Multi-scale modeling of polydisperse multiphase flows using quadrature-based moment methods

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Motivation: Simulation of Gas–Particle Flows

Euler–Lagrange

Anisotropic Gaussian

CHyQMOM

Motivation: Taylor–Green Flow with $St = 5$

Agreement with EL depends on Eulerian closure

Mesoscale Model for Gas–Particle Flows

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

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

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

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

M_0 – mass density of particle phase
M_1 – momentum of particle phase
M_2 – total energy of particle phase

Kinetic equation is coupled to Navier–Stokes equation for gas phase through the moments of VDF (M_0, M_1)

Mesoscale model for polydisperse particles involves $n(t, \mathbf{x}, \mathbf{v}, \xi)$ where ξ is particle mass ...

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Moment Transport Equation

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

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

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

Requirements for VDF Reconstruction

- n^* must be non-negative
- Must work for any set of realizable moments $\mathbf{M}_k$
- Moments of n^* must be equal to M_i for $0 \leq i \leq k$
- Algorithm to find n^* must be fast
- Closure for M_{k+1} should yield hyperbolic moment system

Lattice methods yield negative n^* for some realizable moments

Entropy maximization is relatively slow, but is hyperbolic

QBMM are fast and non-negative, but may be weakly hyperbolic

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Quadrature-Based Moment Methods: Definitions

- Velocity distribution function (1-D) $n(u)$ for $u \in \mathbb{R}$
- Moments of n:

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

  For non-negative $n(u)$, these moments are realizable
- Central moments of n: ($C_0 = 1$, $C_1 = 0$, $0 \leq C_2$= variance)

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

  where mean velocity $\bar{u} := M_1/M_0$. For any $k \geq 0$, C_k depends uniquely on moment vector $\mathbf{M}_k := \{M_0, M_1, \ldots, M_k\}$
- Scaled moments of n: ($S_0 = 1$, $S_1 = 0$, $S_2 = 1$)

$$S_k := C_k / C_2^{k/2} \quad \Longrightarrow \quad q = S_3 \quad \eta = S_4$$

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How do we check realizability?

- Hankel matrix:

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

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

- Theorem: Moment vector $\mathbf{M}_m$ for $m = 2k$ is realizable if $\mathbf{H}_{2i}$ is non-negative for all $i \in \{0, 1, \dots, m\}$
- Boundary of moment space: $|\mathbf{H}_{2m}| = 0$, e.g., $\eta = 1 + q^2$ when $m = 2$. When $\mathbf{M}_{2m}$ is on boundary, then VDF has form

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

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Quadrature Method of Moments

- Given $2 \leq N < \infty$, assume $\mathbf{M}_{2N-1}$ is realizable
- QMOM closure: Let $|\mathbf{H}_{2N}| = 0$ so that

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

- 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 (i.e., M_0 accumulates at isolated points)

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Weakly vs. Fully Hyperbolic Closures

Hyperbolic QMOM

- Assume $\mathbf{M}_4 = \{M_0, M_1, M_2, M_3, M_4\}$ is realizable ($\eta \geq 1 + q^2$)
- HyQMOM closure: 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 $S_5 = (2\eta - q^2)q$, then five eigenvalues of flux Jacobian

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

  are real ($\eta \geq 1 + q^2$) and distinct unless $\eta = 1 + q^2$ ($|\mathbf{H}_4| = 0$)
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VDF Reconstruction with HyQMOM

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

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

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

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

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

Reconstructed $n^*(u)$ is not used to find the numerical flux ...

$p_2 = 0$ when $\eta = 1 + q^2$ (i.e., $|\mathbf{H}_4| = 0$ & QMOM)

Kinetic-Based Flux for Finite-Volume Scheme

- Define the flux $\mathbf{F}(\mathbf{M}_4) := \{M_1, M_2, M_3, M_4, M_5\}$
- Numerical flux must keep moments realizable!
- 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 a Vandermonde system

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- Gaussian moments: 4-node Gauss–Hermite quadrature

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

- Gaussian moments: 4-node Gauss–Hermite quadrature

Kinetic-Based Flux for Finite-Volume Scheme

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

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$$\frac{\partial n(t,x,u)}{\partial t} + u\frac{\partial n(t,x,u)}{\partial x} = 0$$

or

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

closed with HyQMOM

- Exact solution for $n(t,x,u)$ for given $n(0,x,u)$
- Moments initialized differently on $\pm x$ axis
- For $x < 0$, Gaussian VDF with $\bar{u} = +1$, $C_2 = \frac{1}{Ma^2}$
- For $x > 0$, Gaussian VDF with $\bar{u} = -1$, $C_2 = \frac{1}{Ma^2}$
- $Ma = |\bar{u}|/\sqrt{C_2}$ = Mach number
- $Ma = \infty$ is pure trajectory crossing with $\eta = 1 + q^2$ (moment approximation is exact)

