A FILTERED COARSE-GRAIN CFD-DEM APPROACH FOR SIMULATING FLUIDIZED PARTICLES

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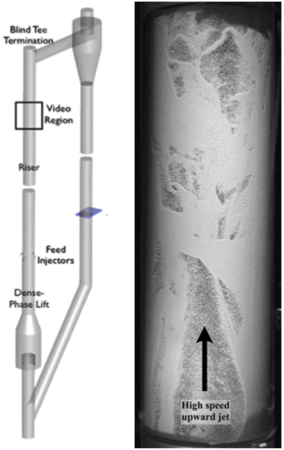
Introduction

- Circulating fluidized beds (CFB) are one of the prominent gas-solid reactors used in the industry
- Contact between the fluid and particles promotes heat and mass transfer
- Efficiency of CFB reactors heavily influenced by riser hydrodynamics
- ***Focus on*** developing scalable coarse-grain DEM models for simulation of risers with polydisperse Geldart group-A particles



Schematic representation of CFB[1]

[1]Shaffer, F, et al., *Powder Technology (2013)*

CFD-DEM gas-phase equations

- Euler–Lagrange (CFD-DEM) approach adopted for many industrial applications
- Volume-filtered Navier–Stokes equations:

$$\frac{\partial}{\partial t}(\varepsilon_f \boldsymbol{u}_f) + \boldsymbol{\nabla} \cdot (\varepsilon_f \rho_f \boldsymbol{u}_f) = 0$$

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f \boldsymbol{u}_f) + \boldsymbol{\nabla} \cdot (\varepsilon_f \rho_f \boldsymbol{u}_f \otimes \boldsymbol{u}_f) = \boldsymbol{\nabla} \cdot (\boldsymbol{\tau} - \boldsymbol{R}_u) + \varepsilon_f \rho_f \boldsymbol{g} + \boldsymbol{F}^{\text{inter}}$$

- Main unclosed terms:
  - Pseudo-turbulent stress tensor, $\boldsymbol{R}_u$
  - Interphase momentum exchange, $\boldsymbol{F}^{\text{inter}}$

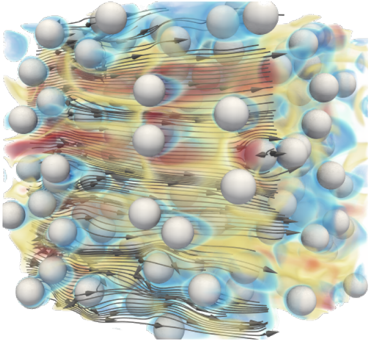
Modeling pseudo-turbulent Reynolds stress

- Subgrid-scale model accounting for pseudo-turbulence (Mehrabadi, et al.[2])
- Pseudo-turbulent kinetic energy:

$$k_f = \frac{1}{2}\langle \boldsymbol{u}_f'' \cdot \boldsymbol{u}_f'' \rangle$$
$$\approx E_f \left[2\varepsilon_p + 2.5\varepsilon_p\left(1-\varepsilon_p\right)^3 \exp\left(-\varepsilon_p \, \mathrm{Re}_p^{1/2}\right)\right]$$

- Pseudo-turbulent stress tensor:

$$\boldsymbol{R}_u = \langle \boldsymbol{u}_f'' \otimes \boldsymbol{u}_f'' \rangle \approx 2k_f\left(\boldsymbol{b} + \frac{1}{3}\boldsymbol{I}\right)$$



Pseudo–turbulence in particle-laden flows[3]

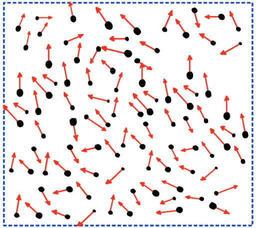
[2] Mehrabadi, et al. *Journal of Fluid Mechanics, 2015*
[3] Lattanzi, et al. *Journal of Fluid Mechanics, 2022*

Particle equation of motion

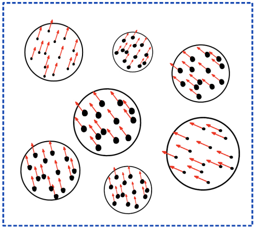
- Particle transport equation in traditional CFD-DEM:

$$\frac{d\boldsymbol{u}_p}{dt} = \boldsymbol{f}_p^{\text{inter}} + \boldsymbol{f}_p^{\text{col}} + \boldsymbol{g}$$

