



# Fluidization/flow of cohesive particles

Sankaran Sundaresan

Princeton University

- Given rules for particle-particle interactions, determine collective flow characteristics
- *van der Waals*
- *Liquid bridge forces*
  - Effective fluid-particle interaction
- *Electrostatics*
  - Effective particulate phase stress
- Use simulations as tools towards this end
  - Discrete Element Method – scope out what is important
    - Simple shapes (spheres)
    - How does complex shapes (roughness) affect outcome

IFPRI Workshop

Jan 14, 2020



- Common challenge

- Particles are very stiff (resolving contact is expensive)
- Young's modulus  $\sim 1$  GPa

- Practical strategy

- Simulate soft particles (jelly beans)
- Soften by 10 – 1000 times

- Softer particles will have exaggerated overlaps

- For **non-cohesive particles**, this exaggerated overlap is of little concern in flows in **inertial regime**, while some care may be needed in quasi-static flows.



- Common challenge

- Particles are very stiff  
(resolving contact is expensive)
- Young's modulus  $\sim 1$  GPa

- Practical strategy

- Simulate soft particles  
(jelly beans)
- Soften by 10 – 1000 times

- Softer particles will have exaggerated overlaps

- For **cohesive particles**, this exaggerated overlap will magnify unphysically the effect of cohesion in flows in dilute inertial regime.
- The model for cohesion needs modification. (Will discuss)



- Common challenge

- Too many particles → too expensive to simulate
  - Fluidized bed (75  $\mu\text{m}$  particles): 1 L of bed ~ **billion particles**
  - Dry powder Inhalation with 75  $\mu\text{m}$  carrier particles and 2  $\mu\text{m}$  API particles: 10 mg sample ~ **100 million particles**

- Practical strategy

- Simulate small, canonical flow problems to develop understanding and continuum constitutive models
- Coarsen DEM so that one has far fewer pseudo-particles to simulate



- Questions that arise:

- How does cohesion affect continuum constitutive models and what types of simulations can allow us to learn this?

Will discuss this for particle phase stress

- How should the pseudo-particles interact with the gas and among themselves in order to correspond to the original system?

Will not go into this issue in this talk

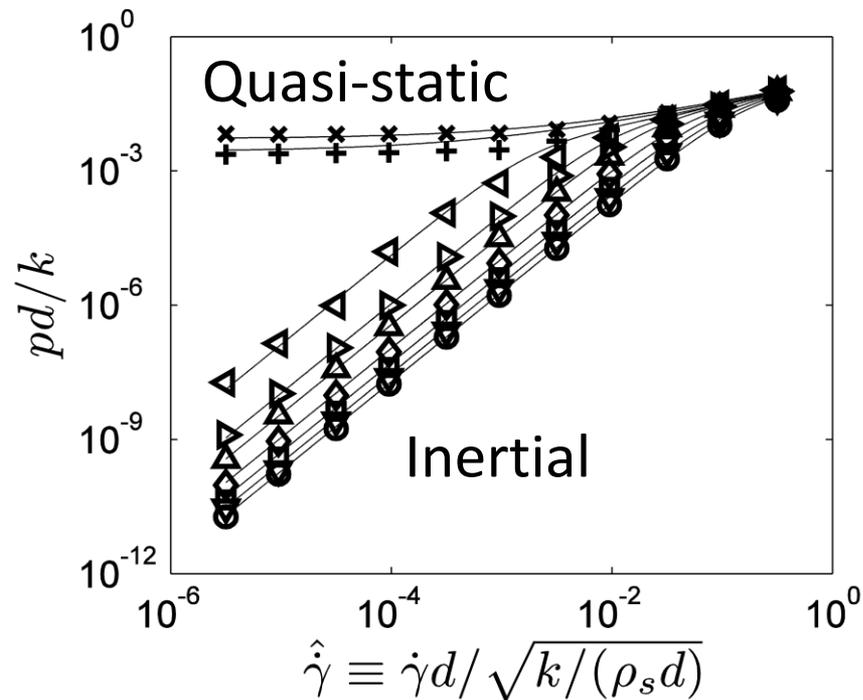
# Outline



- Effect of cohesion on shear flow of dense assemblies
- Modification of cohesion model – softening correction
- Examples of simulations toward continuum constitutive models and/or physical understanding
  - Effect of fines on fluidization
  - Fluidization of monodisperse particles
  - Fluidization of wet particles; tribocharging
- Dry Powder Inhalation – approaches to simplify computations

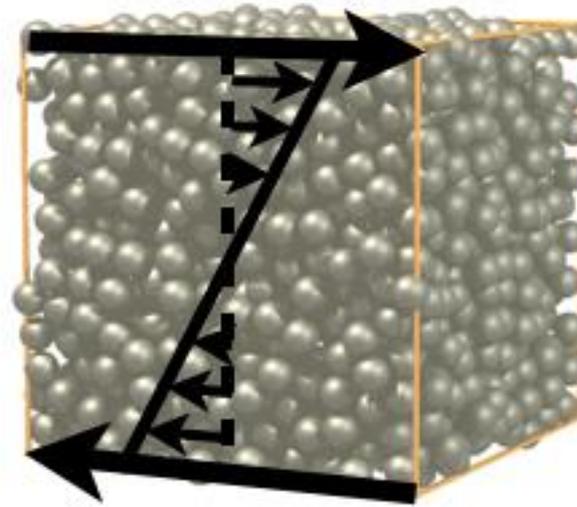
# Pressure in simple shear flow

Scaled pressure for frictional, non-cohesive particles



Scaled shear rate

periodic box



- $\phi = 0.51$
- ▽  $\phi = 0.53$
- $\phi = 0.55$
- ◇  $\phi = 0.57$
- △  $\phi = 0.59$
- ▷  $\phi = 0.6$
- ◁  $\phi = 0.61$
- +  $\phi = 0.62$
- ×  $\phi = 0.63$

