Eulerian Models for Disperse Multiphase Flows

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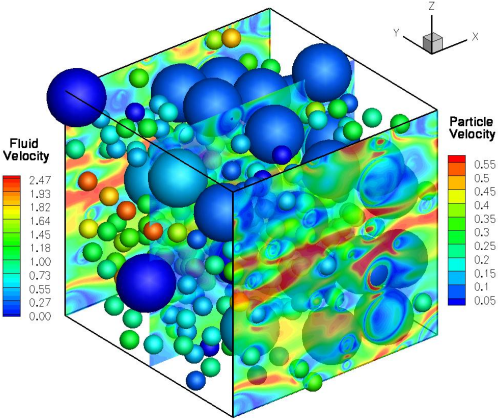
Outline

1. Modeling Disperse Multiphase Flows
2. Conditional HyQMOM
3. Dense Collisional Flows
4. Conclusions & Outlook

Disperse multiphase flow

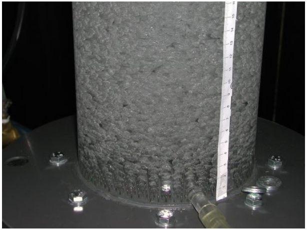
- continuous phase
- disperse phase
- size distribution
- finite particle inertia
- collisions
- variable mass loading
- multiphase turbulence



Bidisperse gas-particle flow (DNS of S. Subramaniam)

Disperse multiphase flows: examples

Bubble columns



Brown-out

Jet break up

Power stations

Volcanos

Spray flames

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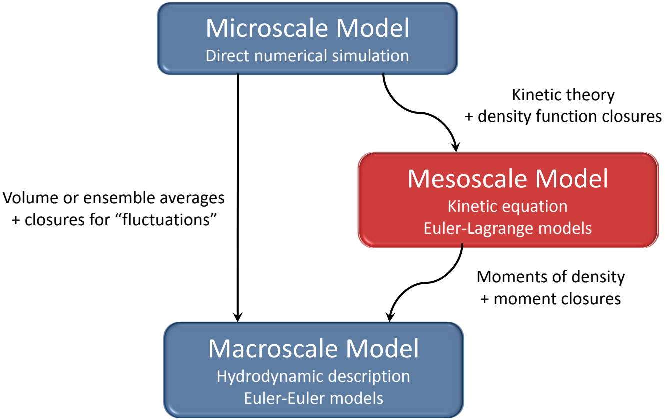
Modeling challenges

- Strong coupling between continuous and disperse phases
- Wide range of particle volume fractions (even in same flow!)
- Inertial particles with wide range of Stokes numbers
- Collision-dominated to collision-less regimes in same flow
- Granular temperature can be very small and very large in same flow
- Particle polydispersity (e.g. size, density, shape) is always present

Need a modeling framework that can handle all aspects!

Overview of kinetic modeling approach



Mesoscale model incorporates more microscale physics in closures!

Types of mesoscale transport (kinetic) equations

- Population balance equation (PBE): $n(t, \mathbf{x}, \xi)$

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}\left[u_i(t, \mathbf{x}, \xi) n\right] + \frac{\partial}{\partial \xi_j}\left[G_j(t, \mathbf{x}, \xi) n\right] = \frac{\partial}{\partial x_i}\left[D(t, \mathbf{x}, \xi)\frac{\partial n}{\partial x_i}\right] + \mathbb{S}$$

with known velocity $\mathbf{u}$, growth $\mathbf{G}$, diffusivity D and source $\mathbb{S}$

- Kinetic equation (KE): $n(t, \mathbf{x}, \mathbf{v})$

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

with known acceleration $\mathbf{A}$ and collision operator $\mathbb{C}$

- Generalized population balance equation (GPBE): $n(t, \mathbf{x}, \mathbf{v}, \xi)$

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

with accelerations $\mathbf{A}$, $\mathbf{G}$ and collision/aggregation $\mathbb{C}$

Eulerian moment transport equations

- PBE: $M_k = \int \xi^k n \, \mathrm{d}\xi$

$$\frac{\partial M_k}{\partial t} + \frac{\partial}{\partial x}\left(\int \xi^k u n \, \mathrm{d}\xi\right) = k \int \xi^{k-1} G n \, \mathrm{d}\xi + \frac{\partial}{\partial x}\left(\int \xi^k D \frac{\partial n}{\partial x} \, \mathrm{d}\xi\right) + \int \xi^k \mathbb{S} \, \mathrm{d}\xi$$

- KE: $M_k = \int v^k n \, \mathrm{d}v$

$$\frac{\partial M_k}{\partial t} + \frac{\partial M_{k+1}}{\partial x} = k \int v^{k-1} A n \, \mathrm{d}v + \int v^k \mathbb{C} \, \mathrm{d}v$$

