + \bar{u}}(u) \) is the Dirac delta function centered at \( u_\alpha + \bar{u} \), and the three weights \( \rho_\alpha \) and the three velocity abscissas \( u_\alpha \) are determined from the first five integer moments of \( f^0 \) by (4), which is equivalent to

\[
C_k = \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha^k \quad \text{for } k \in \{0, 1, 2, 3, 4, 5\}.
\]

(6)

For \( C_2 > 0 \) this yields [19]

\[
\rho_1 = \frac{-C_2^{1/2}}{u_1 \sqrt{4\eta_\alpha - 3q_\alpha^2}}, \quad \rho_2 = 1 + \frac{C_2}{u_1 u_3}, \quad \rho_3 = \frac{C_2^{1/2}}{u_3 \sqrt{4\eta_\alpha - 3q_\alpha^2}},
\]

and

\[
u_1 = C_2^{1/2} \left( \frac{1}{2} (q_u - \sqrt{4\eta_\alpha - 3q_\alpha^2}) \right), \quad \nu_2 = 0, \quad \nu_3 = C_2^{1/2} \left( \frac{1}{2} (q_u + \sqrt{4\eta_\alpha - 3q_\alpha^2}) \right),
\]

(8)

where \( q_u := S_3 \) and \( \eta_\alpha := S_4 \). When \( S_4 = 1 + S_2^2 \), \( \rho_2 = 0 \) and the system reduces to QMOM2 [16]. Otherwise, the weights are strictly positive.

2.2. Application of HyQMOM3 to 1-D kinetic equations

As in [19], consider the kinetic equation:

\[
\partial_t f + u \partial_x f = 0, \quad t > 0, x \in \mathbb{R}, u \in \mathbb{R},
\]

(9)

with initial condition \( f(0, x, u) = f_0(x, u) \). Defining the \( i \)-th-order moment:

\[
M_i(t, x) = \int f(t, x, u)u^i \, du, \quad i = 0, \ldots, 4;
\]

the associated governing equations are easily obtained from (9) after multiplication by \( u^i \) and integration over \( u \):

\[
\begin{align*}
\partial_t M_0 &+ \partial_x M_1 = 0, \\
\partial_t M_1 &+ \partial_x M_2 = 0, \\
\partial_t M_2 &+ \partial_x M_3 = 0, \quad \Rightarrow \quad \partial_t \mathbf{M} + \partial_x \mathbf{F(M)} = 0, \\
\partial_t M_3 &+ \partial_x M_4 = 0, \\
\partial_t M_4 &+ \partial_x M_5 = 0.
\end{align*}
\]

(10)

with \( \mathbf{M} = (M_0, \ldots, M_4)^t \) and \( \mathbf{F(M)} = (F_0, \ldots, F_4)^t = (M_1, \ldots, M_4, M_5)^t \). This model is closed by using HyQMOM3 to model \( M_5 \). The Jacobian matrix for the fluxes \( \frac{\partial F_i}{\partial \mathbf{M}} \) has five real eigenvalues [19]:

\[
\lambda_0 = \bar{u}, \quad \lambda_{1,2,3,4} = \bar{u} + C_2^{1/2} \frac{1}{2} \left( q_u \pm \sqrt{4\eta_\alpha - 3q_\alpha^2} \pm 4\sqrt{(\eta_\alpha - q_\alpha^2)(\eta_\alpha - q_\alpha^2 - 1)} \right).
\]

(11)

and hence (10) is hyperbolic for all realizable moment sets. These eigenvalues are used to define the kinetic-based fluxes.

The spatial fluxes \( \mathbf{F(M)} \) are computed using a kinetic-based definition [11]:

\[
F_i(t, x) = \int_0^\infty f(t, x, u)u^{i+1} \, du + \int_{-\infty}^0 f(t, x, u)u^{i+1} \, du, \quad i = 0, \ldots, 4;
\]

(12)

where the decomposition into positive and negative directions is used to define the flux function as proposed in [1,11,27]. Thus, (12) becomes

\[
F_i(t, x) = M_0 \sum_{\alpha=1}^{4} w_\alpha \left[ \max(0, \lambda_\alpha)^{i+1} + \min(0, \lambda_\alpha)^{i+1} \right], \quad i = 0, \ldots, 4,
\]

(13)

where \( \lambda_\alpha \) are the eigenvalues in (11). The weights \( w_\alpha \) are found by solving the moment problem [19]:
where \( \varphi_{\alpha} = (\lambda_{\alpha} - \bar{u})/C_2^{1/2} \) are the normalized eigenvalues found from (11). These weights are always non-negative [19]. Reconstructing the eigenvalues instead of the abscissas was shown to prevent numerical spikes in the zeroth-order moment in solutions to 1-D Riemann problems [19]. Both reconstructions give identical moments up to order five.

In practice, the quadrature used in the kinetic-based fluxes may result in large eigenvalues that restrict the timestep to a computationally unfeasible value. To prevent this, \( (q_u, \eta_u) \) may need to be modified to limit the eigenvalues (see Sec. 5.1.2 for more details). To design a first-order scheme, the decomposition in (13) is sufficient as it corresponds to an upwind scheme at the kinetic level. For a high-order scheme [31], the spatial fluxes can be found from (13) by employing a high-order spatial reconstruction for \( M_0 w_{\alpha} \) and a first-order reconstruction for the abscissas \( \lambda_{\alpha} \).

3. CHyQMOM\(_9\) for 2-D kinetic equations

As in [19], consider a 2-D phase space with VDF \( f(\nu) \) for \( \nu = (u, v)^T \) and define the bivariate moments

\[
M_{i,j} := \int_{\mathbb{R}^2} f(\nu) u^i v^j \, d\nu, \quad i, j = 0, 1, \ldots, \infty. \tag{15}
\]

For \( M_{0,0} > 0 \), the bivariate central moments are

\[
C_{i,j} := \frac{1}{M_{0,0}} \int_{\mathbb{R}^2} f(\nu)(u - \bar{u})^i (v - \bar{v})^j \, d\nu, \quad i, j = 0, 1, \ldots, \infty; \tag{16}
\]

where \( \bar{u} = M_{1,0}/M_{0,0} \) and \( \bar{v} = M_{0,1}/M_{0,0} \). The ten bivariate moments needed for 2-D CHyQMOM\(_9\) are

\[
M = \begin{bmatrix}
M_{0,0} & M_{0,1} & M_{0,2} & M_{0,3} & M_{0,4} \\
M_{1,0} & M_{1,1} & M_{1,2} & M_{1,3} & M_{1,4} \\
M_{2,0} & M_{2,1} & M_{2,2} & M_{2,3} & M_{2,4} \\
M_{3,0} & M_{3,1} & M_{3,2} & M_{3,3} & M_{3,4} \\
M_{4,0} & M_{4,1} & M_{4,2} & M_{4,3} & M_{4,4}
\end{bmatrix}. \tag{17}
\]

CHyQMOM\(_9\) reproduces all second-order moments, allows for PTC due to the third-order moments, and is hyperbolic due to the fourth-order moments [19].

3.1. Definition of 2-D CHyQMOM\(_9\)

For CHyQMOM\(_9\) [19], the approximate bivariate VDF is

\[
f^a(\nu) := M_{0,0} \sum_{\alpha=1}^{3} \rho_\alpha \delta_{\bar{u}+u_\alpha}(u) \sum_{\beta=1}^{3} \rho_{\alpha\beta} \delta_{\bar{v}+v_{\alpha\beta}}(v) \tag{18}
\]

where the parameters \( \{\rho_1, \rho_2, \rho_3, u_1, u_3\} \) \( (u_2 = 0) \) are determined using HyQMOM\(_3\) from the moments \( \{M_{0,0}, M_{1,0}, M_{2,0}, M_{3,0}, M_{4,0}\} \). In (18), \( \bar{v}_{\alpha} \) and \( v_{\alpha\beta} \) are found from the moments \( \{M_{1,0}, M_{0,1}, M_{2,0}, M_{2,0}, M_{4,0}\} \). The conditional mean, \( \bar{v}_{\alpha} = a_0 + a_1 u_\alpha \), has the following properties:

\[
\sum_{\alpha=1}^{3} \rho_\alpha \bar{v}_{\alpha} = 0, \quad \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha \bar{v}_{\alpha} = C_{1,1}, \tag{19}
\]

and thus \( \bar{v}_{\alpha} = \frac{C_{1,1}}{C_{2,0}} u_\alpha \).

The central moments found from (18) are

\[
C_{i,j} = \sum_{\alpha=1}^{3} \rho_\alpha u_{\alpha}^i \sum_{\beta=1}^{3} \rho_{\alpha\beta} (\bar{v}_{\alpha} + v_{\alpha\beta})^j. \tag{20}
\]

A binomial expansion then leads to
where the conditional central moments are

\[ C_{j|\alpha} := \sum_{\beta=1}^{3} \rho_{\alpha\beta} \nu_{\alpha\beta}^j. \]  

(22)

It follows immediately from (21) that \( C_{0|\alpha} = 1 \). By choosing \( C_{2|\alpha} = C_{1,1}C_{3,0}/C_{2,0} \), we find \( C_{1|\alpha} = 0 \).

The parameters [\( \rho_{u1}, \rho_{u2}, \rho_{u3}, v_{u1}, v_{u2}, v_{u3} \)] in (22) are determined from the conditional moments \( \{1, 0, C_{2|\alpha}, C_{3|\alpha}, C_{4|\alpha}\} \) using HyQMOM3. We compute the conditional variances in the form

\[ C_{2|\alpha} = C_{0,2} (b_0 + b_1 u_{\alpha}) \]  

(23)

where \( u_{\alpha} = u_{\alpha}/C_{2,0}^{1/2} \), from (21) using \( \{C_{0,2}, C_{1,2}\} \) by choosing \( C_{1,2} = C_{1,1}C_{3,0}/C_{2,0} \). This yields \( b_0 = 1 - q_{uv}^2 \) and \( b_1 = q_{uv}/(q_{uv} - q_{uv}^2) \) where \( q_{uv} = C_{1,1}/\sqrt{C_{2,0}C_{3,0}/C_{2,0}^{3/2}} \) and \( q_{v} = C_{3,0}/C_{2,0}^{3/2} \). If one of the conditional variances is negative, then \( b_1 \) is limited such that all conditional variances are non-negative [19].

The conditional moments \( C_{3|\alpha} \) and \( C_{4|\alpha} \) are found from \( \{C_{0,3}, C_{0,4}\} \) by assuming that they depend on \( \alpha \) through \( C_{2|\alpha} \):

\( C_{3|\alpha} = q_{v}^* C_{2|\alpha}^2 \) and \( C_{4|\alpha} = \eta_{v}^* C_{2|\alpha}^2 \). This yields the following relations for \( q_{v}^* \) and \( \eta_{v}^* \):

\[ q_{v}^* = \left[ \sum_{\alpha=1}^{3} \rho_{\alpha} \left( C_{2|\alpha}^{1/2} \right)^{3/2} \right]^{-1} \left[ 2e_{uv} q_{u} + (1 - 3q_{uv}^2)q_{v} \right] \]  

(24)

where \( C_{2|\alpha} = C_{2,0}/C_{2,0} \), and

\[ \eta_{v}^* = \left[ \sum_{\alpha=1}^{3} \rho_{\alpha} \left( C_{2|\alpha} \right)^2 \right]^{-1} \left[ \eta_{v} - e_{uv}^4 \eta_{u} - 6e_{uv}(1 - e_{uv}^2)q_{v} - 4e_{uv}q_{v} q_{uv} q_{u} - 3 \right] \]  

(25)

where the scaled moments are \( \eta_{u} := C_{4,0}/C_{2,0}^{3/2} \) and \( \eta_{v} := C_{4,0}/C_{2,0}^{3/2} \).

In the limit of perfect correlation, \( |q_{uv}| = 1 \), \( q_{v} = q_{uv} q_{u} \) and \( \eta_{v} = e_{uv}^2 \eta_{u} \), and thus \( q_{v}^* = 0 \) and \( \eta_{v}^* = 0 \). For uncorrelated variables, \( \eta_{u} = 0, q_{v} = 0 \) and \( \eta_{v} = \eta_{v} \). Otherwise, the realizability of \( \mu_{u}^4 \) requires that \( \eta_{v}^* \geq 1 + (q_{v}^*)^2 \). If this condition is not met, then \( q_{v}^* \) and \( \eta_{v}^* \) are projected to the realizability curve \( \eta_{v} = 1 + (q_{v}^*)^2 \) along the direction of the Gaussian moments (i.e., \( q_{v}^* = 0 \) and \( \eta_{v}^* = 3 \)). HyQMOM3 can then be applied for each \( \alpha \) to find the remaining parameters. In A.3 we provide a compact method for computing the 2-D ChyQMOM9 parameters based on the method described above.

4. ChyQMOM27 for 3-D kinetic equations

Here we describe the extension of 2-D ChyQMOM9 developed in [19] to a 3-D phase space using ideas from CQMOM [32]. The 27 nodes (i.e. 2-D ChyQMOM9 augmented by three nodes in the third direction) are determined from the following 16 moments:

\[
M = \begin{pmatrix}
M_{0,0,0} & M_{0,0,1} & M_{0,0,2} \\
M_{1,0,0} & M_{1,0,1} & M_{1,0,2} \\
M_{2,0,0} & M_{2,0,1} & M_{2,0,2} \\
M_{3,0,0} & M_{3,0,1} & M_{3,0,2} \\
M_{4,0,0} & M_{4,0,1} & M_{4,0,2}
\end{pmatrix}
\]

(26)

In a 3-D phase space, there are six possible permutations of the conditioning variables. Here we consider only one, corresponding to a VDF of the form \( f(v) = f(w|u, v)f(v|u)f(u) \) where \( v = (u, v, w) \). Nonetheless, the other five permutations can be found by permuting the components of \( v \). For clarity, we will first describe the non-degenerate case where the 2-D approximation \( f^{(2)}(u, v) \) in (18) has nonzero weights for all nine nodes. Thus, we shall assume that the quadrature parameters in the 2-D approximation are known (i.e., they have already been computed as described in Sec. 3).
4.1. Definition of 3-D CHyQMOM27

We define CHyQMOM27 in 3-D phase space using the approximate distribution

\[
f^\alpha(v) = M_{0,0,0} \sum_{\alpha = 1}^{3} \rho_{\alpha} \delta_{v_{\alpha} + u_{\alpha}}(v) \sum_{\beta = 1}^{3} \rho_{\alpha \beta} \delta_{\tilde{v}_{\alpha} + v_{\alpha \beta}}(v) \sum_{\gamma = 1}^{3} \rho_{\alpha \beta \gamma} \delta_{\tilde{w}_{\alpha \beta} + w_{\alpha \beta \gamma}}(w)
\]

(27)

where \( \tilde{v}_{\alpha} \) is the conditional mean of \( v \) given \( u_{\alpha} \) and \( \tilde{w}_{\alpha \beta} \) is the conditional mean of \( w \) given \( u_{\alpha} \). The doubly conditioned mean of \( w \), denoted by \( \tilde{w}_{\alpha \beta} \), is defined below. Hereinafter, we assume that the moments \( M_{i,j,k} \) and central moments \( C_{i,j,k} \) exist, and are nondegenerate (i.e., live in the interior of moment space) [14]. The basic idea for 3-D CHyQMOM27 is to find the 2-D bivariate moments conditioned on \( u = u_{\alpha} \), denoted by \( M_{j,k|\alpha} \). Then, for each \( \alpha \), the 2-D CHyQMOM3 described in Sec. 3.1 is employed to find \( \rho_{\alpha \beta}, v_{\alpha \beta} \) and \( \rho_{\alpha \beta \gamma}, w_{\alpha \beta \gamma} \).

