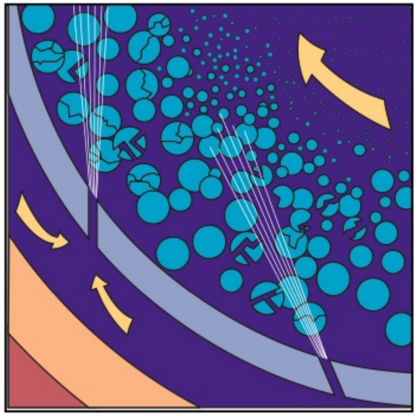
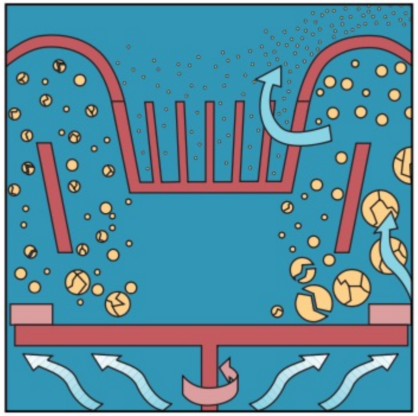
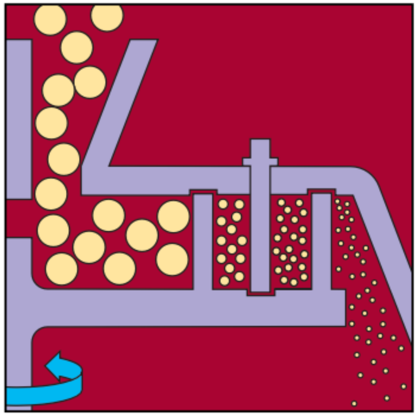
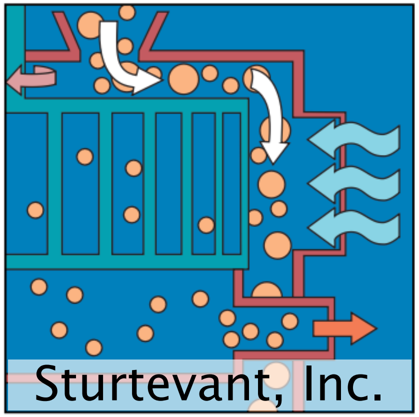
MODELING GAS-PARTICLE TRANSPORT IN MILLS AND CLASSIFIERS (REVIEW)







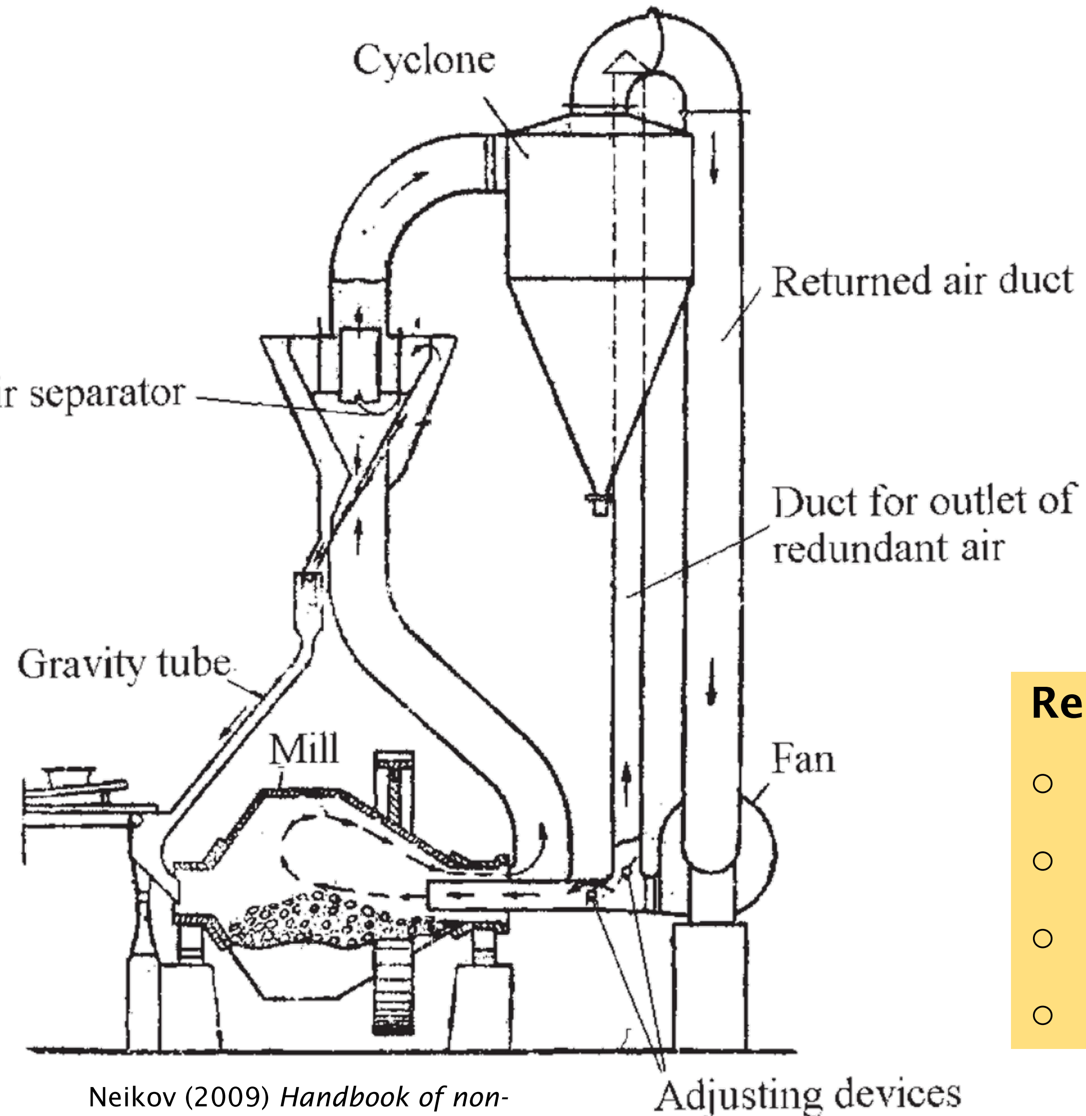


Jesse Capecelatro, University of Michigan

IFPRI 2024 Annual General Meeting

June 15—19, 2024 · Toronto, ON

Pneumatic transport in a representative ball mill



Neikov (2009) *Handbook of non-ferrous metal powders* (pp. 45-62).

Relevant flow phenomena:

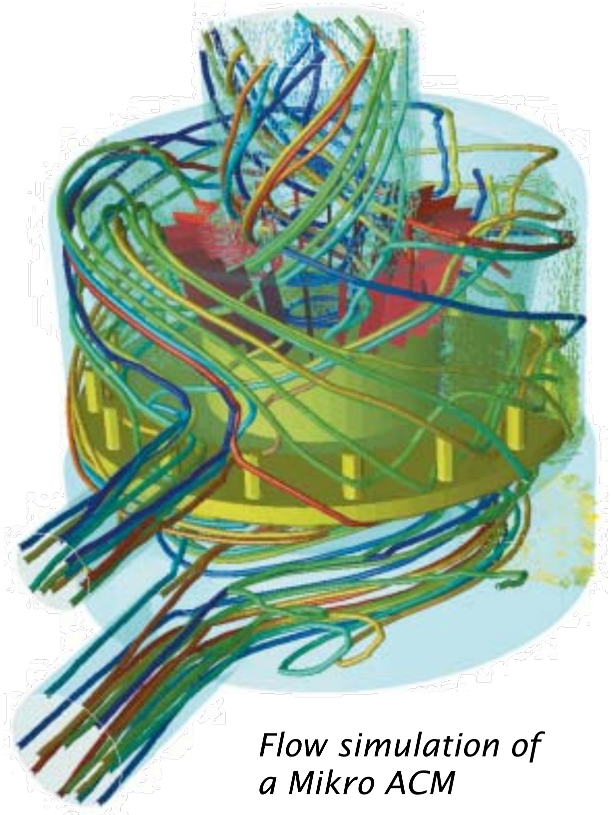
- Flow separation / turbulence
- Particle size segregation
- Preferential concentration
- Deposition/erosion/abrasion

Context & challenges

Complex turbulent two-phase transport of particles in mills and classifiers determines the magnitude and frequency of the breakup of particles and stress exerted on surfaces that determine the overall energy efficiency.

Modeling challenges

- Scales of motion of turbulence
- Varying particle size / shape
- Large number of particles
- Four-way coupling (gas⇄particle + particle ⇄ particle)



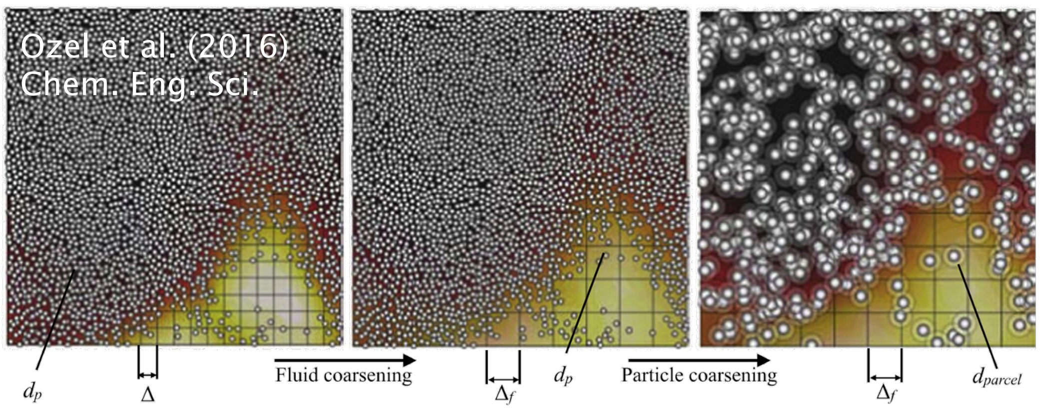
Flow simulation of a Mikro ACM

Modeling approaches (not comprehensive)

High resolution ↕ *Low cost*

- Direct numerical simulation (DNS)
- High-resolution CFD-DEM
- Coarse-grain DEM / MP-PIC (parcels)

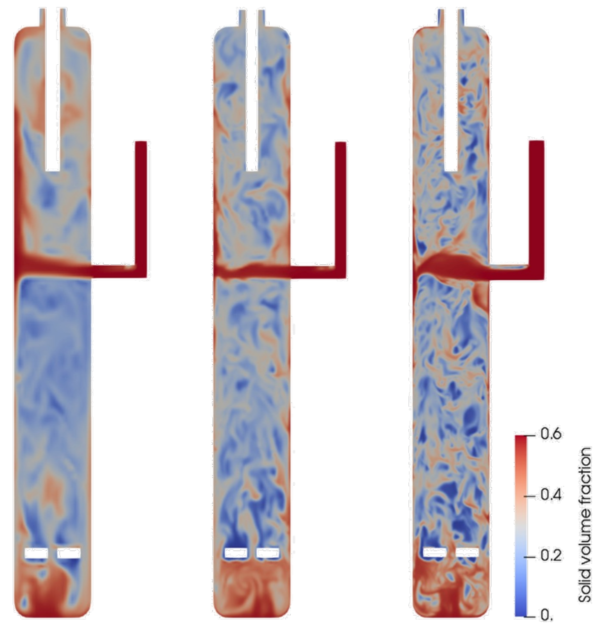
} *Particle (Lagrangian) models*



- Moment methods
- Two-fluid models
- Filtered two-fluid models

} *Continuum (Eulerian) models*

- "Engineering models" (head loss coefficient)



Yu et al. (2020)
Chem. Eng. Sci.

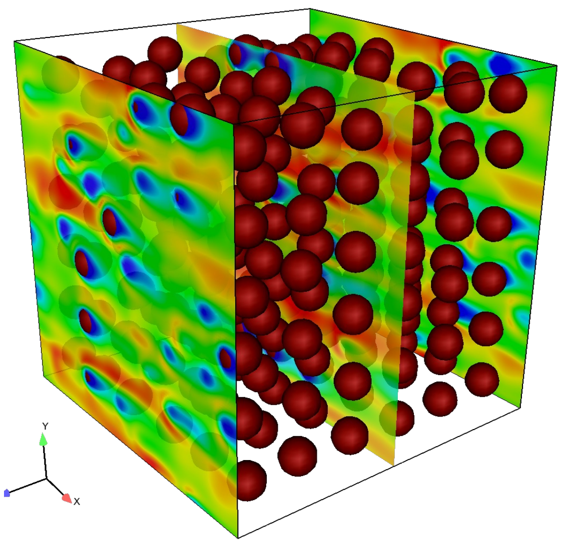
Coarser grids induce loss of local structure representation

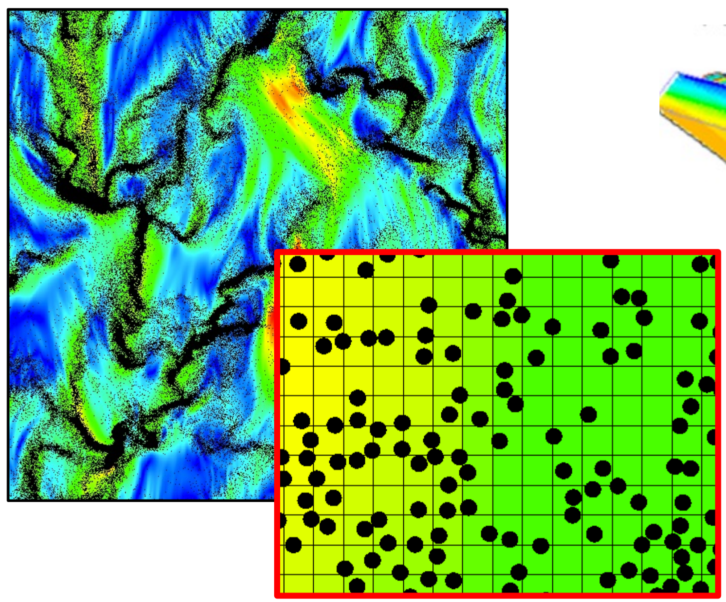
"DNS" ($\Delta x < \eta$) fluid velocity fluctuations are resolved

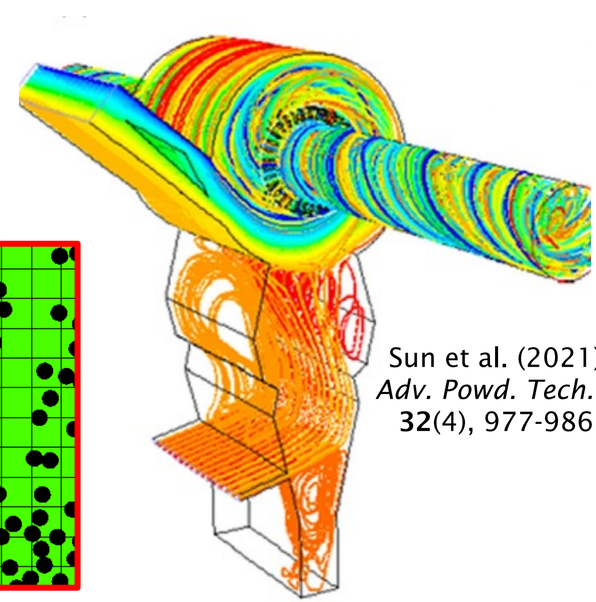
"LES" ($\Delta x > d_p$) fluid velocity resolved at scale larger than particle (need to model drag)

"RANS" ($\Delta x \gg d_p$) average velocity solved (need to reconstruct SGS fluctuations)

Microscale → Mesoscale → Macroscale





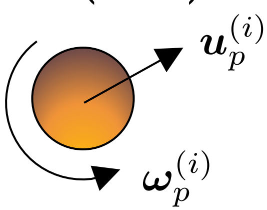


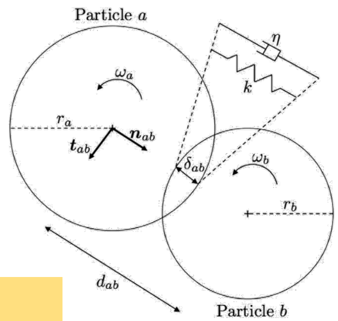
Sun et al. (2021) *Adv. Powd. Tech.*, **32**(4), 977-986.

