Development of a Two-Fluid Drag Law for Clustered Particles using Direct Numerical Simulation

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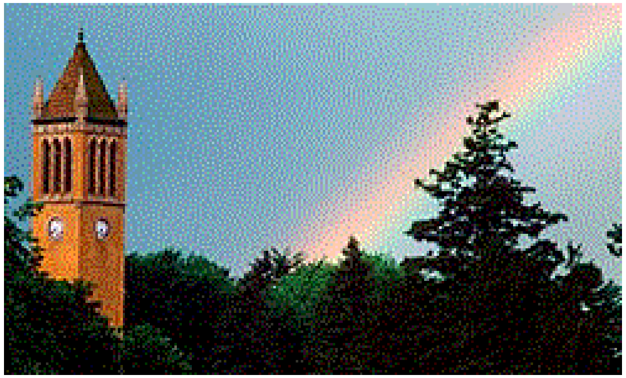

NETL Multiphase Flow Workshop 2013

Acknowledgements

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  - Seckin Gokaltun, Norman Munroe (FIU)
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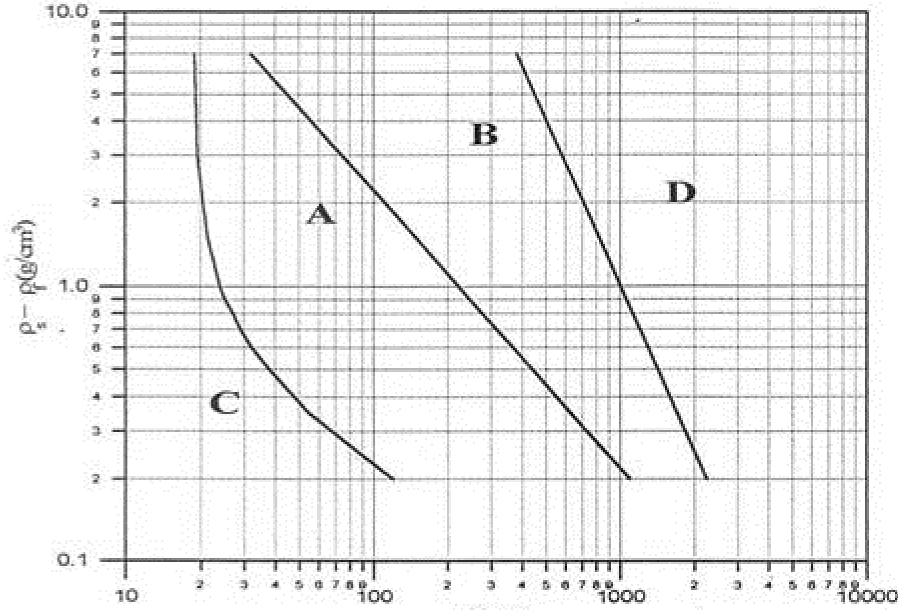
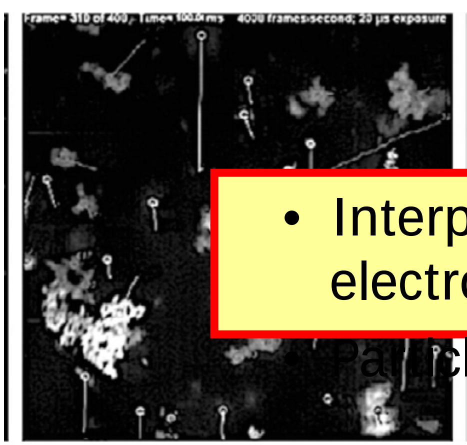
  - Department of Energy (DOE) HBCU/MI Award Grant No: *DE-FE0007260* through the National Energy Technology Laboratory (NETL)
  - National Science Foundation (NSF) CMMI 0927660

- Geldart classification
  - Geldart B particles
    - Higher Re_m and St
    - Uniform particle configuration
  - Geldart A Particles
    - Lower Re_m and St
    - Formation of particle clusters



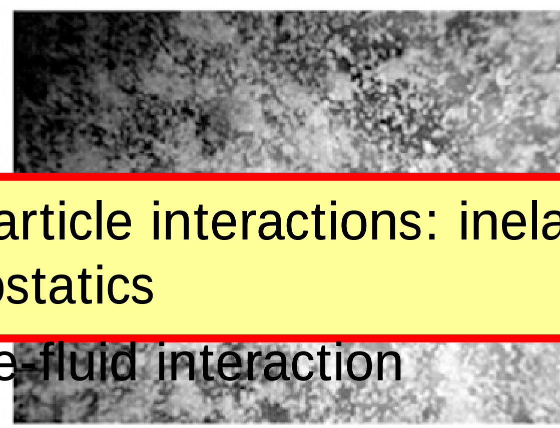
Plascoat™ 571 polyethylene

FCC catalyst in the bed



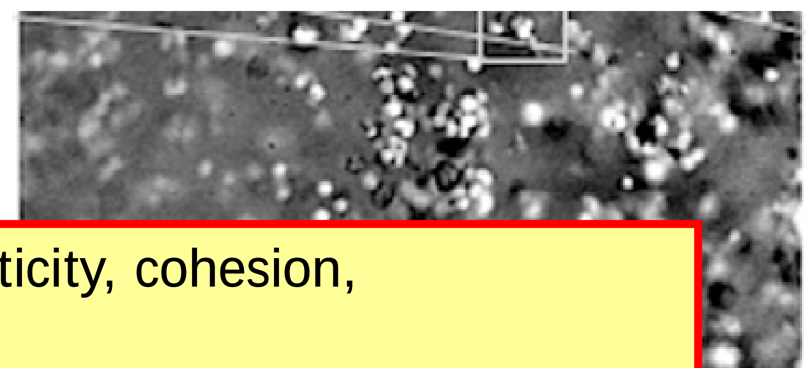
○← 100 µm Diameter

In the free board



○← 100 µm Diameter

In the fluidized bed



○ ← 100 µm Diameter

- Interparticle interactions: inelasticity, cohesion, electrostatics
- Particle-fluid interaction

Cocco et al., Particle clusters in and above fluidized beds, *Powder Technology*, 2010

Collaboration with Experiments at FIU

- Florida International University
  - Dr. Seckin Gokaltun

Bubbling Bed

Filter bag

Acrylic riser 2' X 5"