As described in detail in Appendix A, the first step in modified Q MOM is to compute, for each \( \alpha \), the following nine bivariate moments conditioned on \( u \) (by definition \( M_{0,0|\alpha} = 1 \)):

\[
M_{1,0|\alpha} M_{0,1|\alpha} C_{2,0|\alpha} C_{1,1|\alpha} C_{0,2|\alpha} C_{3,0|\alpha} C_{0,3|\alpha} C_{0,4|\alpha} C_{0,4|\alpha}.
\]

(28)

which are needed for 2-D CHyQMOM9. For the first-order moments, this yields \( M_{1,0|\alpha} = C_{2,0,0}|M_{0,0,0}^{1/2} \) and \( M_{0,1|\alpha} = C_{0,0,2}|M_{0,0,0}^{1/2} \) where \( q_{uv} = C_{1,1,0}|C_{2,0,0}^{1/2} \) and \( q_{uw} = C_{1,0,1}|C_{2,0,0}^{1/2} \) are correlation coefficients. The remaining components in (28) are defined using the conditional variances:

\[
C_{2,0|\alpha} = C_{0,2,0} + 1 - q_{uv}^{2} + q_{uv}(q_{uv} - q_{uw}q_{uv})|\kappa_{uv}^{1/2}, C_{0,2|\alpha} = C_{0,0,2} + 1 - q_{uw}^{2} + q_{uw}(q_{uw} - q_{uw}q_{uw})|\kappa_{uw}^{1/2}.
\]

(29)

For example, the conditional covariance is \( C_{1,1|\alpha} = (C_{2,0,0}|C_{2,0,0}^{1/2})^{1/2} \) where the conditional correlation coefficient is defined as

\[
\rho_{\alpha \beta \gamma} = \sum_{\alpha = 1}^{3} \rho_{\alpha} \rho_{\alpha \beta} \rho_{\alpha \beta \gamma} \sum_{\alpha = 1}^{3} \rho_{\alpha} \rho_{\alpha \beta} \rho_{\alpha \beta \gamma}.
\]

(30)

The skewness coefficients (or scaled moments of order 3) are defined by \( q_{u} := C_{3,0,0}|C_{2,0,0}^{3/2} \), \( q_{u} := C_{0,3,0}|C_{2,0,0}^{3/2} \), and \( q_{w} := C_{0,0,3}|C_{2,0,0}^{3/2} \). To prevent the conditioned statistics from becoming unrealizable, the non-negative limiters \( \kappa_{uv}, \kappa_{uw}, \kappa_{uw} \) are introduced. If the conditioned variances and correlations coefficients are unrealizable, the limiters are decreased from unity until those statistics become realizable. For example, we must have \( q_{uv} \leq 1 \) for all \( \alpha \), otherwise \( \kappa_{uw} \) is decreased.

In a similar manner, \( C_{3,0|\alpha} = C_{2,0|\alpha}|q_{uv}^{1/2} \) and \( C_{0,3|\alpha} = C_{2,0|\alpha}|q_{uw}^{1/2} \) where the conditioned skewness coefficients are defined by

\[
q_{v|\alpha} = \sum_{\alpha = 1}^{3} \rho_{\alpha} C_{2,0|\alpha}^{1/2}, q_{w|\alpha} = \sum_{\alpha = 1}^{3} \rho_{\alpha} C_{2,0|\alpha}^{1/2}.
\]

(31)

Likewise, \( C_{4,0|\alpha} = C_{2,0|\alpha}|q_{uv}^{2} \) and \( C_{0,4|\alpha} = C_{2,0|\alpha}|q_{uw}^{2} \) where the conditional flatness coefficients are defined by

\[
\eta_{v|\alpha} = \sum_{\alpha = 1}^{3} \rho_{\alpha} C_{2,0|\alpha}, \eta_{w|\alpha} = \sum_{\alpha = 1}^{3} \rho_{\alpha} C_{2,0|\alpha}.
\]

(32)

The flatness coefficients (or scaled moments of order 4) are defined by \( \eta_{u} := C_{4,0,0}|C_{2,0,0}^{4/2} \), \( \eta_{u} := C_{0,4,0}|C_{2,0,0}^{4/2} \), and \( \eta_{w} := C_{0,0,4}|C_{2,0,0}^{4/2} \). If \( \eta_{v|\alpha} \) is not realizable, then \( q_{v|\alpha} \) and \( \eta_{v|\alpha} \) are projected to the realizability curve \( \eta_{v|\alpha} = 1 + q_{v|\alpha}^{2} \) along the direction of the Gaussian moments (i.e., \( q_{v|\alpha} = 0 \) and \( \eta_{v|\alpha} = 3 \)). The same is done for \( q_{w|\alpha} \) and \( \eta_{w|\alpha} \).

Given the conditional moments in (28), we can now compute \( \rho_{\alpha \beta \gamma}, \kappa_{uv}, \kappa_{uw}, \kappa_{uw} \) from the formulas for the 2-D CHyQMOM9 described in Sec. 3.1. Finally, the conditioned means in (27) are given by \( \tilde{v}_{\alpha} = \tilde{v} + M_{1,0|\alpha}, \tilde{w}_{\alpha} = \tilde{w} + M_{0,1|\alpha} \) and \( \tilde{w}_{\alpha \beta} = C_{1,1|\alpha}|C_{2,0,0}^{1/2} \).

4.2. Application of CHyQMOM27 to 3-D kinetic equations

Consider a 3-D velocity phase space with VDF \( f(t,x,v) \) for \( x = (x,y,z)^{T} \) and \( v = (u,v,w) \) that satisfies the kinetic equation.
\[ \partial_t f + \mathbf{v} \cdot \partial_x f = 0, \quad t > 0, \ x \in \mathbb{R}^3, \ \mathbf{v} \in \mathbb{R}^3, \]

with initial condition \( f(0, x, v) = f_0(x, v) \). The governing equations for the 16 trivariate moments in (26) are

\[
\begin{align*}
\partial_t M_{0,0,0} + \partial_x M_{1,0,0} + \partial_y M_{0,1,0} + \partial_z M_{0,0,1} &= 0, \\
\partial_t M_{1,0,0} + \partial_x M_{2,0,0} + \partial_y M_{1,1,0} + \partial_z M_{0,1,1} &= 0, \\
\partial_t M_{0,1,0} + \partial_x M_{1,1,0} + \partial_y M_{0,2,0} + \partial_z M_{0,0,2} &= 0, \\
\partial_t M_{0,0,1} + \partial_x M_{1,0,1} + \partial_y M_{0,1,1} + \partial_z M_{0,2,1} &= 0, \\
\partial_t M_{2,0,0} + \partial_x M_{3,0,0} + \partial_y M_{2,1,0} + \partial_z M_{0,2,1} &= 0, \\
\partial_t M_{1,1,0} + \partial_x M_{2,1,0} + \partial_y M_{1,2,0} + \partial_z M_{0,2,2} &= 0, \\
\partial_t M_{0,2,0} + \partial_x M_{1,2,0} + \partial_y 0, \ \partial_t F_z(M) \Rightarrow \partial_t M + \partial_x F_x(M) + \partial_y F_y(M) + \partial_z F_z(M) = 0, \quad \text{(34)}
\]

which requires a closure for seven third-order, six fourth-order, and nine fifth-order moments. These closures are found by using the flux-based quadrature described next. If source terms were present on the right-hand side of (34), they would be closed with 3-D CHyQOMM27 in (27). The 2-D system has been shown to be hyperbolic for small correlations [19], but due to the complexity of the 3-D system, we have not attempted to prove its hyperbolicity. However, our numerical examples in Sec. 6 suggest that the system is hyperbolic.

The 3-D flux \( \mathbf{F} = (F_x, F_y, F_z)^T \) for the 16-moment vector \( \mathbf{M} \) is required to solve the free-transport term. The components of the fluxes for moment \( M_{i,j,k} \) are computed using a kinetic-based definition [11]:

\[
\begin{align*}
F_{x,i,j,k} &= \int_{\mathbb{R}^3} \left( \int_0^\infty f(v)u^{i+1}v^jw^k \, dv \right) \, dw + \int_{\mathbb{R}^3} v \left( \int_0^\infty f(v)u^{i+1}v^jw^k \, dv \right) \, dw, \\
F_{y,i,j,k} &= \int_{\mathbb{R}^3} \left( \int_0^\infty f(v)u^iv^{j+1}w^k \, dv \right) \, dw + \int_{\mathbb{R}^2} v \left( \int_0^\infty f(v)u^iv^{j+1}w^k \, dv \right) \, dw, \\
F_{z,i,j,k} &= \int_{\mathbb{R}^3} \left( \int_0^\infty f(v)u^iv^jw^{k+1} \, dw \right) \, dv + \int_{\mathbb{R}^2} v \left( \int_0^\infty f(v)u^iv^jw^{k+1} \, dw \right) \, dv.
\end{align*}
\]

Each flux component uses a separate density reconstruction in which the flux direction is used to determine the conditioning direction. For example, \( F_{x,i,j,k} \) is computed by first conditioning on the \( u \) component of velocity. After applying 3-D CHyQOMM27, we can assume that flux-based quadrature parameters \( w_{\alpha}, \lambda_{\alpha} \) are known in terms of \( q_u \) and \( \eta_u \). Thus, (35) can be written as

\[
F_{x,i,j,k} = M_{0,0,0} \sum_{\alpha=1}^4 w_\alpha \left[ \max(0, \lambda_\alpha)^{i+1} + \min(0, \lambda_\alpha)^{i+1} \right] \Theta_{u,\alpha}^{i,k}
\]

where \( \Theta_{u,\alpha}^{i,k} \) are the bivariate moments in \( (v, w) \) conditioned on the \( u \) direction. These moments are found from the unconditional moments using the formula (B.5) in Appendix B. The treatment of the other flux components is done analogously by first conditioning on the velocity component in the direction of the flux. The flux in (36) is computed with \( \Theta_{v,\alpha}^{i,k} \), and the flux in (37) with \( \Theta_{w,\alpha}^{i,k} \). In the numerical implementation, the same routine can be used to compute \( F_{x,i,j,k}, F_{y,i,j,k} \) and \( F_{z,i,j,k} \) by simply permuting the order of the trivariate moments.
5. Numerical implementation of CHyQMOM$_{27}$ for gas–particle flows

The CHyQMOM$_{27}$ technique has been implemented in NGA, a CFD code with multiphase capabilities [12]. To solve for two-way coupled flows, we follow a similar procedure for solving the fluid phase with equivalent coupling terms as used by Capcelatro et al. [2]. Considering the finite volume of the particles and forcing from gravity and interphase coupling, the fluid phase is evolved according to a filtered Navier–Stokes equation given in [2],

$$\frac{\partial \alpha_f \rho_f}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f) = 0,$$

$$\frac{\partial \alpha_f \rho_f \mathbf{u}_f}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{u}_f \otimes \mathbf{u}_f) = \nabla \cdot (\mathbf{\sigma}_f - \rho_f \mathbf{l}) - \rho_p M_0 \mathbf{A}_c + \alpha_f \rho_f \mathbf{g},$$

where $\alpha_f = 1 - M_0$ is the fluid volume fraction, $\mathbf{u}_f$ is the fluid velocity, $\rho_f$ is the fluid density, $\rho_p$ is the particle density, $\mathbf{\sigma}_f$ is the fluid viscous stress, $\rho_f$ is the fluid pressure, $\mathbf{A}_c$ is the particle acceleration due to the coupling, $\mathbf{g}$ is gravitational acceleration, $\mathbf{v}_f$ is the bulk fluid viscosity, and $\mathbf{v}_f^*$ is an effective viscosity due to fluid velocity fluctuations around the particles. Equation (59) in Sec. 5.2 discusses the form of $\mathbf{A}_c$. The effective viscosity is computed using Gibilaro’s model [2,20],

$$\mathbf{v}_f^* = \left(\alpha_f^{2.8} - 1\right) \mathbf{v}_f.$$

As per [2,12], the fluid phase is solved using a semi-implicit Crank–Nicolson scheme. For moderately dilute flows for which the collisional fluxes are negligible, the particle-phase VDF evolves as

$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{v} f) + \nabla \cdot (\mathbf{A} f) = \mathcal{C},$$

where $\mathbf{A}$ is the acceleration on the particles due to coupling and gravity, and $\mathcal{C}$ is the collision term. By transformation of (41) into moment space, the evolution of the moment vector is

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot \mathbf{F} + \mathbf{A} = \mathcal{C}$$

where $\mathbf{A}$ and $\mathcal{C}$ are the resulting terms from transforming $\nabla \cdot (\mathbf{A} f)$ and $\mathcal{C}$ into moment space, respectively. We adapt a fractional-step approach to advance the moment vector for the particle phase in time. As used previously by [15,25], we implement an explicit, first-order scheme for convection and semi-analytical updates for the external forces and collisions. We use a directional splitting approach to compute the convection update. We advance sequentially,

$$\frac{\mathbf{M}^* - \mathbf{M}^0}{\Delta t} = -\nabla \cdot \mathbf{F},$$

$$\int_{\mathbf{M}^0} \frac{d\mathbf{M}}{\mathbf{A}} = -\int_t^{t + \Delta t} dt,$$

$$\int_{\mathbf{M}^*} \frac{d\mathbf{M}}{\mathcal{C}} = \int_t^{t + \Delta t} dt,$$

where $\Delta t$ is the timestep, $\mathbf{M}^0$ is the moment vector at the beginning of the timestep, $\mathbf{M}^*$ is the moment vector after the convection sub-step, $\mathbf{M}^{*+1}$ is the moment vector after the external forces sub-step, and $\mathbf{M}^{*+1}$ is the moment vector after the collision sub-step, at the end of the timestep. Section 5.1 discusses the reconstruction of the moment vector fluxes from the CHyQMOM$_{27}$ flux-based quadrature outlined in Appendix B. Section 5.1.1 discusses a modification to the fluxes for specularly reflective walls. Sections 5.2 and 5.3 discuss the implementation of the external forces, and collision sub-steps, respectively.