Particle coarsening

'Fine-grain' CFD-DEM[1]

- Track individual particles w/ models for hydrodynamic forces (e.g., drag) and particle-particle/particle-wall interactions (DEM)



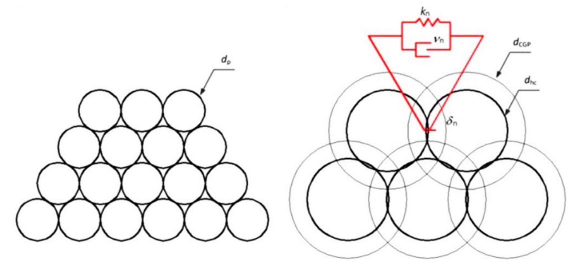


$$m_p \frac{\mathrm{d}\boldsymbol{u}_p^{(i)}}{\mathrm{d}t} = \boldsymbol{F}_{\mathrm{drag}}^{(i)} + \boldsymbol{F}_{\mathrm{col}}^{(i)} + m_p \boldsymbol{g}$$

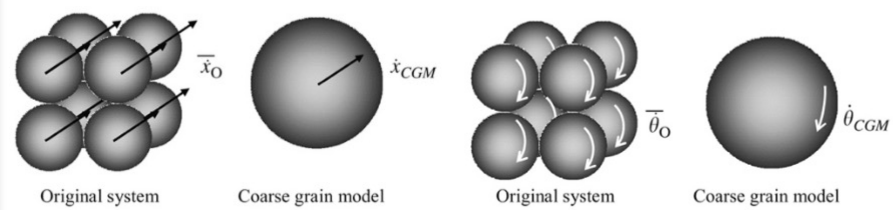
- Transport relies heavily on treatment of hydrodynamic forces
  1. Correct reconstruction of gas velocity
  2. Account for volume fraction (neighbor effects)
- ***Main drawback:*** *Requires tracking every particle in the system!*

Coarse-grained CFD-DEM[2] & MP-PIC[3]

- Track groups of particles (parcels)
- CG-DEM: Handle collisions as larger/softer spheres[4]



- MP-PIC: Collisions computed from particle stress (kinetic theory)
- *Assumes each particle within the parcel has equal properties!*



[1]Tsuji et al. (1993) *Powd. Tech*, **77**(1), 79-87.
[2]Sakai & Koshizuka (2009) *Chem. Eng. Sci.*, **64**(3), 533-539.
[3]Andrews & O'Rourke (1996) *Int. J. Multiphase Flow*, **22**(2), 379-402.
[4]Lu et al. (2014) *Chem. Eng. Sci.*, **120**, 67-87.

Outline of today's talk

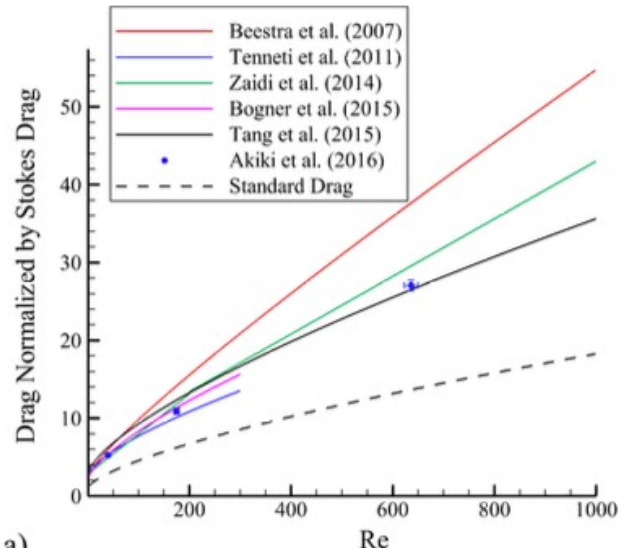
1. **Fluid coarsening**—Coarser grids induce loss of local structure representation
   - Modeling drag in dense suspensions
   - Modeling unresolved turbulence in dilute suspensions
   - Capturing subgrid-scale heterogeneity (clustering)

2. **Particle coarsening**—Reducing the number of particles that must be tracked enables larger system sizes to be simulated and enables larger time steps to extend the process time that can be simulated
   - Coarse graining approaches
   - Applications to mills and classifiers
   - Future directions: filtered CG-DEM

Standard practice in commercial CFD software

Coarsening the grid Δx>d_p requires modeling drag. Typically modeled as a correction to Stokes drag, usually informed from particle-resolved simulations

$$\langle \boldsymbol{F}_D \rangle = 3\pi\mu d_p |\langle \boldsymbol{u} \rangle| \Phi(Re, \varepsilon_p)$$



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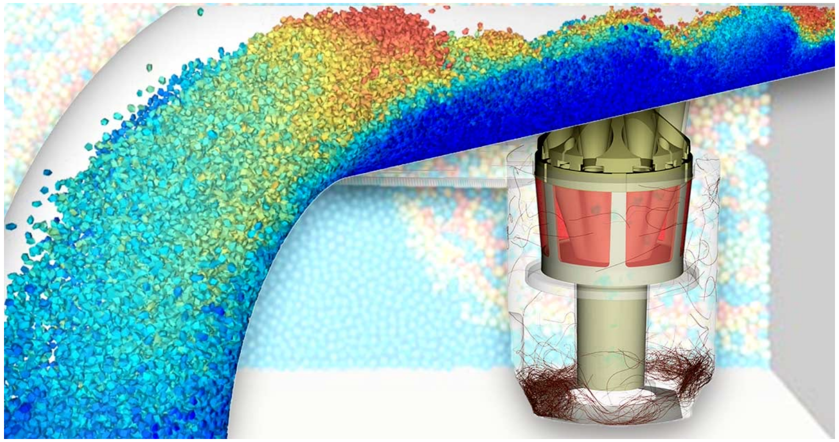

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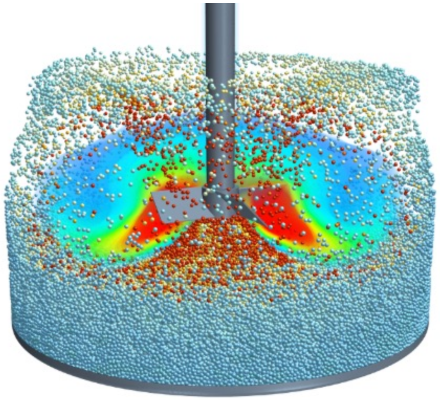

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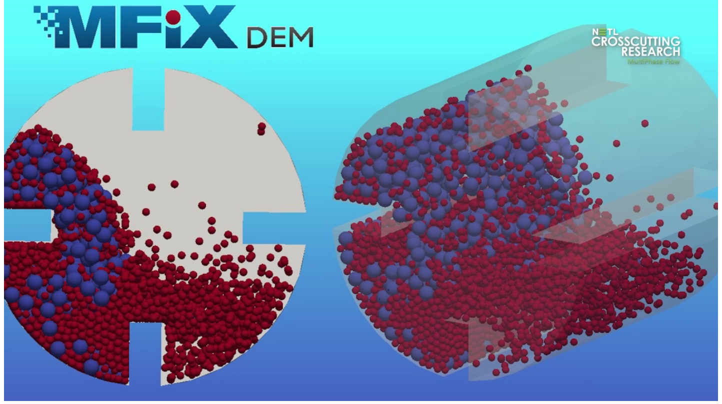
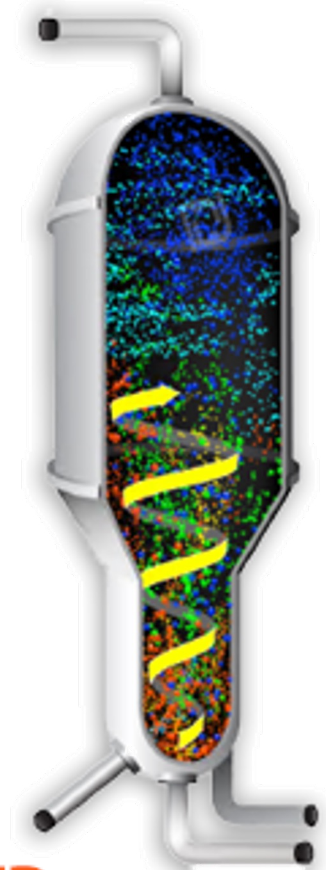




CPFD
Barracuda VR
www.p30download.com

Drag in a dense assembly of particles

It is now well established that a collection of particles exhibit a significant *variation in drag about its mean*.

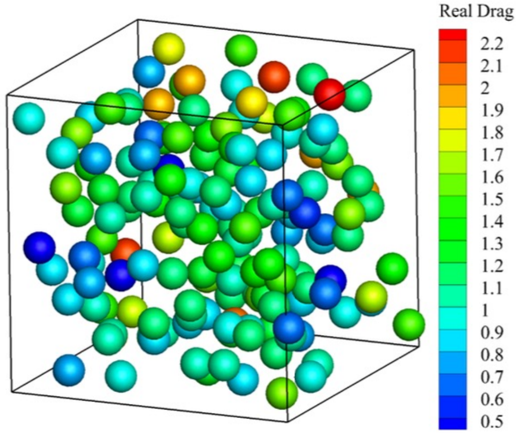
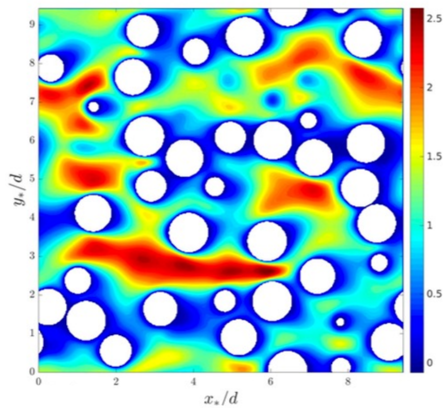
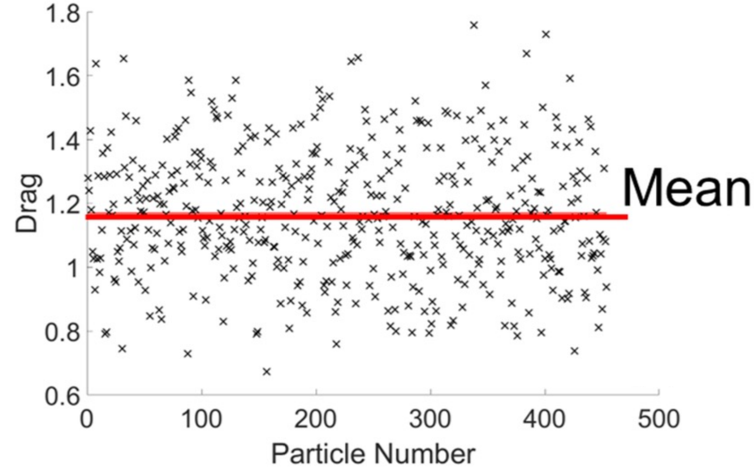
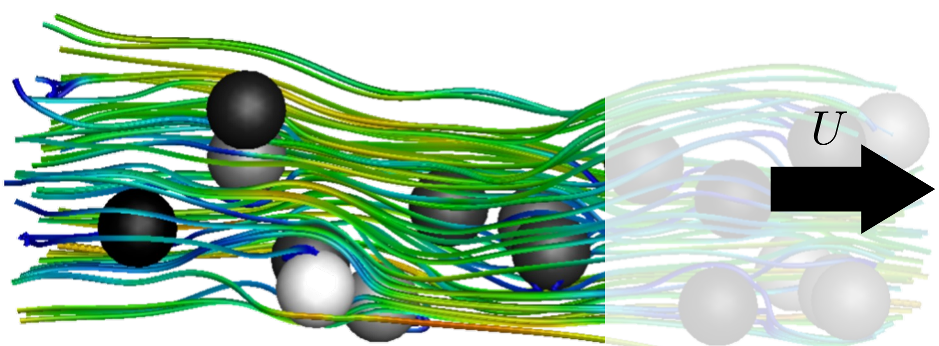


Image via Bala @ UF

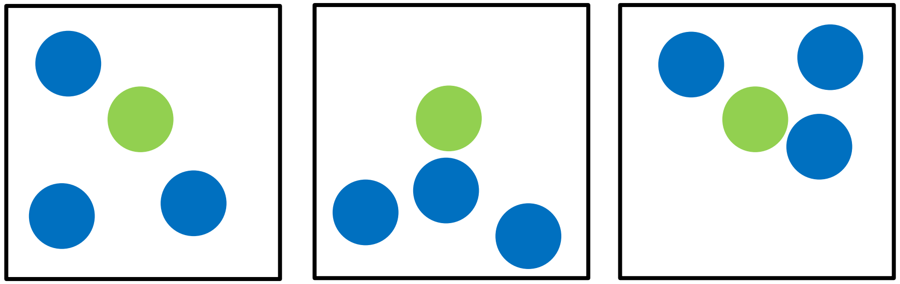




Existing drag laws fail to capture particle *velocity variance* and *dispersion*.



"Neighbor effect"



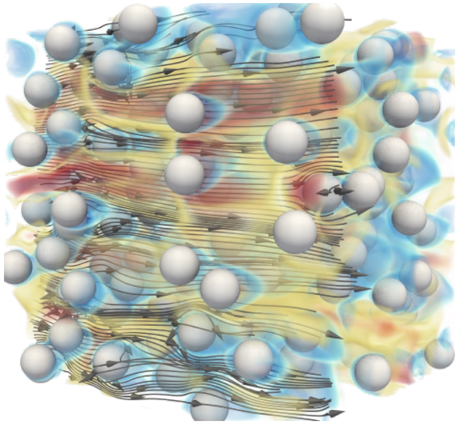
Each case has the same value of Re and ε_p

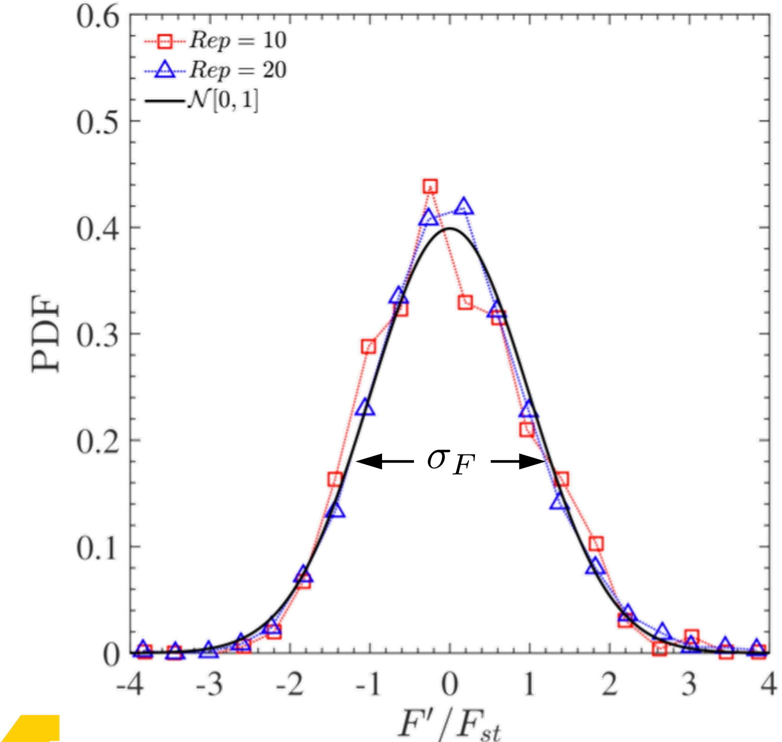
Modeling the drag force stochastically (IFPRI '23 talk)

