Hyperbolic Quadrature Method of Moments

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Motivation: Simulation of fluid–particle flows

E–L

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CHyQMOM$_{27}$

Outline

1. Quadrature-Based Moment Methods
2. Hyperbolic Quadrature Method of Moments
3. Conditional HyQMOM_{3^d}
4. Extension of HyQMOM_N to $3 < N$
5. Conclusions

Kinetic Equation for Fluid–Particle Flows

We wish to approximate solutions for a velocity distribution function (VDF) $f(t, \mathbf{x}, \mathbf{v})$ obeying a kinetic equation of the general form

$$\frac{\partial f}{\partial t} + \frac{\partial v_i f}{\partial x_i} + \frac{\partial}{\partial v_i}\left[A_i(t, \mathbf{x}, \mathbf{v}) f\right] = \mathbb{C}$$

where $\mathbf{A}(t, \mathbf{x}, \mathbf{v})$ is a known acceleration, depending on fluid velocity, and $\mathbb{C}$ is a known particle–particle collision model.

In particular, we are mainly interested in knowing the moments of f ...

Kinetic equation is coupled to Navier–Stokes equation for fluid through the moments of VDF.

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Moment Transport Equation

Velocity moments are defined by $M_k := \int \mathbf{v}^k f \, \mathrm{d}\mathbf{v}$ and obey an unclosed moment equation of the form:

$$\frac{\partial \mathbf{M}_k}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{M}_k)}{\partial \mathbf{x}} = k \int \mathbf{v}^{k-1} \mathbf{A} f \, \mathrm{d}\mathbf{v} + \int \mathbf{v}^k \mathbb{C} \, \mathrm{d}\mathbf{v}$$

with moment vector $\mathbf{M}_k := \{M_0, M_1, \ldots, M_k\}$
and spatial flux $\mathbf{F}(\mathbf{M}_k) := \{M_1, M_2, \ldots, M_k, M_{k+1}\}$.

In this presentation, the main focus is the spatial flux but the same ideas apply to close the source terms for acceleration and collisions.

In particular, the flux Jacobian matrix $\partial \mathbf{F}(\mathbf{M}_k)/\partial \mathbf{M}_k$ must have real, distinct eigenvalues for the moment system to be hyperbolic.

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Closure with Quadrature-Based Moment Methods

Close moment equations by reconstructing density function

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Quadrature-Based Moment Methods: Definitions

- Velocity distribution function (VDF) $f(u)$ for $u \in \mathbb{R}$
- Moments of f:

$$M_k := \int_{\mathbb{R}} f(u) u^k \, \mathrm{d}u$$

  For nonnegative $f(u)$, the moments are realizable.
- Central moments of f: ($C_0 = 1$ and $C_1 = 0$)

$$C_k := \frac{1}{M_0} \int_{\mathbb{R}} f(u)(u - \bar{u})^k \, \mathrm{d}u$$

  where mean velocity $\bar{u} := M_1/M_0$. For any $k \geq 0$, C_k depends uniquely on moment vector $\mathbf{M}_k := \{M_0, M_1, \ldots, M_k\}$.
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$$S_k := C_k / C_2^{k/2}$$

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Definitions

- Hankel matrix:

$$\mathbf{H}_{2n} = \begin{bmatrix} M_0 & M_1 & \dots & M_n \\ M_1 & M_2 & \dots & M_{n+1} \\ \vdots & \vdots & \ddots & \vdots \\ M_n & M_{n+1} & \dots & M_{2n} \end{bmatrix}$$

  is non-negative if $|\mathbf{H}_{2n}| \geq 0$.