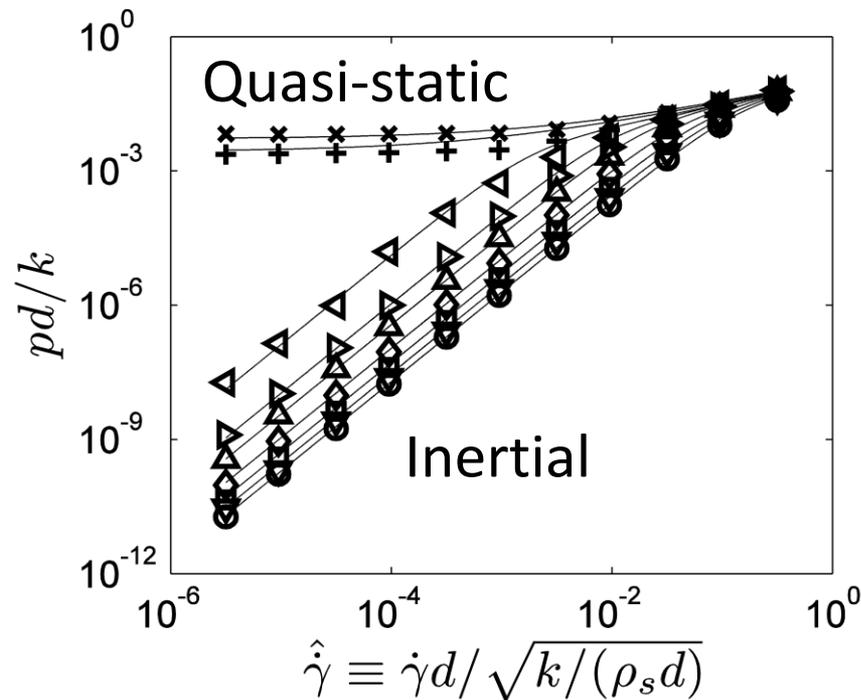
Linear spring-dashpot

Analogous results for Hertzian spring



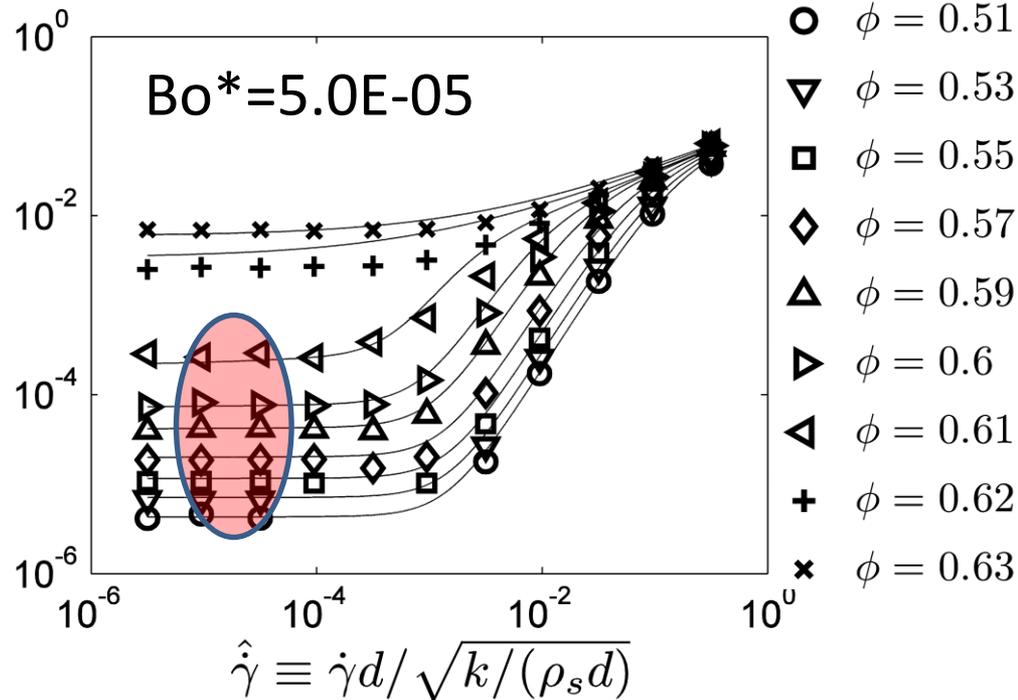
# Pressure in simple shear flow: effect of cohesion

Scaled pressure for frictional, non-cohesive particles



Scaled shear rate

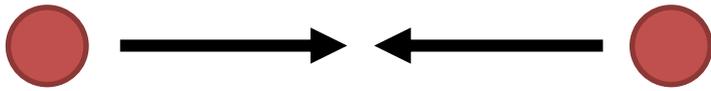
Scaled pressure for frictional, cohesive particles, below the jamming conditions for equivalent non-cohesive particles.



Cohesive yield stress scales with  $F^{max}$

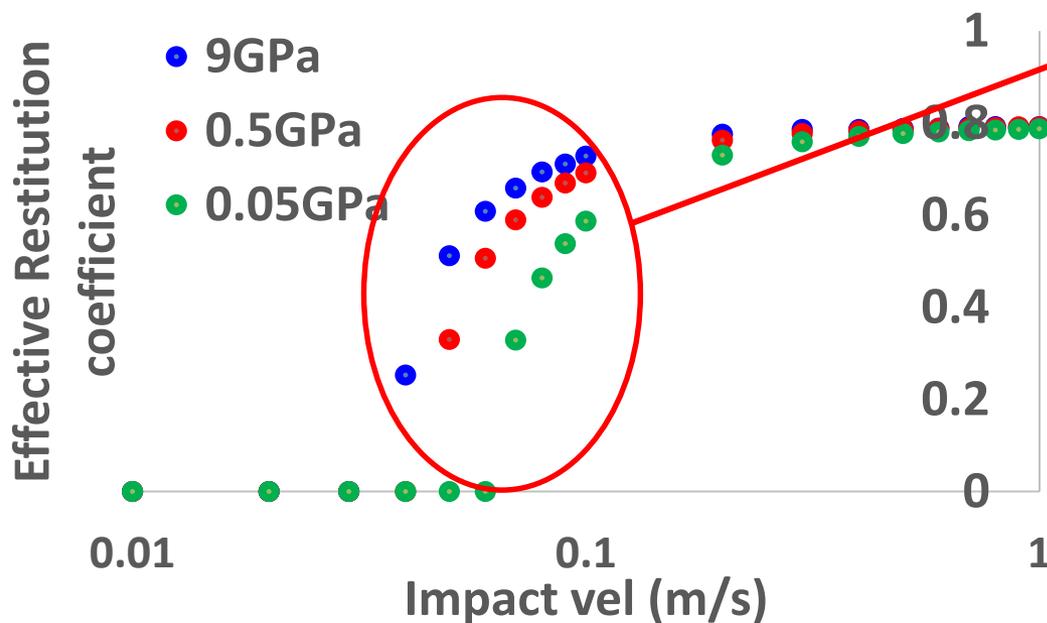
$$Bo^* \equiv F_{vdW}^{max} / kd \approx A / 24ks_{min}^2$$

# Simply softening cohesive particle changes dynamics



$$\text{Effective restitution coefficient} = \frac{\text{relative velocity after collision}}{\text{impact velocity}}$$

