Quadrature-Based Moment Methods for Kinetic Models

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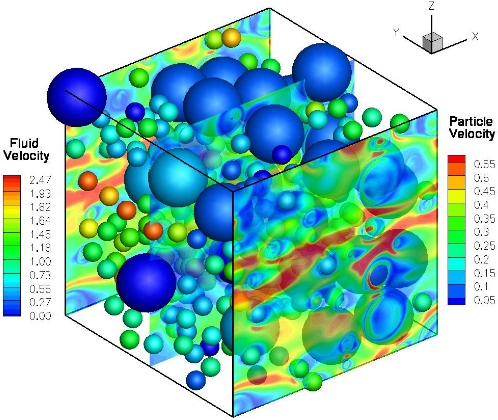
Application: polydisperse multiphase flow

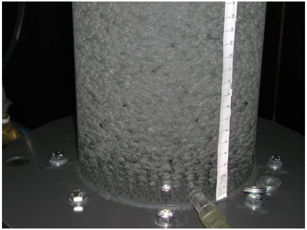
- continuous phase
- disperse phase
- size distribution
- finite particle inertia
- collisions
- variable mass loading
- multiphase turbulence



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

Application: polydisperse multiphase flows

Bubble columns



Brown-out

Jet break up

Power stations

Volcanos

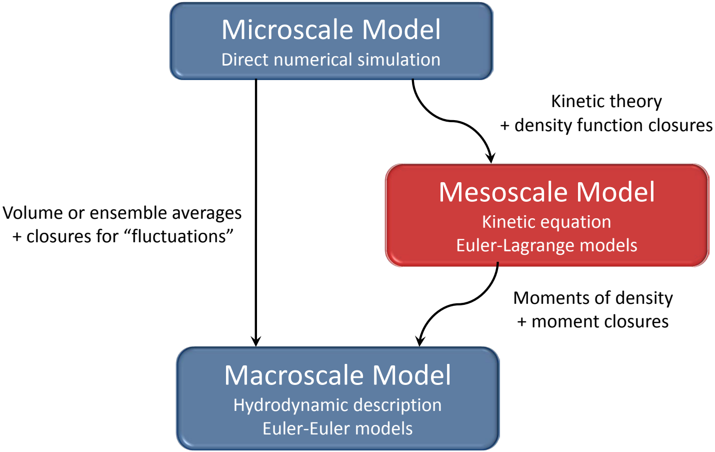
Spray flames

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 $\mathbf{u}$, acceleration $\mathbf{G}$, 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 known accelerations $\mathbf{A}$, $\mathbf{G}$ and collision/aggregation operator $\mathbb{C}$

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

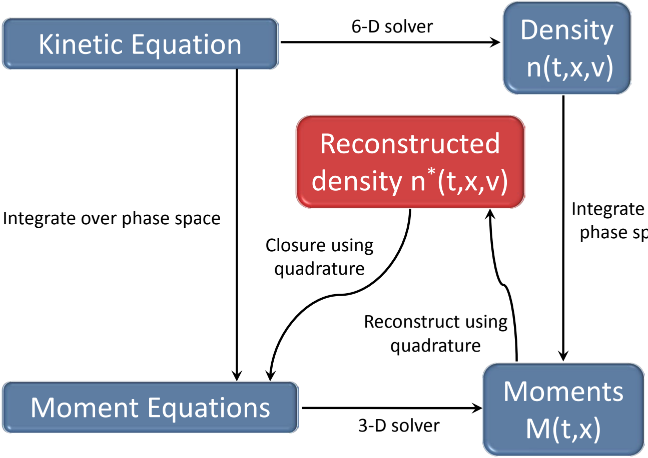
$$\frac{\partial M_k}{\partial t} + \frac{\partial M_{k+1}}{\partial x} = k \int v^{k-1} A n \, \mathrm{d}v + \int v^k \mathbb{C} \, \mathrm{d}v$$

- 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 will usually require mathematical closure

Closure with moment methods



Close moment equations by reconstructing density function

Quadrature-based moment methods (QBMM)