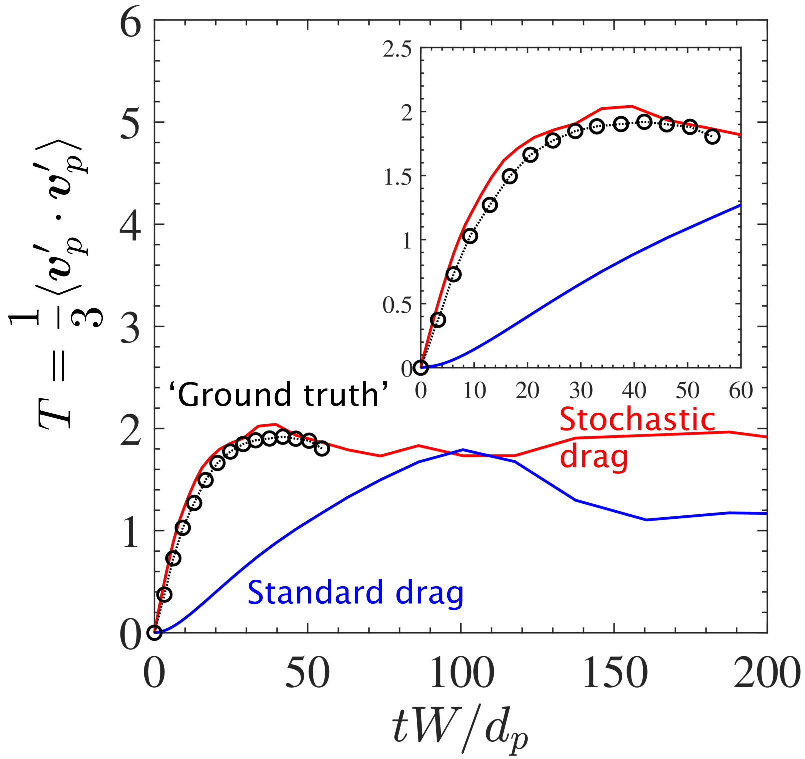
- Do not account for precise neighbor information
- Instead, capture correct *statistics* of residual drag

$$\int \boldsymbol{\tau} \cdot \boldsymbol{n} \mathrm{d}S = \langle \boldsymbol{F}_d \rangle + \boldsymbol{F}_d'' \qquad \langle \boldsymbol{F}_D \rangle = 3\pi\mu d_p |\langle \boldsymbol{u} \rangle| \Phi(Re, \varepsilon_p)$$

$$\mathrm{d}\boldsymbol{F}_{\text{drag}}'' = -\frac{1}{\tau_F} \boldsymbol{F}_{\text{drag}}'' \, \mathrm{d}t + \frac{\sigma_F}{\sqrt{\tau_F}} \mathrm{d}\boldsymbol{W}$$



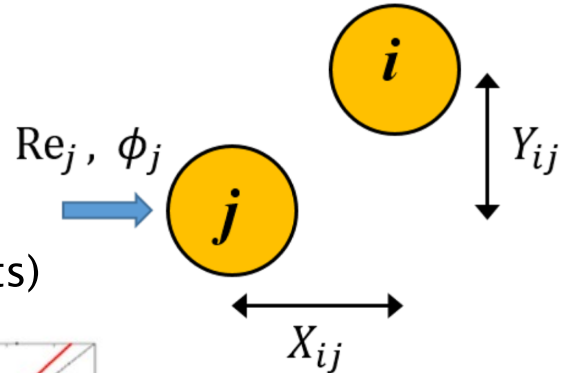




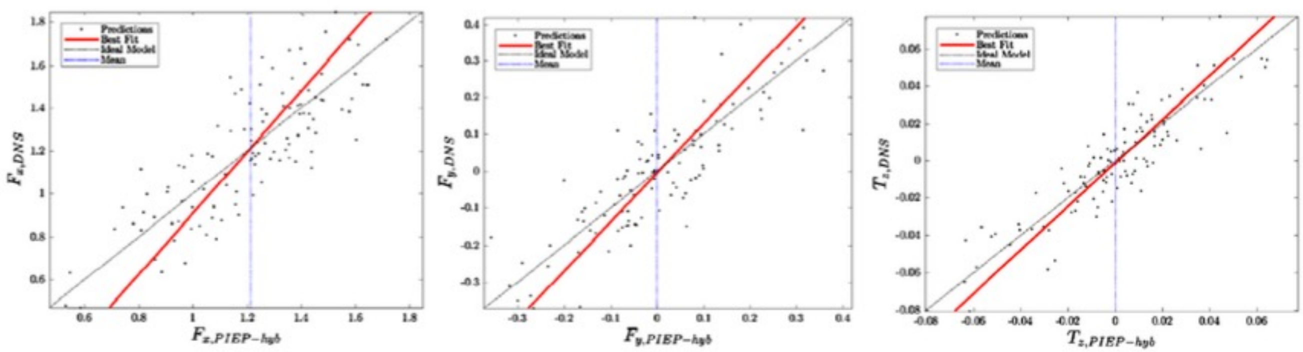
Deterministic approaches to modeling drag

- The force on each particle is deterministically dependent on average (known) quantities: Re, ε_p, and available microscale information
- Example: pairwise interaction extended point particle (PIEP) model[1,2]
- Key idea: assume that the effective flow around a particle can be expressed as a linear superposition of the undisturbed flow and perturbation flow due to each neighboring particle taken one at a time

$$\mathbf{F} \approx \mathcal{F}_{x,0}(Re,\phi)\mathbf{e}_x + \sum_{i=1}^{n}\left[\mathcal{F}_{x,i}(I_i)\,\mathbf{e}_x + \mathcal{F}_i(I_i)\,\hat{\mathbf{r}}_i\right]$$



- Use pre-computed maps or data (regress model coefficients)



Model predictions vs. particle-resolved simulations for Re=40 and ε_p = 0.11

[1]Akiki et al. (2017) *J. Fluid Mech.*, **813**, 882-928.
[2]Moore et al. (2019) *J. Comp. Phys.*, **385**, 187-208.

Example of a machine learning model for the drag force

The hydrodynamic force acting on the i^{th} reference particle considering all the N neighbors can be represented by the following series expansion:

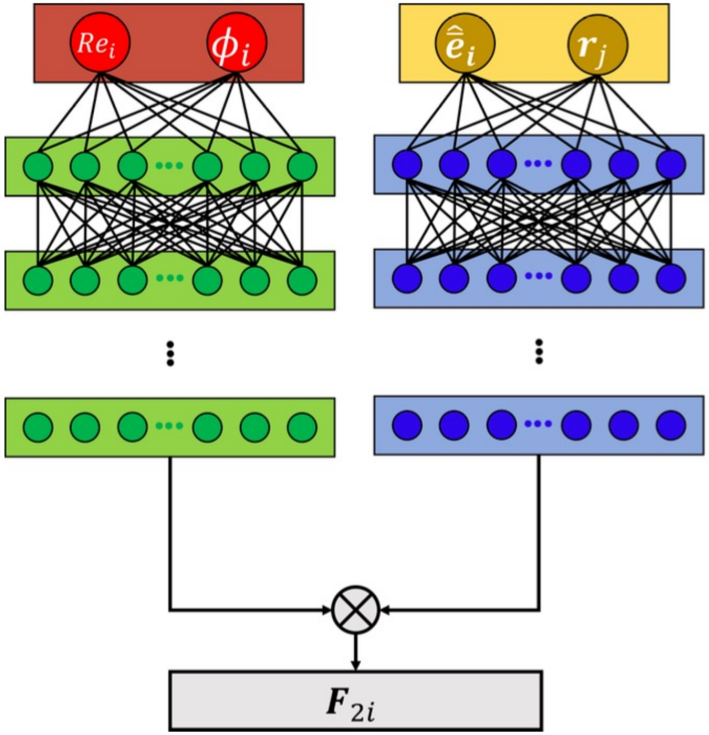
$$\boldsymbol{F}_i(\langle \mathrm{Re} \rangle, \langle \phi \rangle, \{\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N\})$$

$$= \boldsymbol{F}_{1i}(\langle \mathrm{Re} \rangle, \langle \phi \rangle) + \sum_{j=1}^{N} \boldsymbol{F}_{2i}(\langle \mathrm{Re} \rangle, \langle \phi \rangle, \boldsymbol{r}_j) + \sum_{j=1}^{N-1} \sum_{k=j+1}^{N} \boldsymbol{F}_{3i}(\langle \mathrm{Re} \rangle, \langle \phi \rangle, \boldsymbol{r}_j, \boldsymbol{r}_k) + \cdots$$

'Unary term' (effect of neighbors in collective sense)

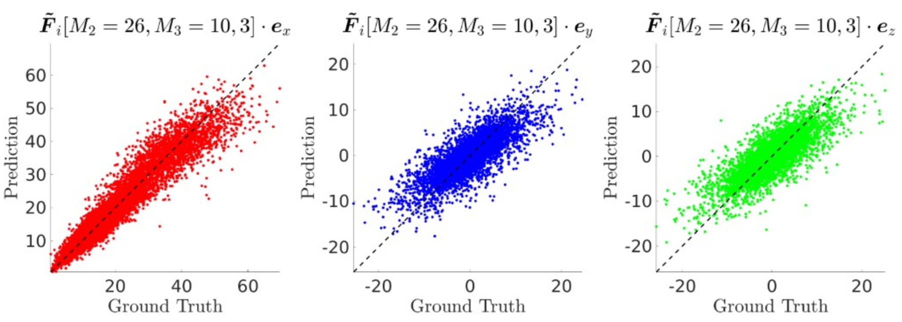
Binary interaction (perturbation due to 1 neighbor at a time)

Trinary interaction (influence of 2 neighbor pairs at a time)



A *sequential learning process*[1] can be used to obtain the binary and trinary terms. Training based on a *force loss function*:

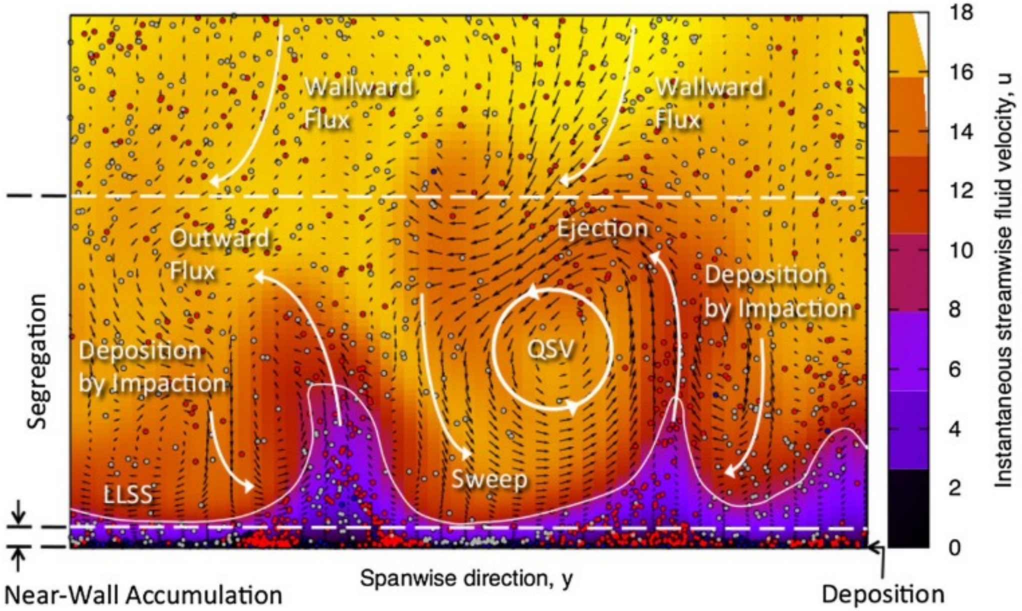
$$\mathcal{L}_{\mathrm{Force}} = \sum_{\mathrm{datasets}} \frac{\sum_{\mathrm{samples}} \frac{|\boldsymbol{F}_{i,\mathrm{PR}} - \boldsymbol{F}_{i,\mathrm{NN}}|^2}{|\langle \boldsymbol{F} \rangle|^2}}{N}$$



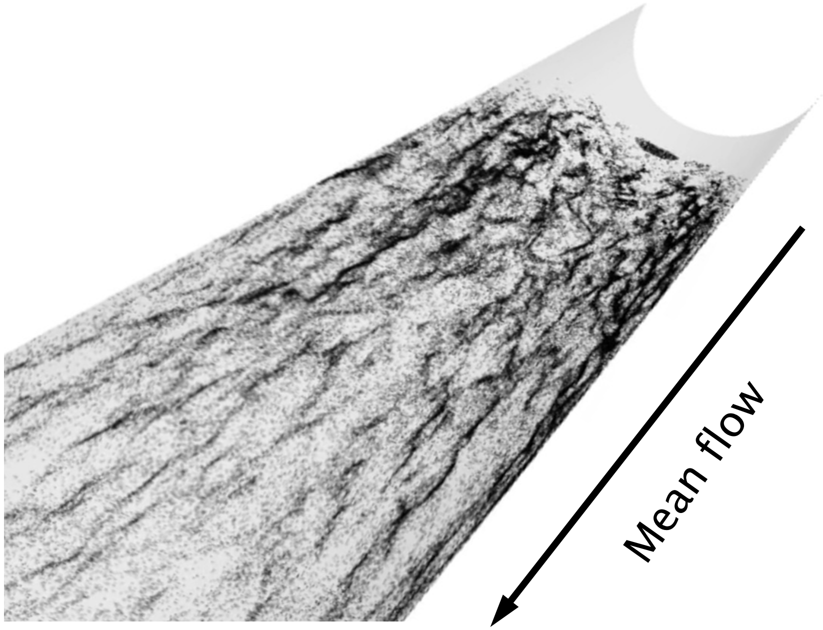
[1]Siddani & Balachandar (2023). Point-particle drag, lift, and torque closure models using machine learning: Hierarchical approach and interpretability. *Physical Review Fluids*, **8**(1), 014303.

Now let's consider dilute suspensions in turbulence

- Particle distribution becomes strongly non-homogeneous in turbulent flows
- Particles sample preferentially the periphery of strong vortical regions and segregate into straining regions
- This has important consequences on deposition and impaction



Transport mechanisms driving concentration build-up in the near-wall region, Soldati & Marchioli (2012) *Advances in Water Resources*, **48**, 18-30.