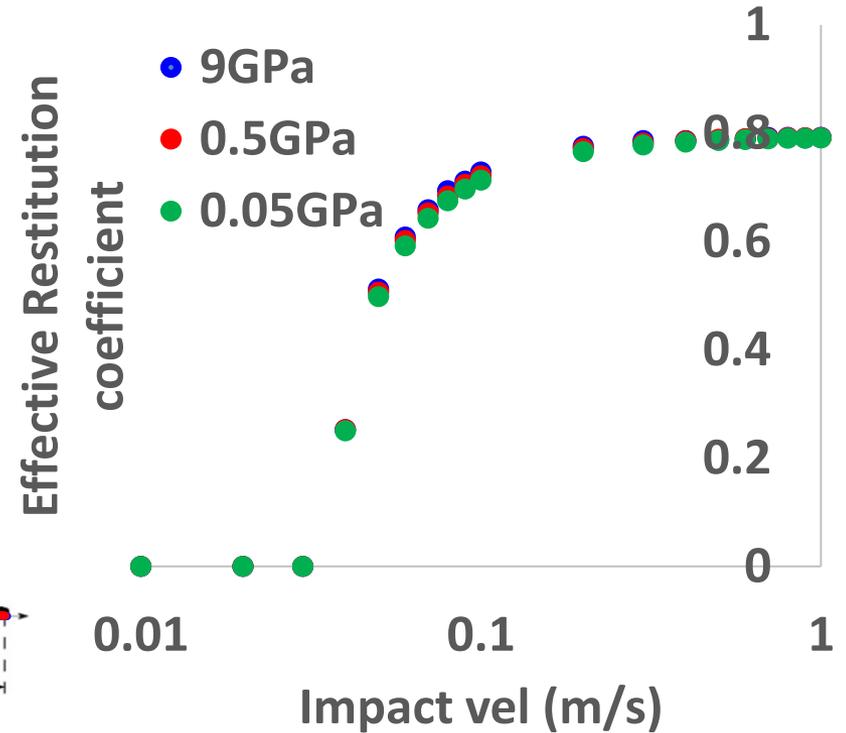
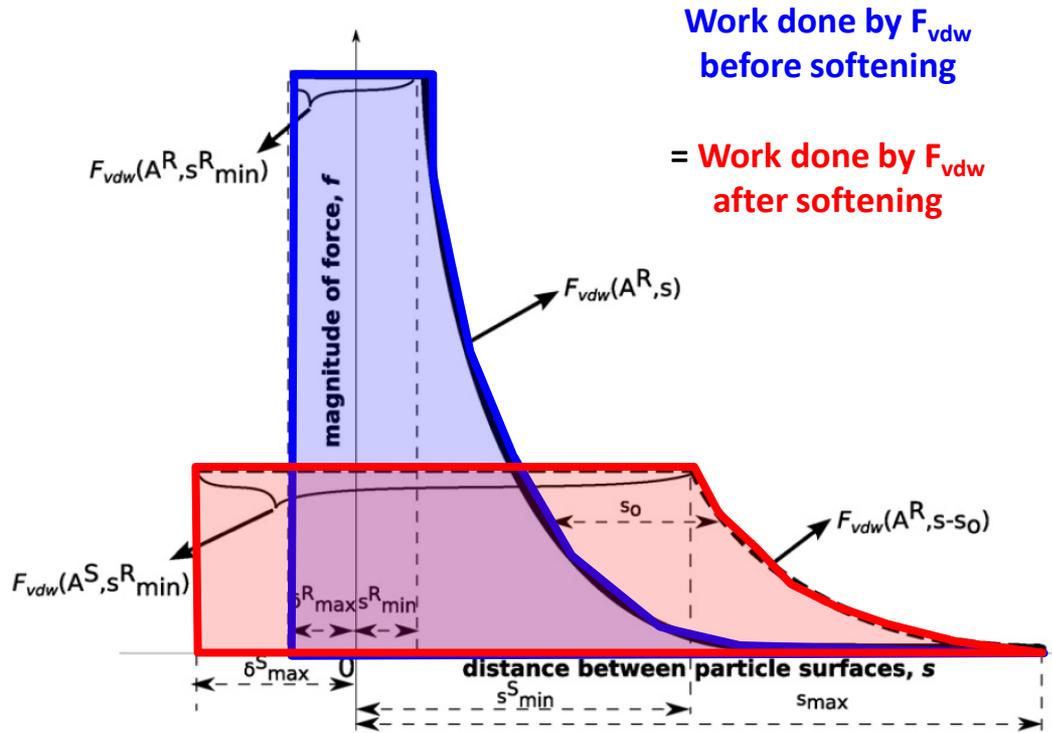
Particle Stiffness (GPa)	Hamaker constant (J)
9	$1 \times 10^{-19}$
0.5	$1 \times 10^{-19}$
0.05	$1 \times 10^{-19}$



Just simply reducing particle stiffness changes particle dynamics

Need to modify the cohesion model in order to conserve particle dynamics

# Modified cohesion model conserves dynamics



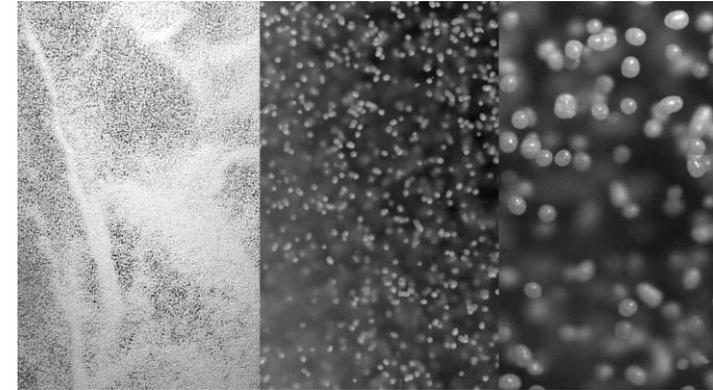
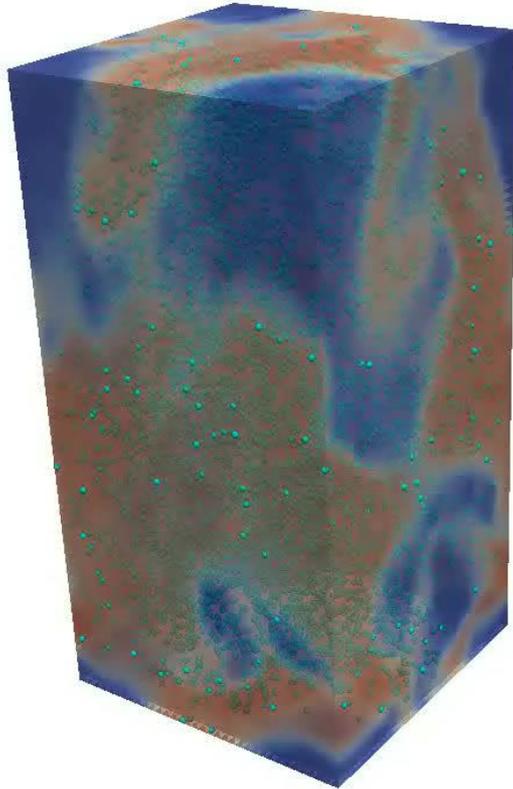
Schematic of the original and modified cohesion model between two particles [1]

The new VDW model conserves the work done by the  $F_{vdw}$

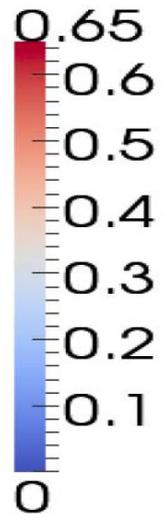
Modified cohesion model conserves collision dynamics