5.1. Reconstruction of fluxes

We implement the first-order and quasi-second-order kinetic-based finite volume schemes (KBFV) for constructing the fluxes from the weights, eigenvalues, and bivariate conditional moments [31]. To demonstrate these schemes, consider the $x$-direction contribution to the divergence of the moment vector flux for a computational cell indexed at $p$:
\[ \partial_t F_x^{(p)} = \frac{1}{\Delta x} \left[ F_x^{(p+1/2)} - F_x^{(p-1/2)} \right], \]  

(44)

where \( F_x^{(p+1/2)} \) is the moment vector flux through the right face of cell \( p \) and \( F_x^{(p-1/2)} \) is the flux through the left face of cell \( p \). By flux splitting, \( F_x^{(p+1/2)} \) is, for example, constructed as

\[
F_{x;i,j,k}^{(p+1/2)} = \sum_{\alpha=1}^{4} \hat{w}_\alpha^{(p+1/2,l)} \max \left( 0, \lambda_\alpha^{(p+1/2,l)} \right)^{i+1} \Theta_{u,\alpha} + \sum_{\alpha=1}^{4} \hat{w}_\alpha^{(p+1/2,r)} \min \left( 0, \lambda_\alpha^{(p+1/2,r)} \right)^{i+1} \Theta_{u,\alpha}.
\]

(45)

where \( \hat{w}_\alpha \) has been substituted for \( M_{0,0,0}w_\alpha \) and the superscripts \( l \) and \( r \) refer to the left and right sides of the right face of cell \( p \). For the first-order upwind and quasi-second-order schemes, \( \lambda_\alpha \) and \( \Theta_{u,\alpha} \) are piece-wise constant, and therefore

\[
\begin{pmatrix} \lambda_\alpha^{(p+1/2,l)} \\ \Theta_{u,\alpha}^{(p+1/2,l)} \end{pmatrix} = \begin{pmatrix} \lambda_\alpha \\ \Theta_{u,\alpha} \end{pmatrix}^{(p+1/2,r)}.
\]

(46)

The first-order upwind scheme also provides a piece-wise constant reconstruction for \( \hat{w}_\alpha \), such that

\[
\hat{w}_\alpha^{(p+1/2,l)} = \hat{w}_\alpha^{(p)}, \quad \hat{w}_\alpha^{(p+1/2,r)} = \hat{w}_\alpha^{(p+1)}. \tag{47}
\]

The quasi-second-order scheme uses a piece-wise linear reconstruction for \( \hat{w}_\alpha \), such that

\[
\hat{w}_\alpha^{(p+1/2,l)} = \hat{w}_\alpha + \frac{\Delta x}{2} S(p), \quad \hat{w}_\alpha^{(p+1/2,r)} = \hat{w}_\alpha^{(p+1)} - \frac{\Delta x}{2} S(p+1)
\]

(48)

where the slope \( S(p) \) is constructed using a minmod limiter as

\[
S(p) = \minmod \left( \frac{\hat{w}_\alpha^{(p)} - \hat{w}_\alpha^{(p-1)}}{\Delta x}, -\frac{\hat{w}_\alpha^{(p+1)} - \hat{w}_\alpha^{(p)}}{\Delta x} \right).
\]

(49)

where

\[
\minmod(x, y) = \text{sign}(x) \left( \frac{1 + \text{sign}(xy)}{2} \right) \min(|x|, |y|).
\]

(50)

Vikas et al. [31] show that these schemes guarantee the realizability of the moment vector, provided the timestep is restricted by

\[
\frac{\Delta t}{\Delta x} \leq \min_{\alpha} \left( \frac{\hat{w}_\alpha^{(p+1/2,l)} \max(\lambda_\alpha^{(p)}, 0) - \hat{w}_\alpha^{(p-1/2,r)} \min(\lambda_\alpha^{(p)}, 0)}{w_\alpha^{(p+1/2,l)}} \right).
\]

(51)

The fluxes through the other cell faces can be constructed analogously.

5.1.1. Implementation of reflective walls

Based on Fox [15], we implement specularly reflective walls with restitution coefficient, \( e_w \). As an example, consider the flux into cell \( p = 1 \) from a left-bounding wall at cell face \( p = 1/2 \). After reverting to a piece-wise constant reconstruction for \( \hat{w}_\alpha^{(p-1)} \), a \( F^{(p+1/2,0)} \) is needed that modifies the wall-normal particle velocity components to the right of the right, \( \lambda_\alpha^{(p+1/2,r)} \), by a factor of \(-e_w\), while keeping \( F_{x;0,0,0}^{(p+1/2)} \), the volume-fraction flux through the wall, null. Since the \( y \) and \( z \) velocities on both sides of the wall must be identical, \( \Theta_{u,\alpha}^{(p)} \) is also the same on both sides of the wall. Under these conditions, we find

\[
F_{x;i,j,k}^{(p+1/2)} = \sum_{\alpha=1}^{4} \frac{\hat{w}_\alpha^{(p+1)}}{e_w} \max \left( 0, -e_w \lambda_\alpha^{(p+1)} \right)^{i+1} \Theta_{u,\alpha}^{(p)} + \sum_{\alpha=1}^{4} \hat{w}_\alpha^{(p+1)} \min \left( 0, \lambda_\alpha^{(p+1)} \right)^{i+1} \Theta_{u,\alpha}^{(p)}. \tag{52}
\]

Similar fluxes at walls aligned in the other directions can be defined.
5.1.2. Eigenvalue limiter for spatial flux

For highly non-equilibrium flows, it may be necessary to modify the third- and fourth-order statistics to limit the eigenvalues such that the timestep imposed by the CFL condition remains computationally feasible. Chalons et al. [8] used a similar limiter modifying the skewness. Since the maximum eigenvalue, $\lambda_{\text{max}}$, and maximum abscissa, $u_{\text{max}}$, scale similarly for large $q_u$ and $\eta_u$, we limit the maximum abscissa for simplicity. From (8) we find

$$u_{\text{max}} = C_2^{1/2} \frac{q_u}{2} + \sqrt{4\eta_u - 3q_u^2}.$$

(53)

When necessary, we force a smaller $u_{\text{max}}$ by modifying $(q_u, \eta_u)$. We have tried several methods of modifying these statistics and found the following method to offer the best balance of control over the eigenvalues and low reconstruction error for $M_3$ and $M_4$.

If $u_{\text{max}}$ is greater than a specified $u_{\text{lim}}$, project $q_u$ and $\eta_u$ along a line towards $(0, 1)$ onto $u_{\text{max}} = u_{\text{lim}}$. Assuming it is positive, the modified $q_u^*$ is the smaller root of

$$q_u^* = \frac{\eta_u - 1}{q_u} \left( \frac{u_{\text{lim}}}{C_2^{1/2}} + \frac{u_{\text{lim}}}{C_2^{1/2}} \right) q_u^* + \frac{u_{\text{lim}}}{C_2^{1/2}} - 1 = 0.$$

(54)

A negative $q_u$ is handled symmetrically. The modified $\eta_u^*$ is found from

$$\eta_u^* = \frac{\eta_u - 1}{q_u^*} q_u^* + 1.$$

(55)

Note that $u_{\text{max}}$ has a lower limit given by

$$\min u_{\text{max}} = C_2^{1/2},$$

(56)

so for large $C_2$, HyQ MOM will fail to yield $q_u$ and $\eta_u$ that gives $u_{\text{max}} \leq u_{\text{lim}}$. When this occurs, choose $(q_u, \eta_u) = (0, 1)$ such that $u_{\text{max}} = C_2^{1/2}$.

5.2. Implementation of external forces

The total acceleration on the particles due to external forces is

$$A = A_c + g.$$

(57)

where $g$ is the acceleration due to gravity and $A_c$ is that due to the fluid–particle coupling. For the coupling, we include Stokes drag, viscous drag exchange, and pressure drag exchange, following Capecelatro et al. [2]. The particle acceleration due to the fluid–particle coupling term is therefore approximated as

$$A_c = \frac{1}{\tau_p} \left( u_f - v \right) + \frac{1}{\rho_p} \nabla \cdot (\sigma_f - p_f I),$$

(58)

where $\tau_p$ is the particle response time, $u_f$ is the fluid velocity, $\sigma_f$ is the fluid viscous stress, and $p_f$ is the fluid pressure, and $I$ is the identity tensor [2].

Transforming $\nabla \cdot (A_c f)$ to moment space gives $A_c$, the moment vector source terms due to the fluid–particle coupling. Due to conservation of mass, the zeroth-order coupling source term is zero. The first-order term, i.e. the particle acceleration due to the coupling, is

$$A_c = \frac{1}{\tau_p} \left( u_f - \frac{M_1}{M_0} \right) + \frac{1}{\rho_p} \nabla \cdot (\sigma_f - p_f I).$$

(59)

The reaction force from $A_c$ is used as a source term in the fluid momentum equation, as shown in (39). The total acceleration from (57) is also separated into two components as $A = A_v + A_f$, so that only $A_v$ is a function of $v$. These components are

$$A_v = -\frac{1}{\tau_p} \cdot v, \quad A_f = \frac{1}{\tau_p} u_f + \frac{1}{\rho_p} \nabla \cdot (\sigma_f - p_f I) + g.$$

(60)

Transforming $\nabla \cdot (A_f)$ to moment space gives the moment vector source term, $A$. From this, the semi-analytical update for the external forces sub-step, in (43), yields


\[ M_0^{\alpha} = M_0^0, \]
\[ M_1^{\alpha} = M_0^\alpha A_f \tau_p (1 - e^{-\Delta t/\tau_p}) + M_1^\alpha e^{-\Delta t/\tau_p}, \]
\[ C_2^{\gamma} = C_2^\gamma e^{-2\Delta t/\tau_p}, \]
\[ C_3^{\gamma} = C_3^\gamma e^{-3\Delta t/\tau_p}, \]
\[ C_4^{\gamma} = C_4^\gamma e^{-4\Delta t/\tau_p}. \]

(61)

For simplicity, this update is shown for a mix of moments \( M_\gamma \) and central moments \( C_\gamma \) of orders \( \gamma = i + j + k \) equal to 0, 1, 2, 3 and 4, respectively. The moments \( M_\gamma^{\alpha} \) are then found using the updated central moments. This integration is accurate for small changes in \( \tau_p \) over the timestep.

5.3. Implementation of collisions

We implement the inelastic BGK collision model of Passalacqua et al. [25]:

\[ C = \frac{1}{\tau_c} (f_{eq} - f), \]

(62)

where \( \tau_c \) is the collision time and \( f_{eq} \) is the inelastic equilibrium distribution,

\[ f_{eq} = \frac{M_0}{[2\pi \Lambda_1]^{1/2}} \exp \left[ -\frac{1}{2} \right] \left( v_i - \frac{M_i}{M_0} \right) \Lambda_{ij}^{-1} \left( v_j - \frac{M_j}{M_0} \right). \]

(63)

In this model, \( \frac{M_i}{M_0} \) is the mean velocity component in direction i, and \( \Lambda \) is a covariance matrix with components

\[ \Lambda_{ij} = \frac{\gamma'}{3} C_{kk} \delta_{ij} + \left( \gamma \omega^2 - 2 \gamma' \omega + 1 \right) C_{i,j}, \]

(64)

and \( C_{kk} \) is the trace of \( C_{i,j} \). Furthermore, \( \gamma' = 1/Pr \) and \( \omega = \frac{1}{2} (1 + e_c) \) where \( Pr \) is the Prandtl number and \( e_c \) is the coefficient of restitution for particle–particle collisions. Following Passalacqua et al. [25], we use \( Pr = 1 \) for this work.

For hard spheres, the collision time is

\[ \tau_c = \frac{(3\pi)^{1/2} d p}{12 g_0 M_0 C_{kk}}, \]

(65)

where \( g_0 \) is the radial distribution function. Following [25], we use the Carnahan–Starling model [7] for \( g_0 \) (recall that \( M_0 \) is the particle-phase volume fraction):

\[ g_0 = \frac{1 - \frac{1}{2} M_0}{(1 - M_0)^3}. \]

(66)

With this collision model, we find the update for the collision sub-step:

\[ M_0^{\alpha+1} = M_0^{\alpha}, \]
\[ M_1^{\alpha+1} = M_1^{\alpha}, \]
\[ M_2^{\alpha+1} = M_2^{\alpha} e^{-\Delta t/\tau_c} + M_2^{eq} (1 - e^{-\Delta t/\tau_c}), \]
\[ M_3^{\alpha+1} = M_3^{\alpha} e^{-\Delta t/\tau_c} + M_3^{eq} (1 - e^{-\Delta t/\tau_c}), \]
\[ M_4^{\alpha+1} = M_4^{\alpha} e^{-\Delta t/\tau_c} + M_4^{eq} (1 - e^{-\Delta t/\tau_c}). \]

(67)

where \( M_\gamma \) and \( M_\gamma^{eq} \) are the moments and equilibrium moments, respectively, of orders 0, 1, 2, 3, and 4, with the latter found from (63). This integration is accurate for small changes in \( \tau_c \) over the timestep.

5.4. Implementation summary

Our solution procedure for the fluid–particle system is summarized as follows:

1. Initialize the solution process.

- Initialize the fluid velocity, pressure, viscosity, density, and particle moment vector.
- Obtain the weights, eigenvalues, and bivariate conditionals moments via flux-based quadrature following Appendix B.
- Select a timestep, \( \Delta t \).
2. Advance the particle phase.
   - Calculate a particle-phase timestep, $\Delta t$, that guarantees realizability using (51).
   - Compute and apply the spatial fluxes to obtain the updated moment vector. See Sec. 5.1 for the construction of these fluxes and Sec. 5.1.1 for the fluxes at walls.
   - Compute the fluid–particle coupling terms. The reaction forces will be applied to the fluid. Apply the external forces, from the fluid–particle coupling and gravity, to the particle moment vector using the semi-analytical expressions described in Sec. 5.2.
   - Apply collisions to the particles moment vector using the semi-analytical expressions described in Sec. 5.3.
   - Obtain the weights, eigenvalues, and bivariate conditional moments via flux-based quadrature following Appendix B.
   - Apply boundary conditions to the results of the quadrature.
   - Repeat until the particle phase has advanced by $\Delta t$.

3. Advance the fluid phase.
   - Compute the fluid volume fraction, $\alpha_f = 1 - M_0$.
   - Compute the effective viscosity using Gibilaro’s model given in (40).
   - Advance (39) by $\delta t$ using a semi-implicit Crank–Nicolson update as per Desjardins et al. [12].

4. Repeat Steps 2 and 3 until the final time.

6. Numerical examples

   We compare CHyQMOM$_{27}$ to the Euler–Lagrange (EL) method in [2] and two previously introduced QBMMs, the anisotropic Gaussian (AG) [28,30] and the tensor product (TP) [16] methods. We use a two-point quadrature per direction for TP and consider both two-point and four-point Gauss–Hermite quadratures per direction for AG. Note that AG is also a hyperbolic closure, albeit a low-order one that controls only up to the second-order moments. TP is a weakly hyperbolic closure that controls moments up to second-order and a subset of the third-order moments.

6.1. 3-D jets

   From the kinetic equation, particle trajectory crossing (PTC) may result in a multi-valued velocity field. Jet crossing is often used to verify numerical methods that attempt to capture this crossing [13,32]. To evaluate CHyQMOM$_{27}$, we first consider two-jet-crossing cases in 3-D. Both cases are run on a mesh of $64^3$ and domain size of $1^3$ with non-mesh-aligned jets.

   For the first case, dropping the external forcing and collision terms, two dilute jets of particles in a vacuum are oriented to intersect in the center of the simulation domain, $(x, y, z) = (0.5, 0.5, 0.5)$. The jet speed and diameters are chosen to be 1 and 10% of the simulation domain length, respectively. The origins of the first and second jets are chosen to be located at $(x, y, z) = (0.2, 0.0, 0.8)$ and $(x, y, z) = (0.0, 0.7, 0.3)$. We considered both first-order and quasi-second-order schemes, using CFL = 0.5 and CFL = 0.25 for each scheme, respectively. Fig. 1 shows the results using CHyQMOM$_{27}$ post-crossing. This reconstruction is capable of correctly computing the 3-D version of jet crossing as the jets successfully pass through each other without interference. Comparing the first-order and quasi-second-order schemes, the latter shows significantly reduced numerical diffusion.

   For the remainder of this paper, all test cases are run with first-order fluxes and with a CFL = 0.5. To test the specularly reflecting wall implementation, our second 3-D jet-crossing case consists of a dilute particle jet in a vacuum oriented to reflect off a wall. This jet is chosen to have a velocity of $(v_x, v_y, v_z) = \frac{1}{0.17}(-0.2, 0.3, -0.2)$, a diameter of 10% of the domain, and an origin at $(x, y, z) = (0.2, 0.0, 0.8)$. Fig. 2 shows results using two different restitution coefficients, $e_w = 1$ and $e_w = 0.5$. As required, the particle jet reflects off the $e_w = 0.5$ wall with a somewhat shallower angle as compared to results from the $e_w = 1$ wall. For both restitution coefficients, the particle jet does not interfere with itself as it reflects off the wall.