- Moment vector $\mathbf{M}_k$ for $k = 2n$ is realizable if $\mathbf{H}_{2m}$ is non-negative for all $m \in \{0, 1, \dots, n\}$.
- Boundary of moment space: $|\mathbf{H}_{2n}| = 0$, e.g., $S_4 = 1 + S_3^2$ when $n = 2$. When $\mathbf{M}_{2n}$ is on boundary, then

$$f(u) = M_0 \sum_{\alpha=1}^{n} p_\alpha \delta_{\bar{u}+u_\alpha}(u)$$

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Quadrature Method of Moments

- Given $2 \leq N < \infty$, assume $\mathbf{M}_k$ exists and is realizable for $k = 2N - 1$.
- QMOM$_N$: Let $|\mathbf{H}_{2N}| = 0$ so that

$$f(u) = M_0 \sum_{\alpha=1}^{N} p_\alpha \delta_{\bar{u}+u_\alpha}(u)$$

- Given $\mathbf{M}_{2N-1}$, use moment-inversion algorithm to compute p_α and u_α.
- $\mathbf{M}_{2N}$ is on boundary of moment space, and closure for M_{2N} yields a weakly hyperbolic moment system:

$$\partial_t \mathbf{M}_{2N-1} + \partial_x \{M_1, M_2, \ldots, M_{2N-1}, M_{2N}\} = 0$$

- M_0 exhibits delta shocks.

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Hyperbolic QMOM

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  is hyperbolic for all realizable $\mathbf{M}_{2N-2}$ when $|\mathbf{H}_{2N-2}| > 0$.
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- In practice, choose S_{2N-1} as function of $\{S_2, S_3, \ldots, S_{2N-2}\}$, e.g., $S_3 = 0$ with $N = 2$.

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Hyperbolic QMOM with $N = 3$

- Assume $\mathbf{M}_4$ exists and is realizable.
- HyQMOM$_3$: Choose M_5 such that moment system

$$\partial_t \mathbf{M}_4 + \partial_x \{M_1, M_2, \ldots, M_4, M_5\} = 0$$

  is hyperbolic for all realizable $\mathbf{M}_4$ when $|\mathbf{H}_4| > 0$.
- If $S_5 = S_3(2S_4 - S_3^2)$, then five eigenvalues of flux Jacobian

$$\bar{u}, \quad \bar{u} + \frac{1}{2}\sqrt{C_2}\left(S_3 \pm \sqrt{4S_4 - 3S_3^2 \pm 4\sqrt{\left(S_4 - S_3^2\right)\left(S_4 - S_3^2 - 1\right)}}\right)$$

  are real because $S_4 \geq 1 + S_3^2$ and distinct unless $S_4 = 1 + S_3^2$ ($|\mathbf{H}_4| = 0$).
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Hyperbolic QMOM with $N = 3$

Given $\mathbf{M}_5$, moment-inversion algorithm yields

$$f^a(u) = M_0 \sum_{\alpha=1}^{3} p_\alpha \delta_{\bar{u}+u_\alpha}(u)$$

$$p_1 = \frac{-\sqrt{C_2}}{u_1\sqrt{4S_4 - 3S_3^2}} \qquad u_1 = \frac{1}{2}\sqrt{C_2}\left(S_3 - \sqrt{4S_4 - 3S_3^2}\right)$$

$$p_2 = 1 + \frac{C_2}{u_1 u_3} \qquad u_2 = 0$$

$$p_3 = \frac{\sqrt{C_2}}{u_3\sqrt{4S_4 - 3S_3^2}} \qquad u_3 = \frac{1}{2}\sqrt{C_2}\left(S_3 + \sqrt{4S_4 - 3S_3^2}\right)$$

N.B. Reconstructed $f^a(u)$ is not used to find the flux ...
and $p_2 = 0$ when $S_4 = 1 + S_3^2$ (i.e., $|\mathbf{H}_4| = 0$ & QMOM$_2$).