Modification is NOT unique

# CFD-DEM simulation: Non-cohesive, monodisperse particles



$$\bar{f} = 0.3$$



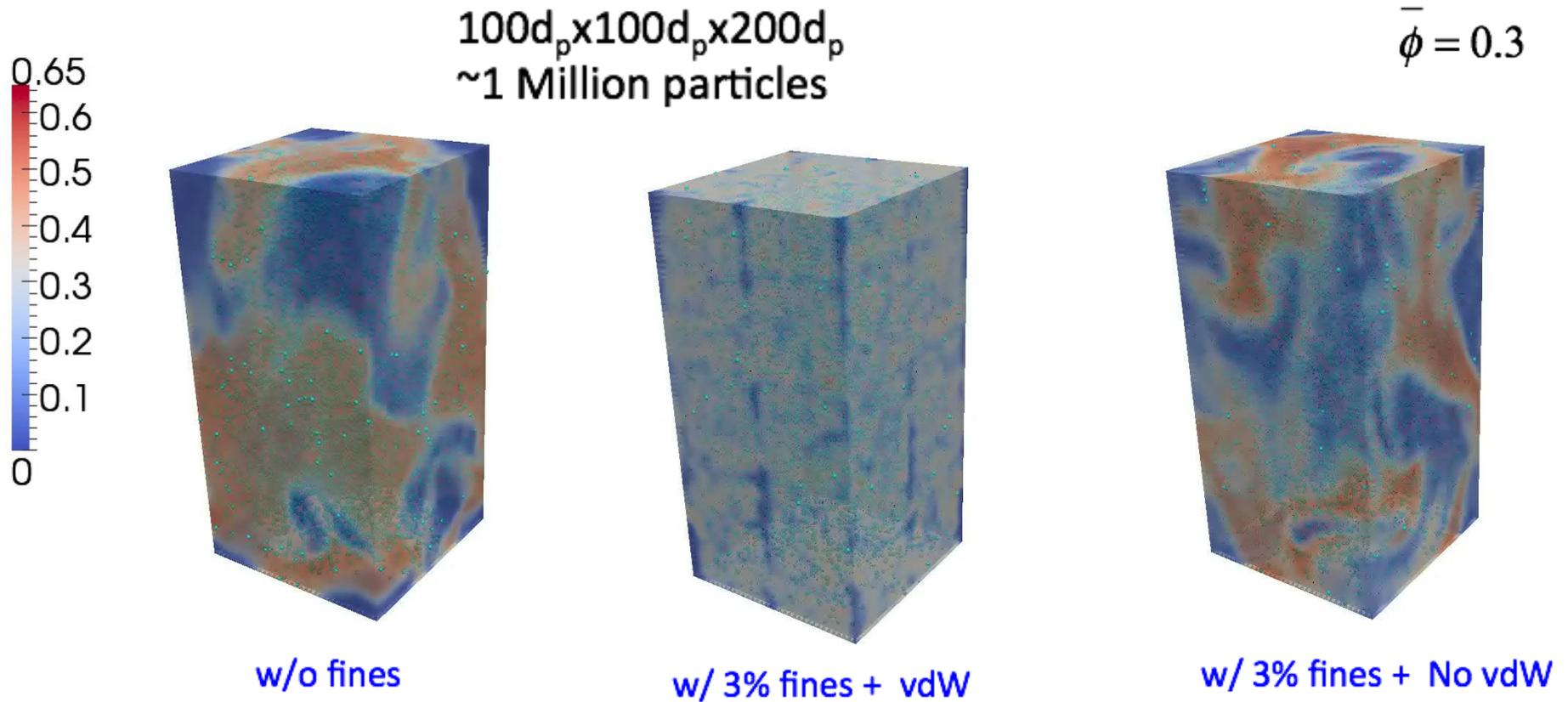
- Filter to get continuum constitutive models
- Add complex particle-particle interactions to probe their effects

$100d_p \times 100d_p \times 200d_p$

~1 Million particles

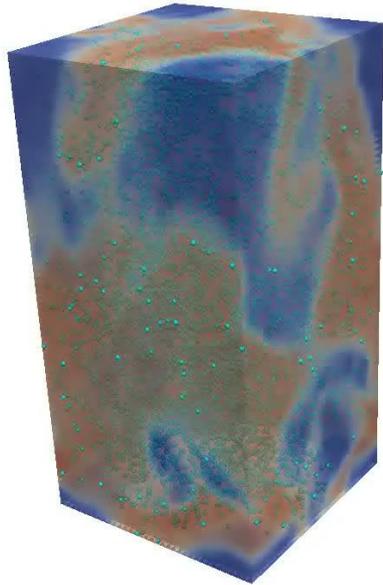
Ozel, et al., Chem. Eng. Sci.,  
155, 258 (2016)

# Effect of fines on fluidization: CFD-DEM simulations



- Appreciable change in hydrodynamics only when fines and vdW forces are included.

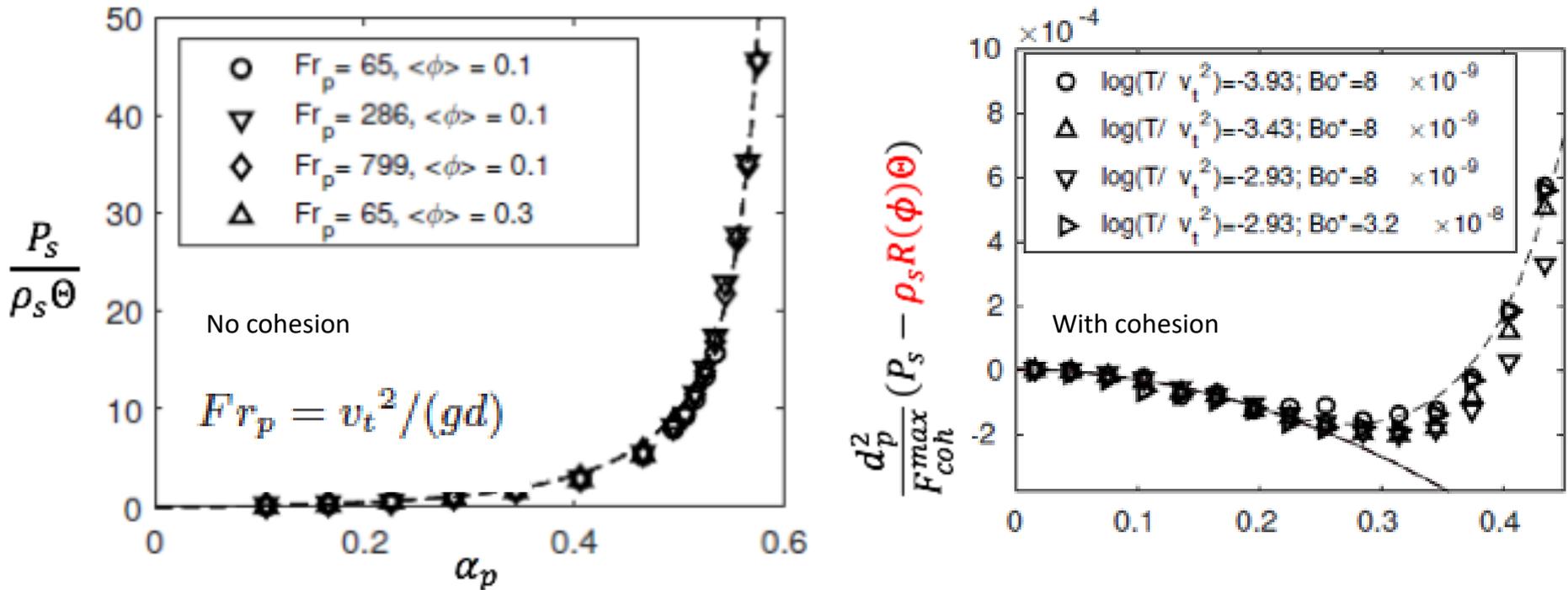
- CFD-DEM simulation snapshots: map to Euler grids and use the results to develop constitutive models



- Perform simulations for different combinations of relevant dimensionless groups and particle volume fractions
- Test the approach for non-cohesive particles against kinetic theory of granular materials
- Extend to cohesive particles