Basic idea: Given a set of transported 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 $n(v)$)

- Recursion formula for $P_N(v)$:

$$P_{\alpha+1}(v) = (v - a_\alpha)P_\alpha(v) - b_\alpha P_{\alpha-1}(v), \quad \alpha = 0, 1, 2, \ldots$$

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

$$\{M_0, M_1, \ldots, M_{2N-1}\} \overset{\text{hard}}{\Longrightarrow} \{a_0, a_1, \ldots, a_{N-1}\}, \{b_1, b_2, \ldots, b_{N-1}\}$$

$$\overset{\text{easy}}{\Longrightarrow} \{n_1, n_2, \ldots, n_N\}, \{v_1, v_2, \ldots, v_N\}$$

Szegö quadrature on unit circle

- If $n(\phi)$ is periodic on the unit circle:

$$\int_{-\pi}^{\pi} g(e^{i\phi}) n(\phi) \, \mathrm{d}\phi = \sum_{\alpha=1}^{N} n_\alpha g(e^{i\phi_\alpha}) + R_N(g)$$

is a Szegö quadrature iff the N nodes $z_\alpha = e^{i\phi_\alpha}$ are zeros of an N^{th}-order para-orthogonal polynomials $B_N(z)$

- Trigonometric moments:

$$\langle \cos(n\phi) \rangle = \int_{-\pi}^{\pi} \frac{1}{2}(z^n + z^{-n}) n(\phi) \, \mathrm{d}\phi, \ \langle \sin(n\phi) \rangle = \int_{-\pi}^{\pi} \frac{1}{2}(z^n - z^{-n}) n(\phi) \, \mathrm{d}\phi$$

are natural choice for reconstruction

- Except for special case [$n(\phi)$ symmetric wrt 0], no fast inversion algorithm is available to find n_α and ϕ_α

1-D quadrature method of moments (QMOM)

Use Gaussian quadrature to approximate unclosed terms in moment equations:

$$\frac{\mathrm{d}\mathbf{M}}{\mathrm{d}t} = \int \mathbf{S}(v) n(v) \mathrm{d}v \approx \sum_{\alpha=1}^{N} n_\alpha \mathbf{S}(v_\alpha)$$

where $\mathbf{M} = \{M_0, M_1, \ldots, M_{2N-1}\}$ and $\mathbf{S}$ is "source term"

- Exact if $\mathbf{S}$ is polynomial of order $\leq 2N - 1$
- 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:

$$n^*(v) = \sum_{\alpha=1}^{N} n_\alpha \delta(v - v_\alpha)$$

$\Longrightarrow$ **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 $\mathbf{M} = \{M_{ijk} : i, j, k \in 0, 1, \dots\}$, find n_α and $\mathbf{v}_\alpha$ such that

$$M_{ijk} = \int v_1^i v_2^j v_3^k n(\mathbf{v}) \mathrm{d}\mathbf{v} = \sum_{\alpha=1}^{N} n_\alpha v_{1\alpha}^i v_{2\alpha}^j v_{3\alpha}^k$$

What moment set to use?

- If $\mathbf{M}$ corresponds to an N-point distribution, then method should be exact
- Avoid brute-force nonlinear iterative solver (poor convergence, ill-conditioned, too slow, . . .)
- Algorithm must be realizable (i.e. non-negative weights, . . .)
- Strategy: choose an optimal moment set to avoid ill-conditioned systems

Brute-force QMOM (2-D phase space)

- Given $3n^2$ bivariate optimal moments ($n = 2$):

$$\begin{matrix} M_{00} & M_{01} & M_{02} & M_{03} \\ M_{10} & M_{11} & M_{12} & M_{13} \\ M_{20} & M_{21} & & \\ M_{30} & M_{31} & & \end{matrix}$$

- Solve 12 moment equations:

$$\sum_{\alpha=1}^{4} |n_\alpha| u_\alpha^i v_\alpha^j = M_{ij}$$

to find $\{n_1, \ldots, n_4; u_1, \ldots, u_4; v_1, \ldots, v_4\}$

- Problem: iterative solver converges slowly (or not at all)
- Problem: system is singular for (nearly) degenerate cases