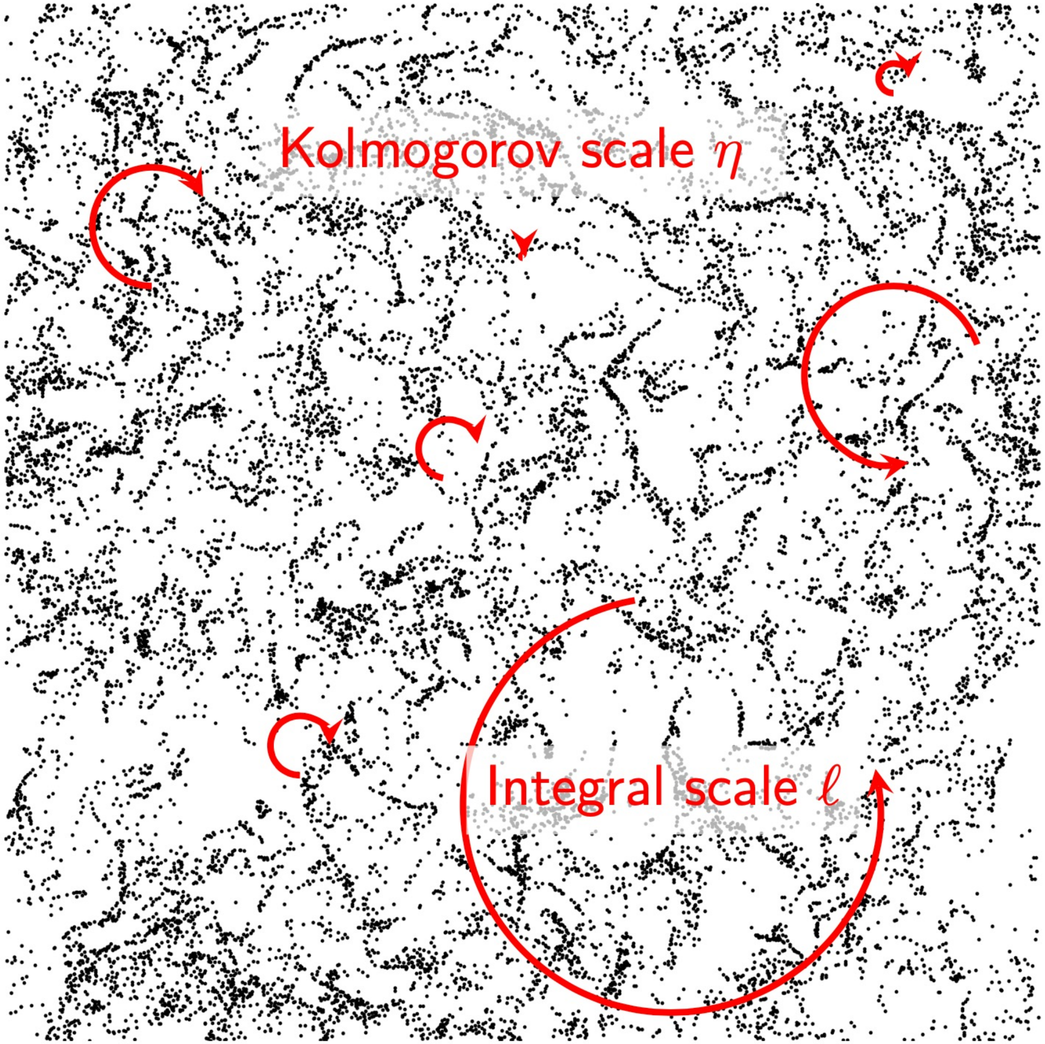
DNS by Yao & Capecelatro (2022) *J. Aerosol Sci.* **166**.

Particles tend to cluster in turbulent flows

- Kolmogorov scales:

  $$\eta = \left(\nu^3/\epsilon\right)^{1/4}, \; \tau_\eta = \sqrt{\nu/\epsilon}$$

- Particle properties:
  - Small: $d_p/\eta \ll 1$
  - Heavy: $\rho_p/\rho_f \gg 1$
  - Dilute: $\langle \varepsilon_p \rangle \ll 1$
- Stokes number: $\mathrm{St}_\eta = \frac{\tau_p}{\tau_\eta}$



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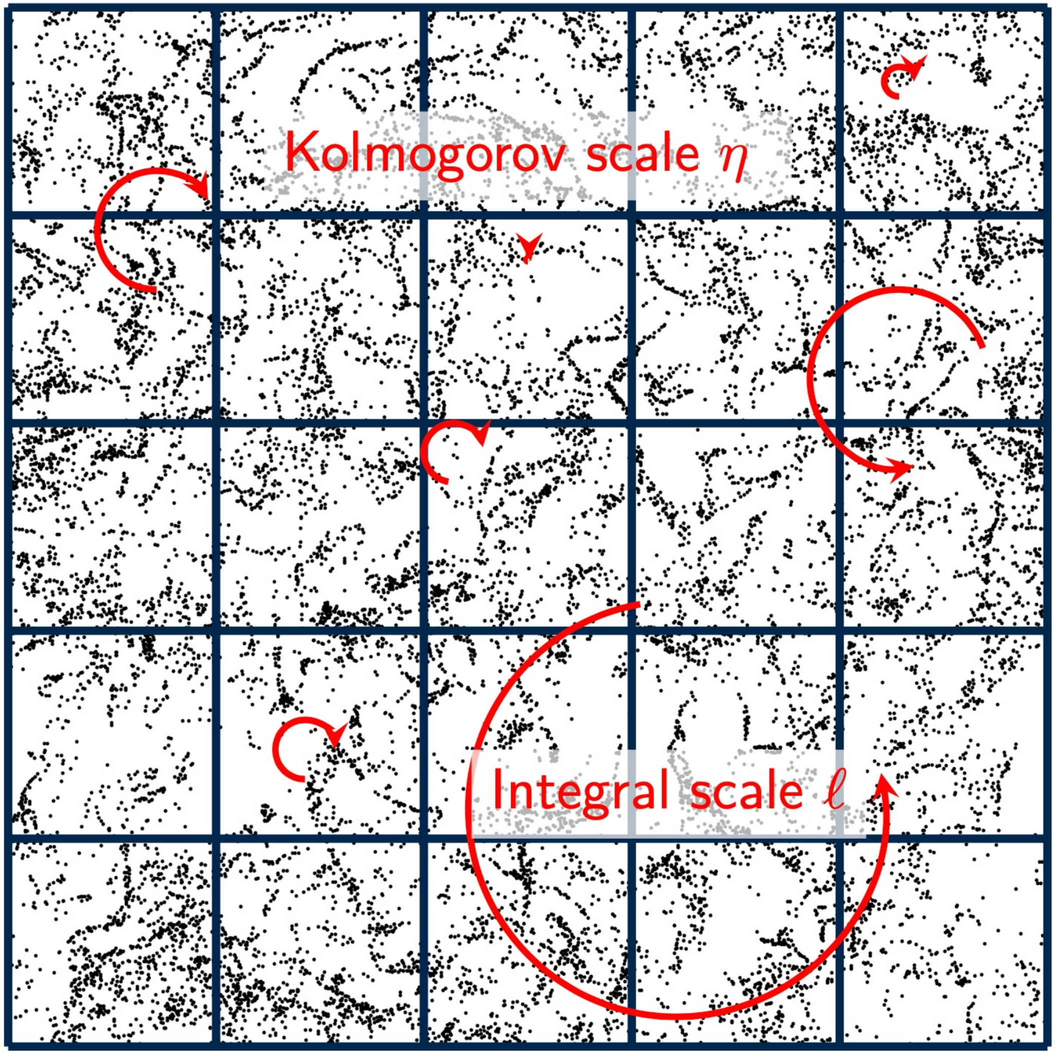
- Stokes number: $\mathrm{St}_\eta = \dfrac{\tau_p}{\tau_\eta}$

- Large-eddy simulation (or RANS):

  $\Delta x > \eta, \; \Delta t > \tau_\eta$

  $\tau_\Delta \sim \left(\Delta x^2/\epsilon\right)^{1/3}$



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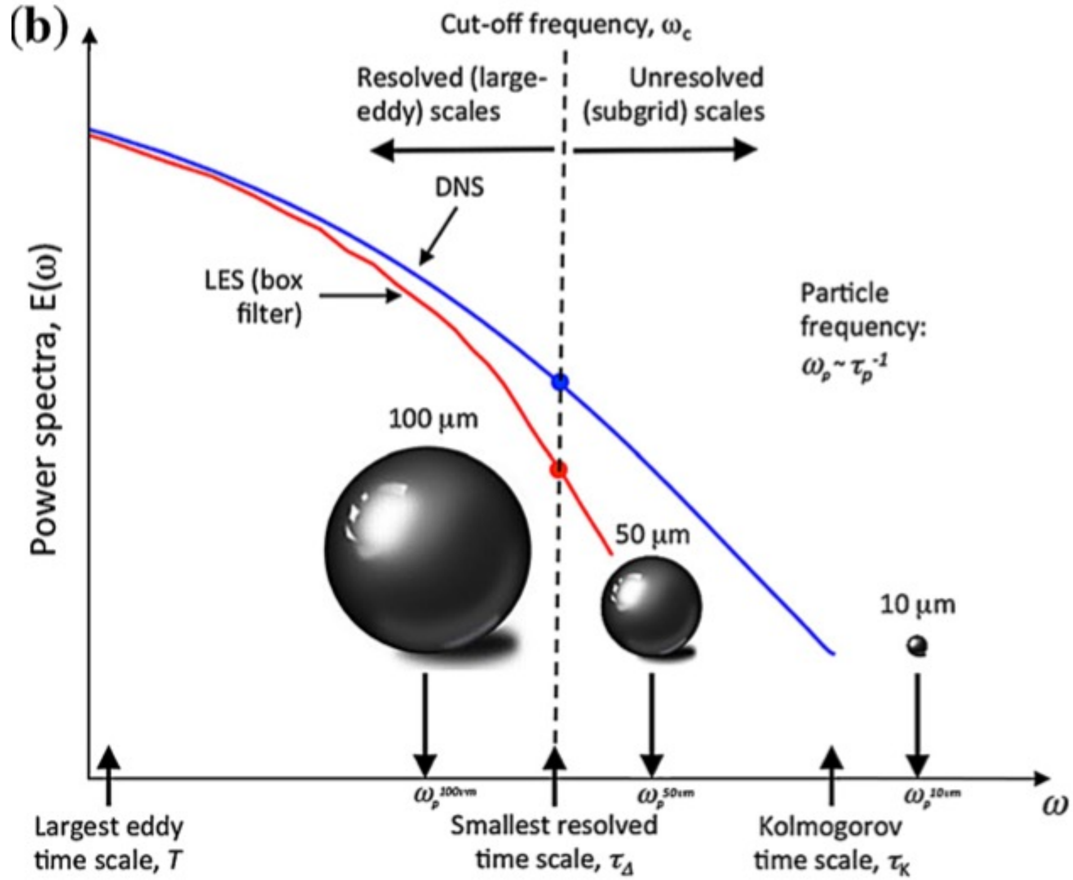


Adapted from Marchioli (2017) *Acta Mechanica*, **228**(3), 741-771.

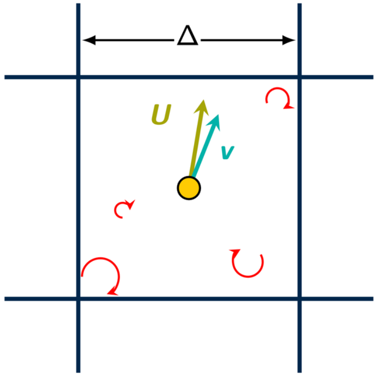
Need to reconstruct subgrid-scale turbulence experienced by particles!

Reconstructing the subgrid-scale ‘velocity seen’

Particle SGS models seek to capture particle kinetic properties *and* preferential concentration determined by the small-scale interaction between particles and turbulence. Requires modeling the **unresolved part of the fluid velocity seen by the particles along their trajectory.**

$$\frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \frac{1}{\tau_p}\left(\boldsymbol{u} - \boldsymbol{v}_p\right), \quad \tau_p = \frac{\rho_p d_p^2}{18\mu}$$

$$\boldsymbol{u} = \overline{\boldsymbol{u}} + \boldsymbol{u}'$$



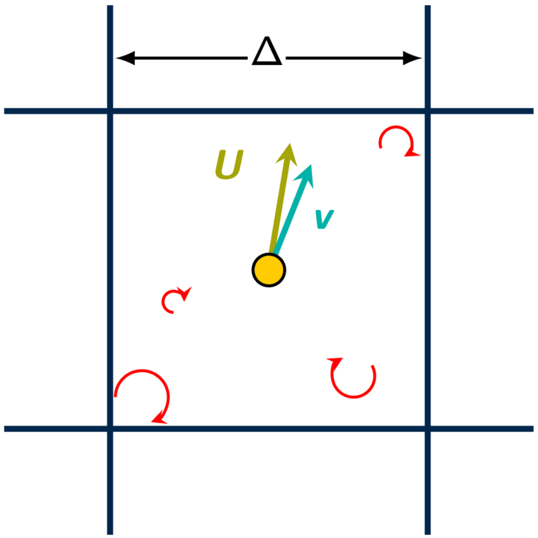
Stochastic Models		Structural Models		
CRW	DRW	ADM	SVS	SOI
Pros • Captures one-point fluid statistics • Insensitive to grid coarsening • Captures correlation in time	**Pros** • Captures one-point fluid statistics • Insensitive to grid coarsening	**Pros** • Low computational cost • No reliance on ad-hoc coefficients, correlations, etc.	**Pros** • Directly constructs spatially heterogeneous velocity field • Captures preferential concentration	**Pros** • Captures SGS velocity field • Works well in combination with ADM
Cons • Unable to capture spatial heterogeneity (e.g., preferential concentration) • Results depend strongly on model timescale	**Cons** • Same cons as CRW • Uncorrelated time increments	**Cons** • Accuracy degrades with grid coarsening • Sensitive to sharp discontinuities (can be unstable)	**Cons** • Computationally expensive • Difficult to use in wall-bounded flows	**Cons** • Reconstructed field may be erroneous • Does not correctly capture clustering for St~1 particles

The continuous random walk model

Random walk models are among the most widely used

$$\frac{\mathrm{d}\boldsymbol{v}_p}{\mathrm{d}t} = \frac{1}{\tau_p}\left(\boldsymbol{u} - \boldsymbol{v}_p\right), \quad \tau_p = \frac{\rho_p d_p^2}{18\mu}$$

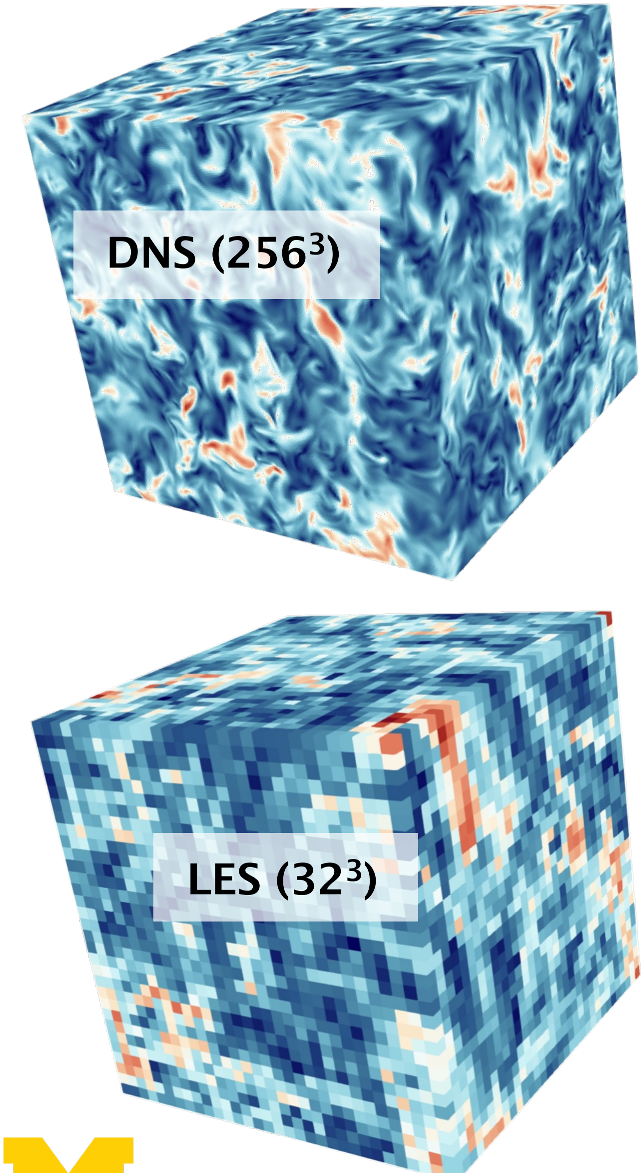
$$\boldsymbol{u} = \overline{\boldsymbol{u}} + \boldsymbol{u}'$$