6.2. 2-D jets

   For simplicity, we perform 2-D jet-crossing simulations to characterize the advantages of CHyQMOM$_{27}$ over previous QBMMs and to evaluate the significance of the $u_{lim}$ parameter. Our first simulation is a two-jet-crossing case performed on a $200^2$ mesh with domain size $1^2$. The jet speeds are chosen to be 1. The jet origins are chosen to be at $(x, y) = (0.8, 0.0)$ for the first jet and $(x, y) = (0.0, 0.3)$ for the second jet. The jets are directed to the center of the domain, $(x, y) = (0.5, 0.5)$. AG is run with a four-point quadrature and $u_{lim}$ is varied for CHyQMOM$_{27}$. The two-jet case does not result in large eigenvalues, so the eigenvalue limiter is not necessary. However, the effects of the limiter can be demonstrated with this case. Fig. 3 shows the post-crossing volume fractions for the three QBMMs. For these snapshots, Fig. 4 shows plots of the reconstructed abscissas in velocity space for the region of crossing, defined as the 4% of domain located in the center. Due to its low-order closure, AG fails to capture the crossing correctly, forcing some volume fraction to deflect rather than pass through. The
reconstructed abscissas are shown to widely disperse in phase space. In contrast, TP captures the crossing without either jet affecting the other and recovers the abscissas exactly. For CHyQMOM\textsubscript{27}, $u_{\text{lim}} = 1$ fails to cross. Resembling the AG result, some interaction between the jets is observed. Higher values of $u_{\text{lim}}$ show successful crossing. Spurious abscissas are seen for CHyQMOM\textsubscript{27}, but they lose weight for increasing $u_{\text{lim}}$.

Three-jet-crossing simulations are next performed to demonstrate the significance of using a hyperbolic closure. The third jet origin is chosen to be at $(x, y) = (0.2, 0)$. Note that none of the three QBMMs considered in this section is capable of capturing the three-jet crossing because all lack the requisite independent quadrature points. A higher-order reconstruction is necessary to recover the exact solution. Additionally, while the eigenvalue limiter was unnecessary for the two-jet crossing, it is needed for three-jet-crossing simulations to remain computationally feasible. These simulations are also performed on a 200×200 mesh. AG is run with a four-point quadrature, and CHyQMOM\textsubscript{27} with various $u_{\text{lim}}$. From the post-crossing volume fractions in Fig. 5, different modes of failure can be seen for the simulation methods. As with the two-jet crossing case, AG allows for some crossing, but the jets are partially deflected away from each other. The crossing for TP and CHyQMOM both fail with CHyQMOM approaching similar results to AG for decreasing $u_{\text{lim}}$. In the limit of zero, the eigenvalue limiter forces the velocity distribution to be symmetric and centered about $\bar{u}$. Therefore a small $u_{\text{lim}}$ forces CHyQMOM to behave more like AG. As the limiter is increased, CHyQMOM allows for further-from-equilibrium dynamics.

TP can be shown to produce $\delta$-shocks in the three-jet-crossing simulations with a grid refinement study. Fig. 6 shows results for the three QBMMs with four levels of grid refinement. Because TP and CHyQMOM\textsubscript{27} were found to give unsteady
solutions, we show the time-averaged volume fractions. Unlike CHyQMOM$_{27}$ and AG, TP exhibits high volume fraction regions in the region after crossing, which become finer under grid refinement. These shocks are further characterized in Fig. 7, in which we plot the time-average of the Laplacian of volume fraction. For TP, large curvature is found for the regions after crossing that become stronger under refinement. This pattern is not as pronounced for AG and CHyQMOM$_{27}$ because $\delta$-shocks are not produced in either scheme.

6.3. Homogeneous cluster-induced turbulent flow

Homogeneous cluster-induced turbulence (CIT) is a canonical particle-laden flow, in which fluid–particle coupling drives turbulent-like fluctuations in the fluid, which in turn lead to particle clustering [3]. Homogeneous CIT simulations are performed in a periodic domain, initially filled homogeneously with particles and fluid. The particles are allowed to fall under gravity while the fluid is kept stationary with an additional source term in the fluid momentum equation. Two-way particle–fluid coupling and particle–particle collision terms are included. The system eventually reaches a statistical steady state after which flow statistics can be computed. Due to the relative simplicity of CIT, it provides an idealized scenario to study particle-laden flows. In this work, we perform pseudo-2D simulations of CIT. The parameters used are shown in Table 1. This configuration was used in a previous verification study of EL and EE methods [26]. For AG simulations [22], the three-point Gauss–Hermite quadrature is used and for CHyQMOM$_{27}$, the eigenvalue limiter is unnecessary and disabled.

Fig. 8 shows representative particle fields from the four simulation methods. Volume fraction is shown for the three Eulerian methods and a sampling of the particle locations for the Lagrangian method. Qualitatively, AG and CHyQMOM$_{27}$ give similar results. TP, however, produces sharp volume fraction regions along the sides of clusters, reminiscent of the shocks observed in the three-jet-crossing case. Overall, the methods show similar clustering behavior.
Fig. 4. Two-jet crossing for various skewness bounds using CHyQMOM27. The abscissas from the quadratures are shown by (●) with transparencies weighted by the abscissa weights. The correct values for the abscissas are shown by (●).

Table 1
Parameters used for CIT simulations. x is the direction of gravity.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle diameter</td>
<td>$d_p$</td>
<td>$90 \times 10^{-6}$ m</td>
</tr>
<tr>
<td>Particle density</td>
<td>$\rho_p$</td>
<td>1000 kg m$^{-3}$</td>
</tr>
<tr>
<td>Fluid density</td>
<td>$\rho_f$</td>
<td>1 kg m$^{-3}$</td>
</tr>
<tr>
<td>Fluid dynamic viscosity</td>
<td>$\mu_f$</td>
<td>$1.8 \times 10^{-5}$ Pas</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>$g$</td>
<td>$-4.0004$ m s$^{-2}$</td>
</tr>
<tr>
<td>Coefficient of restitution</td>
<td>$e$</td>
<td>0.9</td>
</tr>
<tr>
<td>Average particle volume fraction</td>
<td>$\langle M_0 \rangle$</td>
<td>0.01</td>
</tr>
<tr>
<td>Particle response time</td>
<td>$\tau_p$</td>
<td>$0.025$ s</td>
</tr>
<tr>
<td>Stokes settling speed</td>
<td>$\tau_p g$</td>
<td>0.1 m s$^{-1}$</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>$Re_p$</td>
<td>$0.5$</td>
</tr>
<tr>
<td>Domain size</td>
<td>$L_x, L_y, L_z$</td>
<td>$1792$</td>
</tr>
<tr>
<td>Grid spacing</td>
<td>$\Delta x / d_p$</td>
<td>2</td>
</tr>
<tr>
<td>CFL</td>
<td></td>
<td>0.5</td>
</tr>
</tbody>
</table>

For notational symmetry between the fluid and particle phases, we define $\alpha_p = M_0$ and $u_p = M_1 / M_0$. We adapt the phase-averaging (PA) concepts of Fox [18]. The Reynolds average of a quantity $A$ is referred to by $\langle A \rangle$. Similar to Favre averaging, a particle-weighted average is defined as $\langle A \rangle_p = \frac{\langle \alpha_p A \rangle}{\langle \alpha_p \rangle}$. Likewise, the fluid-weighted average is $\langle A \rangle_f = \frac{\langle \alpha_f A \rangle}{\langle \alpha_f \rangle}$. Fluctuations about the Reynolds average, the particle PA, and the fluid PA are given by $A' = A - \langle A \rangle$, $A'' = A - \langle A \rangle_p$, and $A''' = A - \langle A \rangle_f$, respectively. Since CIT is homogeneous and reaches a statistical steady state, Reynolds averages are estimated as averages over the domain and over long times ($\tau_p$=40).
Fig. 5. Three-jet crossing for the three QBMMs. CHyQMOM27 is shown for varying $u_{\text{lim}}$.

To compare EL simulations to the QBMMs used in this study, the particle data must first be converted into particle moments. For an EL simulation with particles $p = 1, 2, ..., n$ located at $x_p$ with velocities $v_p$, the particle moments are estimated as

$$M_{i,j,k}(x) = \sum_p G_h \left( |x - x_p| \right) v_{p,i}^j v_{p,j}^k v_{p,k}^l,$$

where $G_h$ is a Gaussian kernel with bandwidth $h$. A bandwidth of $h/d_p = 10$ is used to compute these moments.

In terms of PA quantities, the particle turbulent kinetic energy (TKE) and fluid TKE are defined as

$$k_p = \frac{1}{2} \left( \mathbf{u}_p^i \cdot \mathbf{u}_p^i \right)_p, \quad k_f = \frac{1}{2} \left( \mathbf{u}_f^i \cdot \mathbf{u}_f^i \right)_f.$$

These quantities have modeling significance for particle-laden flows [3,18], so are important to capture accurately in mesoscale simulations. However, $k_p$ will be sensitive to the bandwidth used to process the EL data. Instead, the total fluctuation energy may be used to compare EL to QBMMs as it does not depend on the bandwidth,

$$\kappa_p = k_p + \frac{1}{2} (C_{i,i})_p,$$

where $C_{i,i}$ is the trace of the second-order central moment tensor, i.e., three times the granular temperature. Table 2 shows various one-point statistics from the simulation methods. Given the large standard deviation of these statistics, we see that all methods produce similar results. The distribution of the clusters is further analyzed by computing a histogram of the
Fig. 6. Three-jet crossing for the three QBMMDs and varying grid resolutions, $n_x$. Time-averaged volume fraction.

Table 2
CIT one-point statistics with the standard deviation of the spatial average time series shown in parentheses.

<table>
<thead>
<tr>
<th></th>
<th>AG</th>
<th>TP</th>
<th>CHyQMOM</th>
<th>EL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume fraction variance</td>
<td>$\frac{\langle u'^2 \rangle}{\langle u \rangle^2}$</td>
<td>2.40 (0.57)</td>
<td>2.23 (0.41)</td>
<td>1.99 (0.33)</td>
</tr>
<tr>
<td>Settling velocity</td>
<td>$-\langle \delta p x \rangle / V_{St}$</td>
<td>3.32 (0.38)</td>
<td>3.45 (0.36)</td>
<td>2.82 (0.40)</td>
</tr>
<tr>
<td>Particle fluctuating energy</td>
<td>$\kappa_p / V_{St}^2$</td>
<td>5.24 (0.55)</td>
<td>5.09 (0.74)</td>
<td>5.05 (0.51)</td>
</tr>
<tr>
<td>Fluid turbulent-kinetic energy</td>
<td>$k_f / V_{St}^2$</td>
<td>9.43 (2.21)</td>
<td>9.73 (1.63)</td>
<td>9.05 (1.83)</td>
</tr>
</tbody>
</table>

volume fraction averaged over time. These results are shown in Fig. 9. For lower volume fractions, we find the distribution of volume fraction to be similar for all methods evaluated. However, AG and TP are found to produce higher volume fraction regions more often than the other methods. This might be indicative of $\delta$-shocks in TP. For AG, the higher volume fractions may be a result of particle clusters failing to cross.
Analogous to energy spectra in single-phase flow, spectral decompositions for volume fraction variance, particle TKE, and fluid TKE are defined as

\[
E_{\alpha_p}(\kappa) = \langle |\mathcal{F}\{\alpha_p\}|^2 \rangle, \\
E_{u_p}(\kappa) = \langle \mathcal{F}\{\sqrt{\alpha_p}u_p''\}^* \otimes \mathcal{F}\{\sqrt{\alpha_p}u_p''\} \rangle, \\
E_{u_p}(\kappa) = \langle \mathcal{F}\{\sqrt{\alpha_p}u_p'''\}^* \otimes \mathcal{F}\{\sqrt{\alpha_p}u_p'''\} \rangle,
\]

(71)

where \(\mathcal{F}\) is the Fourier transform, \(\kappa\) is the wavevector, and * is the complex conjugate. For CIT, we compute spectra in the \(\kappa_x\) and \(\kappa_y\) directions, averaging in the respective other two normal directions and time. For the two velocity spectra, we compute the xx tensor components. These spectra are shown in Fig. 10 for the four simulation methods. We find a similar trend in all of the spectra computed. The spectra computed for EL are sensitive to the Gaussian kernel width, but only for scales smaller than the kernel width. Larger scales are less affected and can be compared results from QBMMs. For the
large scales, the four simulation methods show good agreement. AG and CHyQMOM$_{27}$ have similar spectra for all scales. However, TP shows higher energy in the smallest scales. This may again indicate the presence of $\delta$-shocks in TP that are not evident in CHyQMOM$_{27}$ or AG.

### 6.3.1. Computational cost

Since the computational cost of QBMMs does not depend on the number of particles in the domain, they are expected to scale better than the EL method. This is particularly likely for collisional flows due to the expense of computing particle–particle collisions and evolving the simulation with a timestep restricted by a collisional CFL [2]. In contrast for QBMMs, the BGK model results in a semi-analytical update that does not demand a restrictive timestep and is relatively simple to compute. However, since CHyQMOM$_{27}$ uses a large set of moments with a complicated quadrature, the particle-phase solver is far more expensive per cell than the fluid solver. For a simulation with a relatively small number of particles, EL will be the more efficient choice. As the number of particles increases, CHyQMOM$_{27}$ will become more cost effective than EL.
Fig. 10. Volume fraction (left), particle velocity (middle), and fluid velocity (right) spectra. The top row shows the streamwise spectra and the bottom shows the transverse spectra. Spectra shown for AG (---), TP (----), CHyQMOM (--), and EL (-----).

Fig. 11. CIT timing data for AG (---), TP (----), CHyQMOM (--), and EL (-----). Timing data is shown for varying domain sizes.

Based on the CIT case in Table 1, we evaluate the weak scaling of the four simulation techniques. We run simulations identical to the CIT simulations in the previous section, except varying the domain in the z-direction as $L_z/d_p = 16, 24, 32, \ldots, 96$. Additionally, we revert to a two-node quadrature for AG. As the domain is increased, we increase the number of processors used in the simulations as 72, 108, 144, \ldots, 432. The total computational time for the evolution over $0.104 \tau_p$ is shown in Fig. 11.