Conditional QMOM (2-D phase space)

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

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

- 1-D adaptive quadrature for U direction ($n = 2$)

$$\langle U^k \rangle = M_{k0}, k \in \{0,1,2,3\} \Longrightarrow \text{find weights } \rho_i, \text{ abscissas } u_i$$

- Solve linear systems for conditional moments $\langle V^k | u_i \rangle$:

$$\begin{bmatrix} \rho_1 & \rho_2 \\ \rho_1 u_1 & \rho_2 u_2 \end{bmatrix} \begin{bmatrix} \langle V^k | u_1 \rangle \\ \langle V^k | u_2 \rangle \end{bmatrix} = \begin{bmatrix} \langle V^k \rangle \\ \langle U V^k \rangle \end{bmatrix} = \begin{bmatrix} M_{0k} \\ M_{1k} \end{bmatrix} \quad \text{for } k \in \{1,2,3\}$$

- In principle, CQMOM controls 10 of 12 optimal moments:

$$\begin{matrix} M_{00} & M_{01} & M_{02} & M_{03} \\ M_{10} & M_{11} & M_{12} & M_{13} \\ M_{20} & & & \\ M_{30} & & & \end{matrix}$$

Conditional QMOM (cont.)

- 1-D adaptive quadrature in V direction for each i:

$$\langle V^k | u_i \rangle, k \in \{0,1,2,3\} \Longrightarrow \text{find weights } \rho_{ij}, \text{ abscissas } v_{ij}$$

- Adaptive quadrature sets some $\rho_{ij} = 0$ if subset of conditional moments are not realizable
- Reconstructed density: $n^*(u,v) = \sum_i \sum_j \rho_i \rho_{ij} \delta(u-u_i)\delta(v-v_{ij})$
- Conditioning on $V = v_i$ uses 10 of 12 optimal moments:

$$\begin{matrix} M_{00} & M_{01} & M_{02} & M_{03} \\ M_{10} & M_{11} & & \\ M_{20} & M_{21} & & \\ M_{30} & M_{31} & & \end{matrix}$$

Union of two sets $\Longrightarrow$ optimal moment set

- Extension to higher-dimensional phase space is straightforward

Optimal moment set

Moments needed for all CQMOM permutations $\Longrightarrow$ Optimal moment set

$N = 4$ nodes in 2-D

$$\begin{array}{llll} M_{00} & M_{10} & M_{20} & M_{30} \\ M_{01} & M_{11} & M_{21} & M_{31} \\ M_{02} & M_{12} & & \\ M_{03} & M_{13} & & \end{array}$$

12 moments

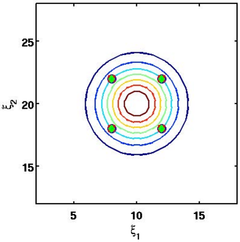
$N = 9$ nodes in 2-D

$$\begin{array}{llllll} M_{00} & M_{10} & M_{20} & M_{30} & M_{40} & M_{50} \\ M_{01} & M_{11} & M_{21} & M_{31} & M_{41} & M_{51} \\ M_{02} & M_{12} & M_{22} & M_{32} & M_{42} & M_{52} \\ M_{03} & M_{13} & M_{23} & & & \\ M_{04} & M_{14} & M_{24} & & & \\ M_{05} & M_{15} & M_{25} & & & \end{array}$$

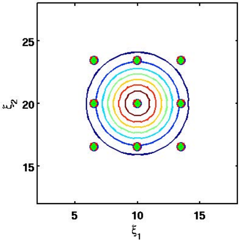
27 moments

Only optimal moment set is transported

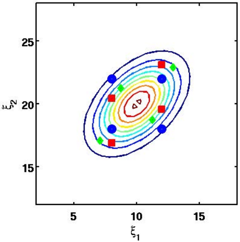
Examples of 2-D quadrature



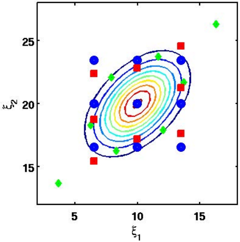
(a) $\rho = 0$ and $N = 4$



(b) $\rho = 0$ and $N = 9$



(c) $\rho = 0.5$ and $N = 4$



(d) $\rho = 0.5$ and $N = 9$

QBMM approximations for bivariate Gaussian with $\rho = 0$ (top) and $\rho = 0.5$ (bottom) for $N = 4$ (left) and $N = 9$ (right).
Brute-force QMOM (green diamond)
Tensor-product QMOM (blue circle)
CQMOM (red square)