High speed camera

Distributor plate

Rotameter

Pressure regulator

Pressure sensors

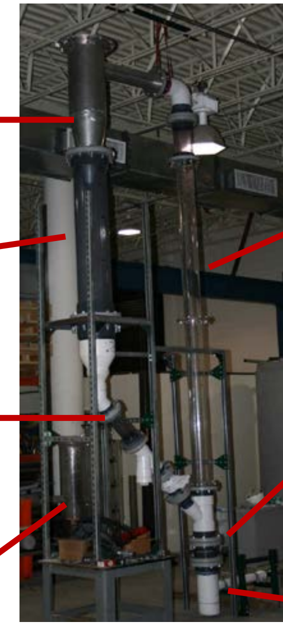
Circulating Fluidized Bed

Cyclonic separator

Stand pipe

Down comer

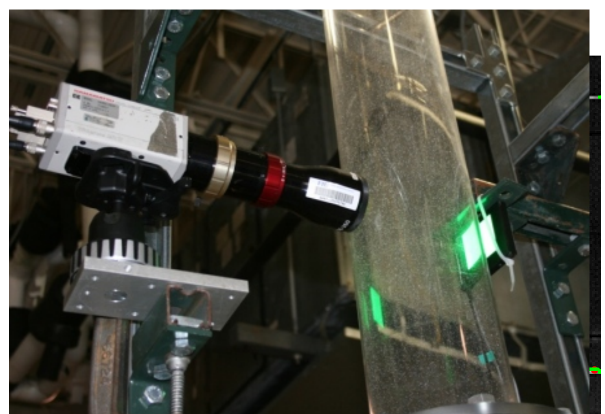
Gate valve

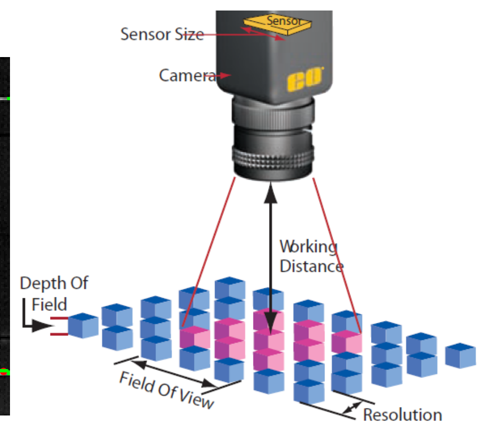


Acrylic Riser 6" X 10'

Distributor plate

Inlet Plenum

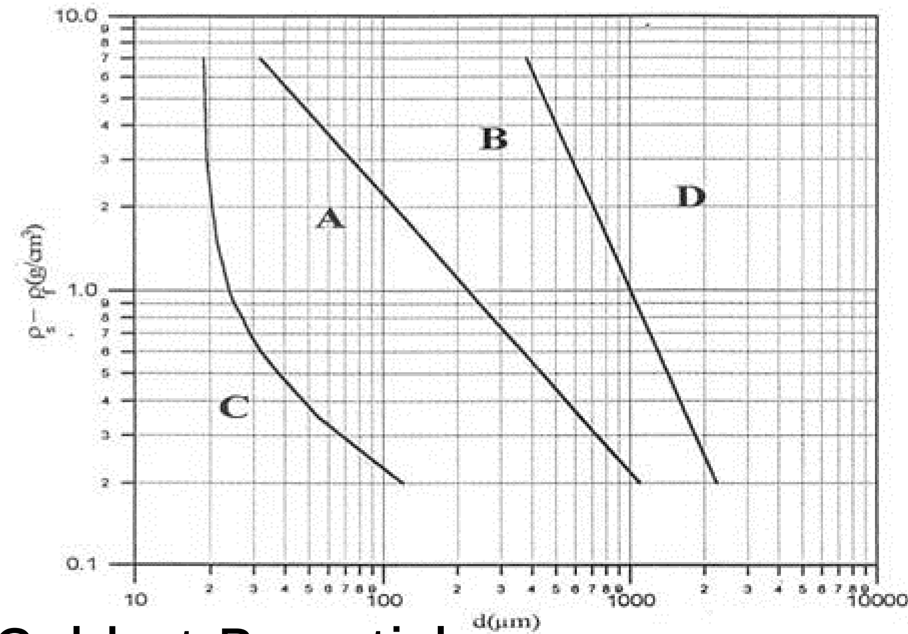




Abbasi Baharanchi, A., Gokaltun, S., Munroe, N., Dulikravich, G., *An Experimental Study Using High Speed Imaging of Clustered Particles for a More Accurate Drag Law in MFIX*, NETL Workshop, 2013.

Motivation

- Geldart classification
  - Geldart B particles
    - Higher Re_m and St
    - Uniform particle configuration
  - Geldart A Particles
    - Lower Re_m and St
    - Formation of particle clusters



- Several drag laws available for Geldart B particles
    - Ergun(1952), Wen-Yu (1966), DNS: Hill et al (2001), van der Hoef et al (2005, 2007),Tenneti et al (2011)
- Comparison of CFD results for <u>*Geldart A*</u> systems forming particle clusters (using uniform configuration drag laws) with experimental results
    - Inaccurate pressure drop/bed expansion

Need for a physics-based clustered drag law

Garg, R., Shahnam, M. and Huckaby, E. D., *Continuum simulations of CO_2 capture by dry regenerable potassium based sorbents*, ICMF 2010: Tampa, FL.

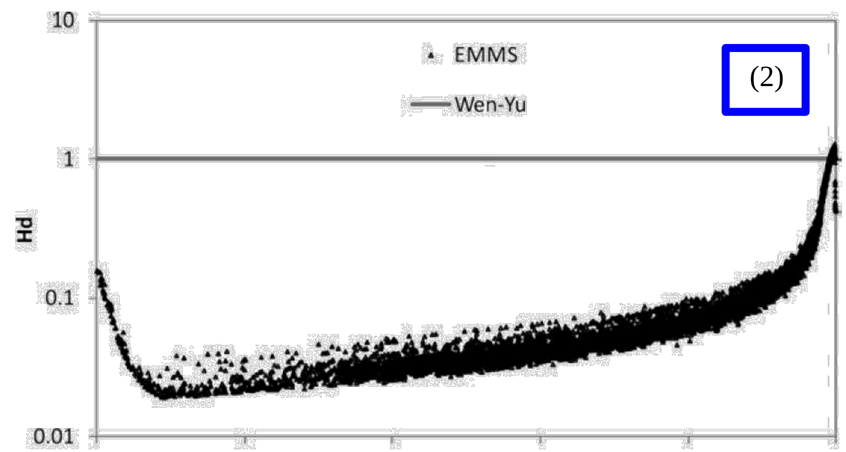
Current Cluster Drag Models

- Current state-of-the-art clustered drag model used in CFD
  - Energy minimization multi scale model[1] (EMMS)
    - Based on the minimum energy required for suspending and transporting dense particle regions
    - Accounts for the effect of heterogeneous structures on drag through a *drag index*

$$\beta = \begin{cases} 150\dfrac{\varepsilon_s(1-\varepsilon_g)\mu_g}{\varepsilon_g d_p^2} + 1.75\dfrac{\rho_g}{d_p}\varepsilon_s\left|\mathbf{v}_g - \mathbf{v}_s\right| & \varepsilon_g < 0.4 \\ \dfrac{3}{4}C_D\dfrac{\rho_g\varepsilon_g\varepsilon_s\left|\mathbf{v}_g-\mathbf{v}_s\right|}{d_p}\varepsilon_g^{-2.65}H_d & \varepsilon_g \geq 0.4 \end{cases}$$

Wen-Yu correlation

Drag index



While EMMS is useful, there is scope for an improved clustered drag law

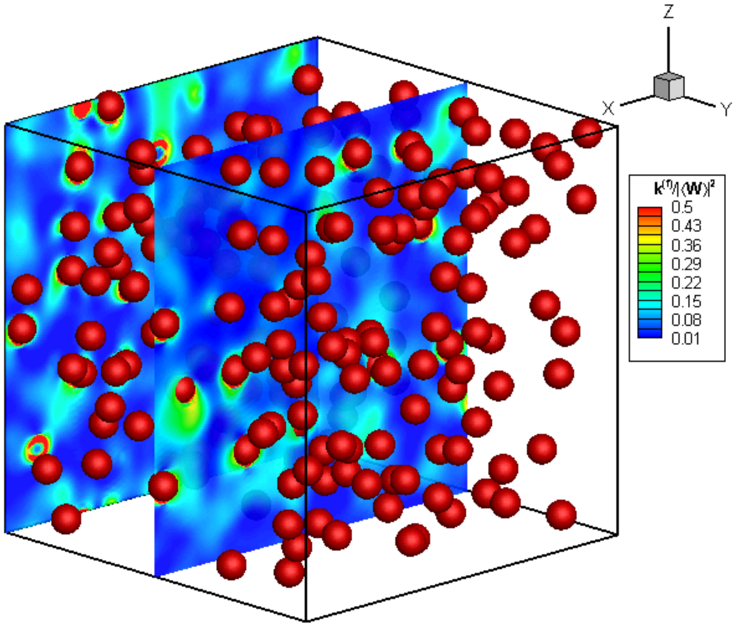
[1] Li, J., Kwauk, M., *Particle-Fluid Two-Phase Flow: the Energy-Minimization Multi-Scale Method; Metallurgy,* Beijing: Industry Press, 1994.