We find that over the range of computational work considered, EL performs the best. AG and CHyQMOM27 perform similarly, but with much higher cost than EL. Finally, TP is found to be much more costly than all other methods. This is likely due to the expensive coordinate rotation applied to the moments in TP [16]. On the other hand, EL scales poorly compared to the QBMMs, and for large problems can be expected to perform worse than CHyQMOM27 and other QBMMs.
Table 3

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle diameter</td>
<td>$d_p$</td>
<td>$200 \times 10^{-6}$ m</td>
</tr>
<tr>
<td>Particle density</td>
<td>$\rho_p$</td>
<td>$2000$ kgm$^{-3}$</td>
</tr>
<tr>
<td>Fluid density</td>
<td>$\rho_f$</td>
<td>$1$ kgm$^{-3}$</td>
</tr>
<tr>
<td>Fluid dynamic viscosity</td>
<td>$\mu_f$</td>
<td>$1.8 \times 10^{-3}$ Pa s</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>$g$</td>
<td>$9.81 \text{ m s}^{-2}$</td>
</tr>
<tr>
<td>Coefficient of restitution (particle–particle)</td>
<td>$e$</td>
<td>$1$ (CHyQMOM27), 0.9 (EL)</td>
</tr>
<tr>
<td>Coefficient of restitution (particle–wall)</td>
<td>$e_w$</td>
<td>$1$ (CHyQMOM27), 0.9 (EL)</td>
</tr>
<tr>
<td>Average particle volume fraction</td>
<td>$\mathbb{V}_0$</td>
<td>$0.01$</td>
</tr>
<tr>
<td>Particle response time</td>
<td>$\tau_p$</td>
<td>$0.2469$ s</td>
</tr>
<tr>
<td>Stokes settling speed</td>
<td>$\tau_s g$</td>
<td>$0.9$ ms$^{-1}$</td>
</tr>
<tr>
<td>Fluid mean flowrate</td>
<td>$\bar{\tau}_{f,x}$</td>
<td>$0.9$ ms$^{-1}$</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>$Re_p$</td>
<td>$10$</td>
</tr>
<tr>
<td>Domain size</td>
<td>$\frac{L_z}{\Delta z}$</td>
<td>$2500$</td>
</tr>
<tr>
<td>Grid spacing (streamwise and depth)</td>
<td>$\Delta x/\Delta p = \Delta z/\Delta p$</td>
<td>$3.125$</td>
</tr>
<tr>
<td>Grid spacing (wall normal)</td>
<td>$\Delta y/\Delta p$</td>
<td>variable</td>
</tr>
<tr>
<td>CFL</td>
<td>$\text{CFL}$</td>
<td>$0.5$</td>
</tr>
</tbody>
</table>

6.4. Particle-laden channel flow

While CIT provides initial validation that CHyQMOM27 recovers a similar solution to EL in the context of coupled fluid-particle flow, the particle phase in CIT is close to equilibrium. In this section, we present CHyQMOM27 simulations using similar parameters as the EL particle-laden channel simulations by Capecelatro et al. [4,5] and examine the behavior of CHyQMOM27 in this coupled and far-from-equilibrium flow. As with homogeneous CIT, we initialize the domain with particles homogeneously suspended in fluid and allow the particles to fall under gravity. For this channel case, however, walls oriented parallel to the direction of gravity are added. Additionally, the fluid is forced upwards, opposing gravity to mimic risers in circulating fluidized beds. To match [4,5], the fluid flowrate is chosen to be equal the Stokes settling speed of the particles. The streamwise and depth direction flows are periodic. Due to the lack of collisional fluxes in CHyQMOM27 the inelastic collisions result in a blowup in the volume fraction for the channel case. Therefore, we revert to the elastic collision model for CHyQMOM27. The parameters used in this simulation are shown in Table 3.

Following [4,5], we perform these simulations on a stretched mesh that is more refined near the walls in the $y$ direction. However, we use a different function to vary $\Delta y$. First, the locations of the wall normal grid cell faces is chosen as

$$
\frac{y_{p - \frac{1}{2}}}{L_y} = \frac{1}{2} \left[ 1 - \cos \left( \frac{p - 1}{ny} \right) \right]
$$

(72)

where $ny = 136$ is number of grid cells in the $y$ direction and $p = 1, 2, 3, \ldots, ny + 1$ are the grid cell indices. Note that the particle diameter is larger than the grid cells near the wall. We modify the grid in (72) by shifting the faces closest to one particle radius away from the wall to be exactly one particle radius away from the wall. With this grid, the modification to the particle moment fluxes due to walls in (52) can be used at those shifted grid cell faces. A schematic of the grid near the wall is shown in Fig. 12.

This simulation is run until it reaches a steady state after about $20\tau_p$. A representative image of the volume fraction is shown in Fig. 13. While it is able to capture the clustering at the walls found in EL simulations by Capecelatro et al. [4–6], CHyQMOM27 also results in an oscillatory volume fraction field. This is likely unphysical because the EL simulations by Capecelatro et al. do not show a similar phenomenon. These oscillations do not appear to be a numerical artifact, but are likely resulting from the solution given by the CHyQMOM27 closure. The oscillations are well resolved and similar unsteadiness is apparent in the three-jet crossing case. The CIT case does not show these oscillations because the particle-phase dynamics remain relatively close to equilibrium. The CHyQMOM27 closure will need additional modeling to achieve better agreement with EL in dilute regions. However, since this work focuses on extending CHyQMOM to 3-D, such modeling is outside the scope of this paper. In addition, these oscillations appear only to occur on small scales, so we may still compare CHyQMOM27 and EL via coarse-grained statistics.

Due to the inhomogeneity of the channel simulation, the Reynolds average, $\langle A \rangle (y)$, is estimated by averaging over the $x$ and $z$ directions and over time ($10\tau_p$). Phase averages are defined identically as for CIT. Statistics for the channel case are shown in Fig. 14. We find the lower-order statistics from the volume fraction distribution, i.e. the mean and the variance, to be similar in both CHyQMOM27 and EL. However, the skewness is found to be much lower for CHyQMOM27. This is likely because we use an elastic collision model whereas an inelastic model would enhance clustering. Despite this discrepancy, the remaining statistics are similar for both methods. The velocity statistics, the particle slip velocity [3], the PA particle velocity, and the PA fluid velocity, likewise are very similar for both methods. However, the particle fluctuation energy and fluid TKE is found to be significantly higher in CHyQMOM27 than in EL. This may be related to the oscillations observed in the volume fraction field, or to larger clusters in CHyQMOM27 compared to EL [26].
7. Conclusions

This work introduces the 3-D extension of CHyQMOM [19], a high-order moment closure to the kinetic equation that preserves hyperbolicity. We implement the 3-node quadrature with flux-based quadrature, a collision operator, and coupling with a fluid solver to simulate collisional gas–particle flows. We compare CHyQMOM$_{27}$ to previous QBMMs, AG and TP, to evaluate the effect of using a higher-order closure and maintaining hyperbolicity. Additionally, we compare these QBMMs to EL to determine the ability of CHyQMOM$_{27}$ to reproduce results from EL. From jet-crossing cases, we find CHyQMOM$_{27}$ can capture dynamics further from equilibrium than AG without producing the δ-shocks found in TP. In CIT simulations, CHyQMOM$_{27}$ and AG agree well with EL, while TP produces stronger clustering behavior indicative of δ-shocks. However, in channel flow simulations, we find CHyQMOM$_{27}$ produces unphysical oscillations in regions where collisions are negligible. CHyQMOM$_{27}$ is shown to be only slightly more computationally costly than AG, while both are much less costly than TP. Although the QBMMs are shown to be more costly than EL for the range of simulations considered, they scale better than EL. This suggests CHyQMOM$_{27}$ may be a practical method for larger simulations. Future work may involve regularization of the CHyQMOM$_{27}$ closure. Struchtrup and Torrilhon have previously introduced a regularization to Grad’s 13-moment equations to smooth the subshocks inherent to the original method by Grad [29]. CHyQMOM$_{27}$ may benefit from a similar procedure.

Conflict of interest statement

There is no conflict of interest.

Acknowledgements

ROF was supported by a grant from the U.S. National Science Foundation (CBET-1437865 and ACI-1440443). RGP and OD were also supported by a grant from the National Science Foundation (CBET-1437903).
Fig. 14. Channel statistics as a function of wall-normal distance for CHyQMOM27 (—) and EL (— – –) [4,5]. In order from left to right and top to bottom, Reynolds-averaged volume fraction, volume fraction variance, volume fraction skewness, x direction slip velocity, PA x direction settling velocity, PA x direction fluid velocity, particle TKE, and fluid TKE.

Appendix A. Modified conditional quadrature method of moments

In the original formulation of CQMOM [32], ideas based on linear algebra were used to compute the conditional univariate moments from the multivariate moments. In this work, a modified version of CQMOM is employed that uses monomial expansions in the quadrature nodes of the conditioning variable. This has several advantages, which includes using a smaller set of moments. The modified CQMOM uses the central moments to determine the expansion coefficients. Below we describe the basic steps using the 3-D velocity moments.

A.1. Modified CQMOM for 3-D velocity moments

Let us assume that the integer velocity moments $M_{i,j,k}$ (as defined using the VDF in the main text) exist for all positive integers $i, j, k$. Let us also assume that $M_{0,0,0} > 0$ so that the central moments $C_{i,j,k}$ also exist. In the following, we will make use of the Hankel matrix $H_{2n}$ for the univariate central moments [14]. For example, for the moments indexed by $i$, the Hankel matrix is
The Hankel matrix is positive if \( |H_{2n}| > 0 \), null if \( |H_{2n}| = 0 \), and negative if \( |H_{2n}| < 0 \). The central moment set \( \{C_{2,0,0}, C_{3,0,0}, \ldots, C_{2n,0,0}\} \) is realizable if \( H_{2n} \) is non-negative. Let \( m \), such that \( 1 \leq m \leq n \), be the smallest integer for which \( H_{2n} \) is null. If \( m \) exists and the moment set is realizable, then \( H_{2n+m+2} \) up to \( H_{2n} \) are also null. We will refer to such cases as degenerate. The corresponding VDF is composed of exactly \( m \) Dirac delta functions with nonzero weights and distinct abscissas [14]. Note that if the VDF is approximated by \( N \) delta functions (e.g., with HyQ MOM \( _N \)), then \( |H_{2N}| = 0 \). Below we will see that \( |H_{2n-2}| > 0 \) is required for CQ MOM, which will be the case for non-degenerate moment sets.

With CQ MOM, one direction is chosen as the conditioning variable. Here we choose the first (u) direction and assume that \( H_{2n-2} \) is positive. Using the central moment set \( \{C_{2,0,0}, C_{3,0,0}, \ldots, C_{2n-1,0,0}\} \), the ChyQ MOM \( _n \) reconstruction of the joint VDF for \( 1 \leq n \) is

\[
f^\alpha(u, v, w) = M_{0,0,0} \sum_{\alpha=1}^{n} \rho_\alpha \delta_{u+u_\alpha}(u) f_\alpha(v, w)
\]

(A.2)

where \( f_\alpha(v, w) \) is the unknown conditional joint VDF. Because \( H_{2n-2} \) is positive, the weights \( \rho_\alpha \) are positive, and the abscissas \( u_\alpha \) are distinct. The univariate central moments are related to these weights and abscissa by

\[
C_{i,0,0} = \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^i \text{ for } i \in \{0, 1, \ldots, 2n-1\}
\]

(A.3)

where \( C_{0,0,0} = 1 \) and \( C_{1,0,0} = 0 \). As noted above, the \( C_{2n,0,0} \) found from (A.3) yields \( |H_{2n}| = 0 \). For ChyQ MOM \( _n \), we restrict the highest-order mixed moment to \( i+j+k=n \), while the highest univariate moments are order \( 2n-2 \) where \( 1 \leq n \) is the number of HyQ MOM \( _n \) abscissas. (The case with \( n = 1 \) is trivial in the present context.) The multivariate central moments found from (A.2) are

\[
C_{i,j,k} = \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^i M_{j,k|\alpha}
\]

(A.4)

where

\[
M_{j,k|\alpha} := \int_{\mathbb{R}^2} f_\alpha(v, w)(v - \tilde{v})^j(w - \tilde{w})^k dvdw
\]

(A.5)

are the unknown bivariate moments of \( v \) and \( w \) conditioned on \( u = u_\alpha \). Comparing (A.4) to (A.3), we see that \( M_{0,0|\alpha} = 1 \). For the first-order conditional moments, we seek expansions of the form

\[
M_{1,0|\alpha} = a_0 + a_1 u_\alpha + a_2 u_\alpha^2 + \cdots + a_{n-1} u_\alpha^{n-1},
\]

\[
M_{0,1|\alpha} = b_0 + b_1 u_\alpha + b_2 u_\alpha^2 + \cdots + b_{n-1} u_\alpha^{n-1},
\]

(A.6)

which, together with (A.4), yield

\[
C_{i,1,0} = a_0 C_{i,0,0} + a_1 C_{i+1,0,0} + a_2 C_{i+2,0,0} + \cdots + a_{n-1} C_{i+n-1,0,0},
\]

\[
C_{i,0,1} = b_0 C_{i,0,0} + b_1 C_{i+1,0,0} + b_2 C_{i+2,0,0} + \cdots + b_{n-1} C_{i+n-1,0,0}
\]

(A.7)

for \( i \in \{0, 1, \ldots, n-1\} \). Using \( M_{1,0|\alpha} \) as an example, the expansion coefficients are found from the linear system:

\[
\begin{pmatrix}
1 & 0 & C_{2,0,0} & \cdots & C_{n-1,0,0} \\
0 & C_{2,0,0} & C_{3,0,0} & \cdots & C_{n,0,0} \\
C_{2,0,0} & C_{3,0,0} & C_{4,0,0} & \cdots & C_{n+1,0,0} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
C_{n-1,0,0} & C_{n,0,0} & C_{n+1,0,0} & \cdots & C_{2n-2,0,0}
\end{pmatrix}
\begin{pmatrix}
a_0 \\
a_1 \\
a_2 \\
\vdots \\
a_{n-1}
\end{pmatrix} =
\begin{pmatrix}
0 \\
C_{1,1,0} \\
C_{2,1,0} \\
\vdots \\
C_{n-1,1,0}
\end{pmatrix}
\]

(A.8)

whose coefficient matrix is the Hankel matrix \( H_{2n-2} \). By assumption, \( H_{2n-2} \) is positive and, hence, (A.8) has a unique solution. It then follows that \( M_{1,0|\alpha} \) and \( M_{0,1|\alpha} \) in the form of (A.7) are computable provided that the bivariate central moments \( \{C_{1,1,0}, C_{2,1,0}, \ldots, C_{n-1,1,0}\} \) and \( \{C_{1,0,1}, C_{2,0,1}, \ldots, C_{n-1,0,1}\} \) are known.
For the higher-order conditional moments, we start by defining the central conditional moments:

\[ C_{j,k|\alpha} := \int_{\mathbb{R}^2} f_{\alpha}(v, w) (v - \tilde{v} - M_{1,0|\alpha})^j (w - \tilde{w} - M_{0,1|\alpha})^k \, dv \, dw \] (A.9)

where \( C_{0,0|\alpha} = 1 \) and \( C_{1,0|\alpha} = C_{0,1|\alpha} = 0 \). Using binomial expansions, these moments are related to \( M_{j,k|\alpha} \) by

\[ M_{j,k|\alpha} = \sum_{j_1=0}^{j} \sum_{k_1=0}^{k} \binom{j}{j_1} \binom{k}{k_1} M_{1,0|\alpha}^{j-j_1} M_{0,1|\alpha}^{k-k_1} C_{j_1,k_1|\alpha}. \] (A.10)

and thus to the central moments by

\[ C_{i,j,k} := \sum_{j_1=0}^{j} \sum_{k_1=0}^{k} \binom{j}{j_1} \binom{k}{k_1} \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^{i} M_{1,0|\alpha}^{j-j_1} M_{0,1|\alpha}^{k-k_1} C_{j_1,k_1|\alpha}. \] (A.11)

As shown next, this expression is the starting point for determining the unknown central conditional moments \( C_{j,k|\alpha} \).