Kinetic-Based Flux with $N = 3$

- Define the flux $\mathbf{F}(\mathbf{M}_4) := \{M_1, M_2, M_3, M_4, M_5\}$
- With eigenvalues λ_α, $\alpha \in 0, \ldots, 4$, the kinetic-based flux is

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

- With $\varphi_\alpha = (\lambda_\alpha - \bar{u})/\sqrt{C_2}$, $w_0 = 0$ ($\varphi_0 = 0$) and the +ve weights satisfy

$$\begin{bmatrix} \varphi_1 & \varphi_2 & \varphi_3 & \varphi_4 \\ \varphi_1^2 & \varphi_2^2 & \varphi_3^2 & \varphi_4^2 \\ \varphi_1^3 & \varphi_2^3 & \varphi_3^3 & \varphi_4^3 \\ \varphi_1^4 & \varphi_2^4 & \varphi_3^4 & \varphi_4^4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ S_3 \\ S_4 \end{bmatrix}$$

- *N.B.* For Gaussian $\mathbf{M}_4$, 4-node Gauss–Hermite quadrature.

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

- With $\varphi_\alpha = (\lambda_\alpha - \bar{u})/\sqrt{C_2}$, $w_0 = 0$ ($\varphi_0 = 0$) and the +ve weights satisfy

$$\begin{bmatrix} \varphi_1 & \varphi_2 & \varphi_3 & \varphi_4 \\ \varphi_1^2 & \varphi_2^2 & \varphi_3^2 & \varphi_4^2 \\ \varphi_1^3 & \varphi_2^3 & \varphi_3^3 & \varphi_4^3 \\ \varphi_1^4 & \varphi_2^4 & \varphi_3^4 & \varphi_4^4 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ S_3 \\ S_4 \end{bmatrix}$$

- *N.B.* For Gaussian $\mathbf{M}_4$, 4-node Gauss–Hermite quadrature.

Kinetic-Based Flux with $N = 3$

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Riemann Problem, $Ma = 1.73$: Moments

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Riemann Problem, $Ma = 1.73$: Scaled moments

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Riemann Problem, $Ma = 1.73$: Flux quadrature

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Riemann Problem, $Ma = 30$: Flux quadrature

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Riemann Problem, $Ma = 30$: Scaled moments

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Remarks on HyQMOM$_3$

- Valid for all realizable $\mathbf{M}_4$.
- Characteristic polynomial of moment system is

$$P(X) = -X^5 + \epsilon X^4 + \delta X^3 + \gamma X^2 + \beta X + \alpha$$

where $(\alpha, \beta, \gamma, \delta, \epsilon) = \left(\frac{\partial M_5}{\partial M_0}, \frac{\partial M_5}{\partial M_1}, \frac{\partial M_5}{\partial M_2}, \frac{\partial M_5}{\partial M_3}, \frac{\partial M_5}{\partial M_4} \right)$.

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Outline

1. Quadrature-Based Moment Methods
2. Hyperbolic Quadrature Method of Moments
3. Conditional HyQMOM$_{3d}$
4. Extension of HyQMOM$_N$ to $3 < N$
5. Conclusions

Conditional HyQMOM$_{3d}$: Definitions

- Velocity distribution function (VDF) $f(\mathbf{v})$ for $\mathbf{v} \in \mathbb{R}^d$ with $d = 2, 3$.
- Moments of f in 2-D:

$$M_{i,j} := \int_{\mathbb{R}^2} f(u, v) u^i v^j \, \mathrm{d}u \, \mathrm{d}v$$

  For non-negative $f(u, v)$, the moments are realizable.
- Central moments of f: ($C_{0,0} = 1$ and $C_{1,0} = C_{0,1} = 0$)

$$C_{i,j} := \frac{1}{M_{0,0}} \int_{\mathbb{R}^2} f(u, v)(u - \bar{u})^i (v - \bar{v})^j \, \mathrm{d}u \, \mathrm{d}v$$

  with mean velocities $\bar{u} := M_{1,0}/M_{0,0}$ and $\bar{v} := M_{0,1}/M_{0,0}$.
  For any $i, j \geq 0$, $C_{i,j}$ depends uniquely on moment vector $\mathbf{M}_k := \{M_{0,0}, M_{1,0}, \ldots, M_{l,m}\}$ with $l + m \leq k = i + j$.
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CHyQMOM$_9$: Reconstructed VDF for $d = 2$