- GPBE: $M_{kl} = \int v^k \xi^l n \, \mathrm{d}v\mathrm{d}\xi$

$$\frac{\partial M_{kl}}{\partial t} + \frac{\partial M_{k+1l}}{\partial x} = k \int v^{k-1} \xi^l A n \, \mathrm{d}v\mathrm{d}\xi + l \int v^k \xi^{l-1} G n \, \mathrm{d}v\mathrm{d}\xi + \int v^k \xi^l \mathbb{C} \, \mathrm{d}v\mathrm{d}\xi$$

Terms in red require mathematical closure

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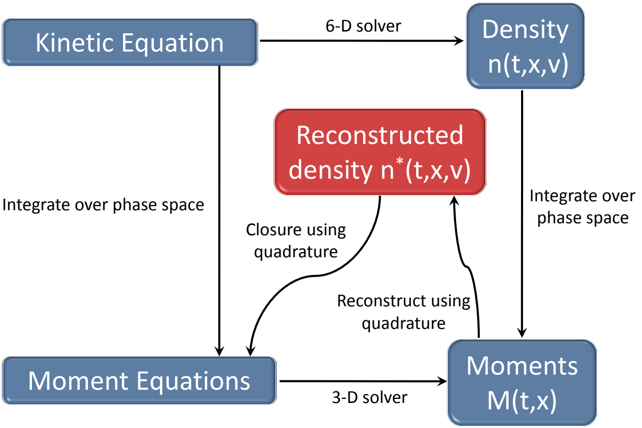
Closure with moment methods



Close moment equations by reconstructing density function

Quadrature-based moment methods (QBMM)

Idea: Given moments, reconstruct the number density function (NDF)

Things to consider:

- Which moments should we choose?
- What method should we use for reconstruction?
- How can we extend method to multivariate phase space?
- How should we design the numerical solver for the moments?

We must be able to demonstrate *a priori* that numerical algorithm is robust and accurate!

Gauss quadrature in 1-D (real line)

- The formula

$$\int g(v)n(v)\,\mathrm{d}v = \sum_{\alpha=1}^{N} n_\alpha g(v_\alpha) + R_N(g)$$

  is a Gauss quadrature iff the N nodes v_α are roots of an N^{th}-order orthogonal polynomial $P_N(v)$ ($\perp$ with respect to $n(v)$)

- Inversion algorithm for moments $M_k = \int v^k n(v)\mathrm{d}v$:

$$\{M_0, M_1, \dots, M_{2N-1}\} \quad \overset{\text{QMOM}}{\Longrightarrow} \quad \{n_1, n_2, \dots, n_N\}, \{v_1, v_2, \dots, v_N\}$$

- Variation: Gauss–Radau quadrature fix v_0 and find n_0 from M_{2N}

$$\int g(v)n(v)\,\mathrm{d}v = \sum_{\alpha=0}^{N} n_\alpha g(v_\alpha) + R_N(g)$$

1-D quadrature method of moments (QMOM)

Approximate unclosed terms in moment equations:

$$\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = \int \mathbf{S}(v)n(v)\mathrm{d}v \approx \sum_{\alpha=0}^{N} n_\alpha \mathbf{S}(v_\alpha)$$

where $\mathbf{M} = \{M_0, M_1, \dots, M_{2N}\}$ and $\mathbf{S}$ is “source term”

- Exact if $\mathbf{S}$ is polynomial of order $\leq 2N$
- Provides good approximation for most other cases with small $N \approx 4$
- Complications arise in particular cases (e.g. spatial fluxes)
- In all cases, moments $\mathbf{M}$ must remain **realizable** for moment inversion

N.B. equivalent to reconstructed N-point distribution function:

$$n^*(v) = \sum_{\alpha=0}^{N} n_\alpha \delta(v - v_\alpha)$$

$\Longrightarrow$ **realizable** if $n_\alpha \geq 0$ for all α

Quadrature in multiple dimensions

No method equivalent to Gaussian quadrature for multiple dimensions!