Starting with the conditional variances, we seek expansions of the form

\[ C_{2,0|\alpha} = C_0 + C_1 u_\alpha + C_2 u_\alpha^2 + \cdots + C_{n-2} u_\alpha^{n-2} \geq 0, \] 
\[ C_{0,2|\alpha} = d_0 + d_1 u_\alpha + d_2 u_\alpha^2 + \cdots + d_{n-2} u_\alpha^{n-2} \geq 0, \] (A.12)

which, together with (A.11), yield

\[ C_{1,2,0} - \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^{1} M_{1,0|\alpha}^2 = C_0 C_{1,0,0} + C_1 C_{1,1,0} + C_2 C_{1,2,0} + \cdots + C_{n-2} C_{1,n-2,0,0}. \] (A.13)

Using \( C_{2,0|\alpha} \) as an example, the expansion coefficients are found from the linear system:

\[
\begin{pmatrix}
1 & 0 & C_{2,0,0} & \cdots & C_{n-2,0,0} \\
0 & C_{2,0,0} & C_{3,0,0} & \cdots & C_{n-1,0,0} \\
C_{2,0,0} & C_{3,0,0} & C_{4,0,0} & \cdots & C_{n,0,0} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
C_{n-2,0,0} & C_{n-1,0,0} & C_{n,0,0} & \cdots & C_{2n-4,0,0}
\end{pmatrix}
\begin{pmatrix}
c_0 \\
c_1 \\
c_2 \\
\vdots \\
c_{n-2}
\end{pmatrix} = \begin{pmatrix}
C_{2,0,0} - \sum_{\alpha=1}^{n} \rho_\alpha M_{1,0|\alpha}^2 \\
C_{1,2,0} - \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha M_{1,0|\alpha}^2 \\
C_{2,2,0} - \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^2 M_{1,0|\alpha}^2 \\
\vdots \\
C_{n-2,2,0} - \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^{n-2} M_{1,0|\alpha}^2
\end{pmatrix} \] (A.14)

whose coefficient matrix is the Hankel matrix \( H_{2n-4} \). By assumption, \( H_{2n-4} \) is positive and, hence, (A.14) has a unique solution. It then follows that \( C_{2,0|\alpha} \) and \( C_{2,0|\alpha} \) in the form of (A.13) are computable provided that the bivariate conditional moments \( \{C_{2,0,0}, C_{2,1,0}, \ldots, C_{n-2,2,0}\} \) and \( \{C_{0,2,0}, C_{1,0,2}, \ldots, C_{n,0,2}\} \) are known.

In general, the realizability constraints \( C_{2,0|\alpha}, C_{2,0|\alpha} \geq 0 \) will not be guaranteed by the solution to (A.14). For example, in the main text with \( n = 3 \), it was necessary to limit \( C_1, d_1 \) to ensure that the conditional variances are non-negative, thereby losing the ability to reproduce exactly the third-order moments \( C_{2,0,0}, C_{1,0,2} \). Furthermore, for a well-defined conditional mean, we expect

\[ C_{2i,2j} \geq \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^{2i} M_{1,0|\alpha}^2 \text{ and } C_{2i,0,2j} \geq \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^{2i} M_{0,1|\alpha}^2 \text{ for } i \in \{0, 1, \ldots, n - 1\} \] (A.15)

with the equality holding when \( C_{2,0|\alpha}, C_{2,0|\alpha} = 0 \). These inequalities represent constraints on the expansion coefficients \( a_k, b_k \). In the main text, we employed \( n = 3 \) and set \( a_2 = b_2 = 0 \) using appropriate choices for \( C_{2,1,0}, C_{2,0,1} \).

Assuming that the conditional variances have been found, we next define scaled conditional moments \( S_{j,k|\alpha} \) by

\[ S_{j,k|\alpha} = \frac{\rho_\alpha^{j/2} u_\alpha^{k/2} M_{1,0|\alpha}^{j/2} M_{0,1|\alpha}^{k/2}}{S_{0,2|\alpha}^{j/2} S_{0,2|\alpha}^{k/2}} \] (A.16)

for \( j + k \geq 2 \) with \( S_{0,0|\alpha} = 1 \), \( S_{1,0|\alpha} = S_{0,1|\alpha} = 0 \) and \( S_{2,0|\alpha} = S_{0,2|\alpha} = 1 \). Thus the central moments are

\[ S_{i,j,k} = \sum_{j_1=0}^{j} \sum_{k_1=0}^{k} \binom{j}{j_1} \binom{k}{k_1} \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^{i} M_{1,0|\alpha}^{j-j_1} M_{0,1|\alpha}^{k-k_1} S_{j_1,k_1|\alpha}. \] (A.17)

For the conditional correlation coefficient, we assume an expansion of the form
\[ S_{1,1\alpha} = e_0 + e_1 u_{\alpha} + e_2 u_{\alpha}^2 + \cdots + e_{n-2} u_{\alpha}^{n-2}, \]  
which yields
\[ C_{i,1,1} - \sum_{\alpha=1}^{n} \rho_{\alpha} u_{\alpha}^i M_{1,0\alpha} M_{0,1\alpha} = \sum_{\alpha=1}^{n} \rho_{\alpha} C_{2,0\alpha}^{1/2} C_{0,2\alpha}^{1/2} \left( e_0 u_{\alpha}^i + e_1 u_{\alpha}^{i+1} + e_2 u_{\alpha}^{i+2} + \cdots + e_{n-2} u_{\alpha}^{i+n-2} \right). \]  

For \( i \in \{0, 1, \ldots, n-2\} \), the resulting linear system yields the coefficients \( e_k \). The coefficient matrix has full rank if \( C_{2,0\alpha} C_{0,2\alpha} > 0 \) for all \( \alpha \). For each \( \alpha \) for which \( C_{2,0\alpha} C_{0,2\alpha} = 0 \), the number of coefficients \( e_k \) must be reduced by one.

In the main text for \( n = 3 \), we set \( e_1 = 0 \) by an appropriate choice for \( C_{1,1,1} \) and solve (A.19) for \( e_0 \) using \( C_{0,1,1} \).

The scaled third-order moments are determined in a similar fashion when \( n \geq 3 \). Taking \( S_{3,0\alpha} \) as an example, we assume an expansion of the form (for \( 3 \leq n \))
\[ S_{3,0\alpha} = f_0 + f_1 u_{\alpha} + f_2 u_{\alpha}^2 + \cdots + f_{n-3} u_{\alpha}^{n-3}, \]  
which yields
\[ C_{i,3,0} - \sum_{\alpha=1}^{n} \rho_{\alpha} u_{\alpha}^i M_{1,0\alpha} \left( M_{1,0\alpha}^2 + 3 C_{2,0\alpha} \right) = \sum_{\alpha=1}^{n} \rho_{\alpha} C_{2,0\alpha}^{3/2} \left( f_0 u_{\alpha}^i + f_1 u_{\alpha}^{i+1} + \cdots + f_{n-3} u_{\alpha}^{i+n-3} \right) \]  
with \( i \in \{0, 1, \ldots, n-3\} \). As described above, the size of this linear system has to be reduced if any \( C_{2,0\alpha} = 0 \). The procedure for determining \( S_{2,1\alpha}, S_{2,2\alpha}, \) and \( S_{0,3\alpha} \) follows the same reasoning. In the main text, \( n = 3 \) so that only the zero-order coefficient \( f_0 \) is needed to determine \( S_{3,0\alpha} \) (and the other third-order moments).

The scaled fourth-order moments are determined in a similar fashion when \( n \geq 4 \). Taking \( S_{4,0\alpha} \) as an example, we assume an expansion of the form (for \( 4 \leq n \), else \( S_{4,0\alpha} - 1 - S_{2,0\alpha}^2 \) is a non-negative constant)
\[ S_{4,0\alpha} = g_0 + g_1 u_{\alpha} + g_2 u_{\alpha}^2 + \cdots + g_{n-4} u_{\alpha}^{n-4} \geq 0, \]  
which yields
\[ C_{i,4,0} - \sum_{\alpha=1}^{n} \rho_{\alpha} u_{\alpha}^i M_{1,0\alpha} \left( M_{1,0\alpha}^2 + 6 M_{1,0\alpha} C_{2,0\alpha} + 4 C_{3,0\alpha} \right) - \sum_{\alpha=1}^{n} \rho_{\alpha} u_{\alpha}^i C_{2,0\alpha}^2 \left( 1 + S_{2,0\alpha}^2 \right) = \sum_{\alpha=1}^{n} \rho_{\alpha} C_{2,0\alpha}^2 \left( g_0 u_{\alpha}^i + g_1 u_{\alpha}^{i+1} + \cdots + g_{n-4} u_{\alpha}^{i+n-4} \right) \]  
with \( i \in \{0, 1, \ldots, n-4\} \). As described above, the size of this linear system has to be reduced if any \( C_{2,0\alpha} = 0 \). The procedure for determining the other fourth-order moments follows the same reasoning. In the main text, \( n = 3 \) so that \( S_{4,0\alpha} \) and \( S_{0,4\alpha} \) are constants found from \( C_{0,4,0} \) and \( C_{0,0,4} \), respectively.

In principle, the procedure for computing the conditional moments can be applied for \( n > 3 \). However, in practice, the realizability constraints will become more difficult to satisfy. In this work, we use \( n = 3 \) with cross moments up to third order. Next we describe how to use the conditional moments \( M_{j,k\alpha} \) to construct a 2-D CHyQ MOM approximation for \( f_{\alpha}(v, w) \) in (A.2) for each \( \alpha \).

### A.2. Conditional moments and statistics for \( n = 3 \)

In A.3, the 2-D formulas resulting from the modified CQ MOM with \( n = 3 \) are presented in a compact form. The following statistics from the trivariate velocity moments appear in these formulas.

**Mean velocities**
\[ \bar{u} = \frac{M_{1,0,0}}{M_{0,0,0}}, \quad \bar{v} = \frac{M_{0,1,0}}{M_{0,0,0}}, \quad \bar{w} = \frac{M_{0,0,1}}{M_{0,0,0}} \]

**Correlation coefficients**
\[ \rho_{uv} = \frac{C_{1,1,0}}{C_{2,0,0}^{1/2} C_{0,2,0}^{1/2}}, \quad \rho_{uw} = \frac{C_{1,0,1}}{C_{2,0,0}^{1/2} C_{0,0,2}^{1/2}}, \quad \rho_{vw} = \frac{C_{0,1,1}}{C_{0,2,0}^{1/2} C_{0,0,2}^{1/2}} \]
Skewness coefficients

\[
\begin{align*}
q_u & = \frac{C_{3,0}}{C_{2,0}^{3/2}} \quad q_v = \frac{C_{3,0}}{C_{2,0}^{3/2}} \quad q_w = \frac{C_{0,3}}{C_{0,2}^{3/2}} \\
q_{uv} & = \frac{C_{1,2}}{C_{2,0} C_{0,2}} = \varepsilon_{uv} q_v \quad q_{uw} = \frac{C_{1,0}}{C_{2,0} C_{0,2}} = \varepsilon_{uw} q_w \\
q_{vw} & = \frac{C_{0,1}}{C_{2,0} C_{0,2}} = \varepsilon_{vw} q_v \quad q_{vu} = \frac{C_{2,1}}{C_{2,0} C_{0,2}} = \varepsilon_{vu} q_u \\
q_{wu} & = \frac{C_{2,0,1}}{C_{0,2} C_{2,0}} = \varepsilon_{wu} q_u \quad q_{vv} = \frac{C_{0,2,1}}{C_{0,2} C_{2,0}} = \varepsilon_{vv} q_v \\
q_{uvw} & = \frac{C_{1,1,1}}{C_{2,0,0} C_{0,2} C_{0,2}} = \varepsilon_{uvw} \eta_w
\end{align*}
\]

Flatness coefficients

\[
\begin{align*}
\eta_u & = \frac{C_{4,0,0}}{C_{2,0}^{2}} \quad \eta_v = \frac{C_{4,0,0}}{C_{2,0}^{2}} \quad \eta_w = \frac{C_{0,4,0}}{C_{2,0}^{2}} \\
\end{align*}
\]

Here we assume that the variances are nonzero in all directions so that all of the above statistics are well defined. Note that closures for the bivariate skewness coefficients have been introduced. These are consistent with the 2-D CHyQMOM₉ reconstruction used in the main text.

The following conditional statistics, found from the \( u \)-conditioned bivariate velocity moments \( M_{j,k}\alpha \) and \( C_{j,k}\alpha \) introduced in A1, are needed. The scaled \( u \) abscissas are defined as \( u_\alpha = C_{2,0,0}^{1/2} u^\alpha \).

\( u \)-conditioned mean velocities

\[
\begin{align*}
\bar{v}_\alpha & = \bar{v} + M_{1,0}\alpha = \bar{v} + C_{0,2,0}^{1/2} \varepsilon_{uv} u_\alpha^\dagger \quad \bar{w}_\alpha = \bar{w} + M_{0,1}\alpha = \bar{w} + C_{0,2,0}^{1/2} \varepsilon_{uw} u_\alpha^\dagger \\
\end{align*}
\]

\( u \)-conditioned variances

\[
\begin{align*}
C_{2,0}\alpha & = C_{0,2,0} \left[ 1 - \varepsilon_{vv}^2 + \varepsilon_{uv} (q_v - \varepsilon_{uv} q_u) u_\alpha^\dagger \right] \quad C_{0,2}\alpha = C_{0,0,2} \left[ 1 - \varepsilon_{uu}^2 + \varepsilon_{uw} (q_w - \varepsilon_{uw} q_u) u_\alpha^\dagger \right]
\end{align*}
\]

\( u \)-conditioned correlation coefficient

\[
\begin{align*}
\varepsilon_{vw}\alpha & = \frac{C_{1,1}\alpha}{C_{2,0,0}^{1/2} C_{0,2,0}^{1/2}} = \frac{1}{S_{1,1}^{1/2} C_{2,0,0}^{1/2}} \left( \varepsilon_{vw} - \varepsilon_{uv} \varepsilon_{uw} \right) \\
\end{align*}
\]

\( u \)-conditioned skewness coefficients

\[
\begin{align*}
q_v\alpha & = \frac{C_{3,0}\alpha}{C_{2,0}^{3/2}} = S_{3,0}\alpha = \frac{3}{3} \left( q_v + 2 \varepsilon_{uv} q_u - 3 \varepsilon_{uw}^2 q_v \right) \\
q_w\alpha & = \frac{C_{0,3}\alpha}{C_{2,0}^{3/2}} = S_{0,3}\alpha = \frac{3}{3} \left( q_w + 2 \varepsilon_{uw} q_u - 3 \varepsilon_{uw}^2 q_w \right) \\
q_{vw}\alpha & = \frac{C_{1,2}\alpha}{C_{2,0,0}^{1/2} C_{0,2,0}^{1/2}} = \varepsilon_{vw}\alpha q_v\alpha \quad q_{wv}\alpha = \frac{C_{2,1}\alpha}{C_{2,0,0}^{1/2} C_{0,2,0}^{1/2}} = \varepsilon_{vw}\alpha q_w\alpha \\
\end{align*}
\]

\( u \)-conditioned flatness coefficients

\[
\begin{align*}
\eta_v\alpha & = \frac{C_{4,0}\alpha}{C_{2,0}^{2}} = S_{4,0}\alpha \\
\eta_w\alpha & = \frac{C_{0,4}\alpha}{C_{2,0}^{2}} = S_{0,4}\alpha \\
\eta_{vw}\alpha & = \frac{C_{2,0,0}^{1/2} \left( \eta_v - \varepsilon_{uv}^4 \eta_u - 6 \varepsilon_{uv}^2 (1 - \varepsilon_{uv}^2) - 6 \varepsilon_{uv} (q_v - \varepsilon_{uv} q_u) q_u \right) - 4 \varepsilon_{0,2,0}^{1/2} \varepsilon_{uv} \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha^\dagger C_{3,0}\alpha}{\sum_{\alpha=1}^{3} \rho_\alpha C_{2,0}\alpha} \\
\end{align*}
\]

\[
\begin{align*}
\eta_{wv}\alpha & = \frac{C_{0,4}\alpha}{C_{2,0}^{2}} = S_{0,4}\alpha \\
\eta_{vw}\alpha & = \frac{C_{2,0,0}^{1/2} \left( \eta_w - \varepsilon_{uw}^4 \eta_u - 6 \varepsilon_{uw}^2 (1 - \varepsilon_{uw}^2) - 6 \varepsilon_{uw} (q_w - \varepsilon_{uw} q_u) q_u \right) - 4 \varepsilon_{0,2,0}^{1/2} \varepsilon_{uw} \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha^\dagger C_{3,0}\alpha}{\sum_{\alpha=1}^{3} \rho_\alpha C_{2,0}\alpha} \\
\end{align*}
\]
We assume that the conditional variances are nonzero in both directions so that all of the above statistics are well defined. However, if one of them is null for a particular value of \( \alpha \), then the formulas derived below can still be used by setting the corresponding abscissas equal to zero. Another possibility (e.g., for PTC) is that all of the conditional variances are very close to zero so that numerically the formulas for the conditional correlation, skewness and flatness coefficients are nearly singular. In such cases, we set \( \eta_{vw|\alpha} = 0 \), \( q_{w|\alpha} = q_{w|\alpha} = 0 \) and \( \eta_{w|\alpha} = \eta_{w|\alpha} = 1 \). As described in \( A.1 \), for \( n = 3 \) the conditioned skewness \( \{ \alpha_{1,0|\alpha}, \alpha_{0,3|\alpha} \} \) and flatness \( \{ \alpha_{1,0,4|\alpha}, \alpha_{0,4,0|\alpha} \} \) coefficients do not depend on \( \alpha \). However, we will keep the explicit \( \alpha \) notation in order to distinguish between the unconditional and conditional statistics (e.g., \( q_{v} \) and \( q_{v|\alpha} \)).

