Simulating Gas-Particle Flows Across All Flow Regimes in an Euler-Euler Framework

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Outline

Motivation : Accurately Simulate Gas-Particle Flow

Two-Fluid Model (TFM)

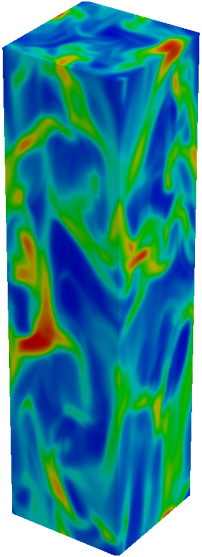
- Widely studied, developed and applied.
- Its hydrodynamic assumption has been proven invalid, especially when particles are dilute.

Quadrature-Based Moment Methods (QBMM)

- Direct numerical reconstruction, less modeling.
- Its explicit nature makes it inefficient when particles are dense.

Objective

- A solution algorithm that combines the best features of TFM and QBMM solvers, which can accurately simulate across all flow regimes.



Gas-Particle Flow Governing Equations

Gas phase: Continuity and momentum transport equations

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

$$\frac{\partial \rho_g \alpha_g \boldsymbol{U}_g}{\partial t} + \nabla \cdot \left(\rho_g \alpha_g \boldsymbol{U}_g \otimes \boldsymbol{U}_g + p_g \mathbf{I} - \rho_g \alpha_g \boldsymbol{\sigma}_g \right) = \rho_g \alpha_g \boldsymbol{g} - \rho_p \alpha_p \boldsymbol{M}_{pg}$$

$$\boldsymbol{M}_{pg} = \frac{1}{\tau_p} \left(\boldsymbol{U}_g - \boldsymbol{U}_p \right) - \frac{1}{\rho_p} \nabla p_g + \frac{\rho_g}{\rho_p} \nabla \cdot \alpha_g \boldsymbol{\sigma}_g$$

Particle phase: Kinetic equation for velocity NDF $f(\mathbf{v})$

$$\frac{\partial f(\mathbf{v})}{\partial t} + \mathbf{v} \cdot \frac{\partial f(\mathbf{v})}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{v}} \cdot f(\mathbf{v}) \mathbf{A} = \mathbb{S}$$

where $\mathbf{A}$ represents acceleration due to forces acting on each particle, $\mathbb{S}$ represents other possible source terms, e.g. particle collisions

Gas-Particle Flow Governing Equations : Velocity Moments

Moments Transport Equation:

$$\frac{\partial \mathbf{M}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S} \qquad M^{\gamma}_{ijk} = \int v_1^i v_2^j v_3^j f(\boldsymbol{v})\, d\boldsymbol{v}$$

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

Particle Continuity Equation:

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

Particle Momentum Equation:

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

Particle Pressure-Tensor Equation:

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

Particle Kinetic, Collisional and Frictional Flux

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:

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

Frictional Flux:

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

Heat Fluxes:

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

Flux-Splitting Scheme

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

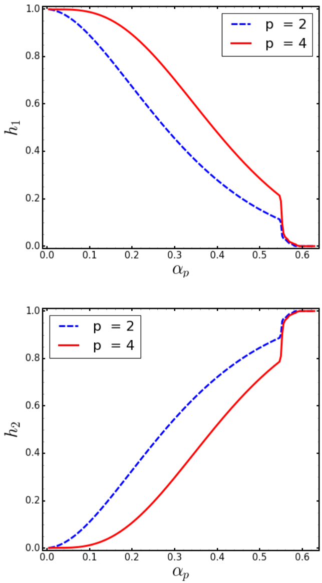
$$h_1 = 1 - h_2$$

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

$$p^\star_{p,c} = 2(1+e)\rho_p \alpha_p^2 g_0 \Theta_p$$

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

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



Hydrodynamic Solver: $\partial \mathbf{M}/\partial t + \nabla \cdot (h_2\mathbf{F} + \mathbf{G} + \mathbf{Z}) = \mathbf{S}$

Particle Volume Fraction:

$$\frac{\partial \alpha_p}{\partial t} + \nabla \cdot \mathbf{h_2} \alpha_p \boldsymbol{U}_p = 0,$$

Particle Velocity:

$$\frac{\partial \alpha_p \boldsymbol{U}_p}{\partial t} + \nabla \cdot \left(\mathbf{h_2} \alpha_p \boldsymbol{U}_p \otimes \boldsymbol{U}_p + \frac{p_p^*}{\rho_p} \boldsymbol{I} - 2\alpha_p \nu_p^* \boldsymbol{S}_p \right) = \alpha_p \boldsymbol{g} + \frac{\alpha_p}{\tau_p} (\boldsymbol{U}_g - \boldsymbol{U}_p) - \frac{\alpha_p}{\rho_p} \nabla p_g + \alpha_p \rho_g \nabla \cdot \alpha_g \boldsymbol{\sigma}_g$$

$$p_p^* = \mathbf{h_2} p_{p,k} + p_{p,c} + p_{p,f} \qquad \nu_p^* = \left(1 + \frac{8\eta \alpha_p g_0}{5} \right) \mathbf{h_2} \nu_{p,k} + \frac{3}{5} \nu_{p,b} + \nu_{p,f}$$