# Effect of cohesion on particle phase stress

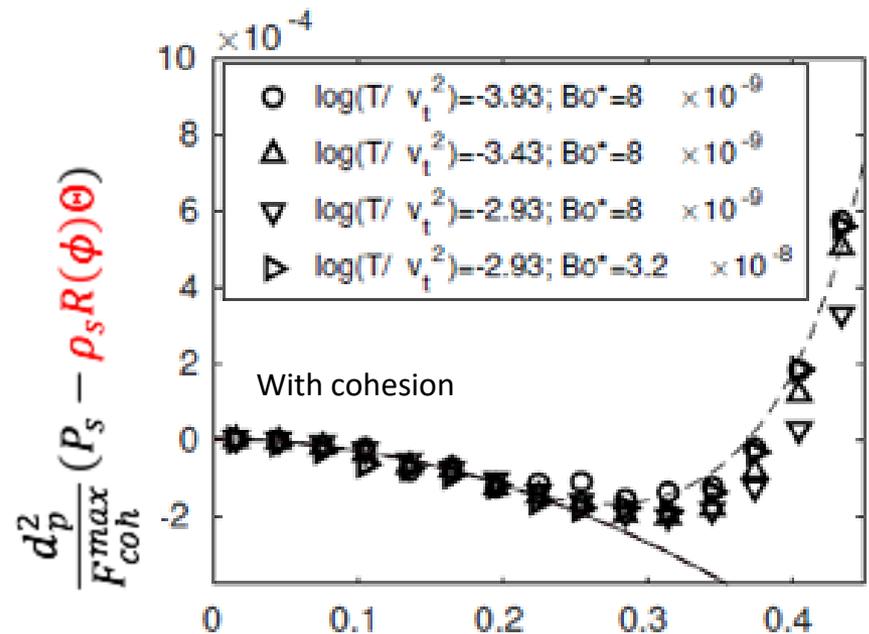
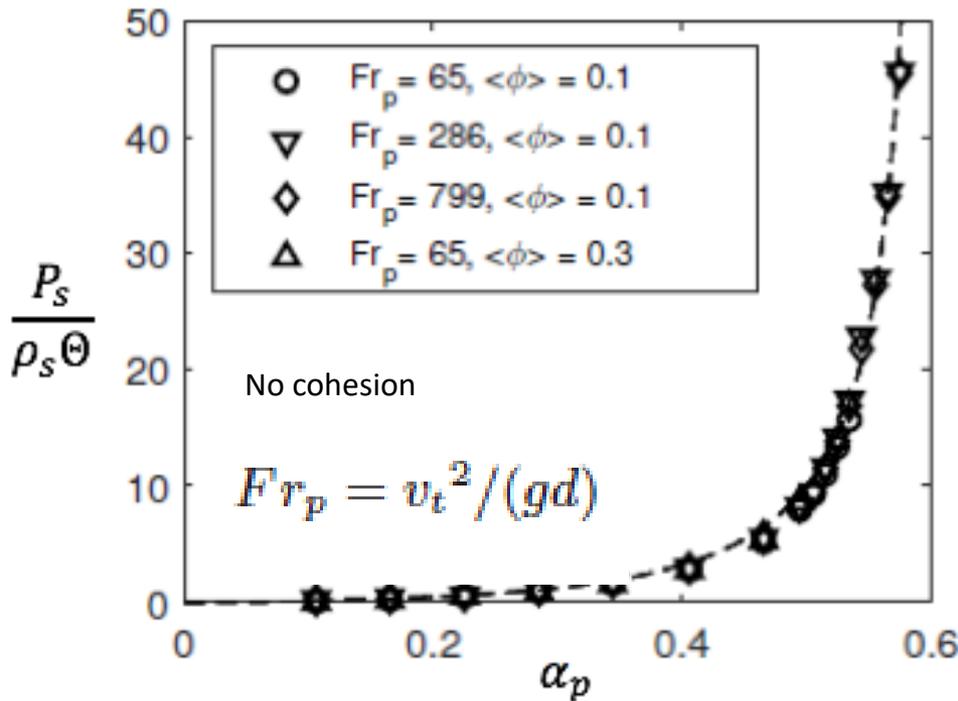
- CFD-DEM simulation snapshots: map to Euler grids and use the results to develop constitutive models



- No cohesion - nearly recover the kinetic theory; only pressure is shown

# Effect of cohesion on particle phase stress

- CFD-DEM simulation snapshots: map to Euler grids and use the results to develop constitutive models



$$p = \rho_s R(\phi) \theta - \alpha \frac{F_{c,max}}{d^2} \phi^2 + \beta \frac{F_{c,max}}{d^2} \frac{(\phi - \phi_b)^2}{\phi_c - \phi}$$

