Project Objectives and Milestones

Objectives:

1. Improve the basic understanding of polydisperse turbulent reacting flows
2. Developing physics-based, mathematically rigorous multiphase flow CFD models
3. Providing input to improve MFiX by widening its applicability

Milestones:

1. FY16Q3 + FY16Q4 : Consistent flux algorithm for size-velocity model for polydisperse particles
2. FY17Q1 : Cutcell technique for complex geometries
3. FY17Q2 : Conditional Hyperbolic Quadrature Method of Moments
Presentation Outline

• Polydisperse Dense Gas-Particle Solver Based on QBMM
  – Background
  – Governing Equations
  – Numerical Method
  – Example Results

• Conditional hyperbolic quadrature method of moments
  – Example Results

• Summary and Future work
Polydisperse Gas-Particle Solver: Motivation

In many commonly encountered engineering applications:

- Polydispersity (e.g., size, density, shape) is present
- "Size" and velocity of disperse phase are closely coupled

Proposed solution: Joint number density function of "size" and velocity of disperse phase can be solved using quadrature-based moment methods (QBMM)
Existing models for polydisperse gas-particle flows

Lagrangian methods
- **Discrete Element Method (DEM)**
  Limitation: Computationally expensive for industrial applications

Eulerian methods
- **Population Balance Equation (PBE) carried by fluid velocity**
  Limitation: Spatial fluxes do not depend on size
- **Class method with separate class velocities**
  Limitation: Computationally expensive for continuous size distribution
- **Direct Quadrature Method of Moments (DQMOM) with a multi-fluid model**
  Limitation: Weights and abscissas are not conserved quantities

Objective:
Develop a robust and accurate moment-based polydisperse flow solver that incorporates microscale physics at reasonable computation cost !!!
Governing Equations: Polydisperse Gas Particle Flows

Gas phase: Continuity and momentum transport equations

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

\[ \frac{\partial}{\partial t} \rho_g \alpha_g \mathbf{U}_g + \nabla \cdot \rho_g \alpha_g \mathbf{U}_g \otimes \mathbf{U}_g = \nabla \cdot \alpha_g \mathbf{\sigma}_g - \alpha_g \nabla p_g + \rho_g \alpha_g \mathbf{g} + \mathbf{M}_{gp} \]

\[ M_{pg} = K_{gp} (\mathbf{U}_g - \mathbf{U}_p) - \alpha_p \nabla p_g + \alpha_p \rho_g \nabla \cdot \alpha_g \mathbf{\sigma}_g \]

Particle phase: Generalized population balance equation

\[ \frac{\partial f (\xi, \mathbf{u})}{\partial t} + \mathbf{u} \cdot \frac{\partial f (\xi, \mathbf{u})}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{u}} \cdot f (\xi, \mathbf{u}) [\mathbf{A} (\xi, \mathbf{u}) + \mathbf{g}] = \mathbf{C} (\xi, \mathbf{u}) \]
Solving GPBE with Quadrature-based moments method

Kinetic Equation → 6-D solver → Density n(t,x,v)

Integrate over phase space → Reconstructed density n*(t,x,v) → Integrate over phase space

Moment Equations → Closure using quadrature → Reconstructed using quadrature

Moments M(t,x) → 3-D solver → Close moment equations by reconstructing density function

Creating Materials and Energy Solutions
Moment sets for solving mas-velocity GPBE

Joint mass-velocity NDF:

\[ f(\xi, u) = n(\xi) \cdot g(u - U(\xi), \Theta(\xi)) \]

\[ g(u - U(\xi), \Theta(\xi)) = \frac{1}{[2\pi\Theta(\xi)]^{3/2}} \exp \left[ -\frac{|u - U(\xi)|^2}{2\Theta(\xi)} \right] \]

Joint mass-velocity moments:

\[ M_s := \int_\Omega \xi^sn(\xi)d\xi, \quad U_s := \int_\Omega \xi^sU(\xi)n(\xi)d\xi, \quad T_s := \int_\Omega \xi^s\Theta(\xi)n(\xi)d\xi, \quad s \in \mathbb{Z} \]
Moments transport equations

Mass moments:

\[ \frac{\partial M_s}{\partial t} + \nabla \cdot \mathbf{U}_s = 0 \]

\(\xi^S\)-mass-weighted velocity:

\[ \frac{\partial \mathbf{U}_s}{\partial t} + \nabla \cdot \left( \mathbf{F}_{u,s} + \mathbf{G}_s + M_s \mathbf{Z}_p \right) = M_s \left( \mathbf{g} - \frac{1}{\rho_p} \nabla p_g + \frac{\rho_g}{\rho_p} \nabla \cdot \alpha_g \mathbf{\sigma}_g \right) + \mathbf{A}_s + \mathbf{C}_s \]