A.3. 2-D conditional weights and abscissas

The 2-D CHyQMOM\(_{9} \) reconstruction of \( f_{\alpha}(v, w) \) can be done by either conditioning on \( v \) or \( w \). Here we present the former:

\[
f_{\alpha}^{2}(v, w) = \sum_{\beta=1}^{3} \rho_{\alpha \beta} \delta_{\alpha \beta}^{v} + \rho_{\alpha \beta}^{v} (v) \sum_{\gamma=1}^{3} \rho_{\alpha \beta \gamma} \delta_{\alpha \beta \gamma} + \rho_{\alpha \beta}^{w} (w) \tag{A.24}
\]

The \( u \)-conditioned weights \( \rho_{\alpha \beta} \) and abscissas \( v_{\alpha \beta} \) in the \( v \) direction are computed using HyQMOM\(_{3} \) from the \( u \)-conditioned univariate moments \( \{1, 0, C_{2,0|\alpha}, C_{3,0|\alpha}C_{4,0|\alpha} \} \) for each \( \alpha \). Using the notation above, this yields

\[
\rho_{\alpha 1} = -1 / v_{\alpha 1}^{\dagger} \sqrt{4 \eta_{\alpha|\alpha} - 3 q_{\alpha|\alpha}^{2}}, \quad \rho_{\alpha 2} = \eta_{\alpha|\alpha} - q_{\alpha|\alpha}^{2} / \eta_{\alpha|\alpha} - q_{\alpha|\alpha}^{2}, \quad \rho_{\alpha 3} = 1 / v_{\alpha 3}^{\dagger} \sqrt{4 \eta_{\alpha|\alpha} - 3 q_{\alpha|\alpha}^{2}}, \tag{A.25}
\]

and \( v_{\alpha \beta} = C_{2,0|\alpha} / v_{\alpha \beta}^{\dagger} \) where

\[
v_{\alpha 1}^{\dagger} = 1 / 2 \left( q_{\alpha|\alpha} - \sqrt{4 \eta_{\alpha|\alpha} - 3 q_{\alpha|\alpha}^{2}} \right), \quad v_{\alpha 2}^{\dagger} = 0, \quad v_{\alpha 3}^{\dagger} = 1 / 2 \left( q_{\alpha|\alpha} + \sqrt{4 \eta_{\alpha|\alpha} - 3 q_{\alpha|\alpha}^{2}} \right). \tag{A.26}
\]

As \( q_{\alpha|\alpha} \) and \( \eta_{\alpha|\alpha} \) do not depend on \( \alpha \), nor do \( \rho_{\alpha \beta} \) and \( v_{\alpha \beta}^{\dagger} \).

The doubly conditioned mean of \( w \) is \( \bar{w}_{\alpha \beta} = C_{0,2|\alpha} \bar{w}_{\alpha \beta} = C_{0,2|\alpha} \bar{q}_{v w|\alpha} v_{\alpha \beta} \). The doubly conditioned variance of \( w \) is

\[
C_{2|\alpha \beta} = C_{0,2|\alpha} C_{2|\alpha \beta} = C_{0,2|\alpha} \left[ 1 - \frac{\rho_{v w|\alpha}^{2}}{C_{2|\alpha \beta}} + \rho_{v w|\alpha} \left( q_{w|\alpha} - \rho_{v w|\alpha} q_{v|\alpha} \right) \kappa_{w|\alpha} v_{\alpha \beta}^{\dagger} \right] \tag{A.27}
\]

where \( \kappa_{w|\alpha} \leq 1 \) is the limiter used to keep \( C_{2|\alpha \beta} \geq 0 \). The doubly conditioned third-order central moment of \( w \) is \( C_{3|\alpha \beta} = C_{3|\alpha \beta}^{\dagger} \eta_{w|\alpha} \) where

\[
C_{3|\alpha \beta} = \frac{\eta_{w|\alpha} - \rho_{v w|\alpha}^{2} q_{w|\alpha} - 3 \rho_{v w|\alpha}^{2} (q_{w|\alpha} - \rho_{v w|\alpha} q_{v|\alpha}) \kappa_{w|\alpha} v_{\alpha \beta}}{\sum_{\beta=1}^{3} \rho_{\alpha \beta} C_{2|\alpha \beta}^{3/2}} \tag{A.28}
\]

The doubly conditioned fourth-order central moment of \( w \) is \( C_{4|\alpha \beta} = C_{4|\alpha \beta}^{\dagger} \eta_{w|\alpha} \) where

\[
\eta_{w|\alpha} = \frac{\eta_{w|\alpha} - \rho_{v w|\alpha}^{4} q_{w|\alpha} - 6 \rho_{v w|\alpha}^{4} \left( q_{w|\alpha} - \rho_{v w|\alpha} q_{v|\alpha} \right) \kappa_{w|\alpha} q_{w|\alpha} \kappa_{w|\alpha} q_{v|\alpha} - 4 \rho_{v w|\alpha} q_{w|\alpha} \kappa_{w|\alpha} q_{w|\alpha} \sum_{\beta=1}^{3} \rho_{\alpha \beta} v_{\alpha \beta}^{\dagger} C_{2|\alpha \beta}^{3/2}}{\sum_{\beta=1}^{3} \rho_{\alpha \beta} C_{2|\alpha \beta}^{3/2}} \tag{A.29}
\]

As described in the main text, \( q_{w|\alpha}^{\ast} \) and \( \eta_{w|\alpha}^{\ast} \) must be checked for realizability (i.e., \( \eta_{w|\alpha}^{\ast} \geq q_{w|\alpha}^{2} + 1 \)), and corrected if needed.

The CHyQMOM\(_{27} \) weights \( \rho_{\alpha \beta \gamma} \) and abscissas \( w_{\alpha \beta \gamma} \) in the third (\( w \)) direction are related to \( q_{w|\alpha}^{\ast} \) and \( \eta_{w|\alpha}^{\ast} \) by

\[
\left\{1, 0, 1, q_{w|\alpha}^{\ast}, \eta_{w|\alpha}^{\ast}\right\} \quad \Longrightarrow \quad \left\{ \rho_{\gamma|\alpha}^{\ast}, w_{\gamma|\alpha}^{\ast} \right\} \quad \Longrightarrow \quad \left\{ \rho_{\alpha \beta \gamma}^{\ast}, w_{\alpha \beta \gamma}^{\ast} = C_{2|\alpha \beta}^{1/2} w_{\alpha \beta \gamma}^{\ast} \right\}
\]

where

\[
\rho_{\gamma|\alpha}^{\ast} = -1 / w_{\gamma|\alpha}^{\dagger} \sqrt{4 \eta_{\gamma|\alpha}^{\ast} - 3 q_{\gamma|\alpha}^{2}}, \quad \rho_{\gamma|\alpha}^{\ast} = \eta_{\gamma|\alpha}^{\ast} - q_{\gamma|\alpha}^{2} / \eta_{\gamma|\alpha}^{\ast} - q_{\gamma|\alpha}^{2}, \quad \rho_{\gamma|\alpha}^{\ast} = 1 / w_{\gamma|\alpha}^{\dagger} \sqrt{4 \eta_{\gamma|\alpha}^{\ast} - 3 q_{\gamma|\alpha}^{2}}\tag{A.30}
\]

and

\[
w_{\gamma|\alpha}^{\dagger} = 1 / 2 \left( q_{w|\alpha}^{\ast} - \sqrt{4 \eta_{w|\alpha}^{\ast} - 3 q_{w|\alpha}^{2}} \right), \quad w_{\gamma|\alpha}^{\ast} = 0, \quad w_{\gamma|\alpha}^{\ast} = 1 / 2 \left( q_{w|\alpha}^{\ast} + \sqrt{4 \eta_{w|\alpha}^{\ast} - 3 q_{w|\alpha}^{2}} \right). \tag{A.31}
\]
Note that the weights do not depend on $\beta$, while the abscissas are scaled by the doubly conditioned variance. In the degenerate case where $\eta_{w|\alpha} = q_{w|\alpha}^2 + 1$, the conditional pdf is two delta functions so that $\rho_{2|\alpha} = 0$. The latter occurs, for example, due to PTC.

Appendix B. Kinetic-based flux with CHyQMOM$_2$

In this appendix, the formulas needed to define the kinetic-based flux in the $u$ direction are presented. The methodology is nearly identical to that in A.1 for $n = 3$. The statistics appearing in the formulas, found from the trivariate velocity moments, are defined in A.2. Here we assume that the variances are nonzero in all directions so that all of the statistics are well defined.

B.1. Kinetic-based VDF reconstruction

The kinetic-based VDF reconstruction in the $x$ direction has the form

$$f_{VW}(v) = M_{0,0,0} \sum_{\alpha=1}^{4} w_{\alpha} \delta_{x\alpha}(u) f_{\alpha}(v, w) \quad (B.1)$$

where the flux eigenvalues are $\lambda_0 = \bar{u}$ and $\lambda_{\alpha} = \bar{u} + C_{2,0,0}^{1/2} \phi_{\alpha}$. The four abscissas $\phi_{\alpha}$ are

$$\phi_{(1,2,3,4)} = \frac{1}{2} \left( q_u \pm \sqrt{4 \eta_u - 3 q_u^2 \pm 4 \left( (\eta_u - q_u^2) (\eta_u - q_u^2 - 1) \right) } \right) \quad (B.2)$$

and the weights $w_{\alpha}$ are found by solving the moment constraints:

$$M_{0,0,0} \begin{bmatrix} 1 & 1 & 1 & 1 \\ \lambda_0 & \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_2 & \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_3 & \lambda_2 & \lambda_1 & \lambda_2 \\ \lambda_4 & \lambda_1 & \lambda_2 & \lambda_3 \\ \lambda_3 & \lambda_2 & \lambda_1 & \lambda_2 \\ \lambda_4 & \lambda_1 & \lambda_2 & \lambda_3 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} \phi_1 & \phi_2 & \phi_3 & \phi_4 \\ \phi_1 & \phi_2 & \phi_3 & \phi_4 \\ \phi_1 & \phi_2 & \phi_3 & \phi_4 \\ \phi_1 & \phi_2 & \phi_3 & \phi_4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ q_u \end{bmatrix} \quad (B.3)$$

where $w_0 = 0$ and $w_{\alpha} \geq 0$. In fact, these weights and abscissas are a 4-node Gaussian quadrature for an unknown distribution function parameterized by $q_u$ and $\eta_u$. For the special case where $q_u = 0$ and $\eta_u = 3$, it is the 4-node Gauss–Hermite quadrature.

B.2. Conditional central moments

The conditional VDF $f_{\alpha}(v, w)$ in (B.1) is unknown. However, we can relate its moments to the trivariate central moments by

$$C_{i,j,k} = C_{2,0,0}^{1/2} \sum_{\alpha=1}^{4} w_{\alpha} \phi_{\alpha}^i M_{j,k|\alpha} \text{ where } M_{j,k|\alpha} := \int_{\mathbb{R}^2} f_{\alpha}(v, w) (v - \bar{v})^j (w - \bar{w})^k dvdw. \quad (B.4)$$

Note that the conditional moments $M_{j,k|\alpha}$ are not central moments because the first-order moments can be nonzero. They are related to the bivariate moments in $(v, w)$ conditioned on the $u$ direction appearing in the main text:

$$\Theta_{u,\alpha}^{j,k} := \sum_{j_1=0}^{j} \sum_{k_1=0}^{k} \binom{j}{j_1} \binom{k}{k_1} \bar{v}^{j-j_1} \bar{w}^{k-k_1} M_{j_1,k_1|\alpha}. \quad (B.5)$$

Thus, explicit formulas are needed for $M_{j,k|\alpha}$ with the ten combinations of $j, k$ in 2-D CHyQMOM$_9$. First, $M_{0,0,0|\alpha} = 1$ and the conditional means are

$$M_{1,0,0|\alpha} = C_{0,0,2}^{1/2} \bar{u} \phi_{\alpha}, \quad M_{0,1,0|\alpha} = C_{0,0,2}^{1/2} \bar{w} \phi_{\alpha}. \quad (B.6)$$

Thus, the central conditional moments are defined by

$$C_{j,k|\alpha} := \int_{\mathbb{R}^2} f_{\alpha}(v, w) \left( v - \bar{v} - C_{0,0,2}^{1/2} \bar{u} \phi_{\alpha} \right)^j \left( w - \bar{w} - C_{0,0,2}^{1/2} \bar{w} \phi_{\alpha} \right)^k dvdw \quad (B.7)$$

where $C_{0,0,0|\alpha} = 1$, $C_{1,0,0|\alpha} = 0$ and $C_{0,1,0|\alpha} = 0$. These central moments are related to $M_{j,k|\alpha}$ by
\[ M_{j,k|\alpha} = \sum_{j_1=0}^{j} \sum_{k_1=0}^{k} \binom{j}{j_1} \binom{k}{k_1} \left( C_{0,2,0,0}^{1/2} \eta_{uv} \eta_{\alpha} \right)^{j_1} \left( C_{0,0,2,0}^{1/2} \eta_{uw} \eta_{\alpha} \right)^{k_1} j_{j_1} C_{j_1,k_1|\alpha}. \]  

(B.8)

Using this expansion to evaluate \( M_{j,k|\alpha} \), we find closures for \( C_{j,k|\alpha} \) as done in A.1. For the second-order moments, we let

\[
\begin{align*}
C_{2.0|\alpha} &= a_0 + a_1 \eta_{\alpha}, \\
C_{0.2|\alpha} &= b_0 + b_1 \eta_{\alpha}, \\
C_{1.1|\alpha} &= \frac{C_{2,0|\alpha}^{1/2} C_{0.2|\alpha}^{1/2}}{C_{0,2,0,0}^{1/2} C_{0,0,2,0}^{1/2}} C_0
\end{align*}
\]