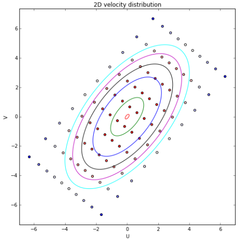
Particle Granular Temperature:

$$\frac{3}{2} \left(\frac{\partial \alpha_p \Theta_p}{\partial t} + \nabla \cdot \mathbf{h_2} \alpha_p \Theta_p \boldsymbol{U}_p \right) = \nabla \cdot (\alpha_p k_\Theta^\dagger \nabla \Theta_p) - \left(\frac{p_p^\dagger}{\rho_p} \mathbf{I} - 2\alpha_p \nu_p^\dagger \mathbf{S}_p \right) : \nabla \boldsymbol{U}_p - 3 \left(\frac{1 - e^2}{2\tau_c} + \frac{1}{\tau_p} \right) \alpha_p \Theta_p$$

$$p_p^\dagger = \mathbf{h_2} p_{p,k} + p_{p,c} \qquad \nu_p^\dagger = \left(1 + \frac{8\eta \alpha_p g_0}{5} \right) \mathbf{h_2} \nu_{p,k} + \frac{3}{5} \nu_{p,b} \qquad k_\Theta^\dagger = \left(1 + \frac{12\eta \alpha_p g_0}{5} \right) \mathbf{h_2} k_{\Theta,k} + \frac{3}{2} \nu_{p,b}$$

Free Transport Solver: $\partial \mathbf{M}/\partial t + \nabla \cdot h_1 \mathbf{F} = \mathbf{0}$

Anisotropic Gaussian Velocity Distribution:



$$g(\boldsymbol{v}) = \frac{\alpha_p}{(2\pi|\mathbf{P}_p|)^{3/2}} \exp\left[-\frac{1}{2}(\boldsymbol{v} - \boldsymbol{U}_p) \cdot \mathbf{P}_p^{-1} \cdot (\boldsymbol{v} - \boldsymbol{U}_p)\right]$$

Granular Stress Tensor Transport

$$\frac{\partial \rho_p \alpha_p \boldsymbol{\sigma}_p}{\partial t} + \nabla \cdot \rho_p \alpha_p \left(\mathbf{h_2} \boldsymbol{U}_p \otimes \boldsymbol{\sigma}_p - \frac{2}{3} k_\Theta^\dagger \nabla \otimes \boldsymbol{\sigma}_p\right) = \rho_p \alpha_p \left(\boldsymbol{S}_{2,flux} - \boldsymbol{S}_2\right)$$

$$\boldsymbol{S}_{2,flux} = \frac{2p_p^\dagger}{\rho_p \alpha_p} \boldsymbol{S}_p - 2\nu_p^\dagger \left[\boldsymbol{S}_p \cdot \nabla \boldsymbol{U}_p + (\nabla \boldsymbol{U}_p)^T \cdot \boldsymbol{S}_p - \frac{2}{3}(\boldsymbol{S}_p : \nabla \boldsymbol{U}_p)\mathbf{I}\right]$$

$$\boldsymbol{S}_2 = \left[\frac{2}{\tau_p} + \frac{(3-e)(1+e)}{2\tau_c}\right] \boldsymbol{\sigma}_p$$

Wall Boundary Conditions

Hydrodynamic solver:

$$\nu_p^* \frac{\partial \boldsymbol{U}_{p,t}}{\partial x_w} = -\mathbf{h_{2,w}} \phi_s \mathcal{V}_w \boldsymbol{U}_{p,t} - \frac{p_{p,f} \tan \phi_w}{\rho_p \alpha_p} \frac{\boldsymbol{U}_{p,t}}{|\boldsymbol{U}_{p,t}|}$$

$$k_\Theta^\dagger \frac{\partial \Theta_p}{\partial \boldsymbol{x}_w} = \mathbf{h_{2,w}} \left[\phi_s \mathcal{V}_w |\boldsymbol{U}_{p,t}|^2 - \frac{3}{2} \left(1 - e_w^2\right) \mathcal{V}_w \Theta_p \right].$$

$$\mathcal{V}_w = (\pi/6) \sqrt{3\Theta_p}$$

Free transport solver:

$$\mathbf{F}_w = \mathbf{h_{1,w}} \int_{\boldsymbol{v} \cdot \boldsymbol{n}_w > 0} \mathbf{G}_r(\boldsymbol{v}) \left(\boldsymbol{v} \cdot \boldsymbol{n}_w\right) d\mathcal{S}_w$$

$$f_r(\boldsymbol{v}) = \phi_s f_{r,d}(\boldsymbol{v}) + (1 - \phi_s) f_{r,s}(\boldsymbol{v})$$

$$f_{r,s}(\boldsymbol{v}) = f_i \left(\boldsymbol{v} - (1 + e_w)(\boldsymbol{v} \cdot \boldsymbol{n}_w)\boldsymbol{n}_w\right)$$

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.