\(\xi^S\)-mass-weighted granular temperature:

\[ \frac{\partial T_s}{\partial t} + \nabla \cdot \left( \mathbf{F}_{\Theta,s} + \frac{2}{3} Q_s \right) = -\frac{2}{3} \mathbf{B}_s - \mathbf{A}_{\Theta,s} - \mathbf{C}_{\Theta,s} \]
Transport equation for $\xi^s$-mass-weighted velocity

\[
\frac{\partial U_s}{\partial t} + \nabla \cdot \left( \mathcal{F}_{u,s} + \mathcal{G}_s + M_s \mathbf{Z}_p \right) = M_s \left( \mathbf{g} - \frac{1}{\rho_p} \nabla \rho_g + \frac{\rho_g}{\rho_p} \nabla \cdot \alpha_g \mathbf{\sigma}_g \right) + \mathcal{A}_s + C_s
\]

Spatial free transport flux:

\[\mathcal{F}_{u,s} = \int_{\Omega} \xi^s U(\xi) \otimes U(\xi) n(\xi) \, d\xi,\]

Spatial flux due to particle kinetics and collision:

\[\mathcal{G}_s = P_s \mathbf{I} - 2\mu_s \mathbf{S}_s, \quad P_s = \int_{\Omega} \xi^s p_p(\xi) n(\xi) \, d\xi, \quad \mu_s = \int_{\Omega} \xi^s \nu_p(\xi) n(\xi) \, d\xi\]

\[p_p(\xi) := \Theta(\xi) + \int_{\Omega} \frac{2}{\eta \alpha(\xi) \epsilon_0(\xi)} \frac{X_{\xi,\xi}^3 \mu_{\xi,\xi}}{X_{\xi,\xi}} E(\xi, \zeta) \, d\zeta\]

\[\nu_p(\xi) := \frac{d(\xi) \sqrt{\pi \Theta(\xi)}}{12} + \int_{\Omega} \frac{2}{\eta \alpha(\xi) \epsilon_0(\xi)} \frac{X_{\xi,\xi}^3 \mu_{\xi,\xi}}{X_{\xi,\xi}} \sqrt{E(\xi, \zeta)} \left[ d(\xi) + d(\zeta) \right] \, d\zeta\]

\[E(\xi, \zeta) = 3\Theta(\xi) + 3\Theta(\zeta) + |U(\xi) - U(\zeta)|^2\]

Spatial flux due to particle friction:

\[\mathbf{Z}_p = p_{p,f} \mathbf{I} - 2\nu_{p,f} \mathbf{S}_p, \quad p_{p,f} = \frac{F_r}{\rho_p \alpha_p} \frac{(\alpha_p - \alpha_{p,fr,min})^{\tau_1}}{(\alpha_{p,fr,max} - \alpha_p)^{\tau_2}} \nu_{p,f} = p_{p,f} \frac{\sin \phi}{\| \mathbf{S}_p \|}\]

Acceleration source term:

\[\mathcal{A}_s := \int_{\Omega} \frac{\xi^s}{\tau_p(\xi)} \left[ U_g - U(\xi) \right] n(\xi) \, d\xi, \quad \tau_p(\xi) := \frac{4 \rho_p d^2(\xi)}{3 \rho_g \gamma_0 C_D(\xi) \text{Re}(\xi)}\]

Collisional source term:

\[C_s := \int_{\Omega} \xi^s C_u(\xi) n(\xi) d\xi, \quad C_u(\xi) := \int_{\Omega} \frac{\eta}{2 \tau_c(\xi, \zeta)} \left[ U(\xi) - U(\zeta) \right] \alpha(\zeta) d\zeta\]
Transport equation for $\xi^S$-mass-weighted granular temperature

$$\frac{\partial T_s}{\partial t} + \nabla \cdot \left( F_{\Theta,s} + \frac{2}{3} Q_s \right) = -\frac{2}{3} B_s - A_{\Theta,s} - C_{\Theta,s}$$

Spatial free transport flux:

$$F_{\Theta,s} := \int_\Omega \xi^S U(\xi) \Theta(\xi) n(\xi) \, d\xi$$

Granular energy production term:

$$B_s := G_s : \nabla U_s,$$

Acceleration source term:

$$A_{\Theta,s} := \int_\Omega \frac{2 \xi^S}{\tau_p(\xi)} \Theta(\xi) n(\xi) \, d\xi,$$

Spatial flux due to particle kinetics and collision:

$$Q_s = -K_s \nabla \Theta_s, \quad K_s = \int_\Omega \xi^S k(\xi) n(\xi) \, d\xi$$

Collisional source term:

$$C_{\Theta}(\xi) = S(\xi) - 3 J(\xi) \Theta(\xi)$$

$$k(\xi) := \frac{15 d(\xi) \sqrt{\pi \Theta(\xi)}}{32} + \int_\Omega \frac{3 \eta \alpha(\xi) \zeta (\xi, \xi) E(\xi, \zeta) \left[ d(\xi) + d(\zeta) \right]}{4 \tau_c(\xi, \zeta)} \, d\xi$$

$$S(\xi) = \int_\Omega \frac{\eta^2 \mu_\xi}{4 \tau_c(\xi, \zeta)} E(\xi, \zeta) n(\zeta) \, d\zeta, \quad J(\xi) = \int_\Omega \frac{\eta}{2 \tau_c(\xi, \zeta)} n(\zeta) \, d\zeta.$$
Numerical method: Quadrature-based closure

\[ f(\xi, u) = n(\xi) \cdot g(u - U(\xi), \Theta(\xi)) \]