- Given a realizable moment set $\mathbf{M} = \{M_{i,j,k} : i, j, k \in 0, 1, \dots\}$, find n_α and $\mathbf{v}_\alpha = (u_\alpha, v_\alpha, w_\alpha)$ such that

$$M_{i,j,k} = \int u^i v^j w^k n(\mathbf{v}) \mathrm{d}\mathbf{v} = \sum_{\alpha=0}^{N} n_\alpha u_\alpha^i v_\alpha^j w_\alpha^k$$

- Avoid brute-force nonlinear iterative solver (poor convergence, ill-conditioned, too slow, . . .)
- Algorithm must be realizable (i.e. non-negative weights, . . .)
- Strategy: choose moment set to solve with 1-D QMOM

Conditional QMOM (2-D phase space)

- Conditional density function and conditional moments (2-D)

$$n(u,v) = f(v|u)n(u) \quad \Longrightarrow \quad M_{k|u} = \int v^k f(v|u)\,\mathrm{d}v$$

- 1-D QMOM for u direction ($n = 2$)

$$M_{k,0}, \quad k \in \{0,1,2,3\} \Longrightarrow \text{find weights } n_\alpha, \text{ abscissas } u_\alpha$$

- Solve linear systems for conditional moments $M_{k|u_\alpha}$:

$$\begin{bmatrix} 1 & 1 \\ u_1 & u_2 \end{bmatrix} \begin{bmatrix} n_1 & \\ & n_2 \end{bmatrix} \begin{bmatrix} M_{k|u_1} \\ M_{k|u_2} \end{bmatrix} = \begin{bmatrix} M_{0,k} \\ M_{1,k} \end{bmatrix} \quad \text{for } k \in \{1,2,3\}$$

- CQMOM controls 10 moments:

$$\begin{matrix} M_{0,0} & M_{0,1} & M_{0,2} & M_{0,3} \\ M_{1,0} & M_{1,1} & M_{1,2} & M_{1,3} \\ M_{2,0} & & & \\ M_{3,0} & & & \end{matrix}$$

Conditional QMOM (cont.)

- 1-D QMOM in v direction for each α:

$$M_{k|u_\alpha}, \quad k \in \{0,1,2,3\} \Longrightarrow \text{find weights } p_{\alpha\beta}, \text{ abscissas } v_{\alpha\beta}$$

- Reconstructed density: $n^*(u,v) = \sum_\alpha \sum_\beta n_\alpha p_{\alpha\beta} \delta(u - u_\alpha) \delta(v - v_{\alpha\beta})$
- Conditioning on $v = v_\alpha$ uses 10 moments:

$$\begin{matrix} M_{0,0} & M_{0,1} & M_{0,2} & M_{0,3} \\ M_{1,0} & M_{1,1} & & \\ M_{2,0} & M_{2,1} & & \\ M_{3,0} & M_{3,1} & & \end{matrix}$$

Union of two sets $\Longrightarrow$ CQMOM moment set

- Extension to higher-dimensional phase space is straightforward

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CQMOM moment set

Moments needed for all CQMOM permutations

$N = 4$ nodes in 2-D

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

12 moments

$N = 9$ nodes in 2-D

$M_{0,0}$	$M_{1,0}$	$M_{2,0}$	$M_{3,0}$	$M_{4,0}$	$M_{5,0}$
$M_{0,1}$	$M_{1,1}$	$M_{2,1}$	$M_{3,1}$	$M_{4,1}$	$M_{5,1}$
$M_{0,2}$	$M_{1,2}$	$M_{2,2}$	$M_{3,2}$	$M_{4,2}$	$M_{5,2}$
$M_{0,3}$	$M_{1,3}$	$M_{2,3}$			
$M_{0,4}$	$M_{1,4}$	$M_{2,4}$			
$M_{0,5}$	$M_{1,5}$	$M_{2,5}$			

27 moments

Entire moment set is transported

Kinetic-based finite-volume methods (KBFVM)

Given **transported moments**, solve

$$\frac{\partial M_{k,l}}{\partial t} + \frac{\partial M_{k+1,l}}{\partial x} = k \int v^{k-1} \xi^l A\, n \,\mathrm{d}v\,\mathrm{d}\xi + l \int v^k \xi^{l-1} G\, n \,\mathrm{d}v\,\mathrm{d}\xi + \int v^k \xi^l \mathbb{C} \,\mathrm{d}v\,\mathrm{d}\xi$$

where RHS is closed using QBMM:

$$\frac{\partial M_{k,l}}{\partial t} + \frac{\partial M_{k+1,l}}{\partial x} = \sum_{\alpha=1}^{\mathcal{N}} \rho_\alpha \left\{ k v_\alpha^{k-1} \xi_\alpha^l A_\alpha + l v_\alpha^k \xi_\alpha^{l-1} G_\alpha + v_\alpha^k \xi_\alpha^l \mathbb{C}_\alpha \right\}$$

Things to consider:

- How do we discretize the spatial fluxes?
- How do we update the moments in time?
- How can we ensure that the moments are always **realizable**?