vdW attraction

only for  $\phi > \phi_b$

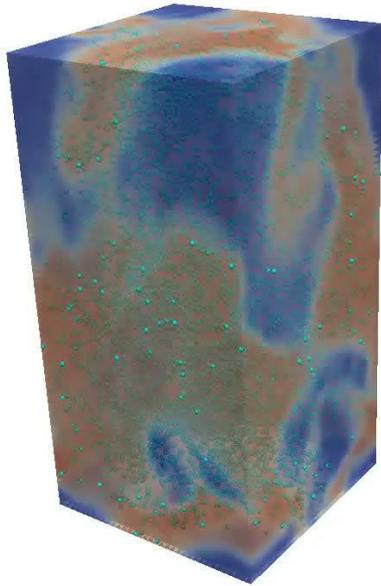
$$f_b = as \frac{qd^2}{F_{c,max}}$$

Force chain

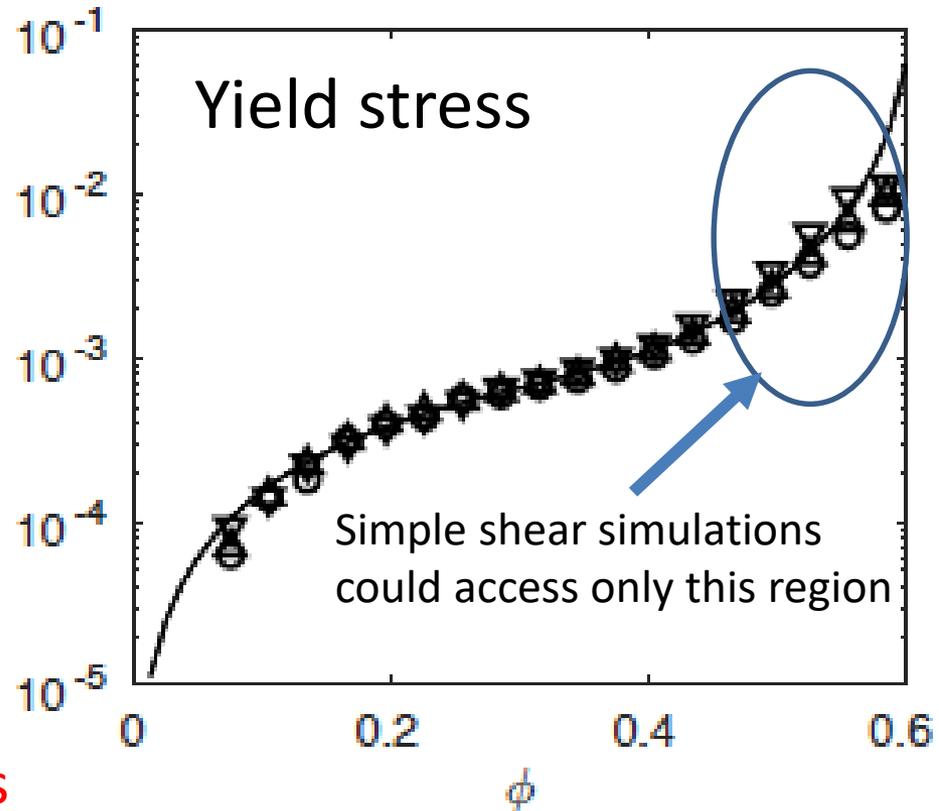
# Effect of cohesion on shear stress



- Shear stress = stress captured by kinetic theory + yield stress



$$\frac{d_p^2}{F_{coh}^{max}} \tau_y$$



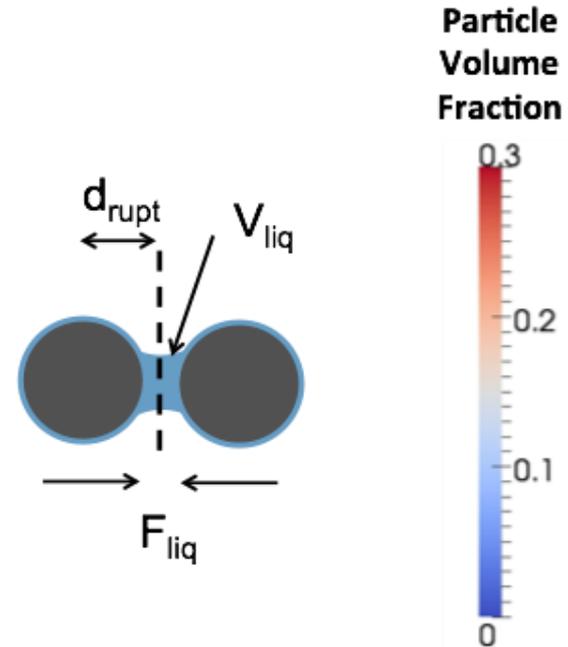
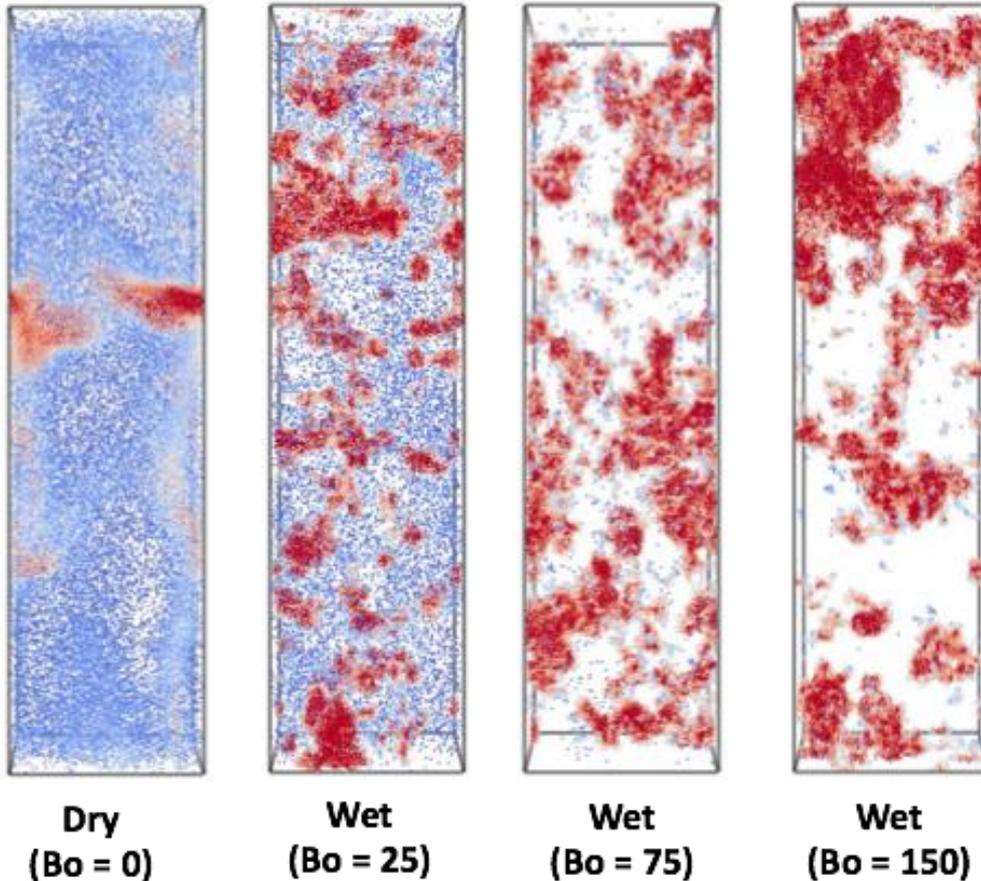
Only maximum force at contact appears in the models for the effects of cohesion

Can also analyze simulation data to probe effective fluid-particle drag

# CFD-DEM of fluidization of wet particles



- Agglomerate size increases with  $Bo$

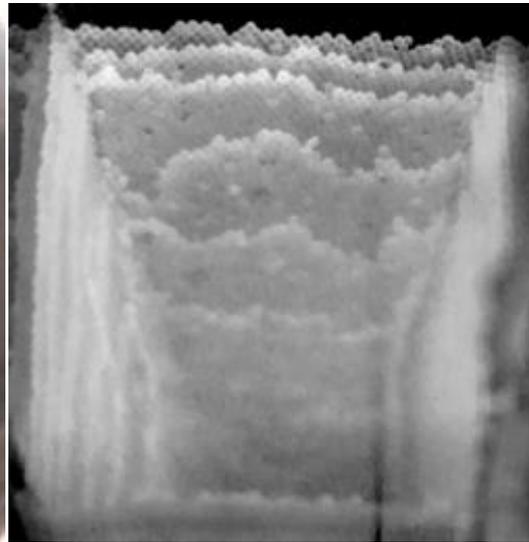


- Continuum drag and stress models
- Agglomerate stability

Girardi, et al, , Chem. Eng. Sci., **144**, 224 (2016)

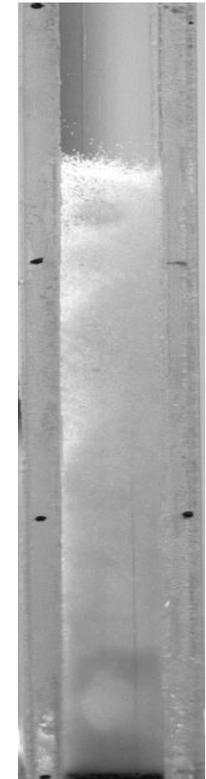
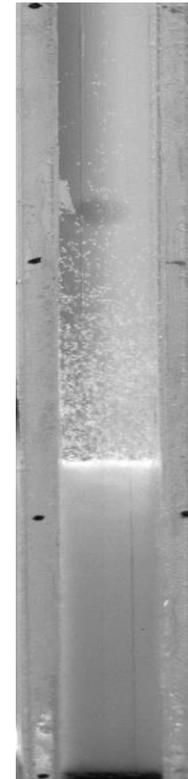
Boyce, et al. , AIChE J., **63**, 2520-2527 (2017)

# Fluidization with tribocharging



RH 20%

RH 60%



Polyethylene particles (276  $\mu\text{m}$ )  
Walls: soda lime glass

$\sim 20 \text{ nC/g}$

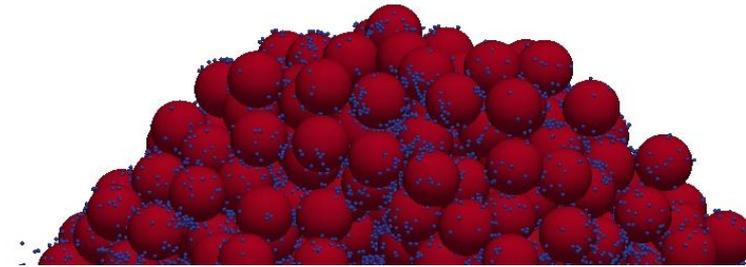
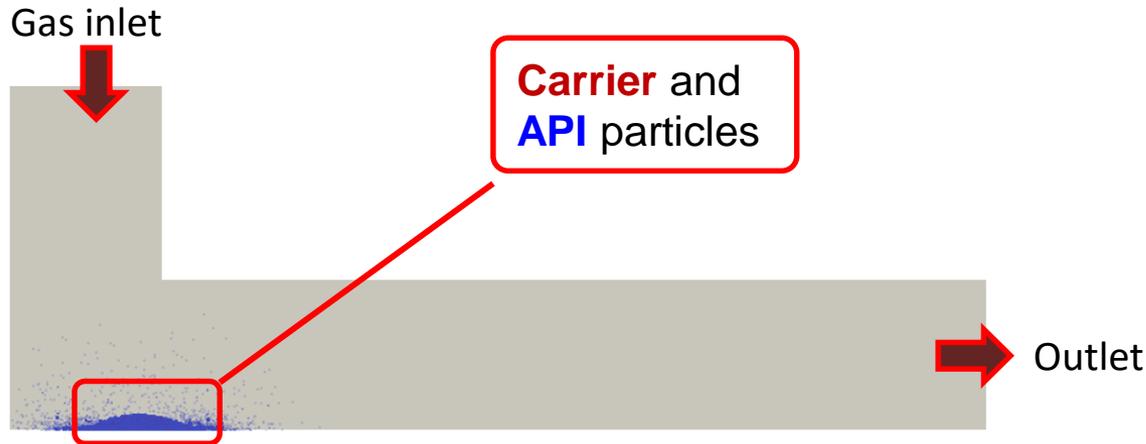
$\sim -3 \text{ nC/g}$