[2] Benyahia, S., *Analysis of Model Parameters Affecting the Pressure Profile in a Circulating Fluidized Bed*, AIChE Journal, 2012, 58 (2).

PR-DNS Simulation Approach

- Particle-resolved direct numerical simulation (PR-DNS) of flow past random configurations of fixed particles
  - periodic domains approximate statistically homogeneous suspensions well[1]
  - impose constant mean pressure gradient
  - volume-averaging to estimate ensemble-averaged quantities

$\langle \mathbf{u}^{(f)} \rangle$

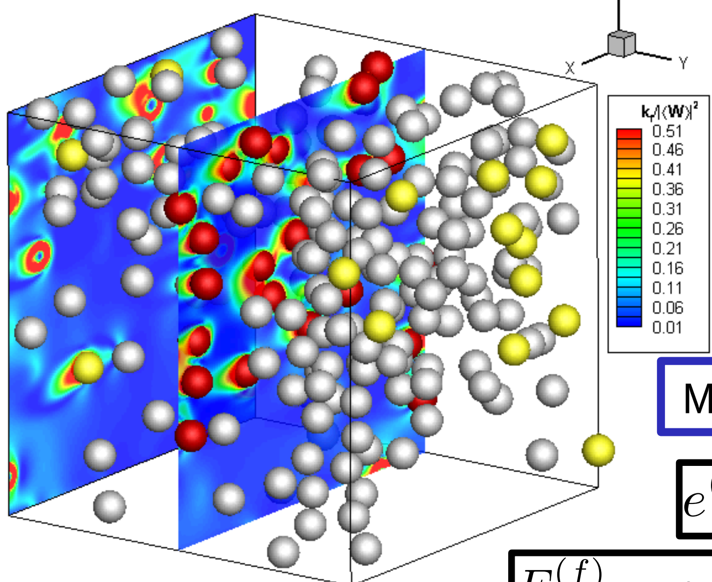


- Demonstrated numerical convergence and accuracy
- Validated in suite of test cases

"[1]Drag law for monodisperse gas–solid systems using particle-resolved direct numerical simulation of flow past fixed assemblies of spheres" S. Tenneti, R. Garg, S. Subramaniam *International Journal of Multiphase Flow*, 37(9), p 1072-1092

Freely evolving non-cohesive suspensions

Freely moving particles undergoing collisions



- Rate of work done by constant mean pressure gradient in maintaining flow

$$\langle \mathbf{W} \rangle \cdot \left\langle \mathbf{S}_M^{(f)} \right\rangle = \Pi^{(f)} + \Pi^{(p)}$$

Mean Slip X Mean Drag | Production of $k^{(f)}$ | Production of $k^{(p)}$

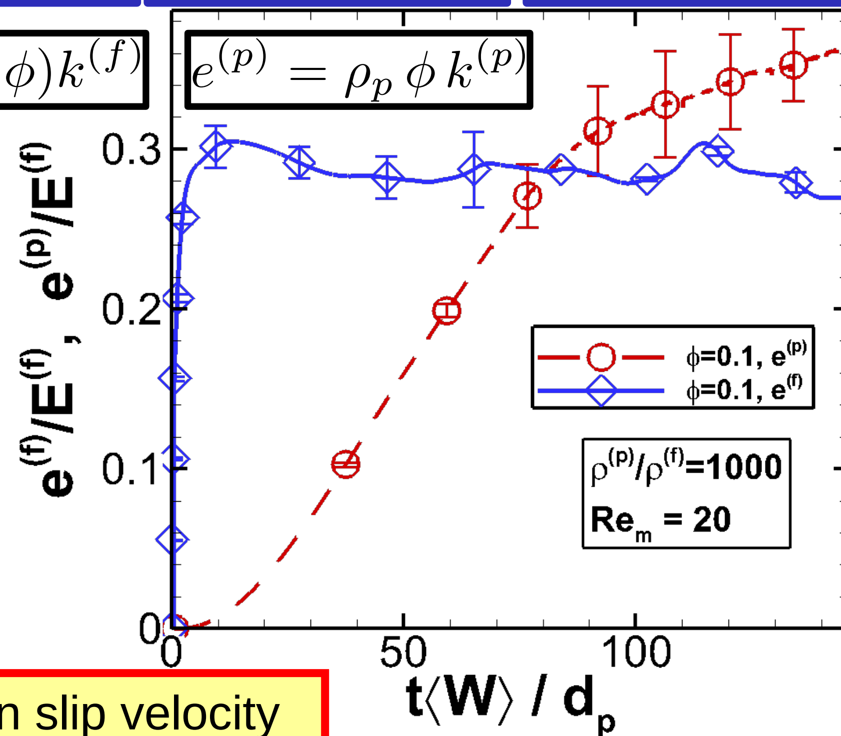
$$e^{(f)} = \rho_f (1-\phi) k^{(f)}$$

$$e^{(p)} = \rho_p \, \phi \, k^{(p)}$$

$$E^{(f)} = \rho_f \langle \mathbf{W} \rangle \cdot \langle \mathbf{W} \rangle / 2$$

$$\underbrace{\rho_f (1-\phi) \frac{dk^{(f)}}{dt}}_{\text{unsteady term}} = \Pi^{(f)} \underbrace{-2\mu_f \langle I_f s_{ij} s_{ij} \rangle}_{\text{viscous dissipation}}$$

$$\underbrace{\rho_p \phi \frac{dk^{(p)}}{dt}}_{\text{unsteady term}} = \Pi^{(p)} \underbrace{-\Gamma_{\mathrm{coll}}^{(p)}}_{\text{collisional dissipation}}$$



Particle velocity fluctuations scale with mean slip velocity

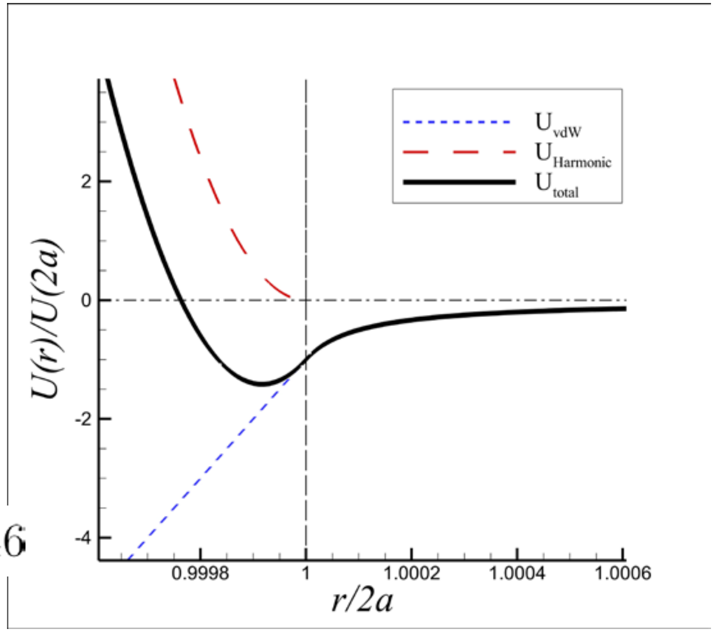
Homogeneous Cooling Cohesive Granular Gas