CQMOM on unit circle

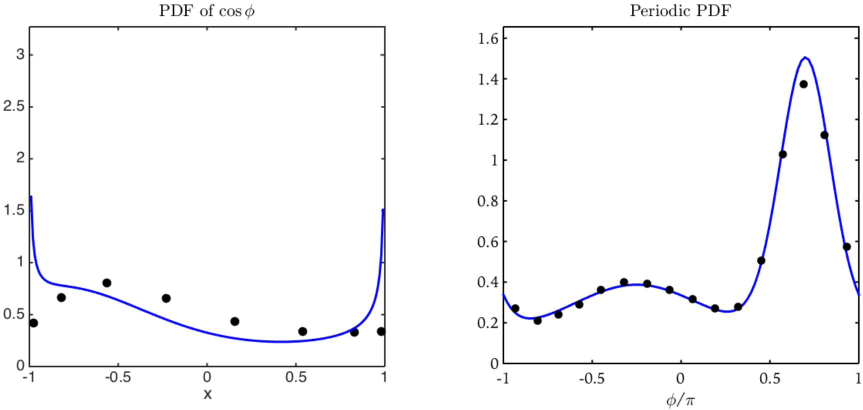
- For $n(\phi)$ on the unit circle, define $x = \cos\phi$ and $y = \sin\phi$
- Conditional pdf is known exactly $n(x, y) = n(x) f(y|x)$

$$f(y|x) = w_1(x)\delta\left(y - \sqrt{1 - x^2}\right) + w_2(x)\delta\left(y + \sqrt{1 - x^2}\right)$$

  with one unknown $w_1(x)$ $(w_2 = 1 - w_1)$

- Apply QMOM with $2N$ moments $\langle \cos^n \phi \rangle$ to find n_α and $x_\alpha = \cos\phi_\alpha$
- CQMOM requires conditional moment $\langle y|x_\alpha \rangle$ to find $w_1(x_\alpha)$
- Apply CQMOM with N moments $\langle \sin\phi \cos^n \phi \rangle$ to find $w_{1\alpha} = w_1(x_\alpha)$
- Gauss/Swegö quadrature for symmetric ndf, otherwise fast, realizable reconstruction

Example of CQMOM on unit circle



8-pt Gauss quadrature 16-pt CQMOM quadrature

Exactly reproduces trigonometric moments up to $N = 8$

Extended quadrature method of moments (EQMOM)

Can we improve reconstructed distribution using kernel density functions?

$$n(v) = \sum_{i=1}^{N} n_i \delta_\sigma(v, v_i)$$

with N weights $n_i \geq 0$, N abscissas v_i but **only one** spread parameter $\sigma \geq 0$

- Gaussian ($-\infty < v < +\infty$):

$$\delta_\sigma(v, v_i) \equiv \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(v - v_i)^2}{2\sigma^2} \right)$$

- Beta ($0 < v < 1$): with $\lambda_i = v_i/\sigma$ and $\mu_i = (1 - v_i)/\sigma$

$$\delta_\sigma(v, v_i) \equiv \frac{v^{\lambda_i - 1}(1 - v)^{\mu_i - 1}}{B(\lambda_i, \mu_i)}$$