Kinetic-based spatial fluxes

Spatial fluxes can use kinetic formulation: e.g. $\partial_t M_{00} + \partial_x M_{10} = 0$

$$\begin{aligned} M_{1,0} &= Q^-_{1,0} + Q^+_{1,0} \\ &= \int_{-\infty}^{0} v \left(\int n^*(v,\xi) \mathrm{d}\xi \right) \mathrm{d}u + \int_0^{\infty} v \left(\int n^*(v,\xi) \mathrm{d}\xi \right) \mathrm{d}v \end{aligned}$$

Using reconstructed n^*, downwind and upwind flux components are

$$Q^-_{1,0} = \sum_{\alpha=1}^{\mathcal{N}} \rho_\alpha v_\alpha \boldsymbol{I}_{(-\infty,0)}(v_\alpha) \qquad Q^+_{1,0} = \sum_{\alpha=1}^{\mathcal{N}} \rho_\alpha v_\alpha \boldsymbol{I}_{(0,\infty)}(v_\alpha)$$

where $I_{\mathbb{S}}(x)$ is the indicator function for the interval $\mathbb{S}$

Kinetic-based fluxes are (weakly) hyperbolic

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Realizable time-stepping schemes

- First-order explicit:

$$\mathbf{M}_i^{n+1} = \mathbf{M}_i^n - \lambda \left[\mathbf{G}\left(\mathbf{M}^n_{i+\frac{1}{2},l}, \mathbf{M}^n_{i+\frac{1}{2},r}\right) - \mathbf{G}\left(\mathbf{M}^n_{i-\frac{1}{2},l}, \mathbf{M}^n_{i-\frac{1}{2},r}\right) \right]$$

- RK2SSP:

$$\begin{aligned}
\mathbf{M}_i^{*} &= \mathbf{M}_i^n - \lambda \left[\mathbf{G}\left(\mathbf{M}^n_{i+\frac{1}{2},l}, \mathbf{M}^n_{i+\frac{1}{2},r}\right) - \mathbf{G}\left(\mathbf{M}^n_{i-\frac{1}{2},l}, \mathbf{M}^n_{i-\frac{1}{2},r}\right) \right] \\
\mathbf{M}_i^{**} &= \mathbf{M}_i^* - \lambda \left[\mathbf{G}\left(\mathbf{M}^*_{i+\frac{1}{2},l}, \mathbf{M}^*_{i+\frac{1}{2},r}\right) - \mathbf{G}\left(\mathbf{M}^*_{i-\frac{1}{2},l}, \mathbf{M}^*_{i-\frac{1}{2},r}\right) \right] \\
\mathbf{M}_i^{n+1} &= \frac{1}{2}\left(\mathbf{M}_i^n + \mathbf{M}_i^{**}\right)
\end{aligned}$$

- High-order FV schemes: Laurent, Nguyen, https://hal.archives-ouvertes.fr/hal-01345689v2

Achieve second order in space and time on unstructured grids

Bubbly flow simulation using QBMM and KBFVM

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Realizable finite-volume scheme on unstructured mesh

Current Status

- QBMM are well suited for fine particles (e.g., aerosols, soot, etc.) where principal closure problem is the source terms (e.g., aggregation, growth, breakage, etc.)
- QBMM combined with KBFVM work well for dilute disperse multiphase flows where spatial transport is due to kinetic fluxes
- However, hardest closure problem is pure kinetic transport where no other physics (e.g., collisions, drag, etc.) modify velocity NDF
- Standard QMOM/CQMOM leads to weakly hyperbolic moment systems (i.e., delta shocks) so a hyperbolic closure would be preferable
- In dense disperse multiphase flows, spatial transport is dominated by collisional fluxes that require an iterative solver

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1 Modeling Disperse Multiphase Flows

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Hyperbolic QMOM

- Approximate velocity NDF by ($N \geq 2$)

$$n(u) \approx M_0 \sum_{\alpha=1}^{N} p_\alpha \delta(u - \bar{u} - u_\alpha)$$

where $\bar{u} = M_1/M_0$, and p_α and u_α are found from central moments:

$$C_i = \frac{1}{M_0} \int_{-\infty}^{+\infty} (u - \bar{u})^i n(u) \, \mathrm{d}u$$

- Fix C_{2N-1} such that moment system is hyperbolic
- Given $\{1, 0, C_2 \ldots, C_{2N-2}\}$ and constraint on C_{2N-1}, apply QMOM

$$\{1, 0, C_2 \ldots, C_{2N-1}\} \overset{\text{QMOM}}{\Longrightarrow} \{p_1, p_2, \ldots, p_N\}, \{u_1, u_2, \ldots, u_N\}$$

Hyperbolic QMOM (cont.)