$Ma = 1.73$: Moments

$Ma = 1.73$: Scaled moments

$Ma = 1.73$: Flux quadrature

$Ma = 30$: Flux quadrature

$Ma = 30$: Scaled moments

Remarks on HyQMOM

- Works for all realizable moment sets $\mathbf{M}_4$
- Reconstructed VDF is always non-negative
- Algorithm is very fast
- Kinetic-based flux similar to off-lattice discrete-velocity solver
- {Kinetic-based flux} + {realizability condition on Δt} = realizable moments
- High-order finite-volume solver possible, but care must be taken to ensure moment realizability

How can we extend HyQMOM to more dimensions?

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Conditional HyQMOM: Definitions

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

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

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

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

  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: Reconstructed VDF for $d = 2$

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

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

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

- 9 discrete velocities on 3×3 'lattice' in 2-D phase space
- HyQMOM with $M_{i,0}$ yields p_α, u_α (i.e., same as 1-D)
- CHyQMOM uses symmetric moment sets to find $p_{\alpha\beta}$, V_α, $v_{\alpha\beta}$

10 moments

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

12 moments

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CHyQMOM (cont.)

- With 10 moments, $V_\alpha = a_0 + a_1 u_\alpha$ is found from

$$\sum_{\alpha=1}^{3} p_\alpha V_\alpha = C_{0,1} = 0 \qquad \sum_{\alpha=1}^{3} p_\alpha u_\alpha V_\alpha = C_{1,1}$$

$\Longrightarrow a_0 = 0$ and $a_1 = C_{1,1}/C_{2,0}$ captures correlation between u and v

- CHyQMOM conditional moments are $\{1, 0, C_{2|\alpha}, C_{3|\alpha}, C_{4|\alpha}\}$ where

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N.B. Conditional moments do not depend on α

- HyQMOM is applied to $\{1, 0, C_{2|\alpha}, C_{3|\alpha}, C_{4|\alpha}\}$ to find $p_{\alpha\beta}$ and $v_{\alpha\beta}$
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CHyQMOM: 10 moments spatial flux

- CHyQMOM 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: 10-moment system with CHyQMOM flux is hyperbolic
- Extension to $d = 3$ follows same logic: CHyQMOM uses either 16 or 23 moments
- 27 discrete velocities on $3 \times 3 \times 3$ 'lattice' in 3-D phase space

Kinetic-Based VDF Reconstruction

- Use five HyQMOM eigenvalues λ_α for u velocities:

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

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

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

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

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

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

leads to realizable moments

Riemann Problem with 3-D Phase Space

$$\frac{\partial n(t,x,\mathbf{v})}{\partial t} + u\frac{\partial n(t,x,\mathbf{v})}{\partial x} = 0$$

or

$$\partial_t \mathbf{M}_4 + \partial_x \bar{\mathbf{M}}_5 = 0$$

closed with 3-D CHyQMOM

- Exact solution for $n(t,x,\mathbf{v})$ for given $n(0,x,\mathbf{v})$
- Moments initialized differently on $\pm x$ axis
- For $x < 0$, Gaussian VDF with $\bar{u} = +1$, $C_{2,0,0} = \frac{1}{Ma^2}$, different covariances
- For $x > 0$, Gaussian VDF with $\bar{u} = -1$, $C_{2,0,0} = \frac{1}{Ma^2}$, different covariances
- Covariance structure must be preserved during transport

Uncorrelated Velocities

Moments

Uncorrelated Velocities

27 quadrature weights and abscissas

Perfectly Correlated Velocities

Moments

Perfectly Correlated Velocities

27 quadrature weights and abscissas

Partially Correlated Velocities

Moments

Partially Correlated Velocities

27 quadrature weights and abscissas

Particle Trajectory Crossing in 2-D

Particle Trajectory Crossing in 2-D with Fluid Drag

Exact solution recovered because M_3 is included

Particle Trajectory Crossing in 3-D

Remarks on CHyQMOM

- Works for any realizable moment set
- Algorithm is very fast
- Correlation structure is preserved during transport
- Binary PTC is captured correctly (but not ternary PTC ...)
- Kinetic-based fluxes using HyQMOM eigenvalues are always realizable
- Open Problem: high-order spatial reconstruction for fluxes on unstructured mesh

Complexity of Gas–Particles Flows

Cluster-Induced Turbulence

Particle-Laden Channel

Particles segregate into clusters

Application of QBMM to Gas–Particle Flows

- Gas phase described by Navier–Stokes solver coupled to particle phase (α_p, momentum exchange)
  1. Initialize fluid and particle fields (moments)
  2. Advance the particle phase using CHyQMOM
  3. Advance the fluid phase
  4. Repeat steps 2 and 3
- Weak coupling suffices for dilute flows, but collisional fluxes require sub-iterations (or implicit method) for convergence in dense flows
- Boundary conditions for wall-bounded flows are important!