Sowinski et al., *Chem. Eng. Sci.* **65**, 2771 (2010)

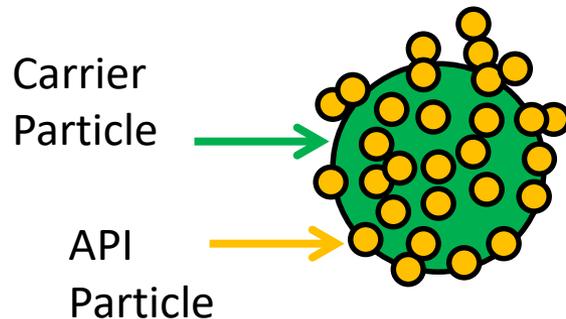
Sippola et al., *J. Fluid Mech.*, **849**, 860 (2018)

CFD-DEM + Poisson solver  
for long-range electric field +  
tribocharging model

# Dry Powder Inhaler



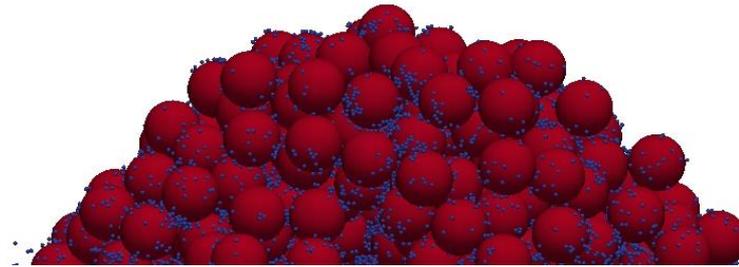
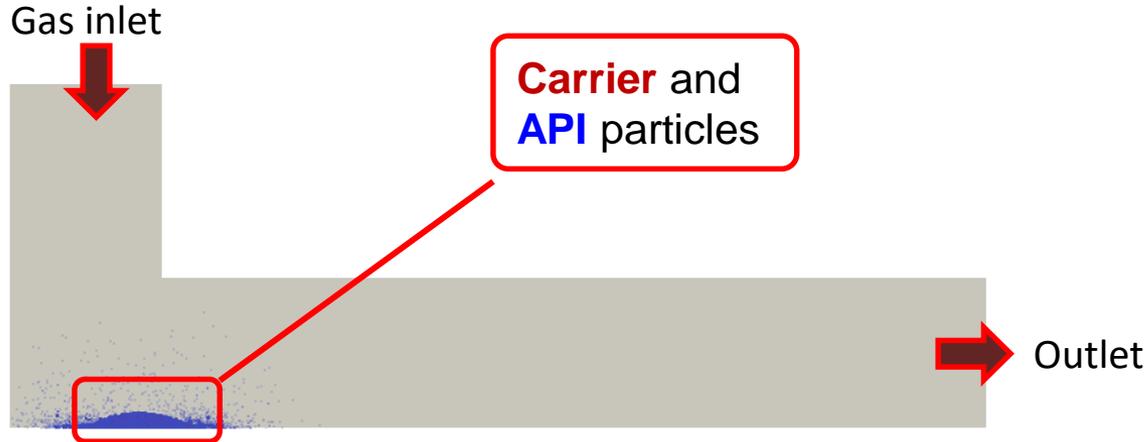
For a 10mg dosage, carrier and API vol% = 95.5:4.5



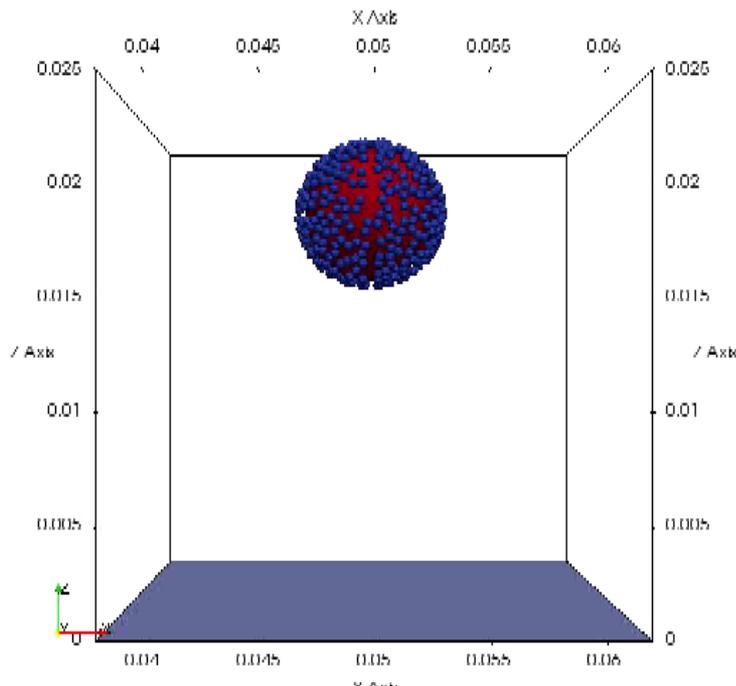
Carrier particle radius ( $\mu\text{m}$ )	API particle radius ( $\mu\text{m}$ )	Number of Carrier Particles	Number of API particles
35	2.5	35k	4.5m
35	1	35k	79m