- Moment closure for kinetic flux in 1-D:

$$\partial_t M_{2N-2} + \partial_x \bar{M}_{2N-1} = 0 \quad \Longrightarrow \quad \bar{M}_{2N-1} = M_0 \sum_{\alpha=1}^{N} p_\alpha (\bar{u} + u_\alpha)^{2N-1}$$

For $N = 3$: $\bar{M}_5 = M_0 \left[p_1 (\bar{u} + u_1)^5 + p_2 \bar{u}^5 + p_3 (\bar{u} + u_3)^5 \right]$

- Theorem: (F. Laurent) Moment system for $\{M_0, M_1, M_2, M_3, M_4\}$ with kinetic flux $\bar{M}_5$ is hyperbolic with 5 distinct eigenvalues

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

where $q = C_3 / C_2^{3/2}$ and $\eta = C_4 / C_2^2$

- HyQMOM is well defined for any realizable set $\{M_0, M_1, M_2, M_3, M_4\}$ (including $\eta > 3$ when $q = 0$), realizability $\eta \geq 1 + q^2 \Longrightarrow$ QMOM

Conditional HyQMOM

- Approximate 2-D velocity NDF by ($N \geq 2$)

$$n(u,v) \approx M_{0,0} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} p_\alpha p_{\alpha\beta} \delta(u - \bar{u} - u_\alpha) \delta(v - \bar{v} - \bar{v}_\alpha - v_{\alpha\beta})$$

where $\bar{v} = M_{0,1}/M_{0,0}$ and abscissas $v_{\alpha\beta}$ and $\bar{v}_\alpha$ are found from central moments:

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

- Example $N^2 = 9$ nodes, CQMOM applied to symmetric moment sets:

10 moments

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

12 moments

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

Conditional HyQMOM (cont.)

- With 10 moments, $\bar{v}_\alpha = a_0 + a_1 u_\alpha$ is found from

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

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

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

$$C_{2|u_\alpha} = C_{0,2} - a_1^2 C_{2,0} \quad C_{3|u_\alpha} = C_{0,3} - a_1^3 C_{3,0} \quad C_{4|u_\alpha} = C_{0,4} - 6a_1^2 C_{2,0} C_{2|u_\alpha} - a_1^4 C_{4,0}$$

N.B. conditional moments do not depend on α

- HyQMOM applied to $\{1, 0, C_{2|u_\alpha}, C_{3|u_\alpha}, C_{4|u_\alpha}\}$ to find $p_{\alpha\beta}$ and $v_{\alpha\beta}$
- With 12 moments, $\bar{v}_\alpha = a_0 + a_1 u_\alpha + a_2 u_\alpha^2$ and $C_{2|u_\alpha} = b_0 + b_1 u_\alpha$

Conditional HyQMOM (cont.)

- CHyQMOM closure for kinetic flux in 1-D spatial and 2-D velocity with 10 moments:

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

- Theorem: (F. Laurent) 10 moment system with kinetic flux is hyperbolic with 10 distinct eigenvectors

- Extension to 3-D phase space follows same logic: Example $N^3 = 27$ nodes uses either 16 or 23 moments

- Test 3-D closure for particle trajectory crossing (PTC) with 16 moments

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Particle trajectory crossing in 1-D

Uncorrelated moments

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16-moment, 27-node CHyQMOM

Particle trajectory crossing in 1-D

Quadrature weights and abscissas

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16-moment, 27-node CHyQMOM

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Particle trajectory crossing in 1-D

Perfectly correlated moments

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16-moment, 27-node CHyQMOM

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Particle trajectory crossing in 1-D

Quadrature weights and abscissas

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16-moment, 27-node CHyQMOM

Particle trajectory crossing in 1-D

Partially correlated moments

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16-moment, 27-node CHyQMOM

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Particle trajectory crossing in 1-D

Quadrature weights and abscissas

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16-moment, 27-node CHyQMOM

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Particle trajectory crossing in 2-D

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10-moment, 9-node CHyQMOM

Particle trajectory crossing in 3-D

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16-moment, 27-node CHyQMOM

CHyQMOM future developments

- CHyQMOM can be extended to higher-order velocity moments (e.g., $N = 4$), but 16 moments already suffices to capture PTC in 3-D
- Size-conditioned CHyQMOM for inertial particles with different sizes is needed for aggregation, growth, breakage, etc.
- CHyQMOM combined with KBFVM works well for dilute disperse multiphase flows where spatial transport is due to kinetic fluxes
- For dense disperse multiphase flows, need to combine CHyQMOM with implicit solver for collisional fluxes
- For KBFVM need realizable high-order spatial reconstructions for fluxes

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Gas–particle flow model for monodisperse particles

Particle-phase KE

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \frac{\partial n}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{A} n = \mathbb{C}$$

- $n(t, \mathbf{x}, \mathbf{v})$: number density function (NDF)
- $\mathbf{v}$: particle velocity
- $\mathbf{A}$: particle acceleration (drag, gravity, ...)
- $\mathbb{C}$: rate of change of n due to particle–particle collisions