EQMOM algorithm

$2N + 1$ moments of $n(v)$ (denote by m_k) for beta-EQMOM:

$$m_0 = m_0^*$$
$$m_1 = m_1^*$$
$$m_2 = \frac{1}{1+\sigma}\left(\sigma m_1^* + m_2^*\right)$$
$$m_3 = \frac{1}{(1+2\sigma)(1+\sigma)}\left(2\sigma^2 m_1^* + 3\sigma m_2^* + m_3^*\right)$$
$$m_4 = \frac{1}{(1+3\sigma)(1+2\sigma)(1+\sigma)}\left(6\sigma^3 m_1^* + 11\sigma^2 m_2^* + 6\sigma m_3^* + m_4^*\right) \equiv m_{2N}^\dagger(\sigma)$$

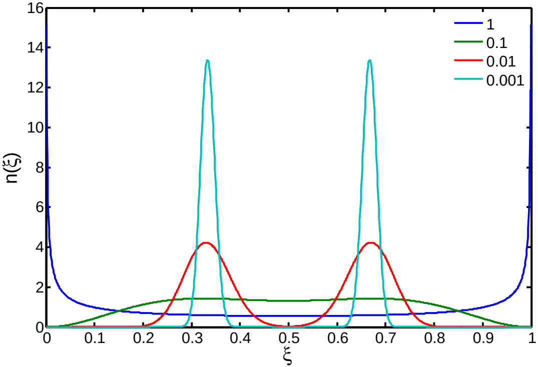
$$m = A(\sigma)m^*$$
$$m^* = A(\sigma)^{-1}m$$

with $m_k^* \equiv \sum_{i=1}^N n_i v_i^k$ (i.e. QMOM moments)

Given m_k for $k = 0, \ldots, 2N$

1. Guess σ
2. Solve for m^* for $k = 0, \ldots, 2N-1$
3. Solve for n_i and v_i using 1-D quadrature with m_k^* for $k = 0, \ldots, 2N-1$
4. Compute m_{2N}^* and resulting estimate $m_{2N}^\dagger$
5. Iterate on σ until $m_{2N} = m_{2N}^\dagger$

Example: beta-EQMOM with $N = 2$



$n_1 = n_2 = 1/2$, $\xi_1 = 1/3$, $\xi_2 = 2/3$ for different values of σ

First $2N$ moments always exact with max σ : $m_{2N} \geq m^{\dagger}_{2N}(\sigma)$

Converges to exact NDF as $N \to \infty$ (Gavriliadis and Athanassoulis 2002)

Closure with EQMOM

Unclosed integrals (given n_i, v_i and σ):

$$\int g(v)n(v)\mathrm{d}v = \sum_{i=1}^{N} n_i \int g(v)\delta_\sigma(v, v_i)\mathrm{d}v$$

Use Gaussian quadrature with known weights w_{ij} and abscissas v_{ij}:

$$\int g(v)\delta_\sigma(v, v_i)\mathrm{d}v = \sum_{j=1}^{M_i} w_{ij} g(v_{ij})$$

where M_i can be chosen arbitrarily large to control error

Dual-quadrature representation of EQMOM:

$$n(v) = \sum_{i=1}^{N}\sum_{j=1}^{M_i} n_i w_{ij} \delta\left(v - v_{ij}\right) \quad (M_i = 1 \text{ when } \sigma = 0)$$

$\Longrightarrow$ exact for polynomials of order $\leq 2N$

EQMOM on unit circle

- For $n(\phi)$ on the unit circle, define $x = \cos\phi$ and $y = \sin\phi$, and

$$n(x,y) = \sum_{\alpha=1}^{N} n_\alpha \delta_{\sigma_\phi}(x, x_\alpha) f_\alpha(y|x)$$

where the kernel density $\delta_{\sigma_\phi}(x, x_\alpha)$ is periodic wrt ϕ

- Conditional pdf is known exactly, but with constant weights:

$$f_\alpha(y|x) = w_{1\alpha}\delta\left(y - \sqrt{1-x^2}\right) + w_{2\alpha}\delta\left(y + \sqrt{1-x^2}\right)$$

with $w_{2\alpha} = 1 - w_{1\alpha}$

- Apply EQMOM with $2N+1$ moments $\langle \cos^n \phi \rangle$ to find n_α, x_α and σ_ϕ
- Apply CQMOM with N moments $\langle \sin\phi \cos^n \phi \rangle$ to find $w_{1\alpha}$