- Soft-sphere DEM of cohesive particles: van der Waals interaction and linear-spring-dashpot on contact

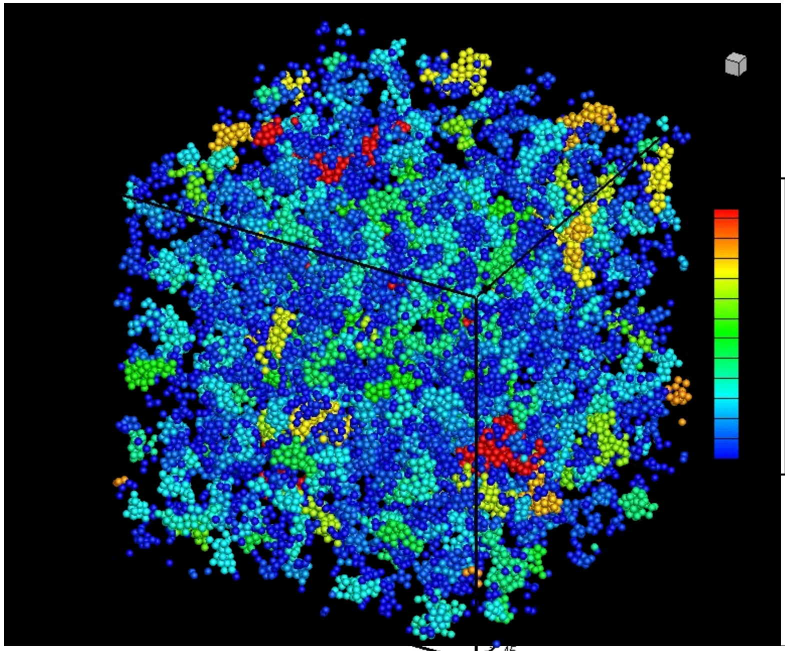
(Eric Murphy)

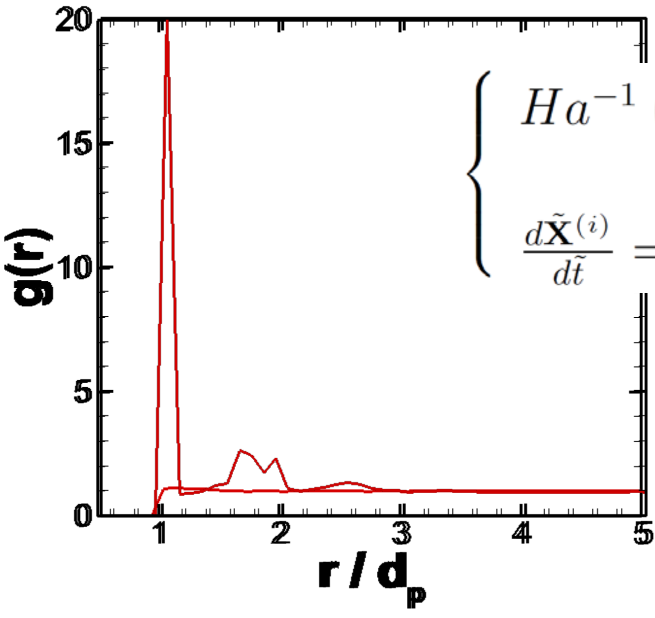
$$Ha = \frac{A}{\rho \pi d_p^2 d_0 T}$$

Ha is the ratio of adhesion energy to particle kinetic energy (granular temperature)



$$\phi = 0.084,\ Ha = 2.4,\ d_0/d_p = 10^{-4},\ L/d_p = 50,\ N = 20146$$



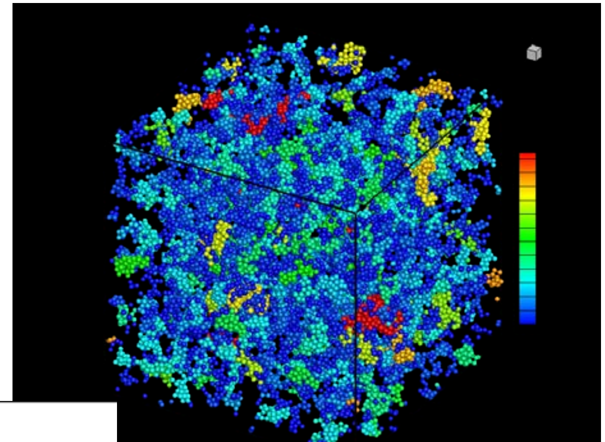


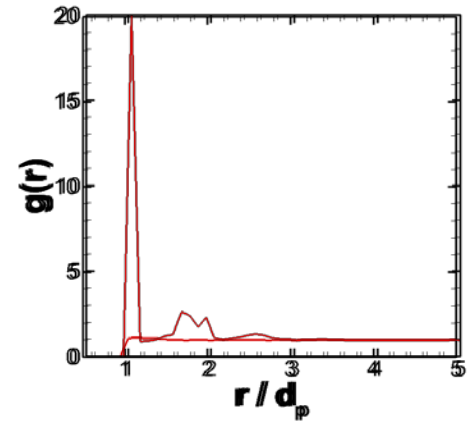
$$\begin{cases} Ha^{-1}\left(\frac{d_0}{d_p}\right)^2 \frac{d\tilde{\mathbf{V}}^{(i)}}{d\tilde{t}} + 1 = 0 \\ \frac{d\tilde{\mathbf{X}}^{(i)}}{d\tilde{t}} = \tilde{\mathbf{V}}^{(i)} \end{cases}$$

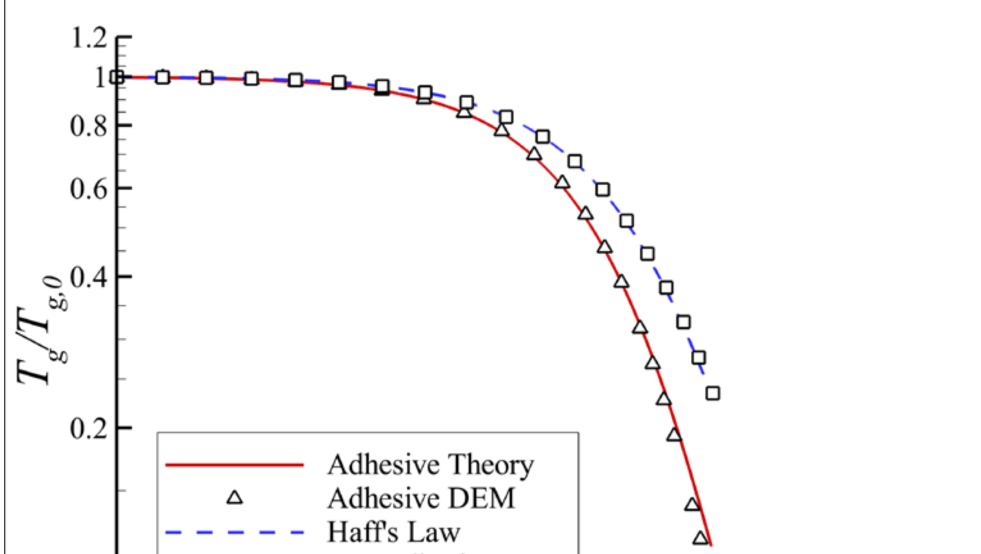
$$\begin{cases} \tilde{t} = \frac{t\sqrt{T}}{d_0} \\ \tilde{\mathbf{X}}^{(i)} = \frac{\mathbf{X}^{(i)}}{d_0} \\ \tilde{\mathbf{V}}^{(i)} = \frac{\mathbf{V}^{(i)}}{\sqrt{T}} \\ Ha = \frac{A}{\rho \pi d_p^2 d_0 T} \end{cases}$$