- Major drawback: requires tracking each individual particle
- Alternatively, n_{pp} particles lumped into 'parcels'
- Common approaches:
  - CG-DEM
    - → Collisions modeled using soft-sphere approach with modified restitution coefficient
    - → Assume uniform particle properties within parcels
  - MP-PIC



Particles



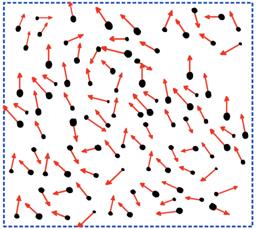
Parcels

Particle equation of motion

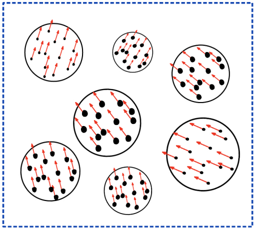
- Particle transport equation in traditional CFD-DEM:

$$\frac{d\boldsymbol{u}_p}{dt} = \boldsymbol{f}_p^{\text{inter}} + \boldsymbol{f}_p^{\text{col}} + \boldsymbol{g}$$

- Major drawback: requires tracking each individual particle
- Alternatively, n_{pp} particles lumped into 'parcels'
- Common approaches:
  - CG-DEM
  - MP-PIC
    - → Collisions modeled using a stochastic approach based on solid stress
    - → Assume uniform particle properties within parcels
    - → Does not converge to deterministic equations in the limit $n_{pp} \to 1$



Particles



Parcels

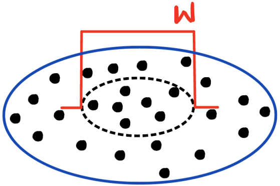
Objective of current work

To develop a rigorous coarse-grain CFD-DEM framework that converges to underlying deterministic equations in the limit $n_{pp} = 1$, with closures that account for variations within the parcel

Coarse-grain modeling using local particle filtering

- Particles are lumped into parcels with n_{pp} particles per parcel
- Parcel properties determined via local averaging using a particle-based filter
- Filtering kernel, W, defined for parcel i:

$$\sum_{j=1}^{n_{pp}} \mathcal{V}_p^{(j)} W(|\widehat{\boldsymbol{x}}_p^{(i)} - \boldsymbol{x}_p^{(j)}|) = 1$$



Box filter over a parcel

- Notation:
  - $j \rightarrow$ particle index
  - $\mathcal{V}_p \rightarrow$ volume of the particle
  - $\boldsymbol{x}_p \rightarrow$ particle position
  - $W \rightarrow$ kernel function

Parcel properties obtained using local particle filtering

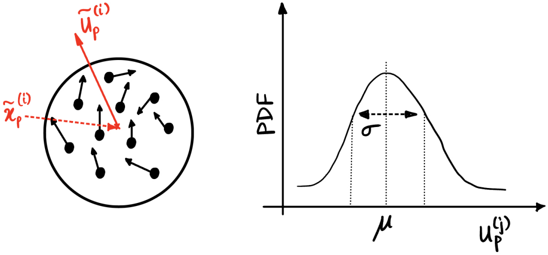
- Position and velocity of parcel i:

$$\widehat{\boldsymbol{x}}_p^{(i)} = \sum_{j=1}^{n_{pp}} \boldsymbol{x}_p^{(j)} \mathcal{V}_p^{(j)} W_{ij}$$

$$\frac{\mathrm{d}\widehat{\boldsymbol{x}}_p^{(i)}}{\mathrm{d}t} = \widehat{\boldsymbol{u}}_p^{(i)} = \sum_{j=1}^{n_{pp}} \boldsymbol{u}_p^{(j)} \mathcal{V}_p^{(j)} W_{ij}$$

- Velocity distribution within parcels is characterized by a mean velocity and granular temperature

$$\theta_p = \frac{1}{3}\widehat{\boldsymbol{u}_p'' \cdot \boldsymbol{u}_p''}$$



PDF of velocity of particles in a parcel

$$\mu = \widehat{\boldsymbol{u}}_p^{(i)} \quad \sigma = \sqrt{3\theta_p}$$

Parcel equation of motion

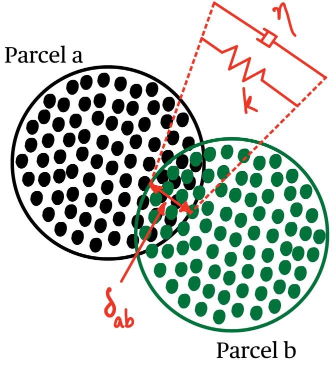
Parcel transport equation:

$$\frac{d\widehat{\boldsymbol{u}}_p}{dt} = \widehat{\boldsymbol{f}}_p^{\text{inter}} + \widehat{\boldsymbol{f}}_p^{\text{col}} + \boldsymbol{g}$$