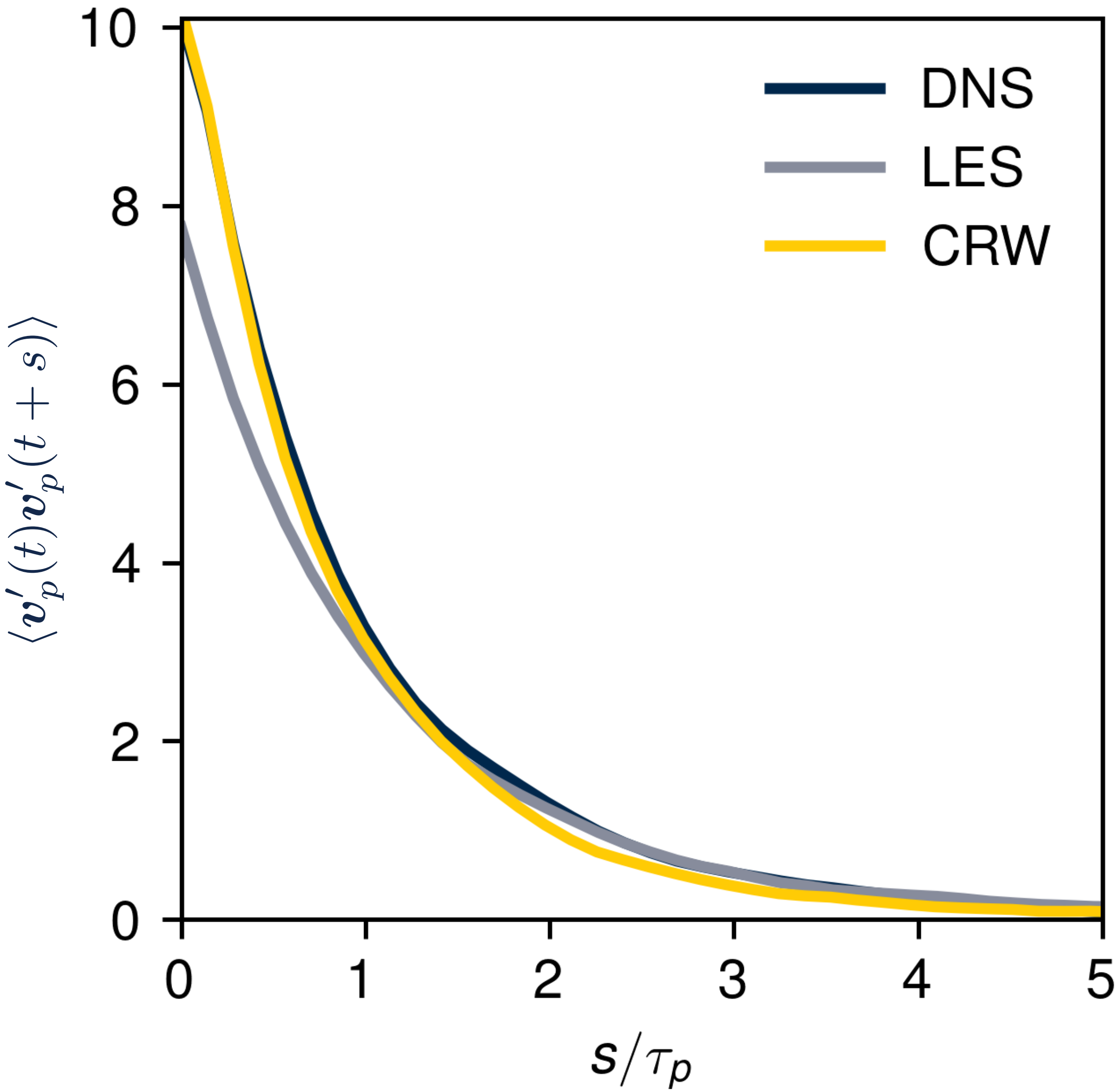


$$\mathrm{d}\boldsymbol{u}' = \underbrace{a(\boldsymbol{x})\boldsymbol{u}\,\mathrm{d}t}_{\text{Drift}} + \underbrace{b(\boldsymbol{x})\,\mathrm{d}\boldsymbol{W}}_{\text{Diffusion}}$$

- Drift: relaxation back to mean, $a(\boldsymbol{x}) = -\tau_{\mathrm{sgs}}^{-1}$
- Diffusion: random forcing, $b(\boldsymbol{x}) = \sqrt{C\epsilon_{\mathrm{sgs}}}$, $\mathrm{d}\boldsymbol{W} \sim \mathcal{N}(0, \sqrt{\Delta t})$

Preferential concentration in homogeneous turbulence





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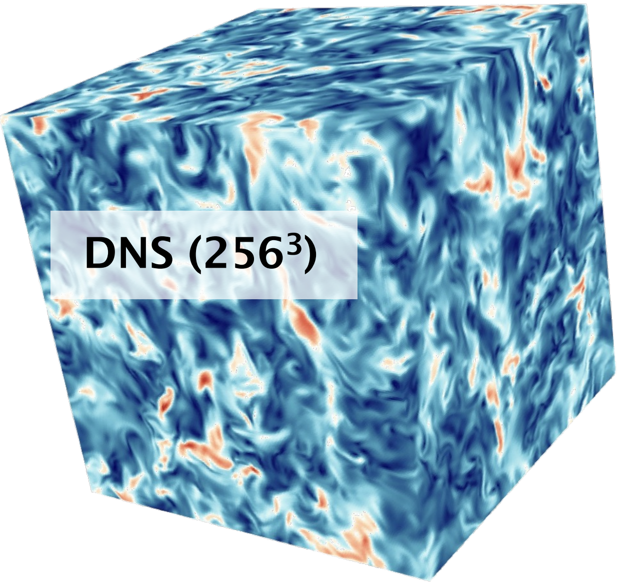
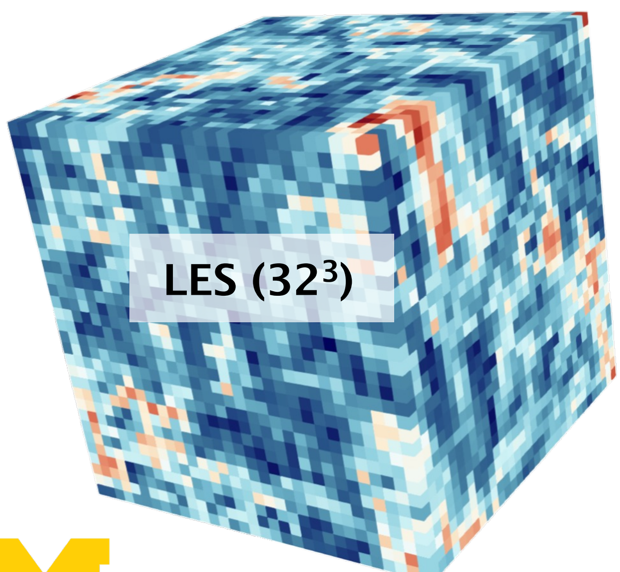
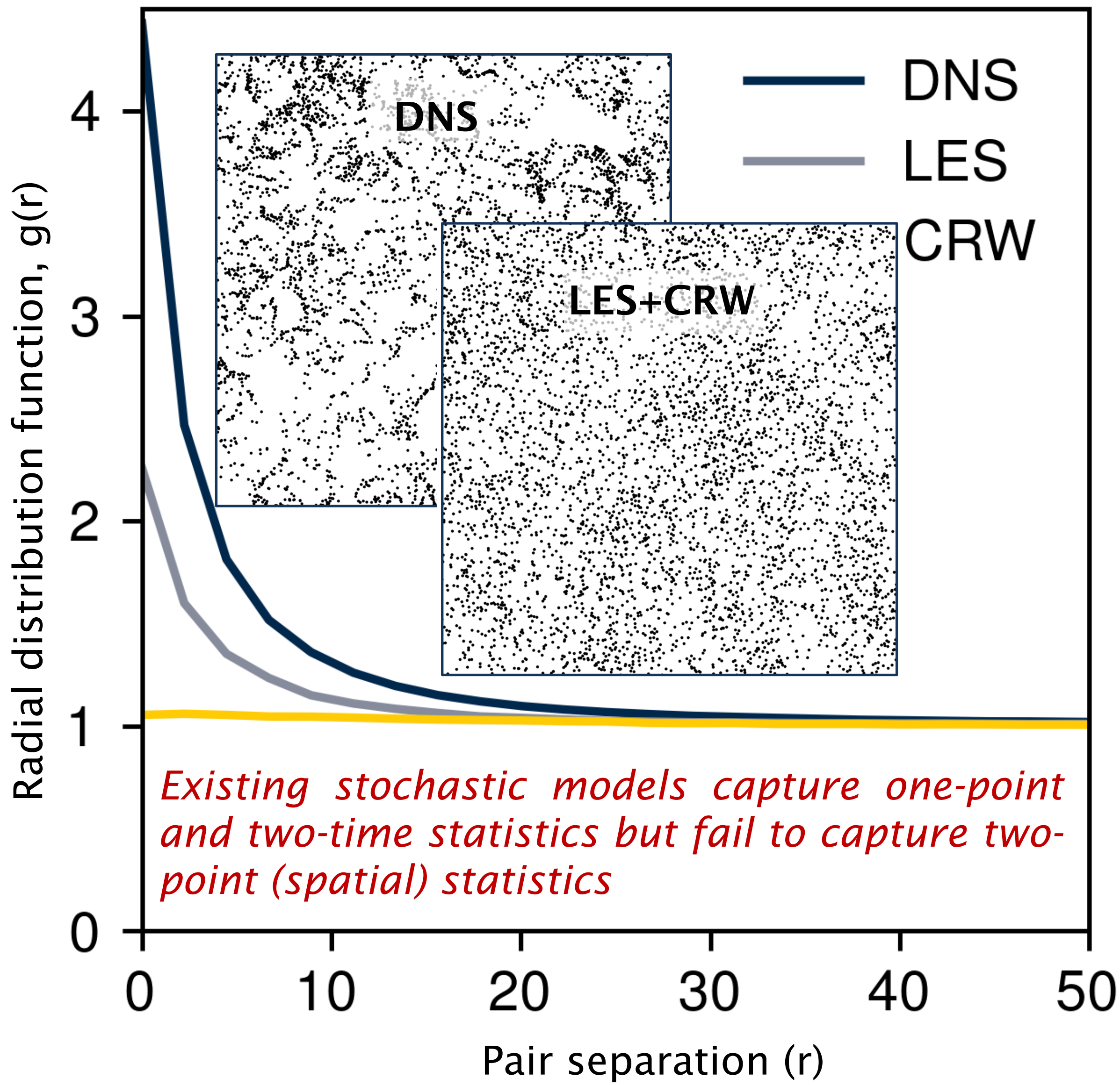




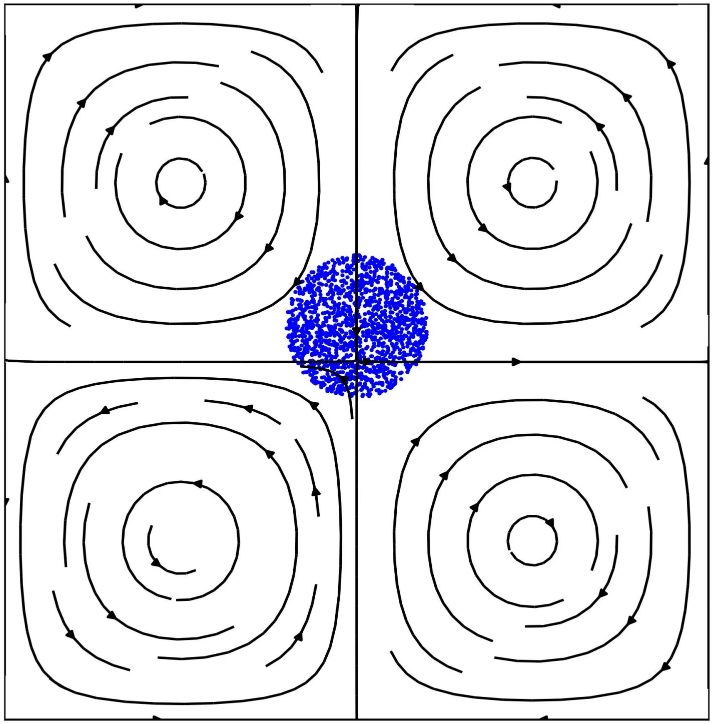


Taylor-Green vortex as a model CFD cell

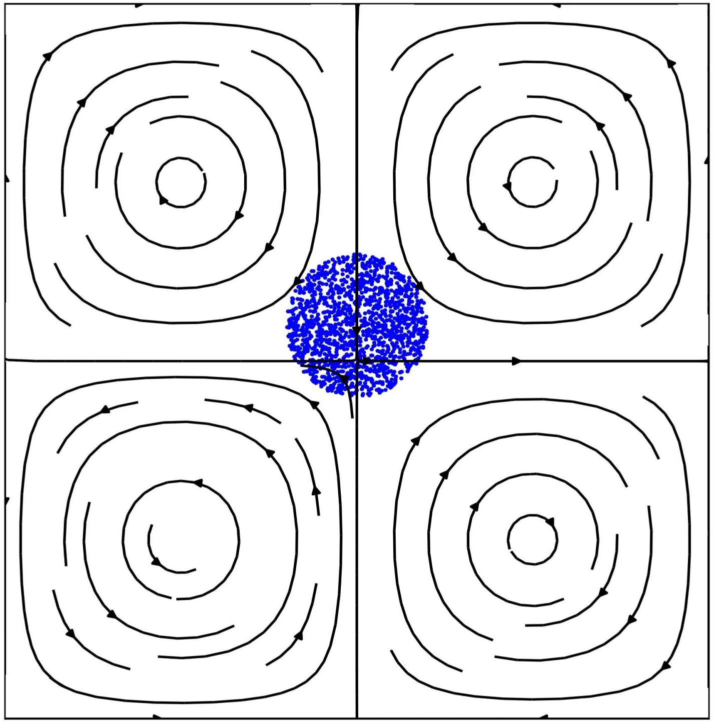
Continuous random walk (CRW) → Homogeneous dispersion!

$$\mathrm{d}\boldsymbol{u} = -\frac{\boldsymbol{u}}{\tau_L} + \sigma_{sg}\sqrt{\frac{2}{\tau_L}}\mathrm{d}\boldsymbol{W} \rightarrow \mathrm{d}\boldsymbol{v}_p = \frac{\boldsymbol{u}-\boldsymbol{v}_p}{\tau_p}\mathrm{d}t \rightarrow \mathrm{d}\boldsymbol{x}_p = \boldsymbol{v}_p\mathrm{d}t$$

Exact solution (using $\boldsymbol{u}$)



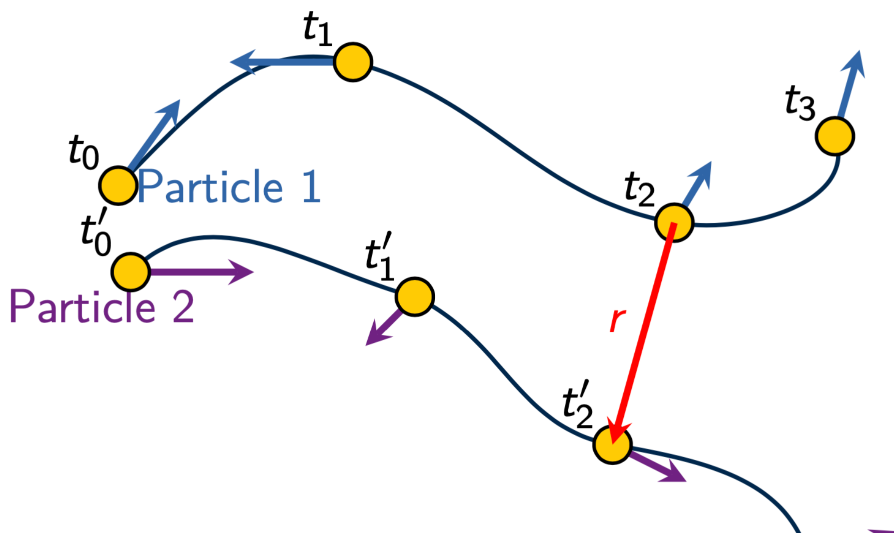
CRW (using one-point info)

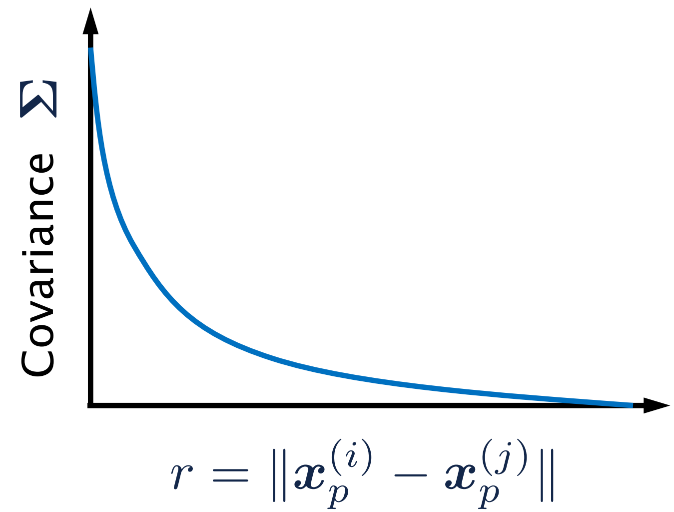


A promising approach to embed spatial information

- How to capture instantaneous spatial distribution in LES/RANS?

$$\mathrm{d}\boldsymbol{u}' = -\boldsymbol{A}\mathrm{d}t + \boldsymbol{B}\cdot\mathrm{d}\boldsymbol{W} \quad \boldsymbol{\Sigma} = \boldsymbol{B}\boldsymbol{B}^T$$





- **Key idea:** leverage what is available
  In each grid cell we know:
  - One-point fluid information (k, ϵ, etc.)
  - Two-point particle information (relative particle positions, velocities, etc.)