Homogeneous Cooling Cohesive Granular Gas

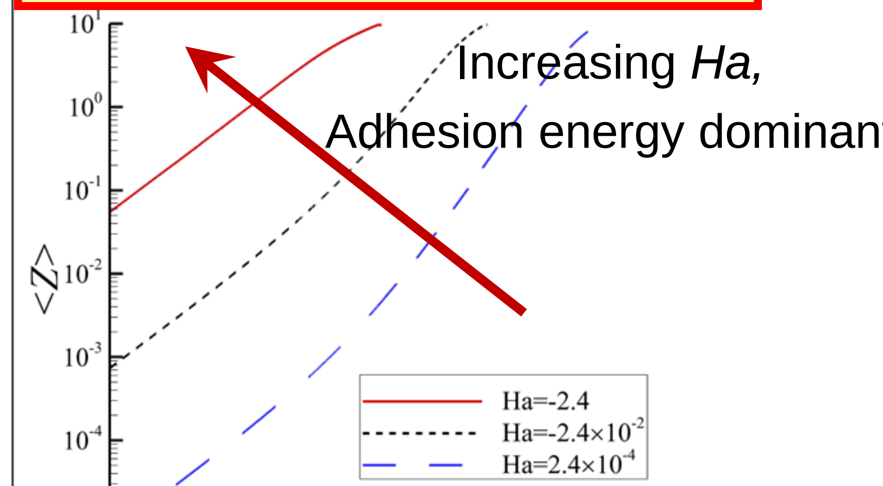
- Pseudo-Liouville Operator Analysis
  - Temperature decay
  - Coordination number
- Soft-sphere DEM of cohesive particles







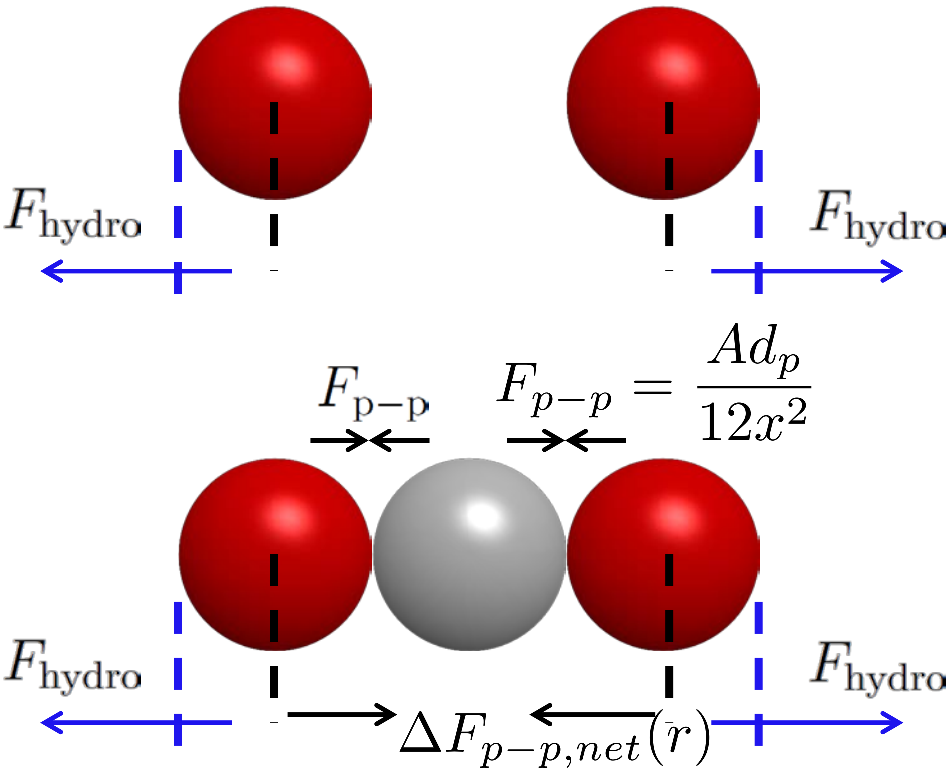
Average coordination number



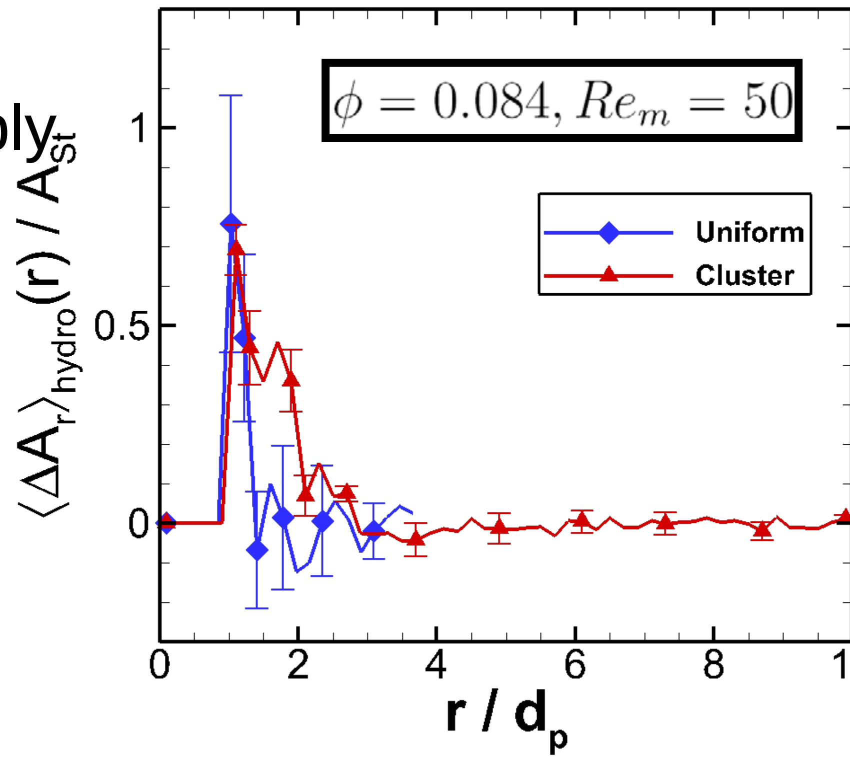
Structure of clusters depends on *Ha*: the ratio of adhesion energy to particle kinetic energy (granular temperature)

Cohesive Suspensions: Flow Physics

- Compare hydrodynamic forces between a pair of particles in uniform and clustered arrangements in a fixed assembly