Multivariate EQMOM

Example: 2-D case ⇒ Extended CQMOM

$$n(u,v) = n(u)f(v|u) = \sum_{\alpha=1}^{N} n_\alpha \delta_{\sigma_u}(u, u_\alpha) \left(\sum_{\beta=1}^{N_\alpha} n_{\alpha\beta} \delta_{\sigma_{v,\alpha}}(v, v_{\alpha\beta}) \right)$$

with N abscissas u_α, $\mathcal{N} = \sum_{\alpha=1}^{N} N_\alpha$ weights $w_{\alpha\beta} = n_\alpha n_{\alpha\beta} \geq 0$ and $\mathcal{N}$ abscissas $v_{\alpha\beta}$, but **only one** parameter $\sigma_u \geq 0$ and N parameters $\sigma_{v,\alpha}$

Define moments:

$$M_{ij} = \int u^i v^j n(u,v) \, \mathrm{d}u \, \mathrm{d}v = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N_\alpha} w_{\alpha\beta} m_{1,i}^{(\alpha)} m_{2,j}^{(\alpha\beta)}$$

where

$$m_{1,i}^{(\alpha)} \equiv \int u^i \delta_{\sigma_u}(u, u_\alpha) \, \mathrm{d}u \qquad m_{2,j}^{(\alpha\beta)} \equiv \int v^j \delta_{\sigma_{v,\alpha}}(v, v_{\alpha\beta}) \, \mathrm{d}v$$

are known functions of the EQMOM parameters

Algorithm for 2-D ECQMOM

- 1-D EQMOM for moments in u:

$$M_{i0} = \sum_{\alpha=1}^{N} n_\alpha m_{1,i}^{(\alpha)} \quad \text{for } i = 0, \dots, 2N \Longrightarrow n_\alpha,\ u_\alpha \text{ and } \sigma_u$$

- Use CQMOM to find conditional moments $\langle V^j \rangle_\alpha \equiv \sum_{\beta=1}^{N_\alpha} n_{\alpha\beta} m_{2,j}^{(\alpha\beta)}$ from the bivariate moments (i.e. solve linear system):

$$\sum_{\alpha=1}^{N} n_\alpha m_{1,i}^{(\alpha)} \langle V^j \rangle_\alpha = M_{ij} \quad \text{for } i = 0, \dots, N-1$$

- For each α, apply 1-D EQMOM to conditional moments:

$$\{1, \langle V \rangle_\alpha, \dots, \langle V^{2N_\alpha} \rangle_\alpha\} \quad \Longrightarrow \quad n_{\alpha\beta},\ v_{\alpha\beta} \text{ and } \sigma_{v,\alpha}$$

- Uses the extended optimal moment set

Extended optimal moment set

All CQMOM permutations $\Longrightarrow$ Extended optimal moment set

$\mathcal{N} = 4$ nodes in 2-D

M_{00}	M_{10}	M_{20}	M_{30}	M_{40}
M_{01}	M_{11}	M_{21}	M_{31}	M_{41}
M_{02}	M_{12}			
M_{03}	M_{13}			
M_{04}	M_{14}			

16 moments

$\mathcal{N} = 9$ nodes in 2-D

M_{00}	M_{10}	M_{20}	M_{30}	M_{40}	M_{50}	M_{60}
M_{01}	M_{11}	M_{21}	M_{31}	M_{41}	M_{51}	M_{61}
M_{02}	M_{12}	M_{22}	M_{32}	M_{42}	M_{52}	M_{62}
M_{03}	M_{13}	M_{23}				
M_{04}	M_{14}	M_{24}				
M_{05}	M_{15}	M_{25}				
M_{06}	M_{16}	M_{26}				