Fluid-phase equations

$$\frac{\partial}{\partial t}\alpha_g \rho_g + \nabla \cdot \alpha_g \rho_g \mathbf{U}_g = 0$$

$$\frac{\partial}{\partial t}\alpha_g \rho_g \mathbf{U}_g + \nabla \cdot \alpha_g \rho_g \mathbf{U}_g \mathbf{U}_g = \nabla \cdot \alpha_g \boldsymbol{\tau}_g + \beta_g + \alpha_g \rho_g \mathbf{g}$$

- $\alpha_g = 1 - \alpha_p$: gas volume fraction
- β_g: mean particle drag

Boltzmann–Enskog inelastic, hard-sphere collision integral

Boltzmann–Enskog collision integral:

$$\mathbb{C} = \frac{6}{\pi d_p} \int_{\mathbb{R}^3} \int_{\mathbb{S}^+} \left[\chi\, f^{(2)}(\mathbf{x}, \mathbf{v}_1''; \mathbf{x} - d_\text{p}\mathbf{n}, \mathbf{v}_2'' - \; f^{(2)}(\mathbf{x}, \mathbf{v}_1; \mathbf{x} + d_\text{p}\mathbf{n}, \mathbf{v}_2) \right] |\mathbf{g} \cdot \mathbf{n}| \, \mathrm{d}\mathbf{n} \mathrm{d}\mathbf{v}_2$$

where $f^{(2)}$ is two-particle density and

- d_p particle diameter
- $\mathbf{g}$ relative velocity vector
- $\mathbf{n}$ unit vector along the direction of particles centers
- $\mathbb{S}^+$ unit half sphere where $\mathbf{g} \cdot \mathbf{n} > 0$
- χ factor relating pre- and post-collisional velocities

Closure yields two terms: point collisions + collisional flux

Complexity of solutions to kinetic equation

3-D Periodic flow

J. S. Capecelatro & O. Desjardins, Cornell

- Average volume fraction: $\alpha_{\mathrm{p}} = 0.01$
- $\rho_{\mathrm{p}}/\rho_{\mathrm{g}} = 1500$, $\mathrm{Re}_{\mathrm{p}} = 1$
- elastic collisions
- full 2-way coupling

Eulerian model should yield identical results
(if closure is accurate)!

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Governing equations: Particle velocity moments

Ten velocity moments (dilute regime):

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S} \qquad M^{\gamma}_{ijk} = \int u^i v^j w^k f(\boldsymbol{v}) \mathrm{d}\boldsymbol{v}$$

$$M^0_{000} = \alpha_p, \quad \begin{bmatrix} M^1_{100} \\ M^1_{010} \\ M^1_{001} \end{bmatrix} = \alpha_p \boldsymbol{U}_p, \quad \begin{bmatrix} M^2_{200} & M^2_{110} & M^2_{101} \\ M^2_{110} & M^2_{020} & M^2_{011} \\ M^2_{101} & M^2_{011} & M^2_{002} \end{bmatrix} = \alpha_p \boldsymbol{U}_p \otimes \boldsymbol{U}_p + \alpha_p \mathbf{P}_p.$$

Particle-phase equations (dense regime $\Longrightarrow 3\Theta_p = trace(\mathbf{P}_p)$):

$$\frac{\partial \rho_p \alpha_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \boldsymbol{U}_p = 0$$

$$\frac{\partial \rho_p \alpha_p \boldsymbol{U}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\boldsymbol{U}_p \otimes \boldsymbol{U}_p + \mathbf{P}_p + \mathbf{G}_p + \mathbf{Z}_p \right) = \rho_p \alpha_p \boldsymbol{g} + \rho_p \alpha_p \boldsymbol{M}_{pg}$$

$$\frac{\partial \rho_p \alpha_p \mathbf{P}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\boldsymbol{U}_p \otimes \mathbf{P}_p + \mathbf{Q}_p + \mathbf{H}_p \right) + \rho_p \alpha_p \left[(\mathbf{P}_p + \mathbf{G}_p) \cdot \nabla \boldsymbol{U}_p + (\nabla \boldsymbol{U}_p)^T \cdot (\mathbf{P}_p + \mathbf{G}_p) \right]$$
$$= \rho_p \alpha_p \mathbf{E}_{pg} + \rho_p \alpha_p \mathbf{C}_p$$

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Kinetic, collisional and frictional fluxes: Dense regime