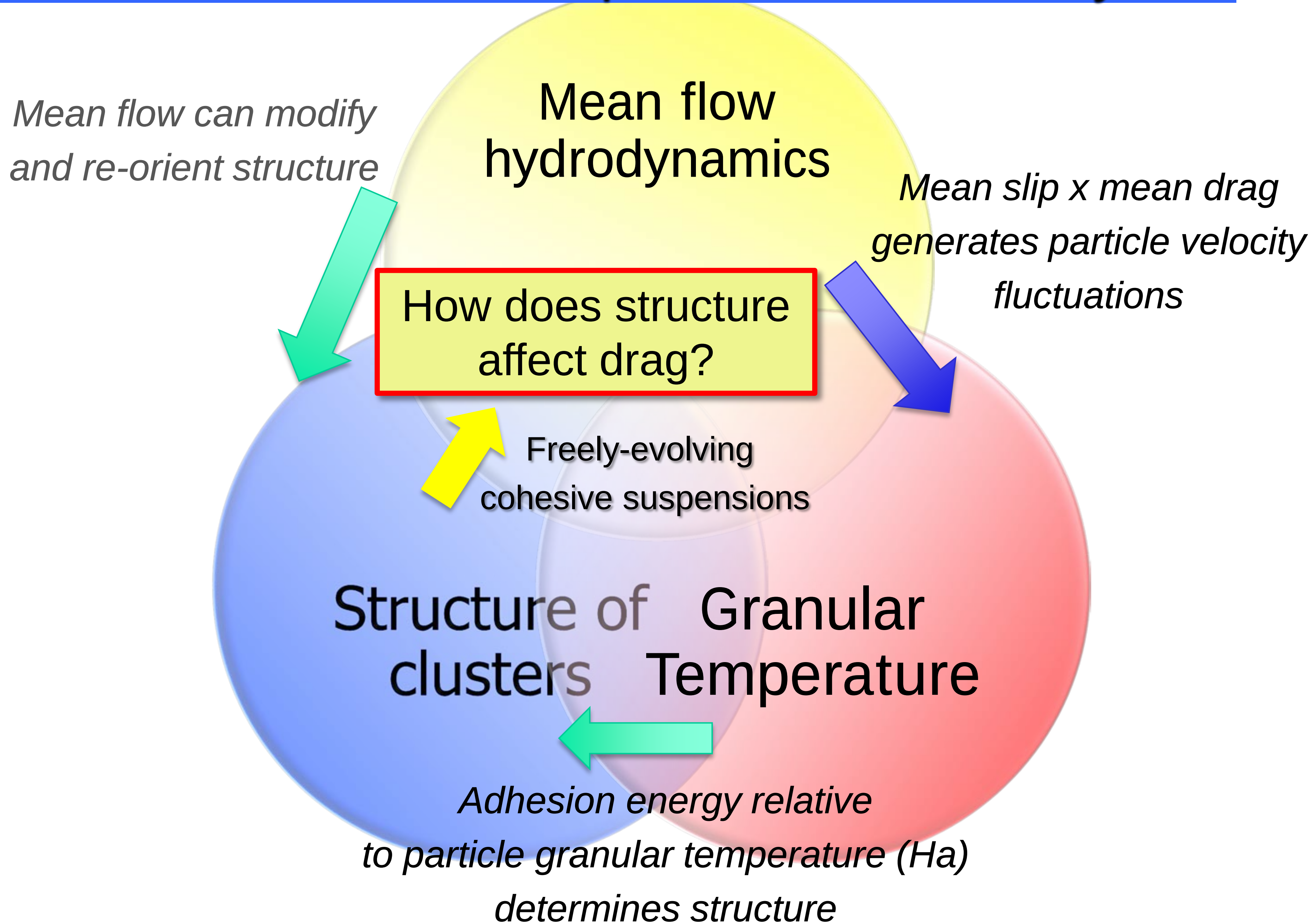
Relative radial acceleration



Particles remain as aggregates if the net cohesive forces overcome the hydrodynamic forces at separation *r*

Difference between uniform and clustered hydrodynamic relative acceleration (force) must be overcome by net cohesive force

Cohesive Suspensions: Flow Physics

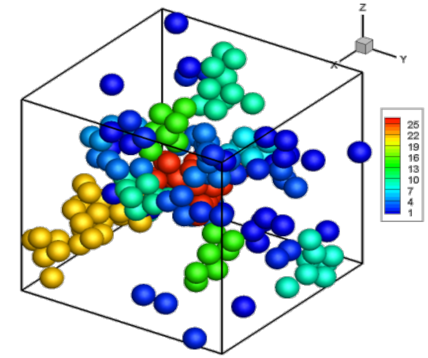


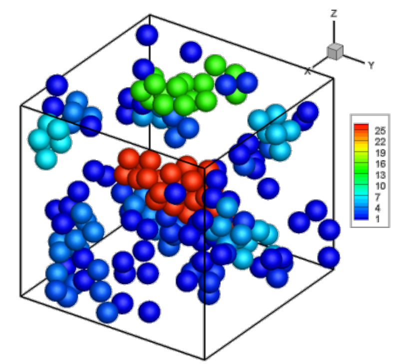
PR-DNS of Clustered Gas-Solid Systems

- ***Type I***: PR-DNS of homogeneous freely evolving gas-solid suspensions of cohesive particles
  - Computationally very expensive owing to range of time and length scales
- ***Type II***: PR-DNS of homogeneous freely evolving clustered gas-solid flow (eliminates cluster formation time)
  A. With cohesive forces allowing rearrangement: study restructuring of clusters in flow
  B. Rigid clusters: study re-orientation of clusters in flow
- ***Type III***: PR-DNS of homogeneous fixed assemblies of clustered particles

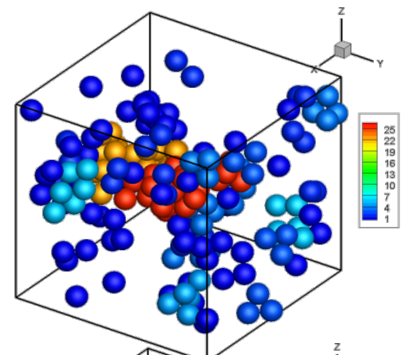
Generation of Particle Clusters

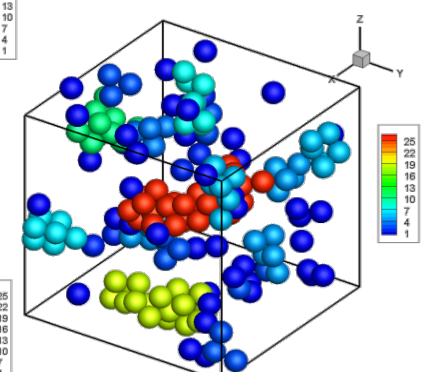
- ❑ Selection of particle sub-ensembles
  - ➢ Cocco et al. (2010) *Powder Tech.*
    - ✓Mean number of particles in a cluster is 26
    - ✓75% of particles in clusters
    - ✓25% of particles as single

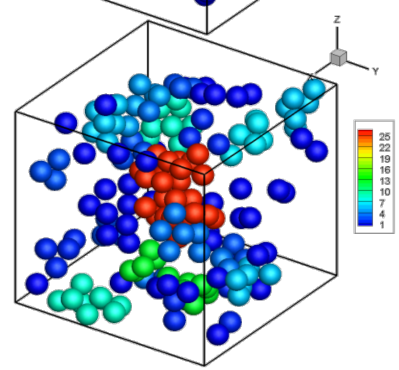


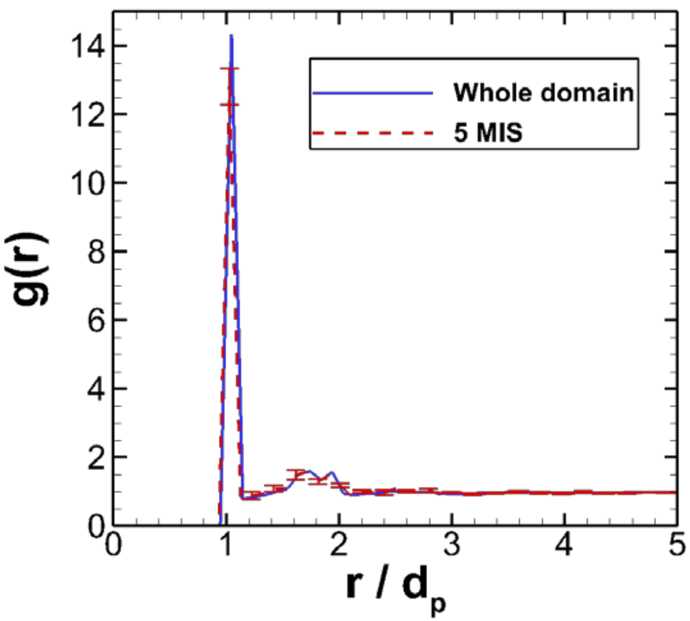


- ❑ Choosing 5 sub-ensembles with $\mathcal{L}/d_p = 10$
  - ➢ Consistent $\phi, \quad g(r)$