Mass NDF:

\[ n(\xi) = \sum_{\alpha=0}^{N} w_\alpha \delta(\xi - \xi_\alpha), \]

Mass-conditioned velocity and granular temperature:

\[ U_s = \sum_{\alpha=0}^{N} w_\alpha \xi^s \alpha U_\alpha, \quad \Theta_s = \sum_{\alpha=0}^{N} w_\alpha \xi^s \alpha \Theta_\alpha, \]
Solution Algorithm: Separate the Mean and Deviation

Variable decomposition:

\[ \mathbf{U}_\alpha = \mathbf{U}_p + \mathbf{V}_\alpha, \ \Theta_\alpha = \Theta_p + \Psi_\alpha \]

\[ \mathcal{U}_s = M_s U_p + \mathcal{V}_s, \quad \mathcal{V}_s = \sum_{\alpha=0}^{N} w_\alpha \xi_\alpha \mathcal{V}_\alpha, \quad \mathcal{T}_s = M_s \Theta_p + \mathcal{W}_s, \quad \mathcal{W}_s = \sum_{\alpha=0}^{N} w_\alpha \xi_\alpha \Psi_\alpha \]

“Mean” Transport:

\[ \frac{\partial M_1}{\partial t} + \nabla \cdot M_1 \mathbf{U}_p = 0 \]

\[ \frac{\partial M_1 U_p}{\partial t} + \nabla \cdot M_1 \mathbf{U}_p \otimes \mathbf{U}_p + \nabla \cdot \left( P_1 \mathbf{I} - 2 \mu_1 \mathbf{S}_p \right) + \nabla \cdot M_1 \mathbf{Z}_p = M_1 \rho_g + K_{gp} \left( \mathbf{U}_g - \mathbf{U}_p \right) - \frac{M_1}{\rho_p} \nabla p_g + \frac{M_1 \rho_g}{\rho_p} \nabla \cdot \alpha_g \sigma_g \]

\[ \frac{\partial M_1 \Theta_p}{\partial t} + \nabla \cdot M_1 \mathbf{U}_p \Theta_p - \frac{2}{3} \nabla \cdot K_1 \Theta_p = -\frac{2}{3} \left( P_1 \mathbf{I} - 2 \mu_1 \mathbf{S}_p \right) : \nabla \mathbf{U}_p - 2 K_{gp} \Theta_p + \mathcal{S}_1 - 3 \mathcal{J}_1 \Theta_p \]

“Deviation” Transport:

\[ \frac{\partial M_s}{\partial t} + \nabla \cdot \mathcal{V}_s = 0 \]

\[ \frac{\partial \mathcal{V}_s}{\partial t} + \nabla \cdot \left( \mathcal{F}_{u,s} + \mathcal{G}'_s \right) = \mathcal{A}_s' + C_s \]

\[ \frac{\partial \mathcal{W}_s}{\partial t} + \nabla \cdot \left( \mathcal{F}_{\Theta,s} + \frac{2}{3} \mathcal{Q}'_s \right) = -\frac{2}{3} \mathcal{B}_s' - \mathcal{K}_{\Theta,s} - C_{\Theta,s} \]
Overall Solution Algorithm

1. Initialized all variables.
2. Reconstruct mass NDF and conditioned velocity using moment-inversion algorithm.
3. Use a kinetic-based solver to solve particle “Deviation” transport.
4. Reconstruct mass NDF and conditioned velocity again, and calculate parameters used in the “Mean” transport.
5. Use a two-fluid solver to solve particle “Mean” transport and gas phase velocity and pressure fields.
6. Solve for the mass-moment transport new mean velocity and update the mass-weighted velocity and granular temperature.
7. Repeat from step 2 until convergence, and then advance in time.
Example results: polydisperse fluidized bed

- Volume Fraction
- Mean Diameter
- Granular Temp
- Vertical Velocity
On-going effort

- Particle aggregation and breakage
  \[ \tilde{S}_k^{(N)}(x, t) = \tilde{B}_k^a(x, t) - \tilde{D}_k^a(x, t) + \tilde{B}_k^b(x, t) - \tilde{D}_k^b(x, t), \]

- Chemical reaction -- biomass gasification

- "Validation" with Goldschmidt et al. (2003) experiments

- Perform detailed Euler-Lagrangian simulations to enhance the effective viscosity and conductivity models.
Conditional hyperbolic quadrature method of moments (CHyQMOM)

Advantage: Hyperbolic, Smaller moments set, Symmetric, Robust !!!
Summery and Future work

**Summery :**

1. A new solution algorithm is proposed to solve dense polydispersed gas-particle flows.
2. It was implemented, and then tested in a dense fluidized bed case.
3. It was demonstrated that the new algorithm is computationally robust, and can be used to model various physical and chemical processes.

**Milestones :**

1. FY17Q3 : Cutcell technique for complex geometries + Implement the already validated new gas-particle turbulence model in MFiX.
2. FY17Q4 : Consolidate previous DQMOM and QMOMK implementation into current MFiX-QBMM module.
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Questions?