33 moments

Only extended optimal moment set is transported

ECQMOM on unit sphere

- For $n(\phi, \theta)$ on the unit sphere, ECQMOM reconstruction is

$$n(\phi,\theta) = \sum_{\alpha=1}^{N} n_\alpha \delta_{\sigma_\theta}(\theta, \theta_\alpha) \left(\sum_{\beta=1}^{N_\alpha} n_{\alpha\beta} \delta_{\sigma_{\phi,\alpha}}(\phi, \phi_{\alpha\beta}) \right)$$

  with periodic kernel density functions for $\theta \in [0, \pi]$ and $\phi \in [-\pi, \pi]$
- Define $z = \cos\theta$ and conditional pdf $f(\phi|z)$
- Apply EQMOM for $2N + 1$ moments $\langle z^n \rangle$ to find n_α, θ_α and σ_θ
- Use CQMOM to find trigonometric moments involving ϕ conditioned on $z_\alpha = \cos\theta_\alpha$
- For each α, apply EQMOM on unit circle to conditional moments to find $n_{\alpha\beta}$, $\phi_{\alpha\beta}$, $\sigma_{\phi\alpha}$ and $w_{1\alpha\beta}$

Summary of QBMM

- Extended optimal moment set $\Longrightarrow$ reconstruct NDF with fast, robust algorithm
- NDF must be realizable and moment-inversion algorithm must be robust
  - CQMOM is always realizable by construction
  - EQMOM gives a smooth NDF with low computational cost
- Current "best" moment-inversion algorithms:
  - 1-D phase space $\Longrightarrow$ EQMOM
  - Multivariate phase space $\Longrightarrow$ multivariate ECQMOM
- Dual-quadrature representation used to close source terms
- Given smooth NDF, high-order kinetic-based transport solvers can be derived to ensure realizability

Kinetic-based finite-volume methods (KBFVM)

Given a set of **extended optimal moments**, solve

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

where RHS is closed using QBMM:

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

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. $\partial_t M_{00} + \partial_x M_{10} = 0$

$$\begin{aligned} M_{10} &= Q_{10}^- + Q_{10}^+ \\ &= \int_{-\infty}^{0} u \left(\int n^*(u,v) \mathrm{d}v \right) \mathrm{d}u + \int_{0}^{\infty} u \left(\int n^*(u,v) \mathrm{d}v \right) \mathrm{d}u \end{aligned}$$

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

$$Q_{10}^- = \sum_{\alpha=1}^{\mathcal{N}} n_\alpha u_\alpha I_{(-\infty,0)}(u_\alpha) \qquad Q_{10}^+ = \sum_{\alpha=1}^{\mathcal{N}} n_\alpha u_\alpha I_{(0,\infty)}(u_\alpha)$$

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

Kinetic-based fluxes are always hyperbolic

Finite-volume method: definitions

- 1-D advection problem:

$$\frac{\partial \mathbf{M}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{M})}{\partial x} = 0$$

where $\mathbf{M} = \int \mathbf{K}(v)n(v)\mathrm{d}v$ and $\mathbf{F}(\mathbf{M}) = \int v\mathbf{K}(v)n(v)\mathrm{d}v$

- Finite-volume representation of moment vector:

$$\mathbf{M}_i^n \equiv \frac{1}{\Delta x}\int_{x_i}^{x_{i+1}} \mathbf{M}(t_n, x)\mathrm{d}x$$

- Finite-volume formula:

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

where $\mathbf{G}\left(\mathbf{M}_l, \mathbf{M}_r\right) = \int v^+\mathbf{K}(v)n_l(v)\mathrm{d}v + \int v^-\mathbf{K}(v)n_r(v)\mathrm{d}v$

Realizability and spatial fluxes

- Flux functions: given $\mathbf{M}_i^n$ define $\mathbf{G}(\mathbf{M}_l, \mathbf{M}_r)$ to achieve high-order spatial accuracy but keep $\mathbf{M}_i^{n+1}$ realizable!
- Discrete distribution function: Define

$$\mathbf{M}_i^{n+1} \equiv \int \mathbf{K}(v) h_i(v) \mathrm{d}v$$

and finite-volume formula can be written as

$$h_i(v) = \lambda |v^-| n^n_{i+\frac{1}{2},r} + \lambda v^+ n^n_{i-\frac{1}{2},l} + n_i^n - \lambda |v^-| n^n_{i-\frac{1}{2},r} - \lambda v^+ n^n_{i+\frac{1}{2},l}$$