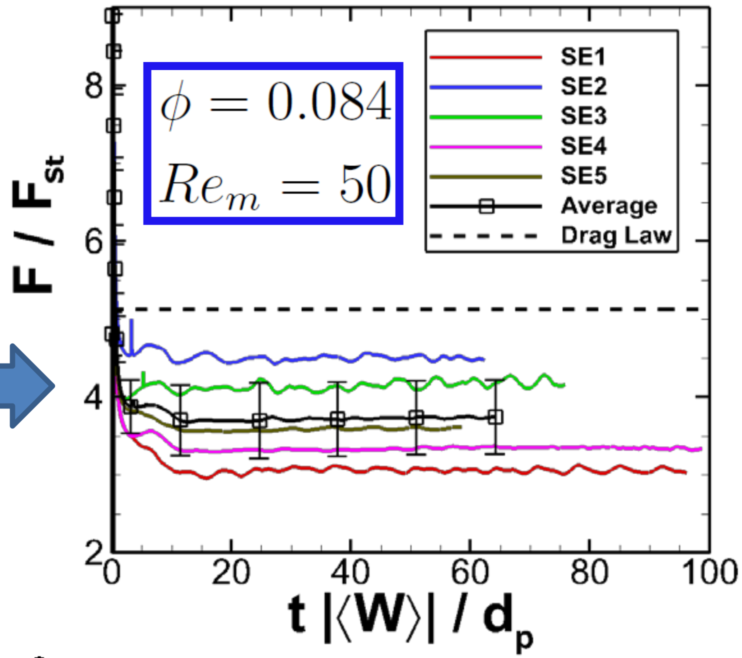


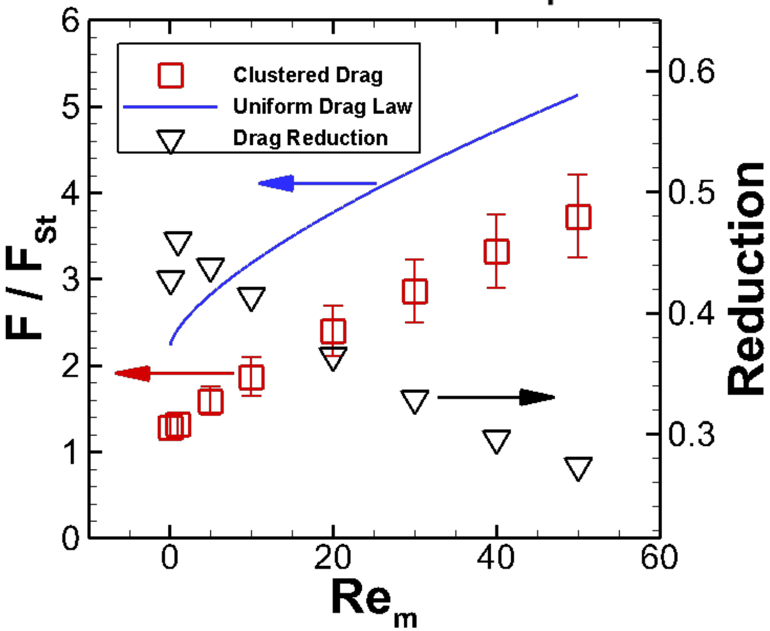




Sub-ensembles represent statistical properties of the whole domain

Direct Numerical Simulation

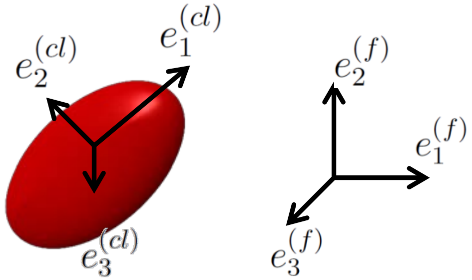




- Drag reduction is observed in clustered configurations
- Maximum reduction occurs at lower Re_m
- Higher volume fraction simulations are in progress

Cluster Drag: Dependencies

- Solid-phase volume fraction and mean-slip Reynolds number
  - ✓ Similar to uniform particle configuration drag law $\phi,\ Re_m$
- Cluster size R_g
- Anisotropy in clusters $\mathbf{e}^{(f)} \otimes \mathbf{e}^{(cl)}$
  - ✓ Alignment of cluster principal axis and mean flow unit vector