Kinetic flux:

$$\boldsymbol{U}_p \otimes \boldsymbol{U}_p + \mathbf{P}_p$$

$$\mathbf{P}_p = \Theta_p \mathbf{I} - \boldsymbol{\sigma}_p = \Theta_p \mathbf{I} - 2\nu_{p,k}\boldsymbol{S}_p$$

$$\boldsymbol{S}_p = \frac{1}{2}\left[\nabla \boldsymbol{U}_p + (\nabla \boldsymbol{U}_p)^T - \frac{2}{3}(\nabla \cdot \boldsymbol{U}_p)\,\mathbf{I}\right]$$

Collisional flux (pressure infinite for finite $\alpha_p \approx 0.63$):

$$\mathbf{G}_p = \frac{p_{p,c}}{\rho_p \alpha_p}\mathbf{I} - 2\nu_{p,c}\boldsymbol{S}_p$$

Frictional flux (pressure infinite for finite $\alpha_p \approx 0.63$, null when $\alpha_p < 0.55$):

$$\mathbf{Z}_p = \frac{p_{p,f}}{\rho_p \alpha_p}\mathbf{I} - 2\nu_{p,f}\boldsymbol{S}_p$$

Energy fluxes: $\boldsymbol{U}_p \otimes \mathbf{P}_p + \mathbf{Q}_p + \mathbf{H}_p = \boldsymbol{U}_p \otimes \mathbf{P}_p - \frac{2}{3}k_\Theta \nabla \otimes \mathbf{P}_p$

Kinetic flux-splitting scheme for all flow regimes

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$$

$$h_1 + h_2 = 1$$

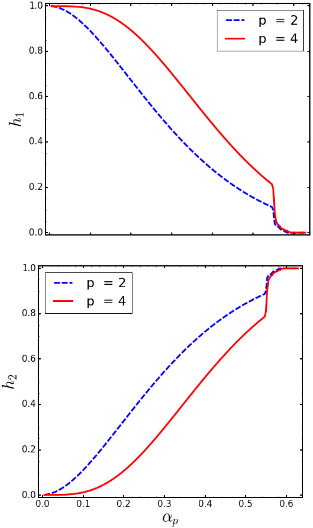
$$h_2 = \left(\frac{p_{p,c} + p_{p,f}}{p_{p,k} + p_{p,c} + p_{p,f} + \varepsilon} \right)^p$$

Step 1: KBFVM

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot h_1 \mathbf{F} = \mathbf{0}$$

Step 2: Hydrodynamic solver

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot (h_2 \mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$$



Solution Procedure

1. Initialize all variables $\mathbf{M}$, $\{\alpha_p, \boldsymbol{U}_p, \Theta_p, \boldsymbol{\sigma}_p\}$, and $\{\alpha_g, \boldsymbol{U}_g, p_g\}$
2. Calculate h_1 and h_2
3. **Explicit** Free-transport solver:
   - Compute kinetic-based moment fluxes to transport the moments
   - Update $\{\alpha_p, \boldsymbol{U}_p, \Theta_p, \boldsymbol{\sigma}_p\}$ using moments $\mathbf{M}$
4. **Iterative** Hydrodynamic solver:
   - Solve $\{\alpha_p, \boldsymbol{U}_p, \Theta_p\}$ hydrodynamic transport equations
   - Solve gas-phase velocity and pressure, $\{\boldsymbol{U}_g, p_g\}$, equations
5. Solve $\boldsymbol{\sigma}_p$ transport equation
6. Update moment set $\mathbf{M}$ using $\{\alpha_p, \boldsymbol{U}_p, \Theta_p, \boldsymbol{\sigma}_p\}$
7. Advance in time by repeating from Step 2 until simulation is complete