(black part ≥ 0, red part can be negative)

- Sufficient condition for realizable moments: $h_i(v) \geq 0$ for all v and i

Realizable, high-order, spatial fluxes

- First order: $n^n_{i-\frac{1}{2},r} = n^n_{i+\frac{1}{2},l} = n^n_i$ so that
  $h = \lambda|v^-|n^n_{i+1} + \lambda v^+ n^n_{i-1} + \left(1 - \lambda|v^-| - \lambda v^+\right) n^n_i \quad \Rightarrow \frac{1}{|v^-|+v^+} \geq \lambda$
  Moments are realizable, but scheme is diffusive ...
- Quasi-higher order: Let $n^n_i = \sum_\alpha \rho^n_{\alpha,i}\delta(v - v^n_{\alpha,i})$
  and define

$$n^n_{i-\frac{1}{2},r} = \sum_\alpha \rho^n_{\alpha,i-\frac{1}{2},r}\delta(v - v^n_{\alpha,i})$$
$$n^n_{i+\frac{1}{2},l} = \sum_\alpha \rho^n_{\alpha,i+\frac{1}{2},l}\delta(v - v^n_{\alpha,i})$$

so that

$$h = \lambda|v^-|n^n_{i+\frac{1}{2},r} + \lambda v^+ n^n_{i-\frac{1}{2},l} + \sum_\alpha \left(\rho^n_{\alpha,i} - \lambda|v^-|\rho^n_{\alpha,i-\frac{1}{2},r} - \lambda v^+ \rho^n_{\alpha,i+\frac{1}{2},l}\right)\delta(v - v^n_{\alpha,i})$$

$$\Longrightarrow \quad \min_\alpha \left(\frac{\rho^n_{\alpha,i}}{|v^-_{\alpha,i}|\rho^n_{\alpha,i-\frac{1}{2},r} + v^+_{\alpha,i}\rho^n_{\alpha,i+\frac{1}{2},l}}\right) \geq \lambda$$

Use high-order, finite-volume schemes only for the weights

Realizable time-stepping schemes

- First-order explicit:

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

  is realizable

- Second-order Runga-Kutta (RK2) is not realizable
- RK2SSP:

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

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

$$\mathbf{M}_i^{n+1} = \frac{1}{2}\left(\mathbf{M}_i^n + \mathbf{M}_i^{**} \right)$$

  is realizable

Achieve second order in space and time on unstructured grids

Bubbly flow

Loading movie…

Quasi-second-order *realizable* finite-volume scheme on unstructured mesh

Summary of KBFVM

- When solving moment transport equations, we must guarantee realizability
- First-order FV methods are realizable, but too diffusive
- Standard high-order FV methods lead to unrealizable moments
- Kinetic-based flux functions can be designed to be realizable
- Use dual-quadrature representation with high-order spatial reconstruction
- High-order time-stepping schemes are also possible
- KBFVM provide robust treatment of shocks/discontinuous solutions

Final remarks

- Mesoscopic models have direct link with underlying physics and result in a kinetic equation
- QBMM solves kinetic equation by reconstructing distribution function from moments
- Reconstruction requires realizable moments
- Numerical schemes must ensure that moments are always realizable
- QBMM on unit sphere can be used for radiation transport

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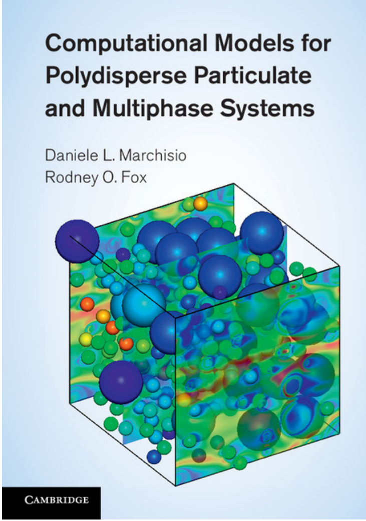

Thanks for your attention!

Questions?

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