Example Simulations : Models in Hydrodynamic Solver

Drag :

$$\tau_p = \frac{4\rho_p d_p^2}{3\rho_g \nu_g C_D Re_p}, \qquad Re_p = \frac{\alpha_g d_p |\boldsymbol{U}_g - \boldsymbol{U}_p|}{\nu_g}, \qquad C_D = \max\left[\frac{24}{Re_p}\left(1 + Re_p^{0.687}\right), 0.44\right]\alpha_g^{-2.65}$$

Particle Collision :

$$\eta = \frac{1}{2}(1+e), \qquad g_0 = \frac{1 - \frac{1}{2}\alpha_p}{(1-\alpha_p)^3}, \qquad \tau_c = \frac{d_p}{6\alpha_p g_0 \sqrt{\Theta_p/\pi}}, \qquad \Delta^* = \eta^2 \Theta_p \mathbf{I} + (1-\eta)^2 \mathbf{P}_p$$

Particle Pressure :

$$p_{p,k} = \rho_p \alpha_p \Theta_p, \qquad p_{p,c} = 4\rho_p \eta \alpha_p^2 g_0 \Theta_p - \rho_p \alpha_p \nu_{p,b} \nabla \cdot \boldsymbol{U}_p, \qquad p_{p,f} = Fr \frac{\left(\alpha_p - \alpha_{p,fr,min}\right)^r}{\left(\alpha_{p,max} - \alpha_p\right)^s}$$

Particle Viscosity :

$$\nu_{p,b} = \frac{8\eta\alpha_p g_0 d_p \sqrt{\Theta_p}}{3\sqrt{\pi}}, \qquad \nu_{p,k} = \frac{1}{2}\Theta_p \left[\frac{1}{\tau_p} + \frac{\eta(2-\eta)}{\tau_c}\right]^{-1} \left[1 + \frac{8}{5}\eta(3\eta-2)\alpha_p g_0\right]$$

$$\nu_{p,c} = \frac{8\eta\alpha_p g_0}{5}\nu_{p,k} + \frac{3}{5}\nu_{p,b}, \qquad \nu_{p,f} = \frac{p_{p,f}}{\rho_p \alpha_p \|\boldsymbol{S}_p\|}\sin\phi$$

Particle Conductivity :

$$k_{\Theta,k} = \frac{5}{2}\Theta_p \left[\frac{3}{\tau_p} + \frac{4\eta(41-33\eta)}{\tau_c}\right]^{-1} \left[1 + \frac{12}{5}\eta^2(4\eta-3)\alpha_p g_0\right] \qquad k_{\Theta,c} = \frac{12\eta\alpha_p g_0}{5}k_{\Theta,k} + \frac{3}{2}\nu_{p,b}$$

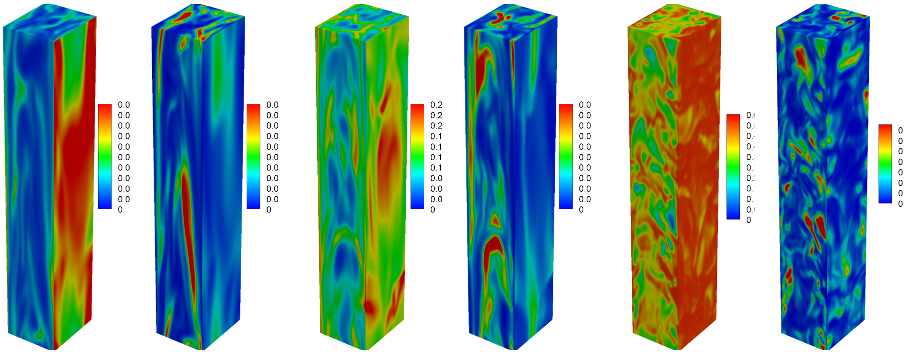
Example Simulations : 2D Fluidized Bed, p = 4