- Collisions modeled as a mass-spring-dashpot system using soft-sphere approach
- Coefficient of restitution modified to account for the dissipation of granular energy[5]

$$\frac{\ln e_{CG}}{\ln e} = \sqrt{n_{pp}} \frac{\sqrt{1 - \frac{(\ln e)^2}{(\ln e)^2 + \pi^2}}}{\sqrt{1 - \frac{n_{pp}(\ln e)^2}{(\ln e)^2 + \pi^2}}}$$

- Upper limit on n_{pp} imposed $(e = 0.8 \Rightarrow n_{pp} \leq 199)$



[5] Benyahia, S. and Galvin, J.E., Industrial & Engineering Chemistry Research (2010)

Filtered drag force acting on parcels

➢ Filtered drag force:

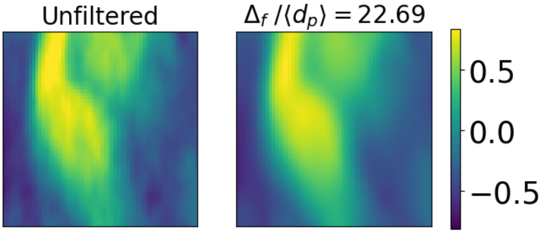
$$\widehat{\boldsymbol{f}}_{drag}^{(i)} = \widehat{(\beta[\boldsymbol{u}_f^{(i)} - \boldsymbol{u}_p^{(i)}])} = \sum_{j=1}^{n_{pp}} \beta(\varepsilon_f^{(j)}, \mathrm{Re}_p^{(j)})[\boldsymbol{u}_f^{(j)} - \boldsymbol{u}_p^{(j)}]\mathcal{V}_p^{(j)} W_{ij}$$

$$= \beta(\overline{\varepsilon}_f^{(i)}, \mathrm{Re}_{CG}^{(i)})[\widetilde{\boldsymbol{u}}_f^{(i)} - \widehat{\boldsymbol{u}}_p^{(i)}]\,(1 + H)$$

➢ Eulerian-based filtering:

$$\widetilde{\boldsymbol{u}}_f = \overline{\varepsilon_f \boldsymbol{u}_f} / \overline{\varepsilon_f}$$

$$\overline{\varepsilon}_f(\boldsymbol{x}) = \int_\Omega \mathcal{G}(\boldsymbol{y}) \varepsilon_f(\boldsymbol{x} - \boldsymbol{y}) d\boldsymbol{y}$$



Filtered velocity field

Drag correction factor

- Drag correction factor:

$$H = \frac{\overline{\beta[\boldsymbol{u}_f^{(i)} - \boldsymbol{u}_p^{(i)}]}}{\beta(\bar{\varepsilon}_f^{(i)}, \mathrm{Re}_{CG}^{(i)})[\widetilde{\boldsymbol{u}}_f^{(i)} - \widehat{\boldsymbol{u}}_p^{(i)}]} - 1$$

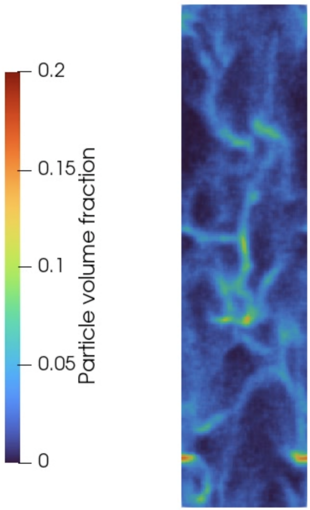
  - $H = 0$: drag obtained using resolved quantities require no correction
  - $H > 0$: drag overestimated when computed using resolved quantities
  - $H < 0$: drag underestimated when computed using resolved quantities

- Similar closure appears in filtered two-fluid method[5,6,7]