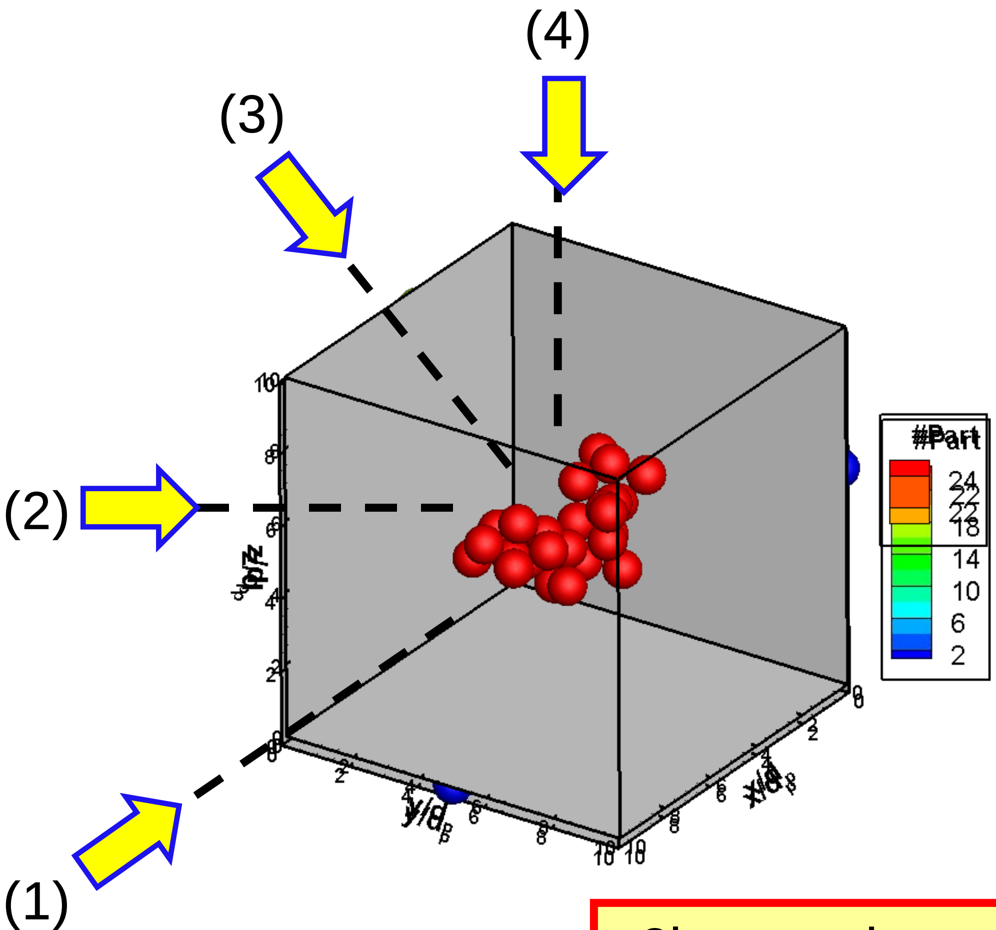


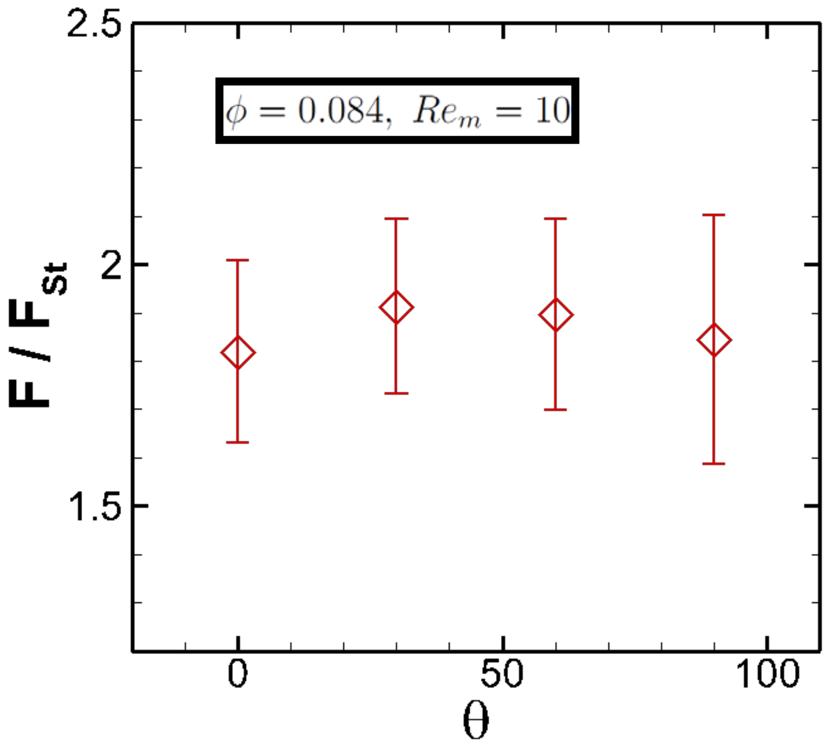
- The ratio of frontal area to the wetted area of a cluster $\dfrac{A_{\text{frontal}}}{A_{\text{wetted}}}$
- Tentative proposal for cluster drag law

$$F_{cl} = f\left(\frac{\langle \Delta A_r \rangle_{\text{hydro}}}{A_{\text{p-p}}}, \phi, Re_m, \frac{R_g}{d_p}, \mathbf{e}^{(f)} \otimes \mathbf{e}^{(cl)}, \frac{A_{\text{frontal}}}{A_{\text{wetted}}}\right)$$

Analysis of Drag Force

❑ Cluster alignment to the mean flow

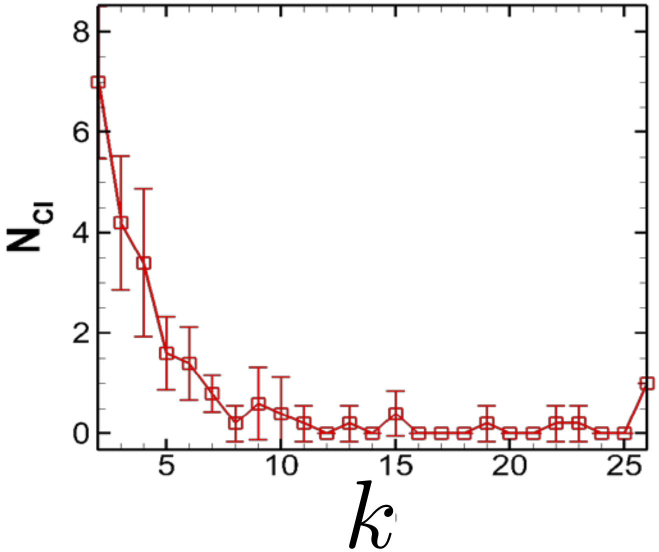




- Cluster orientation does not affect the total drag force significantly

Analysis of Drag Force

❑ Distribution of drag in clusters in simulated cases



$$P(N_p = k)$$

Cluster size distribution

$$F_{\text{Equi.}} = F_{\text{Uni.}}\left(\tilde{Re}_m, \tilde{\phi}\right)$$

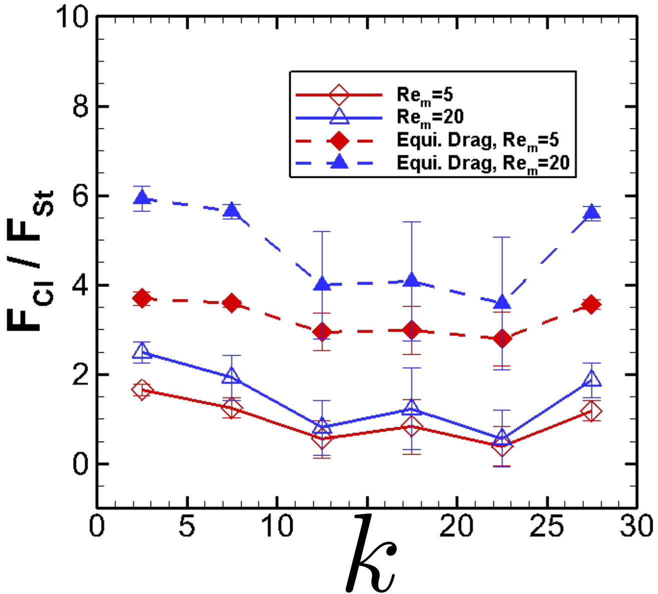
$$\tilde{d}_p = d_p\, N_p^{1/3} \qquad \tilde{\phi} = \phi$$

$$\tilde{Re}_m = Re_m \frac{\tilde{d}_p}{d_p}$$

$$\langle F_{Cl} \rangle = \sum_k \langle F_{Cl} \mid N_p = k \rangle P(N_p = k)$$

$$\langle F_{\text{Cl}} \mid N_p = k \rangle = C(\ldots) F_{\text{Uni.}}(\tilde{Re}_m, \tilde{\phi})$$

Porosity parameter



- $F_{equi.}$ is proportional to the cluster drag by a porosity parameter
- Can the total drag can be computed by knowing the porosity parameter and cluster size distribution? Preliminary results are promising!

Summary

- ❑ Conclusion
  - ➢ Flow physics in clustering particle suspensions: interplay of
    - ✓ Granular temperature arising from mean flow hydrodynamics
    - ✓ Ratio of adhesive energy to particle granular temperature: affects structure of clusters
    - ✓ Particle clusters affect mean drag and mean flow hydrodynamics
  - ➢ Drag reduction is observed in gas-solid flows with clusters compared to uniform particle configurations (fixed assemblies)
- ❑ Future work
  - ➢ Gain better physical understanding of cohesive suspensions using PR-DNS (provide agg./breakage kernels for kinetic/PBE)
  - ➢ Compare cluster statistics with experimental results; tune parameters as necessary to reproduce
  - ➢ Develop a physics-based drag law for particle clusters based on PR-DNS results