- Approximate 2-D velocity VDF by (v conditioned on u)

$$f^a(u,v) = M_{0,0} \sum_{\alpha=1}^{3} p_\alpha \delta_{\bar{u}+u_\alpha}(u) \sum_{\beta=1}^{3} p_{\alpha\beta} \delta_{\bar{v}+V_\alpha+v_{\alpha\beta}}(v)$$

where abscissas $v_{\alpha\beta}$ and V_α are found from central moments.

- CHyQMOM$_9$ uses symmetric moment sets:

10 moments

$M_{0,0}$	$M_{1,0}$	$M_{2,0}$	$M_{3,0}$	$M_{4,0}$
$M_{0,1}$	$M_{1,1}$			
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12 moments

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N.B. Conditional moments do not depend on α.

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CHyQMOM$_9$: 10 moments spatial flux

- CHyQMOM$_9$ closure for flux in 1-D spatial and 2-D velocity:

$$\partial_t M_{1,1} + \partial_x \bar{M}_{2,1} = 0 \quad \Longrightarrow \quad \bar{M}_{2,1} = M_{0,0} \sum_{\alpha=1}^{3} p_\alpha (\bar{u} + u_\alpha)^2 (\bar{v} + V_\alpha)$$

$$\partial_t M_{0,2} + \partial_x \bar{M}_{1,2} = 0 \Longrightarrow \bar{M}_{1,2} = M_{0,0} \sum_{\alpha=1}^{3} p_\alpha (\bar{u} + u_\alpha) \sum_{\beta=1}^{3} p_{\alpha\beta} (\bar{v} + V_\alpha + v_{\alpha\beta})^2$$

- Theorem: (F. Laurent) 10 moment system with closed flux is hyperbolic with 10 distinct eigenvectors.
- Extension to $d = 3$ follows same logic: CHyQMOM$_{27}$ uses either 16 or 23 symmetric moment sets.

Kinetic-Based VDF Reconstruction

- Use five HyQMOM$_3$ eigenvalues λ_α for u velocities:

$$f^k(u,v) = M_{0,0} \sum_{\alpha=0}^{4} w_\alpha \delta_{\lambda_\alpha}(u)\, p(v|u=\lambda_\alpha)$$

where conditional PDF $p(v|u=\lambda_\alpha)$ is found as before.

- Kinetic-based flux uses $f^k(u,v)$, e.g.,

$$F_{x;i,j} = \int_{\mathbb{R}} \left(\int_0^\infty f^k(u,v) u^{i+1} v^j \,\mathrm{d}u \right) \mathrm{d}v + \int_{\mathbb{R}} \left(\int_{-\infty}^0 f^k(u,v) u^{i+1} v^j \,\mathrm{d}u \right) \mathrm{d}v$$

- Discrete flux with conditional moment $\mathcal{V}_\alpha^j := \int_{\mathbb{R}} v^j p(v|u=\lambda_\alpha)\mathrm{d}v$:

$$F_{x;i,j} = M_{0,0} \sum_{\alpha=0}^{4} w_\alpha \left[\max(0,\lambda_\alpha)^{i+1} + \min(0,\lambda_\alpha)^{i+1} \right] \mathcal{V}_\alpha^j$$

Particle Trajectory Crossing in 1-D

Uncorrelated moments

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16-moment CHyQMOM$_{27}$

Particle Trajectory Crossing in 1-D

Quadrature weights and abscissas

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16-moment CHyQMOM$_{27}$

Particle Trajectory Crossing in 1-D

Perfectly correlated moments

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16-moment CHyQMOM$_{27}$

Particle Trajectory Crossing in 1-D

Quadrature weights and abscissas

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16-moment CHyQMOM$_{27}$

Particle Trajectory Crossing in 1-D

Partially correlated moments

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16-moment CHyQMOM$_{27}$

Particle Trajectory Crossing in 1-D

Quadrature weights and abscissas

Loading movie...