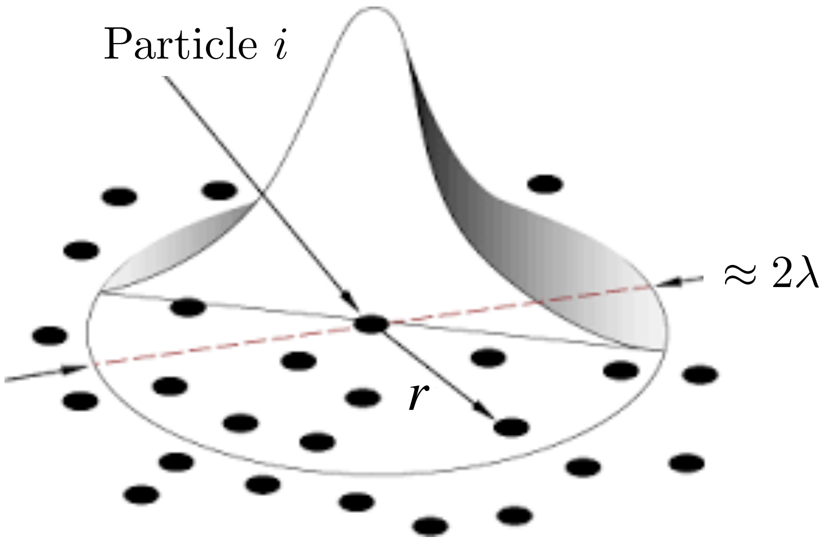
- *Replace white noise with spatially correlated noise*

Towards a two-point Lagrangian stochastic model

- We propose a model of the form:

$$b_j\,\mathrm{d}\boldsymbol{W}_{ij} \approx \widetilde{b\,\mathrm{d}\boldsymbol{W}}_i = \frac{\sum_{j=1}^{N}\rho(r)b_j\mathrm{d}\boldsymbol{W}_j}{\sqrt{\sum_{j=1}^{N}\rho(r)^2}}$$

  - $\rho(r)$: "smoothing kernel" that controls spatial correlation



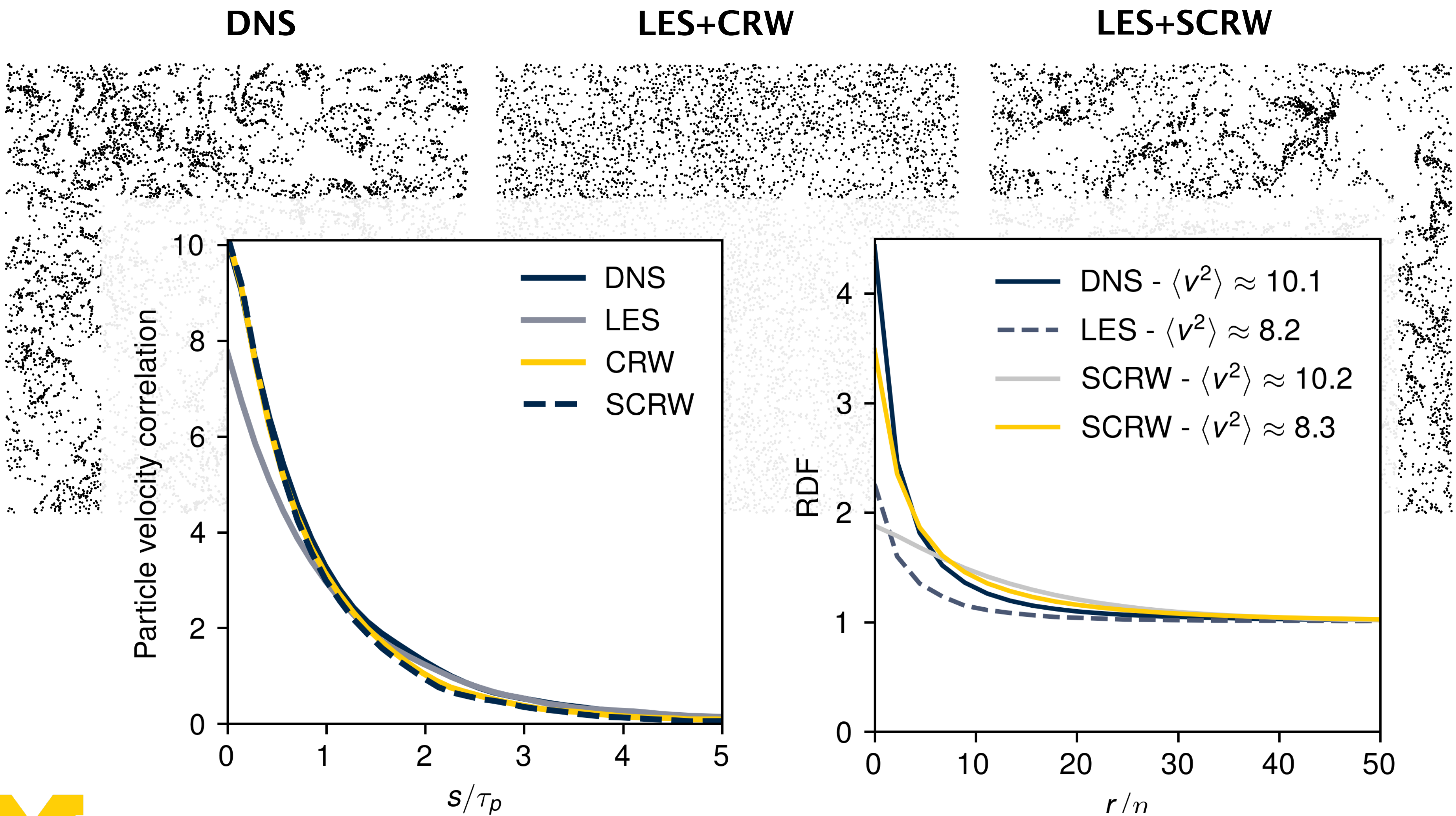
- The spatial structure of velocity fluctuations described by the *structure function*
  - From Kolmogorov's theory the structure function scales like:

$$\langle \Delta u^2 \rangle = \begin{cases} \frac{\langle\epsilon\rangle}{15\nu} r^2 & : r \ll \eta \\ C\left[\langle\epsilon\rangle r\right]^{2/3} & : \eta \ll r \ll \ell \\ 2u_{\mathrm{rms}}^2 & : r > \ell \end{cases}$$

    - Pair separation: $r = |\boldsymbol{x}^{(i)} - \boldsymbol{x}^{(j)}|$
    - Kolmogorov constant: $C \approx 2$

Spatially-correlated random walk

SGS model that captures one-point *and* two-point statistics!



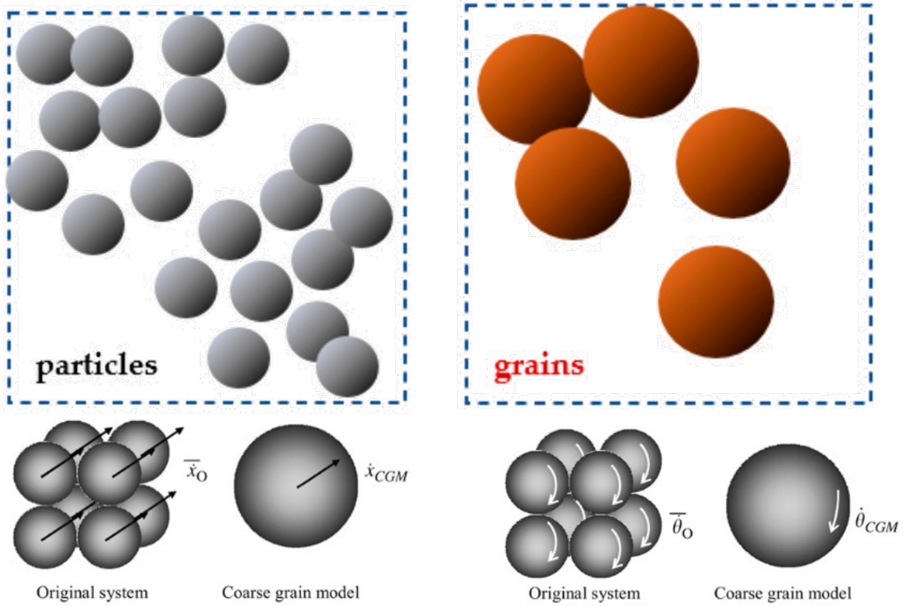
Outline of today's talk

1. **Fluid coarsening**—Coarser grids induce loss of local structure representation
   - Modeling drag in dense suspensions
   - Modeling unresolved turbulence in dilute suspensions
   - Capturing subgrid-scale heterogeneity (clustering)

2. **Particle coarsening**—Reducing the number of particles that must be tracked enables larger system sizes to be simulated and enables larger time steps to extend the process time that can be simulated
   - Coarse graining approaches
   - Applications to mills and classifiers
   - Future directions: filtered CG-DEM

Coarse-grain DEM

- In CG-DEM, several particles are lumped together to form grains (parcels)[1]
  - Coarse-grain factor: $f = d_g/d_p$
  - Coarse-grain number: $n_{CG} = n_p/n_g$
  - Mass is conserved:
    $$\sum_{N_g} m_g = \sum_{N_p} m_p$$

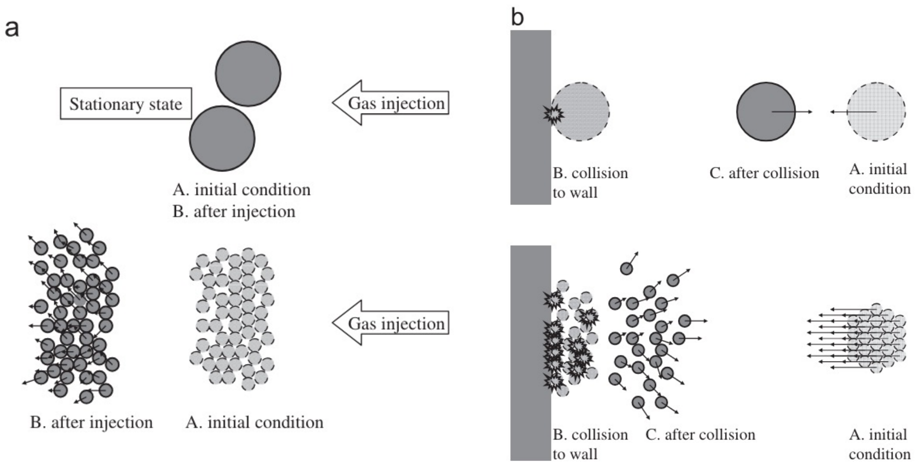


- Equation of motion of each grain:
  $$m_g \frac{\mathrm{d}\boldsymbol{u}_g}{\mathrm{d}t} = \boldsymbol{F}_{g,\mathrm{drag}} + \boldsymbol{F}_{g,\mathrm{col}} + m_g \boldsymbol{g}$$
  - Drag: $\boldsymbol{F}_{g,\mathrm{drag}} = n_{CG} \boldsymbol{F}_{p,\mathrm{drag}}$
  - Coefficient of restitution: $\frac{\ln e_g}{\ln e_p} = \sqrt{n_{CG}} \frac{\sqrt{1 - \frac{(\ln e_p)^2}{(\ln e_p)^2 + \pi^2}}}{\sqrt{1 - \frac{n_{CG}(\ln e_p)^2}{(\ln e_p)^2 + \pi^2}}}$
  - Spring and damper: $k = m_{ij} \frac{\pi^2 + (\ln e_g)^2}{\tau_c^2}$; $\eta = -2\ln(e_g) \frac{\sqrt{m_{ij} k}}{\pi^2 + (\ln e_g)^2}$
  - Sliding friction: $\mu_g = \frac{\mu_p}{\sqrt{f}}$

[1]Di Renzo et al. (2021) Coarse-grain DEM modelling in fluidized bed simulation: A review. *Processes*, **9**(2), 279.