[5] Igci, Y, et al., *Industrial & Engineering Chemistry Research (2008)*
[6] Parmentier, J, et al., *AIChE Journal (2012)*
[7] Milioli, C, et al., *AIChE Journal (2013)*

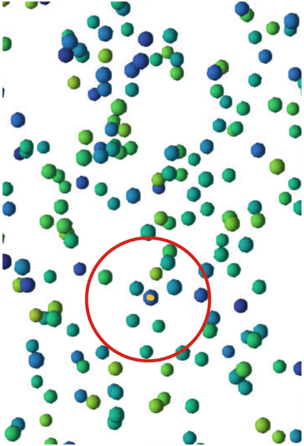
Modeling drag correction factor

- Simulations of "cluster-induced turbulent" flow in a triply periodic domain with monodisperse and polydisperse distribution of Geldart group-A particles
  - Particle mean diameter : $75\ \mu m$
  - Particle density : $2250\ kg/m^3$
  - Particle volume fraction : 0.02
  - No. of particles $\sim$ 2.1M
  - Domain : $960d_p \times 240d_p \times 240d_p$
  - $dx = dy = dz = 3d_p$



Modeling drag correction factor

- ➢ Simulations of “cluster-induced turbulent” flow in a triply periodic domain with Geldart group-A particles
- ➢ Efficient, embarrassingly parallel, detection of particles within parcels using KDTree algorithm

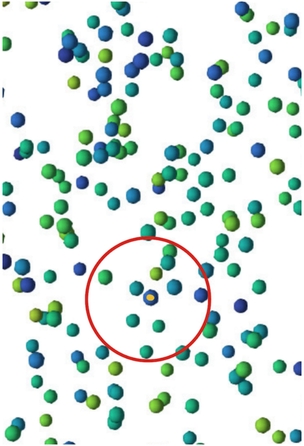


Zoomed-in view of particles in flow

Modeling drag correction factor

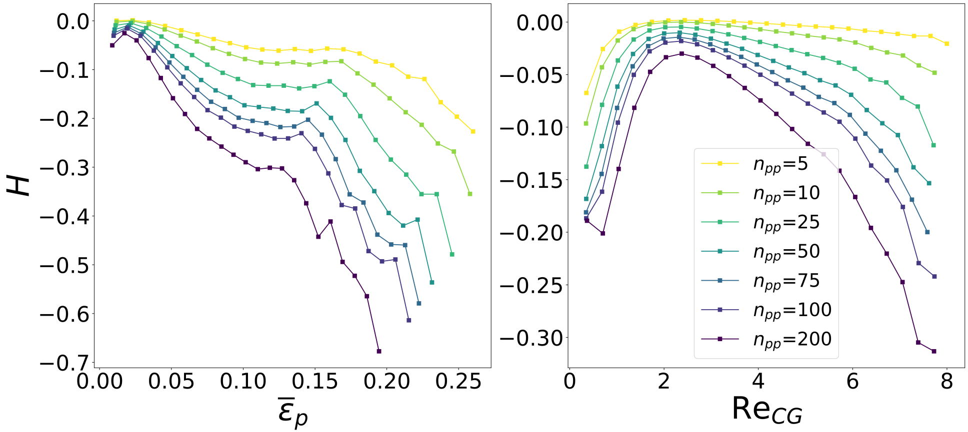
- Simulations of "cluster-induced turbulent" flow in a triply periodic domain with Geldart group-A particles
- Efficient, embarrassingly parallel, detection of particles within parcels using KDTree algorithm
- Filtered quantities obtained using a volume-weighted box filter

$$\widehat{\boldsymbol{u}}_p^{(i)} = \sum_{j=1}^{n_{pp}} \boldsymbol{u}_p^{(j)} \mathcal{V}_p^{(j)} W_{ij} = \frac{\sum_{j=1}^{n_{pp}} \boldsymbol{u}_p^{(j)} \mathcal{V}_p^{(j)}}{\sum_{j=1}^{n_{pp}} \mathcal{V}_p^{(j)}}$$



Zoomed-in view of particles in flow

Variation of drag correction factor with monodisperse particles



Parcels with polydisperse particles

- Solid mass and volume are conserved within each parcel

$$m_{CG} = \sum_{j=1}^{n_{pp}} m_p^{(j)} \ , \quad \mathcal{V}_{CG} = \sum_{j=1}^{n_{pp}} \mathcal{V}_p^{(j)}$$