16-moment CHyQMOM$_{27}$

Particle Trajectory Crossing in 2-D

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10-moment CHyQMOM$_9$

Particle Trajectory Crossing in 2-D with Fluid Drag

10-moment CHyQMOM$_9$

Particle Trajectory Crossing in 3-D

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16-moment CHyQMOM$_{27}$

Remarks on CHyQMOM$_{27}$

- Valid for all realizable moment sets.
- With $N = 3$, binary PTC is captured correctly (but not ternary PTC ...)
- Far from Gaussian, some high-order cross moments are not used when conditional moments are not realizable.
- Kinetic-based fluxes using HyQMOM$_3$ eigenvalues are always realizable (e.g. +ve weights).
- Open Problem: kinetic-based fluxes on unstructured meshes.
- Open Problem: high-order spatial reconstruction for fluxes.

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Remarks on CHyQMOM$_{27}$

- Valid for all realizable moment sets.
- With $N = 3$, binary PTC is captured correctly (but not ternary PTC ...)
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HyQMOM$_N$: How to choose S_{2N-1}?

- Scaled characteristic polynomial is

$$P(X) = -X^{2N-1} + \cdots + \epsilon X^4 + \delta X^3 + \gamma X^2 + \beta X + \alpha$$

where $\alpha := \dfrac{\partial M_{2N-1}}{\partial M_0} = 0 \iff 2N-3 = \sum_{n=3}^{2N-2}(n-2)\frac{\partial \ln S_{2N-1}}{\partial \ln S_n}$.

- Define $p_M := \sum_\beta \kappa_\beta S_3^{i_3} S_4^{i_4} \cdots S_{M+2}^{i_{M+2}}$ where κ_β are constants and sum over all allowable sets of $\{0 \le i_n \in \mathbb{N} : M = \sum_{n=3}^{M+2}(n-2)i_n\}$.
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- For $N = 4$, 2-parameter solution exists:

$$S_7 = 3S_3S_6 - S_4S_5 + 2S_3S_4^2 - 3S_3^2S_5 + a\frac{3}{4}(4S_4 - 3S_3^2)(S_3^3 - 2S_4S_3 + S_5)$$
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- $a = 2$ recovers the previous case.
- $a = 0$ and $b = 0$ recovers the HyQMOM$_4$ case.
- $a = 0$ and $b = 1$ gives a 1-parameter solution $\beta = 0$.

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Observations: Flux-based quadrature for $N = 4$

- Flux-based quadrature computed using non-zero eigenvalues φ_α and S_k:

$$\begin{bmatrix} \varphi_1 & \varphi_2 & \cdots & \varphi_6 \\ \varphi_1^2 & \varphi_2^2 & \cdots & \varphi_6^2 \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1^6 & \varphi_2^6 & \cdots & \varphi_6^6 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_6 \end{bmatrix} = \begin{bmatrix} 0 \\ S_2 \\ \vdots \\ S_6 \end{bmatrix}$$

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Riemann, $N = 4$, $Ma = 0.9$: Weights and Abscissas

Loading movie...

Riemann, $N = 4$, $Ma = 0.9$: Scaled Moments

Loading movie...

Riemann $Ma = 0.9$: $N = 3$ versus $N = 4$

HyQMOM$_3$

HyQMOM$_4$

Small, negative weights for HyQMOM$_4$, but moments remain realizable

Remarks on HyQMOM$_N$

- Valid for all realizable moment sets $\mathbf{M}_{2N-2}$?
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OpenQBMM Project (www.openqbmm.org)

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Thanks for your attention!

Questions?