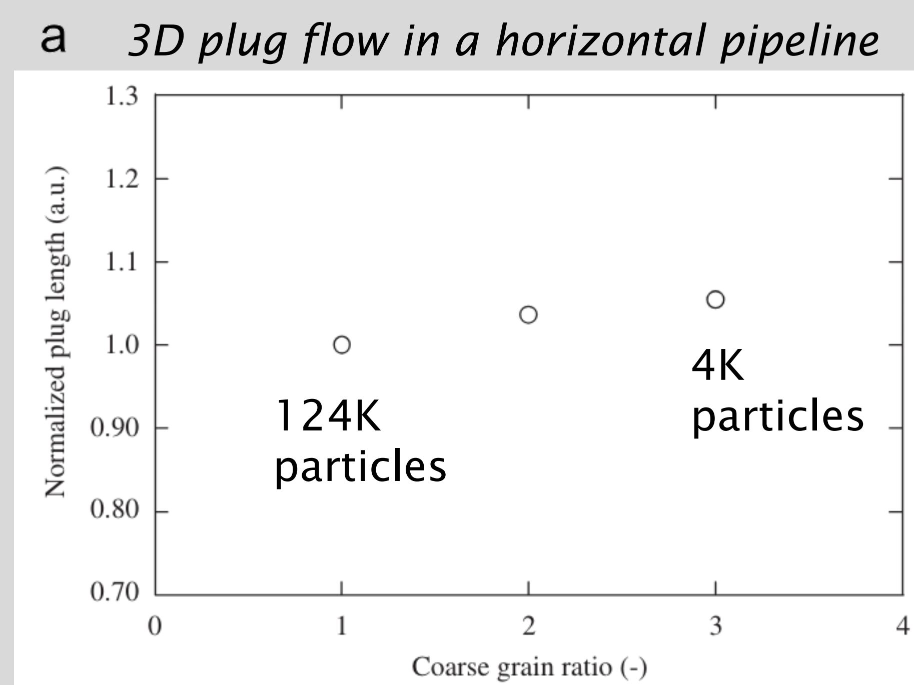
Coarse grain DEM applied to a horizontal pipeline

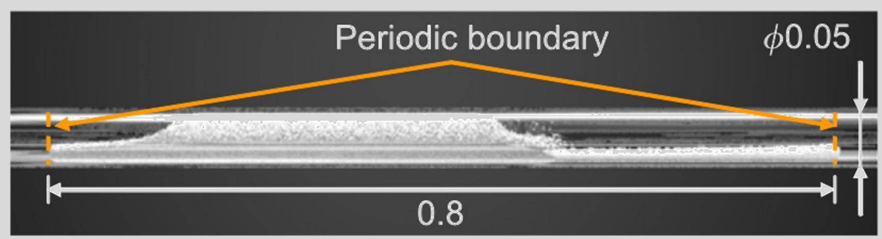
- CG-DEM: Cannot simply replace small particles with fewer large ones



- The contact force is modeled under the assumption that the kinetic energy of a coarse grain particle agrees with that of a group of the original particles

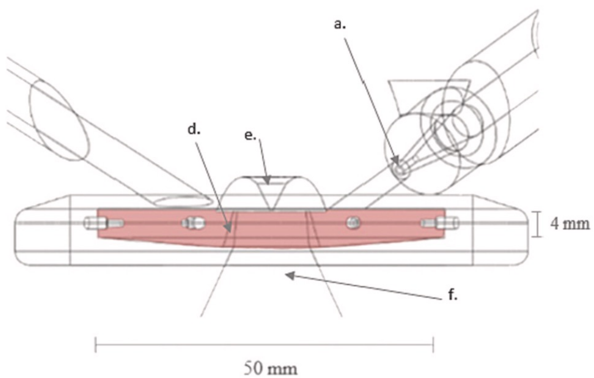
- Drag is modeled by balancing the coarse grain particle and the group of the original particles

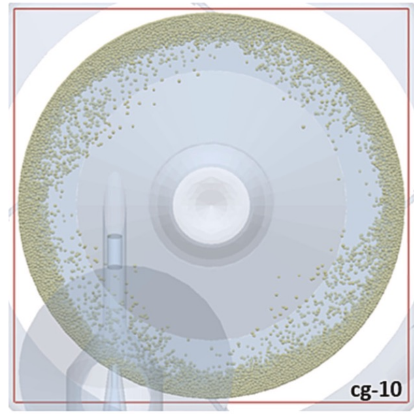


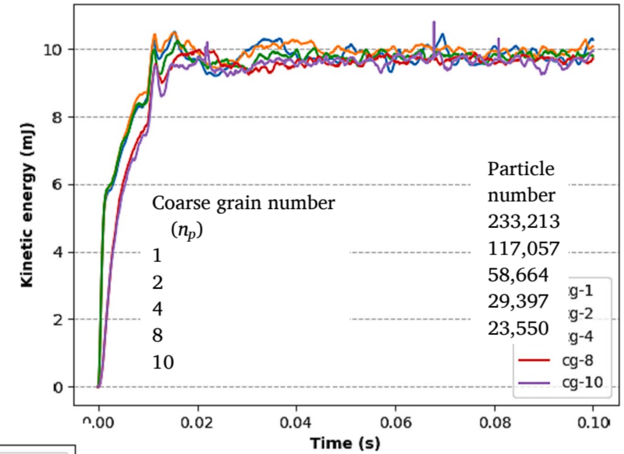


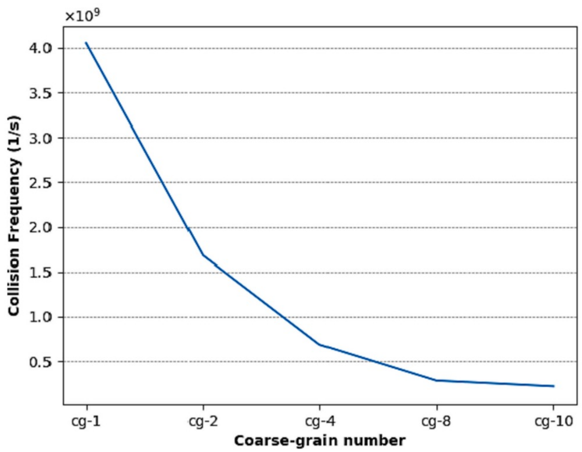
Sakai, M., & Koshizuka, S. (2009). Large-scale discrete element modeling in pneumatic conveying. *Chemical Engineering Science*, **64**(3), 533-539.

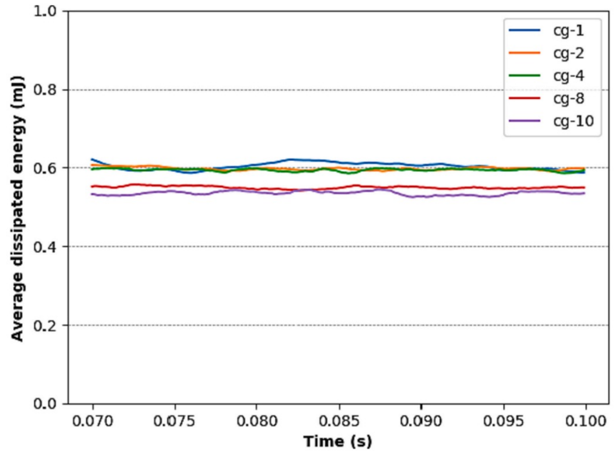
Coarse grain DEM applied to a spiral jet mill











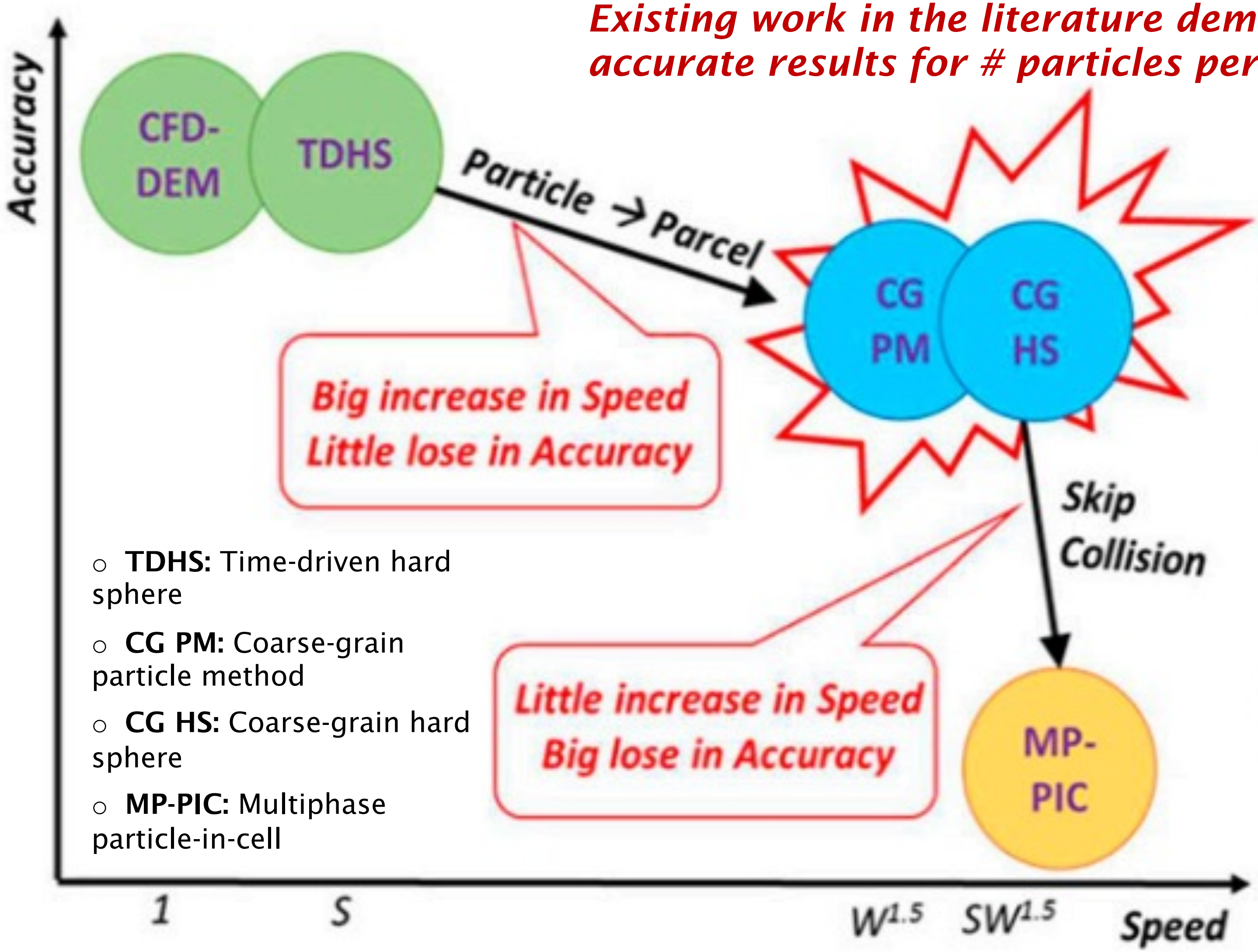
CG number	# particles
1	233,213
2	117,057
4	58,664
8	29,397
10	23,550

- *"As the particle number is reduced 2-fold and 4-fold, respectively, and interparticle collision rate is reduced 60% each time"*
- Increasing the CG number beyond 4 further led to a decrease in the average rate of dissipated energy for each particle system

Scott et al. (2022). Application of coarse-graining for large scale simulation of fluid and particle motion in spiral jet mill by CFD-DEM. *Powder Technology*, **411**, 117962.

Assessment of discrete particle methods for fluidized beds

Existing work in the literature demonstrates accurate results for # particles per parcel < 10



- **TDHS:** Time-driven hard sphere
- **CG PM:** Coarse-grain particle method
- **CG HS:** Coarse-grain hard sphere
- **MP-PIC:** Multiphase particle-in-cell

Lu et al. (2017) *Ind. & Eng. Chem. Research*, **56**(27), 7865-7876.

Eulerian-based two-fluid models

- Avoid cost of tracking individual particles by solving hydrodynamic equations for each phase:

$$\frac{\partial}{\partial t}\left(\rho_f\, \alpha_f\right) + \nabla.\left(\rho_f\, \alpha_f\, \vec{v_f}\right) = 0$$

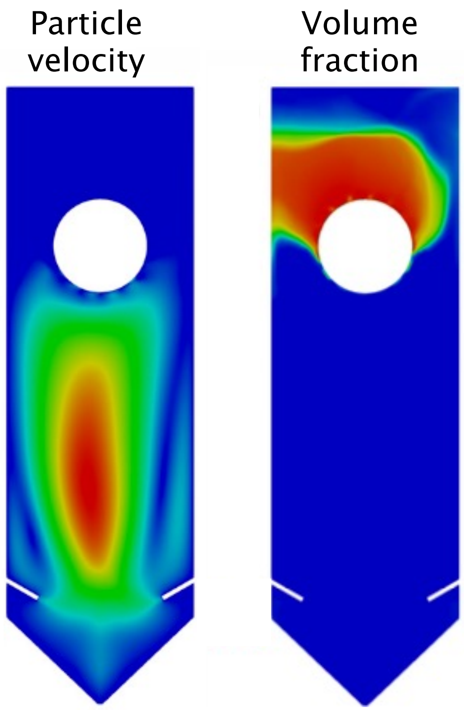
$$\frac{\partial}{\partial t}\left(\rho_s\, \alpha_s\right) + \nabla.\left(\rho_s\, \alpha_s\, \vec{v_s}\right) = 0$$

$$\frac{\partial}{\partial t}\left(\alpha_f\, \rho_f\, \vec{v_f}\right) + \nabla.\left(\alpha_f\, \rho_f\, \vec{v_f}\ \vec{v_f}\right) = -\alpha_f\, \nabla p + \nabla.\bar{\bar{\tau}}_f + \alpha_f\, \rho_f\, \vec{g} + \left[\beta\left(\vec{v_s} - \vec{v_f}\right)\right]$$

$$\frac{\partial}{\partial t}\left(\alpha_s\, \rho_s\, \vec{v_s}\right) + \nabla.\left(\alpha_s\, \rho_s\, \vec{v_s}\ \vec{v_s}\right) = -\alpha_s\, \nabla p - \nabla p_s + \nabla.\bar{\bar{\tau}}_s + \alpha_s\, \rho_s\, \vec{g} + \left[\beta\left(\vec{v_f} - \vec{v_s}\right)\right]$$

- Solid-phase constitutive equations (e.g., granular viscosity) from kinetic theory of granular flow
- Assumes highly collisional + no trajectory crossing (can alleviate these assumptions by solving for higher order moments)
- Commonly applied to fluidized bed reactors, less common for mills/classifiers (limited validation data)
- Capturing size segregation and particle breakage less straight forward compared to Lagrangian approaches

Fluidized bed opposed gas jet mill (RANS+TFM)



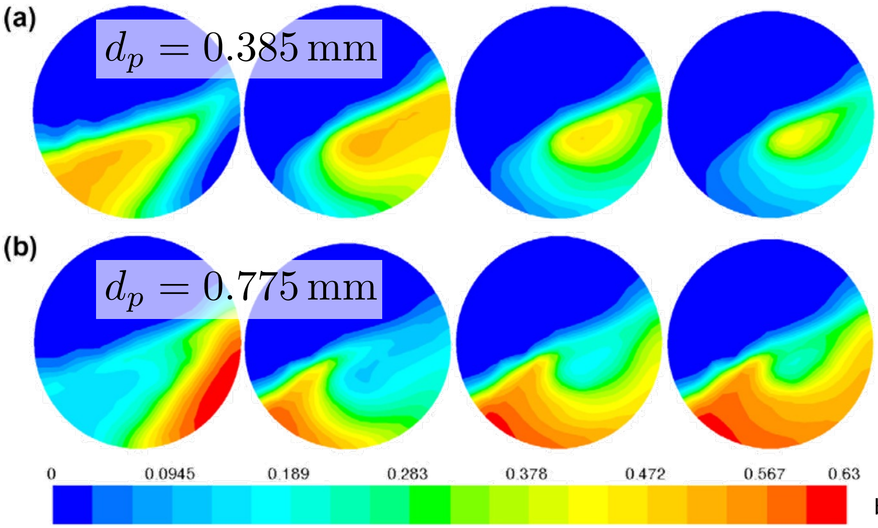
Araújo dos Santos et al. (2020) Eulerian multiphase simulation of the particle dynamics in a fluidized bed opposed gas jet mill. *Processes*, **8**(12), 1621.