Cluster-Induced Turbulence

Particle diameter	d_p	90×10^{-6} m
Particle density	ρ_p	$1000\,\mathrm{kg\,m^{-3}}$
Fluid density	ρ_f	$1\,\mathrm{kg\,m^{-3}}$
Fluid viscosity	μ_f	1.8×10^{-5} Pa s
Gravitational constant	g	$4.0004\,\mathrm{m\,s^{-2}}$
Coefficient of restitution	e	0.9
Average particle volume fraction	$\langle M_0 \rangle$	0.01
Particle response time	$\tau_p = \frac{\rho_p d_p^2}{18\mu_f}$	0.025 s
Stokes settling speed	$\mathcal{V}_{St} = \tau_p g$	$0.1\,\mathrm{m\,s^{-1}}$
Particle Reynolds number	$Re_p = \frac{\mathcal{V}_{St} d_p}{\nu_f}$	0.5
Domain size	$\frac{\mathcal{L}_x}{d_p} = 4\frac{\mathcal{L}_y}{d_p} = 56\frac{\mathcal{L}_z}{d_p}$	1792
Grid spacing	$\Delta x / d_p$	2
CFL		0.5

Euler-Lagrange simulations available for validation

EL versus CHyQMOM for CIT

		CHyQMOM	EL
Volume fraction variance	$\langle \alpha'^2 \rangle / \langle \alpha \rangle^2$	1.99 (0.33)	2.00 (0.30)
Settling velocity	$-\langle u_{p,x} \rangle_p / \mathcal{V}_{St}$	2.82 (0.40)	2.96 (0.40)
Particle energy	$\kappa_p / \mathcal{V}_{St}^2$	5.05 (0.51)	5.09 (0.61)
Fluid TKE	$k_f / \mathcal{V}_{St}^2$	9.05 (1.83)	8.42 (1.61)

Particle-Laden Channel Flow

Particle diameter	d_p	200×10^{-6} m
Particle density	ρ_p	$2000\,\mathrm{kg\,m^{-3}}$
Fluid density	ρ_f	$1\,\mathrm{kg\,m^{-3}}$
Fluid viscosity	μ_f	1.8×10^{-5} Pa s
Gravitational constant	g	$3.645\,\mathrm{m\,s^{-2}}$
Coefficient of restitution	e	1
Coefficient of restitution	e_w	1
Average particle volume fraction	$\overline{M}_0$	0.01
Particle response time	$\tau_p = \frac{\rho_p d_p^2}{18\mu_f}$	0.2469 s
Stokes settling speed	$\mathcal{V}_{St} = \tau_p g$	$0.9\,\mathrm{m\,s^{-1}}$
Fluid mean flowrate	$\overline{u}_{f,x}$	$0.9\,\mathrm{m\,s^{-1}}$
Particle Reynolds number	$Re_p = \frac{\mathcal{V}_{St} d_p}{\nu_f}$	10
Domain size	$\frac{\mathcal{L}_x}{d_p} = 10\frac{\mathcal{L}_y}{d_p} = \frac{20}{3}\frac{\mathcal{L}_z}{d_p}$	2500
Grid spacing (streamwise and depth)	$\Delta x/d_p = \Delta z/d_p$	3.125
Grid spacing (wall normal)	$\Delta y/d_p$	variable
CFL		0.5

Euler-Lagrange simulations available for validation

EL versus CHyQMOM for Channel

EL black, CHyQMOM blue

Volume fraction

VF Skewness

Particle velocity

Particle energy

VF variance

Slip velocity

Fluid velocity

Fluid TKE

Future Directions for Quadrature-Based Moment Methods

- Size-conditioned CHyQMOM for inertial particles with different sizes is needed for aggregation, growth, breakage, etc.
- Realizable high-order spatial reconstructions for fluxes (on unstructured meshes ...)
- Hybrid solvers for polydisperse flows capable of dealing efficiently with dilute and dense regimes in same flow
- More physics in mesoscale model (e.g., pseudo-turbulence, buoyancy, added mass, lift, etc.) to handle wider range of flows

OpenQBMM Project (www.openqbmm.org)

Quadrature-based moment methods for CFD in OpenFOAM

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Thanks for your attention!

Questions?