2-D bubbling fluidized bed

α_p h_2 $U_{p,y}$ Θ_p $\sigma_{p,xy}$

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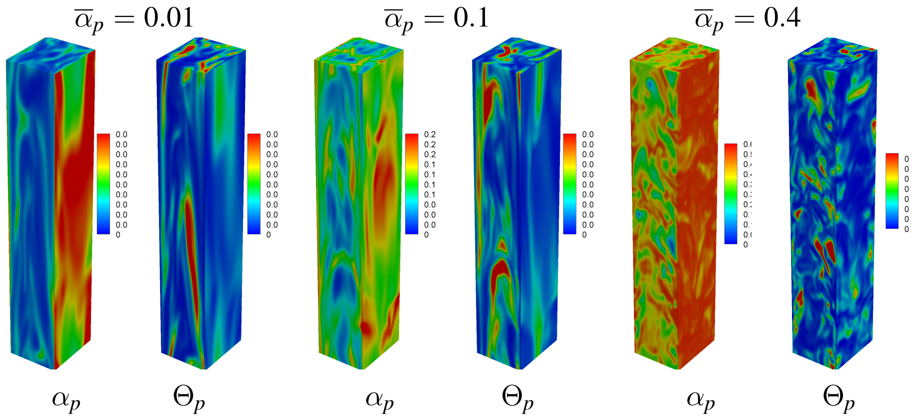
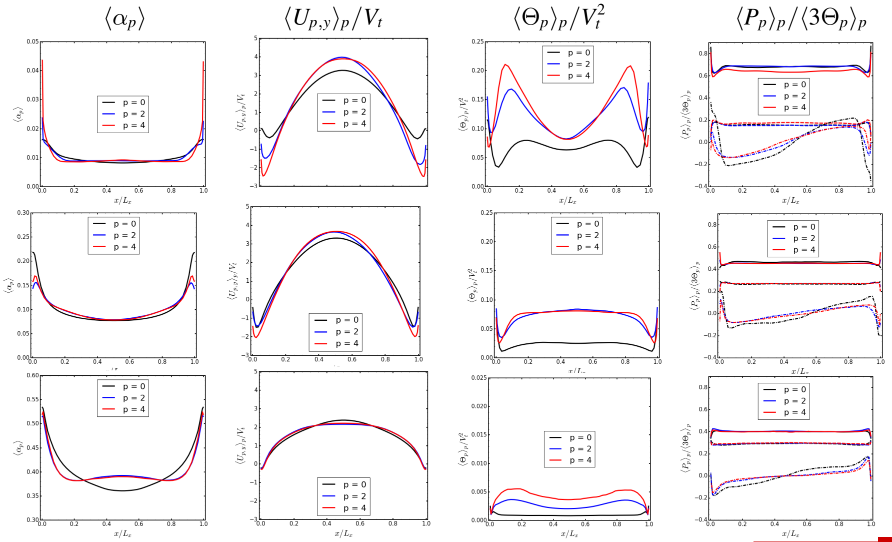
3-D wall-bounded vertical channel: Instantaneous fields



Wall-bounded vertical channel: Statistical results



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Future developments

- Dense–dilute flow solver will be extended to fourth-order velocity moments using CHyQMOM to capture PTC
- Dense–dilute flow solver will be extended to polydisperse particles (e.g., sprays) using size-conditioned CHyQMOM
- Dense–dilute flow solver will be adapted to monokinetic flows, such as disperse bubbly flow, using size-conditioned CHyQMOM and additional interphase forces (e.g., virtual mass, lift, etc.)

Outline

1 Modeling Disperse Multiphase Flows

2 Conditional HyQMOM

3 Dense Collisional Flows

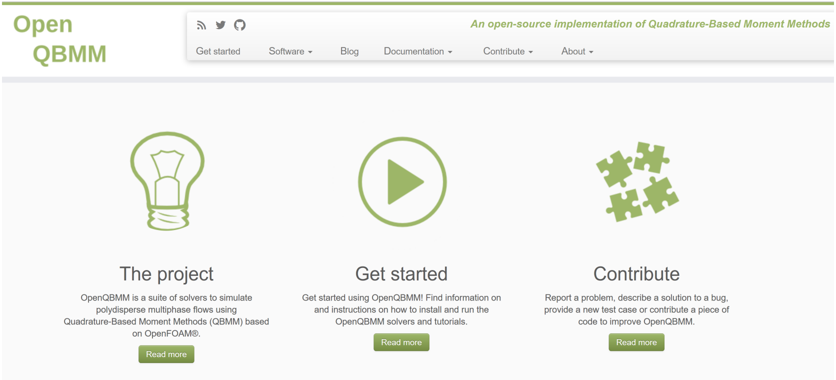
4 Conclusions & Outlook

Conclusions & Outlook

- Mesoscale models have direct link with underlying physics and result in a kinetic equation
- QBMM solves kinetic equation by reconstructing distribution function from moments
- For fine particles, QBMM provides an accurate closure for source terms
- For inertial particles, use CHyQMOM for velocity NDF reconstruction for dilute flows
- For dense flows, CHyQMOM is used for kinetic flux and source terms, while a "two-fluid" hydrodynamic solver is used for collisional fluxes
- Extension to size-conditioned CHyQMOM will allow for polydisperse inertial particles

OpenQBMM project (www.openqbmm.org)

Please contribute to the advancement of computational fluid dynamics!



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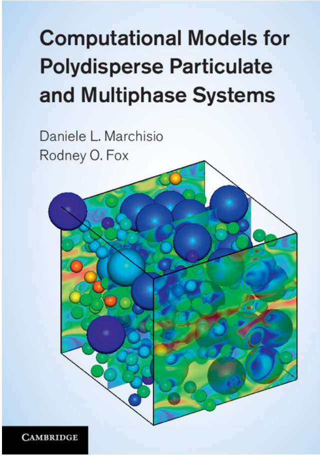

Thanks for your attention!

Questions?