Capturing size segregation using Eulerian models

- Directly extending the two-fluid model to polydisperse flows requires binning the size distribution and solving equations for each bin (very expensive)
- Example: particle segregation in a rotating drum[1]
- 3 continuum phases are considered: solids phase 1, solids phase 2, and gas phase. The solids pressure consists of a kinetic term and a collision term:

$$p_{si} = \alpha_{si}\rho_{si}\theta_{si} + 2\frac{d_{sjsi}^3}{d_{si}^3}(1+e_{sjsi})\alpha_{si}\alpha_{sj}\rho_{si}g_{0,sjsi}\theta_{si} \qquad \alpha_g + \sum_{i=1}^{2}\alpha_{si} = 1$$

- Size-induced particle segregation in a 20 RPM rotating drum[1]



Volume fraction of small & large particles

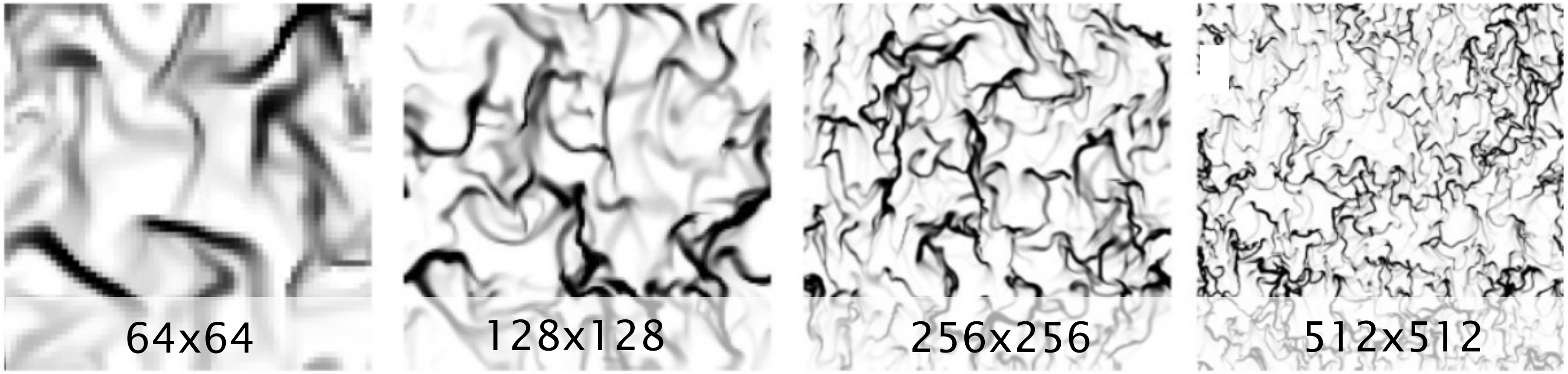
Challenges with Eulerian models:

- Expensive to bin each size class
- One value of velocity in each cell (cannot capture trajectory crossing)
- **Promising approach:** CFD+population balance equation using moment method closure to track *moments* of the distribution function[2]

[1] Huang et al. (2013) Numerical studies of particle segregation in a rotating drum based on Eulerian continuum approach. *Advanced Powder Technology*, **24**(1), 364-372.
[2] Marchisio & Fox (2013) *Computational models for polydisperse particulate and multiphase systems*. Cambridge University Press

Filtered two-fluid models

- Performing simulations with $\Delta x \gg d_p$ results in subgrid-scale heterogeneity
- Two-fluid models assume one value of velocity, volume fraction, etc. per grid cell!
- Filtering the two-fluid equations reveals need for sub-filter closure (e.g., drag)[1]



- Applying a low pass filter to the solids momentum equation:

$$\left[\frac{\partial(\rho_s\bar{\phi}_s\bar{\mathbf{v}})}{\partial t} + \nabla\cdot(\rho_s\bar{\phi}_s\bar{\mathbf{v}}\bar{\mathbf{v}})\right] = -\nabla\cdot\Sigma_s - \bar{\phi}\nabla\cdot\bar{\boldsymbol{\sigma}}_g + \bar{\mathbf{F}} + \rho_s\bar{\phi}_s\mathbf{g}$$

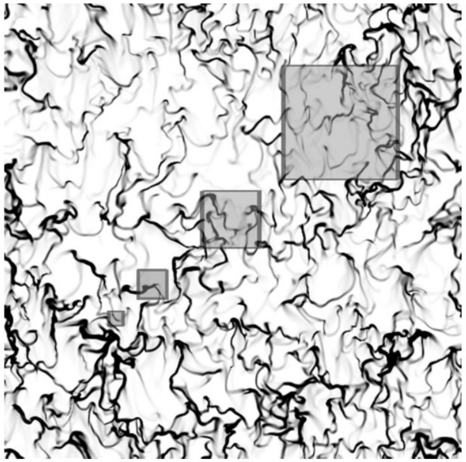
- Filtered drag: $\overline{\boldsymbol{F}} = \overline{\beta\left(\boldsymbol{u}_g - \boldsymbol{v}_p\right)} = \beta^*\left(\overline{\boldsymbol{u}}_g - \overline{\boldsymbol{v}}_p\right) \rightarrow \beta^* = \dfrac{\overline{\beta\left(\boldsymbol{u}_g - \boldsymbol{v}_p\right)}}{\overline{\boldsymbol{u}}_g - \overline{\boldsymbol{v}}_p}$

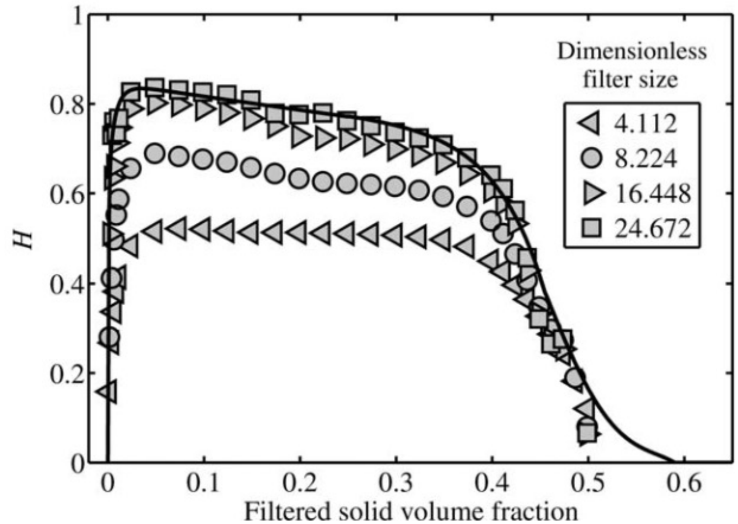
- Correction: $H = 1 - \beta^*/\beta\left(\overline{\phi}_s, \overline{\mathrm{Re}}_p\right)$

[1] Igci et al. (2008) Filtered two-fluid models for fluidized gas-particle suspensions. *AIChE Journal*, 54(6), 1431-1448.

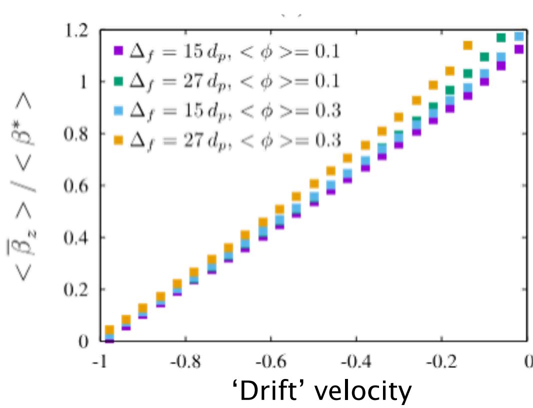
Sub-filtered drag is important

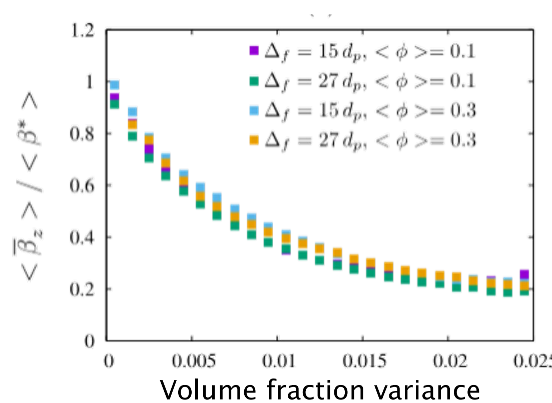
- Sub-filtered drag is significant[1]





- What should a model of the sub-filtered drag depend on?
  - Filtered volume fraction[2,3]
  - Volume fraction variance[3]
  - Drift velocity[2,3]
  - Other?
- Recent work is turning to ML to model sub-filtered drag





[1]Milioli et al. (2013) *AIChE Journal*, **59**(9), 3265-3275.
[2]Parmentier et al. (2012) *AIChE Journal*, **58**(4), 1084-1098.
[3]Ozel et al. (2017) *Physics of Fluids*, **29**(10).

A promising direction: Filtered CFD-DEM

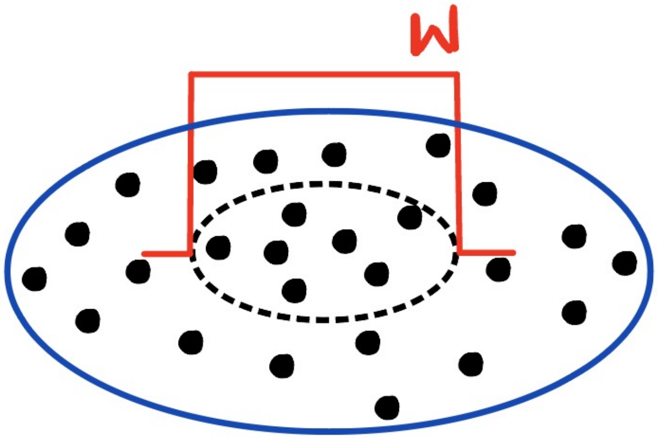
Applying a low-pass filter to the DEM equations reveals unclosed terms that are typically neglected in CG-DEM[1]

- Parcel position: $\widetilde{\boldsymbol{x}}_p^{(i)} = \sum_{j=1}^{N_{pp}} \boldsymbol{x}_p^{(j)} V_p^{(j)} W_{ij}$
- Parcel velocity: $\widetilde{\boldsymbol{u}}_p^{(i)} = \frac{\mathrm{d}\widetilde{\boldsymbol{x}}_p^{(i)}}{\mathrm{d}t} = \sum_{j=1}^{N_{pp}} \boldsymbol{u}_p^{(j)} V_p^{(j)} W_{ij}$
- Filtered momentum equation:

$$m_p \frac{\mathrm{d}\widetilde{\boldsymbol{u}}_p^{(i)}}{\mathrm{d}t} = \widetilde{\boldsymbol{F}}_{\text{drag}}^{(i)} + \widetilde{\boldsymbol{F}}_{\text{col}}^{(i)} + m_p \boldsymbol{g}$$

$$\widetilde{\boldsymbol{F}}_{\text{drag}}^{(i)} = \sum_{j=1}^{N_{pp}} \beta\left(\varepsilon_p^{(j)}, \mathrm{Re}_p^{(j)}\right)\left[\boldsymbol{u}_f^{(j)} - \boldsymbol{u}_p^{(j)}\right] V_p^{(j)} W_{ij}$$

$$\approx \boldsymbol{F}_{\text{drag}}^{(i)}\left(\widetilde{\varepsilon}_p^{(i)}, \widetilde{\mathrm{Re}}_p^{(i)}\right) + \Delta \boldsymbol{F}_{\text{drag}}^{(i)}$$



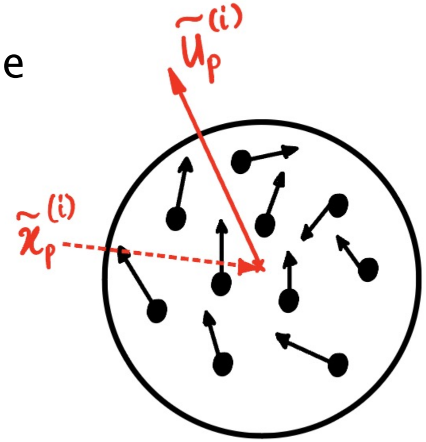
Notation:
- N_{pp} is # particles/parcel
- j is particle index
- V_p is the particle volume
- X_p is the partice position
- W is the filter kernel

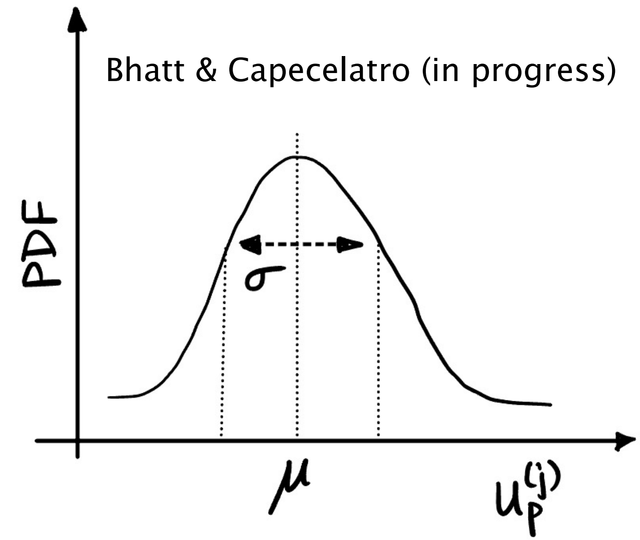
[1]Bhatt & Capecelatro (in progress)

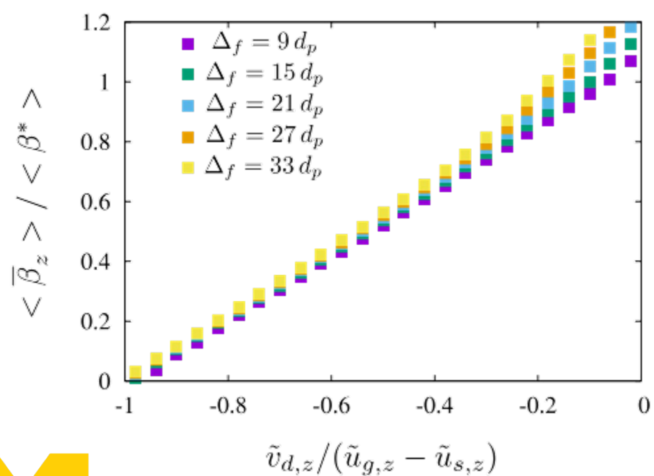
A promising direction: Filtered CFD-DEM

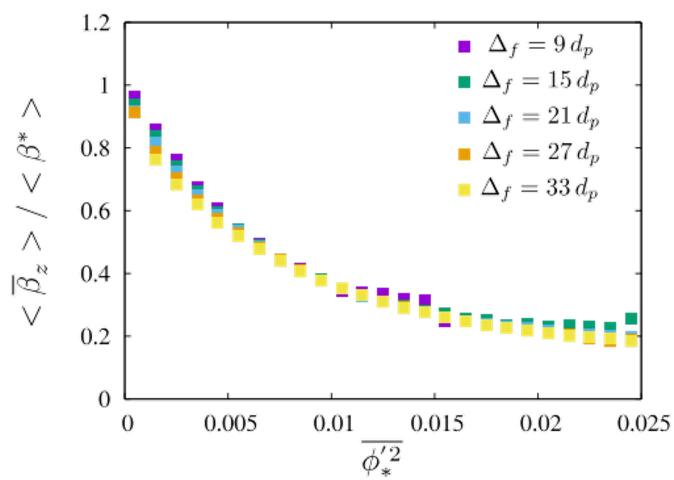
Applying a low-pass filter to the DEM equations reveals unclosed terms that are typically neglected in CG-DEM

- Significant particle-to-particle variation may exist at the sub-filter level
- Each parcel contains a *distribution* in velocity and granular temperature
- Sub-filter drag laws mostly developed for Euler-Euler (two-fluid) models. Previous works show that neglecting this term can be detrimental!









Ozel, A., Gu, Y., Milioli, C. C., Kolehmainen, J., & Sundaresan, S. (2017). Towards filtered drag force model for non-cohesive and cohesive particle-gas flows. *Physics of Fluids*, **29**(10).

Concluding remarks

1. CFD-DEM is a popular choice for modeling transport in mills and classifiers (typically coupled with RANS)
2. Recent advancements have been made to improve hydrodynamic interactions in dense assemblies (capturing neighbor effects) using deterministic/stochastic approaches and more recently ML
3. In many cases, gas-phase turbulence is unresolved, need to reconstruct subgrid-scale velocity fluctuations. Commonly done using stochastic (random walk) models (but they fail to capture spatial heterogeneity)
4. Everything above requires tracking each individual particle! Coarse-grained DEM is gaining popularity to reach industry-relevant scales
5. Standard CG-DEM approaches degrade accuracy once the number of particles per parcel > 10
6. A rigorous derivation of the filtered DEM equations reveal unclosed terms that are often neglected. This points to a route towards *scalable* CG-DEM!
7. Eulerian-based models based on kinetic theory of granular flows are promising. Momentum methods represent attractive approach to capture breakage/size segregation. Filtered two-fluid models are needed to capture SGS heterogeneity.

Questions?