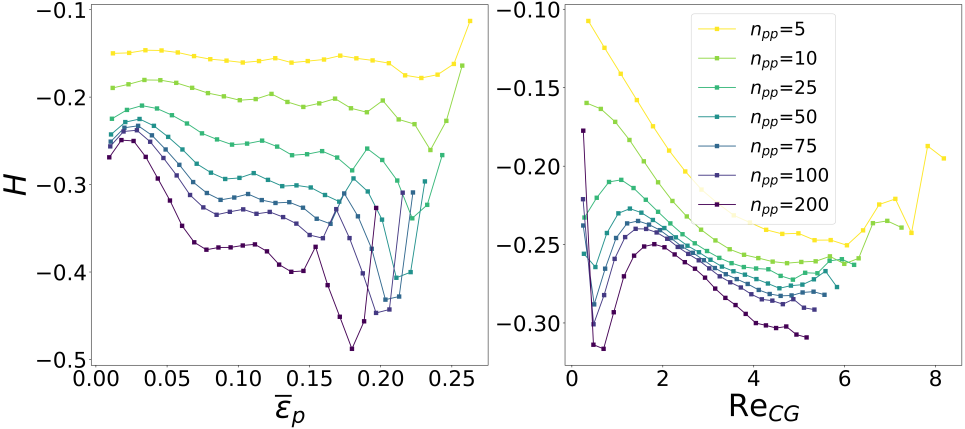
- Equivalent diameter of the particles in the parcels computed using volume constraint

$$d_{p,\text{eff}} = \left(\frac{\sum_{j=1}^{n_{pp}} d_p^3}{n_{pp}} \right)^{1/3}$$

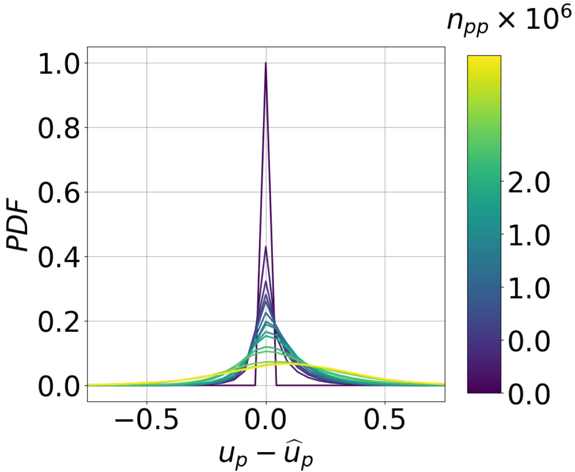
- Reynolds number of parcels computed using the effective diameter

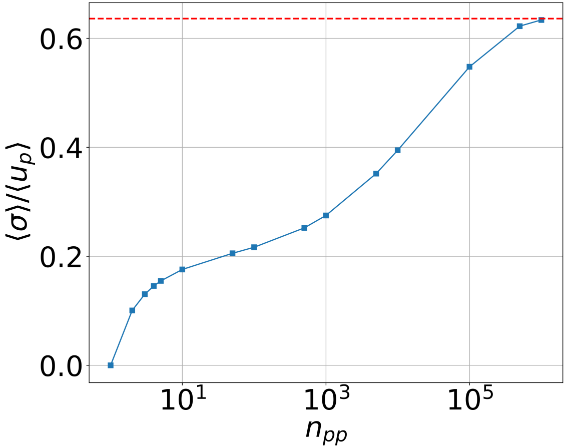
$$\mathrm{Re}_{CG} = \frac{\rho_f |\widetilde{\boldsymbol{u}_f} - \widehat{\boldsymbol{u}}_p| d_{p,\text{eff}}}{\nu}$$

Variation of drag correction factor with polydisperse particles



Velocity variation within parcels





Conclusion

Summary

- A rigorous formulation of a scalable filtered coarse-grain CFD-DEM is presented
- Unclosed sub-filter terms arise and require modeling
- Sub-filter drag force quantified with simulations of "cluster induced turbulent" flows

Future work

- Symbolic regression will be employed to obtain closed-form algebraic models
- Formulation will be extended to capture high-order particle statistics within parcels like granular temperature, in addition to exchanging particles between parcels
- Borrow ideas from moment methods for the formulation

Thank you!