(B.9)

where the intercepts \((a_0, b_0 \geq 0 \text{ and } c_0^2 \leq 1)\) and slopes are found by forcing (B.4) to be exact. The resulting closures are

\[
\begin{align*}
M_{2,0|\alpha} &= C_{0,2,0}^{1/2} \eta_{uv} \eta_{\alpha}^2 + C_{2,0|\alpha} \text{ where } C_{2,0|\alpha} = C_{0,2,0}^{1/2} \left[ 1 - \eta_{uv}^2 + \eta_{uv} (q_v - \eta_{uv} q_u) \eta_{uv} \right], \\
M_{0,2|\alpha} &= C_{0,2,0}^{1/2} \eta_{uw} \eta_{\alpha}^2 + C_{0,2|\alpha} \text{ where } C_{0,2|\alpha} = C_{0,2,0}^{1/2} \left[ 1 - \eta_{uw}^2 + \eta_{uw} (q_w - \eta_{uw} q_u) \eta_{uw} \right],
\end{align*}
\]

(B.10) and (B.11)

\[
M_{1,1|\alpha} = C_{0,2,0}^{1/2} \eta_{uv} \eta_{\alpha}^2 + \left[ \frac{\eta_{uv} \eta_{uw} \eta_{\alpha}^2 + \frac{1}{2} \sum_{\alpha=1}^{4} \eta_{uv} \eta_{uw} \eta_{\alpha} \eta_{uv} \eta_{uw} \eta_{\alpha}}{C_{0,2,0}^{1/2} C_{0,0,2,0}^{1/2}} \right].
\]

(B.12)

As in the main text, to ensure that \( C_{2,0|\alpha} \geq 0 \) and \( C_{0,2|\alpha} \geq 0 \), limiters \((0 \leq \eta_{uv}, \eta_{uw} \leq 1)\) may be required for the slopes in (B.10) and (B.11). Also, \( c_0^2 \leq 1 \) requires that \( C_{0,2,0} C_{0,0,2} (\eta_{uv} - \eta_{uv} \eta_{uw})^2 \eta_{uv} \leq \left( \sum_{\alpha=1}^{4} \eta_{uv} \eta_{uw} \right)^2 \), which is controlled by the limiter \( \eta_{uv} \).

For the third-order moments, the closures are

\[
M_{3,0|\alpha} = C_{0,2,0}^{3/2} \eta_{uv} \eta_{\alpha}^3 + 3C_{0,2,0}^{1/2} \eta_{uv} \eta_{\alpha} C_{2,0|\alpha} + C_{3,0|\alpha} \text{ where } C_{3,0|\alpha} = q_v \eta_{uv}^{3/2|\alpha}
\]

(B.13)

\[ q_v = \frac{q_v - \eta_{uv} q_u - 3 \eta_{uv}^2 (q_v - \eta_{uv} q_u) \eta_{uv}}{\sum_{\alpha=1}^{4} \eta_{uv} \eta_{uw} \eta_{\alpha} \left[ 1 - \eta_{uv}^2 + \eta_{uv} (q_v - \eta_{uv} q_u) \eta_{uv} \right]^{3/2}}. \]

and

\[
M_{0,3|\alpha} = C_{0,2,0}^{3/2} \eta_{uw} \eta_{\alpha}^3 + 3C_{0,2,0}^{1/2} \eta_{uw} \eta_{\alpha} C_{2,0|\alpha} + C_{0,3|\alpha} \text{ where } C_{0,3|\alpha} = q_w \eta_{uw}^{3/2|\alpha}
\]

(B.14)

\[ q_w = \frac{q_w - \eta_{uw} q_u - 3 \eta_{uw}^2 (q_w - \eta_{uw} q_u) \eta_{uw}}{\sum_{\alpha=1}^{4} \eta_{uw} \eta_{uv} \eta_{\alpha} \left[ 1 - \eta_{uw}^2 + \eta_{uw} (q_w - \eta_{uw} q_u) \eta_{uw} \right]^{3/2}}. \]

For the fourth-order moments, the closures are

\[
M_{4,0|\alpha} = C_{0,2,0}^{4} \eta_{uv} \eta_{\alpha}^4 + 6C_{0,2,0}^{2} \eta_{uv} \eta_{\alpha}^2 C_{2,0|\alpha} + 4C_{1,1|\alpha}^{1/2} \eta_{uv} \eta_{uw} \eta_{\alpha} C_{3,0|\alpha} + C_{4,0|\alpha} \text{ where } C_{4,0|\alpha} = \eta_{uv} \eta_{uw}^{2|\alpha}
\]

(B.15)

\[ \eta_{uv} = \frac{\eta_{uv} - \eta_{uv} \eta_u - 6 \eta_{uv}^2 \left[ 1 - \eta_{uv}^2 + \eta_{uv} (q_v - \eta_{uv} q_u) \eta_{uv} \right] - 4 \eta_{uv} q_v \sum_{\alpha=1}^{4} \eta_{uv} \eta_{uw} \eta_{\alpha} \eta_{uv} \eta_{uw} \eta_{\alpha} \left( \frac{C_{2,0}^{2} \eta_{uv} \eta_{uw} \eta_{\alpha}}{C_{0,2,0}^{2}} \right)^{3/2}}{(1 - \eta_{uv}^2)^2 + \eta_{uv}^2 (q_v - \eta_{uv} q_u)^2 \eta_{uv}^2}, \]

and

\[
M_{0,4|\alpha} = C_{0,2,0}^{4} \eta_{uw} \eta_{\alpha}^4 + 6C_{0,2,0}^{2} \eta_{uw} \eta_{\alpha}^2 C_{2,0|\alpha} + 4C_{1,1|\alpha}^{1/2} \eta_{uw} \eta_{uv} \eta_{\alpha} C_{3,0|\alpha} + C_{0,4|\alpha} \text{ where } C_{0,4|\alpha} = \eta_{uw} \eta_{uv}^{2|\alpha}
\]

(B.16)

\[ \eta_{uw} = \frac{\eta_{uw} - \eta_{uw} \eta_u - 6 \eta_{uw}^2 \left[ 1 - \eta_{uw}^2 + \eta_{uw} (q_w - \eta_{uw} q_u) \eta_{uw} \right] - 4 \eta_{uw} q_w \sum_{\alpha=1}^{4} \eta_{uw} \eta_{uv} \eta_{\alpha} \eta_{uw} \eta_{uv} \eta_{\alpha} \left( \frac{C_{2,0}^{2} \eta_{uw} \eta_{uv} \eta_{\alpha}}{C_{0,2,0}^{2}} \right)^{3/2}}{(1 - \eta_{uw}^2)^2 + \eta_{uw}^2 (q_w - \eta_{uw} q_u)^2 \eta_{uw}^2}. \]

The statistics \( q_v, q_w, \eta_{uv}, \eta_{uw} \) must be checked for realizability, and corrected if needed. Also, the formulas for these coefficients can be nearly singular if all conditional variances for \( v \) and/or \( w \) are very small. In such cases, we set \( q_v, q_w = 0 \) and \( \eta_{uv}, \eta_{uw} = 1 \).

In summary, once the moments \( M_{j,k|\alpha} \) have been computed from (B.6)–(B.16), they are employed in (B.5) to find \( \theta_{l,k|\alpha}^{1,l} \). These results are finally used in (38) to compute the kinetic-based flux component in the \( x \) direction.
Appendix C. Extension of CHyQMOM27 to all third-order moments

In this appendix, we describe the extension of CHyQMOM27 to include all third-order moments in 2-D and 3-D velocity phase space. The flux-based quadrature is constructed using the same procedure as in Appendix B starting from the results presented here.

C.1. 2-D CHyQMOM9 with 12 moments

The extension of 2-D CHyQMOM9 uses the 12-moment set

\[
M = \begin{bmatrix}
M_{0,0} & M_{0,1} & M_{0,2} & M_{0,3} & M_{0,4} \\
M_{1,0} & M_{1,1} & M_{1,2} & \\
M_{2,0} & M_{2,1} & \\
M_{3,0} & \\
M_{4,0} &
\end{bmatrix}.
\]

(C.1)

This moment set is of interest because all third-order moments (which control the energy flux) are included. At the same time, the degenerate cases with exactly one or two velocity abscissas needed to handle PTC at arbitrary angles are allowed. The algorithm for computing 2-D CHyQMOM9 is the same as in the main text, except for the differences described next. More details are given in Appendix A.

Using the central moments found from (C.1), the conditional mean is expanded as \( \bar{\nu}_\alpha = a_0 + a_1 u_\alpha + a_2 u_\alpha^2 \) where

\[
\begin{align*}
\sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha &= 0, & \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha \bar{\nu}_\alpha &= C_{1,1}, & \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha^2 \bar{\nu}_\alpha &= C_{2,1}.
\end{align*}
\]

(C.2)

This yields a linear system for the coefficients:

\[
\begin{bmatrix}
1 & 0 & C_{2,0} \\
0 & C_{2,0} & C_{3,0} \\
C_{2,0} & C_{3,0} & C_{4,0}
\end{bmatrix}
\begin{bmatrix}
a_0 \\
a_1 \\
a_2
\end{bmatrix} =
\begin{bmatrix}
0 \\
C_{1,1} \\
C_{2,1}
\end{bmatrix}.
\]

(C.3)

which has a unique solution if \( H_4 \) is positive (i.e., \( C_{2,0} > 0 \) and \( S_{4,0} > 1 + S_{2,0}^2 \)). In the case where \( C_{2,0} = 0 \), \( \bar{\nu}_\alpha = 0 \); and when \( C_{2,0} > 0 \) but \( S_{4,0} = 1 + S_{2,0}^2 \), \( \bar{\nu}_\alpha = \frac{C_{1,0}}{C_{2,0}} u_\alpha \). These two cases correspond to \( \rho_2 = 1 \) and \( \rho_2 = 0 \), respectively. The definition of \( \bar{\nu}_\alpha \) as quadratic, as opposed to linear, in \( u_\alpha \) is the main difference from the main text. The third-order moment \( C_{2,1} \) is needed to define \( a_2 \). From a numerical perspective, using a quadratic function is slightly more difficult because one must deal with situations where the coefficient matrix in (C.3) is ill-conditioned or even singular. Such cases occur when the moments are on the boundary of moment space (i.e. PTC).

Next, the conditional variance \( C_{2|\alpha} \) has the form given in (23) with the two coefficients found from

\[
\begin{align*}
\sum_{\alpha=1}^{3} \rho_\alpha C_{2|\alpha} &= C_{0,2}, & \sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha^2 &= C_{3,0}, & \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha C_{2|\alpha} &= C_{1,2} - \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha \bar{\nu}_\alpha^2.
\end{align*}
\]

(C.4)

If one of the conditional variances is negative, then \( b_1 \) is limited such that all conditional variances are non-negative. As in the main text, the conditional moments \( C_{3|\alpha} \) and \( C_{4|\alpha} \) are found from \( \{C_{0,3}, C_{0,4}\} \) by assuming that they depend on \( \alpha \) through \( C_{2|\alpha} \). This yields

\[
q^*_\nu = \left[ \sum_{\alpha=1}^{3} \rho_\alpha C_{2|\alpha}^2 \right]^{-1} \begin{bmatrix}
C_{0,3} - \sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha^3 - 3 \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha C_{2|\alpha} \\
\sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha^2 C_{2|\alpha} - 4 q^*_\nu \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha C_{2|\alpha}^2
\end{bmatrix},
\]

\[
\eta^*_\nu = \left[ \sum_{\alpha=1}^{3} \rho_\alpha C_{2|\alpha}^2 \right]^{-1} \begin{bmatrix}
C_{0,4} - 6 \sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha^4 - 2 \sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha^2 C_{2|\alpha}^2 - 3 \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha C_{2|\alpha}^3 \\
\sum_{\alpha=1}^{3} \rho_\alpha \bar{\nu}_\alpha C_{2|\alpha}^2 - 2 q^*_\nu \sum_{\alpha=1}^{3} \rho_\alpha u_\alpha C_{2|\alpha}^3
\end{bmatrix}.
\]

(C.5)

Realizability requires that \( q^*_\nu \geq 1 + (q^*_\nu)^2 \). If this condition is not met, then \( q^*_\nu \) and \( \eta^*_\nu \) are projected to the realizability curve \( \eta^*_\nu = 1 + (q^*_\nu)^2 \) in the direction of the Gaussian moments (i.e., \( q^*_\nu = 0 \) and \( \eta^*_\nu = 3 \)). The limiting case where all conditional variances are very small is handled as described in the main text.
C.2. 3-D CHyQMOM\textsubscript{27} with 23 moments

The 3-D CHyQMOM\textsubscript{27} can be extended to control the following set of 23 moments:

\[
\mathbf{M} = \begin{pmatrix}
M_{0,0,0} & M_{0,1,0} & M_{0,0,1} & M_{0,2,0} & M_{0,0,2} & M_{0,1,1} & M_{0,0,3} \\
M_{1,0,0} & M_{1,1,0} & M_{1,0,1} & M_{1,2,0} & M_{1,0,2} & M_{1,1,1} & M_{1,0,3} \\
M_{2,0,0} & M_{2,1,0} & M_{2,0,1} & M_{2,1,1} & M_{2,0,2} & M_{2,0,3} & M_{2,0,4} \\
M_{3,0,0} & M_{3,1,0} & M_{3,0,1} & M_{3,0,2} & M_{3,0,3} & M_{3,0,4} & M_{3,0,5} \\
M_{4,0,0} & M_{4,1,0} & M_{4,0,1} & M_{4,0,2} & M_{4,0,3} & M_{4,0,4} & M_{4,0,5}
\end{pmatrix}.
\]

The algorithm for computing 3-D CHyQMOM\textsubscript{27} is the same as in the main text, except that more terms are used in the expansions for the conditional moments \(M_{j,k,a}\) to make use of the additional third-order moments. Specifically, we must compute the following 11 bivariate moments conditioned on \(u\) (by definition \(M_{0,0,a} = 1\)):

\[
M_{1,0,a} | M_{0,1,a} | C_{0,2,a} | C_{1,1,a} | C_{0,2,a} | C_{2,1,a} | C_{1,2,a} | C_{0,3,a} | C_{0,4,a} | C_{0,4,a}.
\]

These moments are then employed in the 2-D algorithm described in C.1. The method for computing them is given in A.1 for the case \(n = 3\). In particular, the conditional third-order moments \(C_{2,1,a}\) and \(C_{1,2,a}\) are found from (A.17) using \(C_{0,2,1}\) and \(C_{0,1,2}\), respectively. The expansions for \(S_{2,1,a}\) and \(S_{1,2,a}\) (see (A.16)) thus include only the zero-order coefficients. Finally, the limiting cases where the conditional variances are all very small are handled as described in the main text.

CHyQMOM\textsubscript{27} with 16 moments and CHyQMOM\textsubscript{23} with 23 moments privilege the coordinate axes and are not rotationally invariant. Therefore, it may also be desirable to transport the full set of fourth-order moments. In this case, the mixed, fourth-order, conditioned moments are needed to compute the fluxes for the additional moments. As with the other conditioned statistics, additional polynomials of the abscissas must be found to fit these statistics. Another interesting possibility worth exploring would be to use independent sums of rotationally invariant third- and fourth-order moments as is done in Grad’s 13-moment closure [29].

References