α_p h_2 $\boldsymbol{U}_{p,y}$ Θ_p $\boldsymbol{\sigma}_{p,xy}$

3D Wall-bound Vertical Channel : Instantaneous Fields

$$d_p = 100\mu\text{m} \ , \ \rho_p = 1000 \text{ kg/m}^3 \ , \ \rho_g = 1 \text{ kg/m}^3 \ , \ \nu_g = 1.8 \times 10^{-5} \text{ m}^2/\text{s} \ ,$$
$$e = 0.9 \ , \ e_w = 0.9 \ , \ \phi = 0.25 \ , \ \phi_s = 0.1 \ , \ \phi_w = 0.25, \ p = 4$$

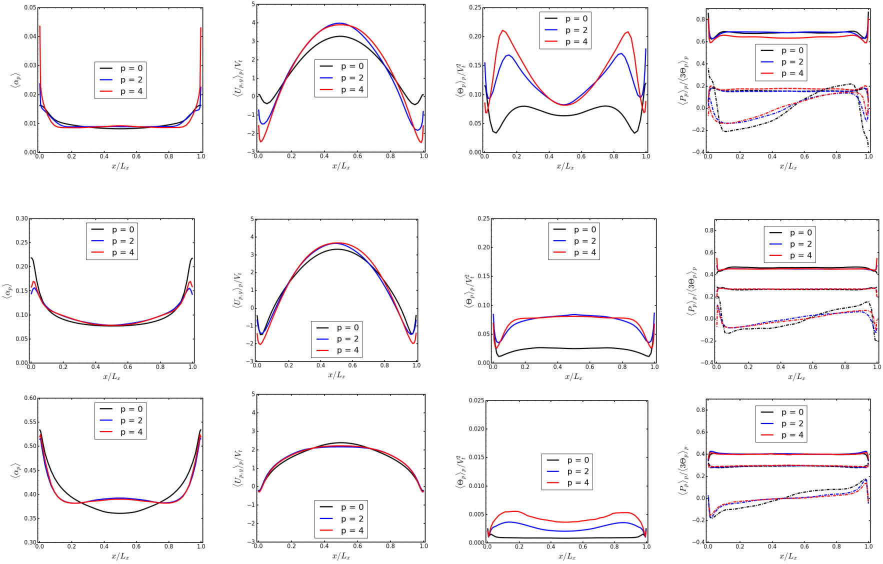
$\overline{\alpha}_p = 0.01$ $\overline{\alpha}_p = 0.1$ $\overline{\alpha}_p = 0.4$



α_p Θ_p α_p Θ_p α_p Θ_p

Wall-bound Vertical Channel : Statistical results

$\langle \alpha_p \rangle$, $\langle U_{p,y} \rangle_p / V_t$, $\langle \Theta_p \rangle_p / V_t^2$, $\langle P_p \rangle_p / \langle 3\Theta_p \rangle_p$



Extension to Polydisperse Systems

Joint size-velocity NDF :

$$n(\xi, \boldsymbol{v}) = \; f(\xi) \;\; g(\boldsymbol{v}|\xi)$$

Free transport solver:

Size distribution $f(\xi)$: $\{M^0_{0000}, M^0_{0001}, M^0_{0002}, M^0_{0003}\} \rightarrow \{w_1, w_2, \xi_1, \xi_2\}$

Size conditioned velocity distribution $g(\boldsymbol{v}|\xi)$: $\boldsymbol{U}_n, \Theta_n, \boldsymbol{\sigma}_n$.

Hydrodynamic solver:

Direct QMOM, i.e. treat quadrature node as particle phase

$$\frac{\partial w_n}{\partial t} + \nabla \cdot (\mathbf{h_2} w_n \boldsymbol{U}_n) = 0$$

$$\frac{\partial \rho_n \alpha_n}{\partial t} + \nabla \cdot (\mathbf{h_2} \rho_n \alpha_n \boldsymbol{U}_n) = 0$$

$$\rho_n \alpha_n = w_n \xi_n = w_n (\rho_n \frac{1}{6} \pi d_n^3)$$

Conclusions

- A solution algorithm is proposed to accurately treat all fluid-particle regimes occurring simultaneously.
- This algorithm is based on splitting the free-transport flux solver dynamically and locally in the flow. Hydrodynamic solver is employed in close-packed to moderately dense regions, while in dilute to very dilute regions a kinetic-based finite-volume solver is used in conjunction with QBMM.
- To illustrate the accuracy and robustness of the proposed solution algorithm, it is implemented for particle velocity moments up to second order.
- By varying the average particle volume fraction in the flow domain, it is demonstrated that the flow solver can handle seamlessly all flow regimes present in fluid-particle flows.

Future Work

- Enable MFIX-QBMM to handle complex geometries by using Cutcell technique in MFIX.
- Implement Hyperbolic Quadrature Method of Moments (HQMOM) to better capture particle trajectory crossing (PTC).
- Implement and validate gas-particle turbulence model in MFIX.
- Consolidate previous QBMM implementations into current MFIX-QBMM module: DQMOM and QMOMK.

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Thank you for your attention !!!

Questions ?