Costly for CFD-DEM simulation

# Dry Powder Inhaler



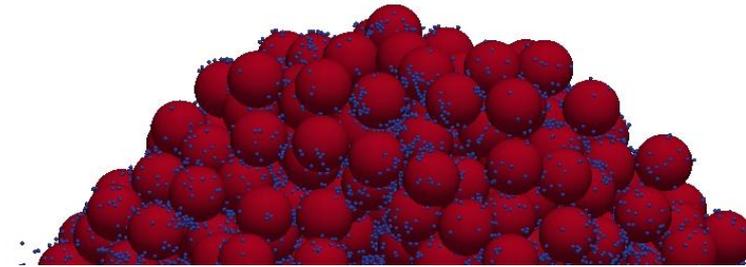
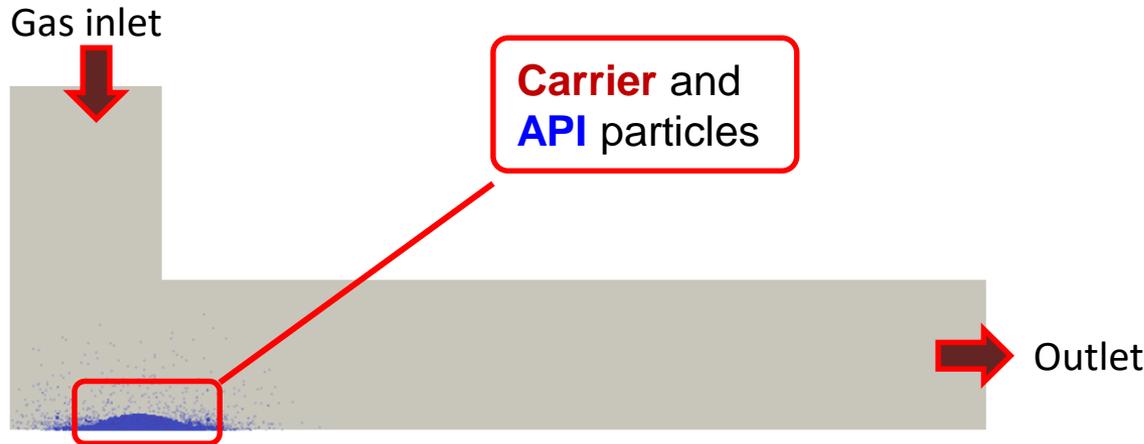
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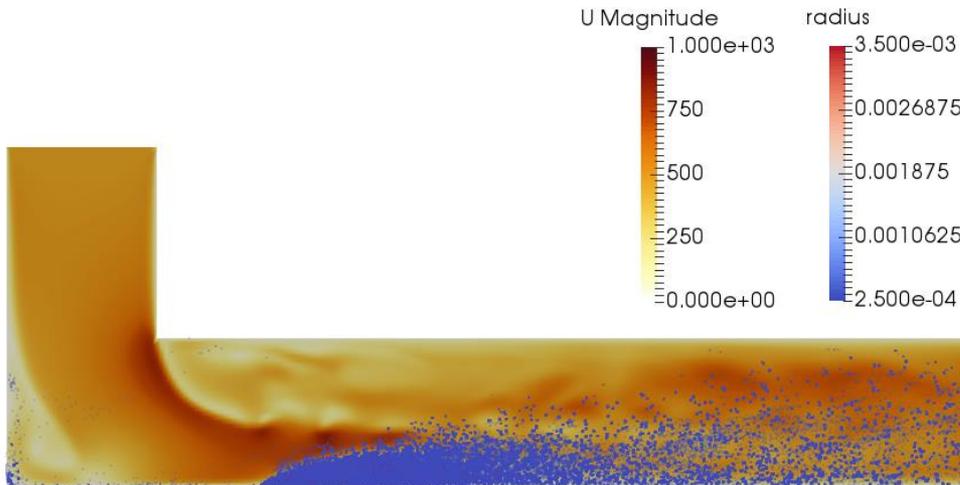
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Costly for CFD-DEM simulation

# Two-stage strategy: softening and coarsening



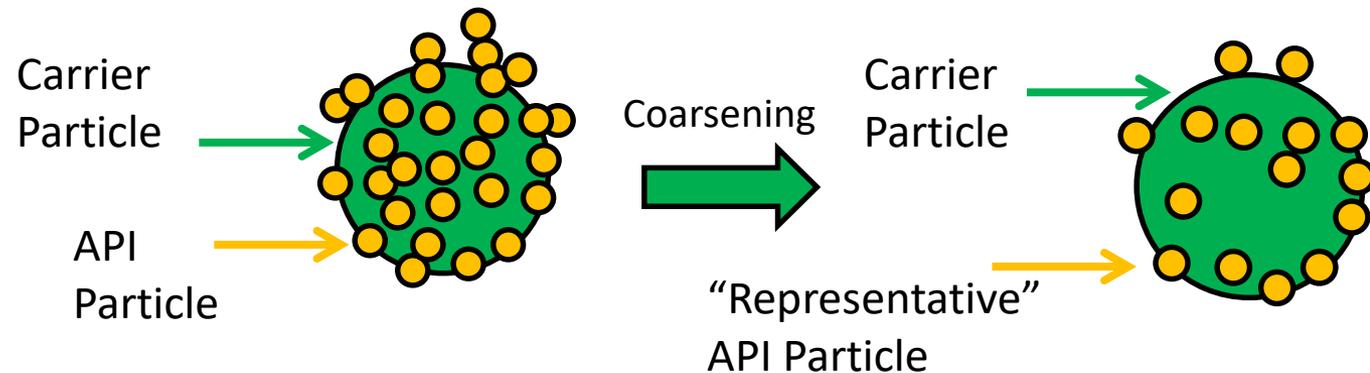
## Softening Approach

Reducing particle stiffness increases the DEM time step, thus making the simulation faster

Particle Stiffness (GPa)	Softening	DEM Time step (s)
9	Original	$2 \times 10^{-9}$
0.5	18	$1 \times 10^{-8}$
0.05	180	$3 \times 10^{-8}$

## Coarsening Approach

Model API particles by “representative” particles, each representing N primary particles



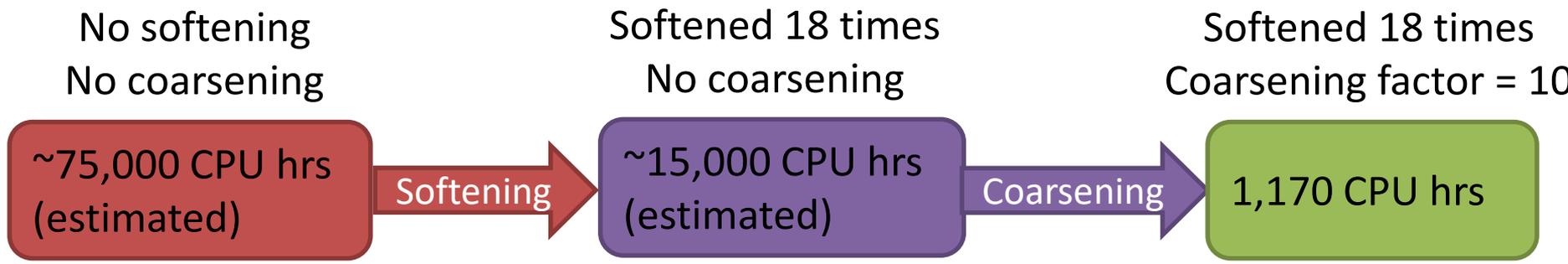
This approach further reduces computational cost as fewer particles are tracked in the simulation



# Savings in computational cost and quality of predictions

CPU hours (= No processors used × No of hours used) is used to measure computational cost

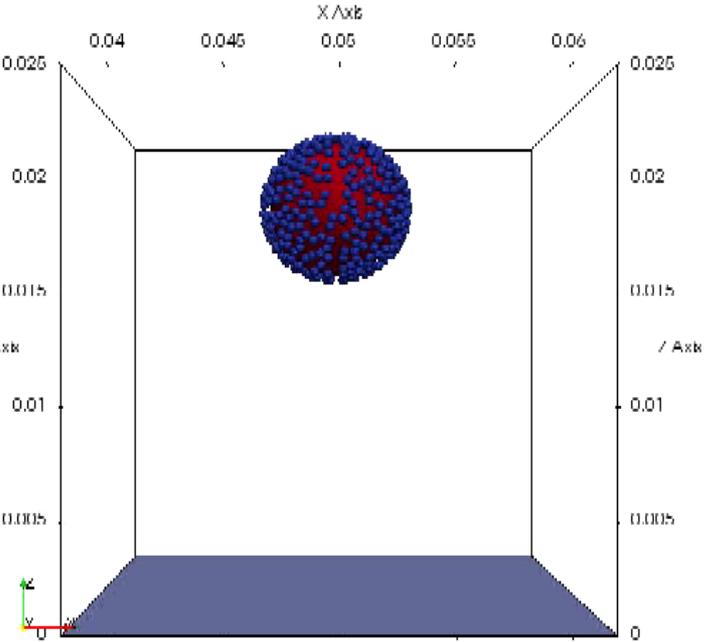
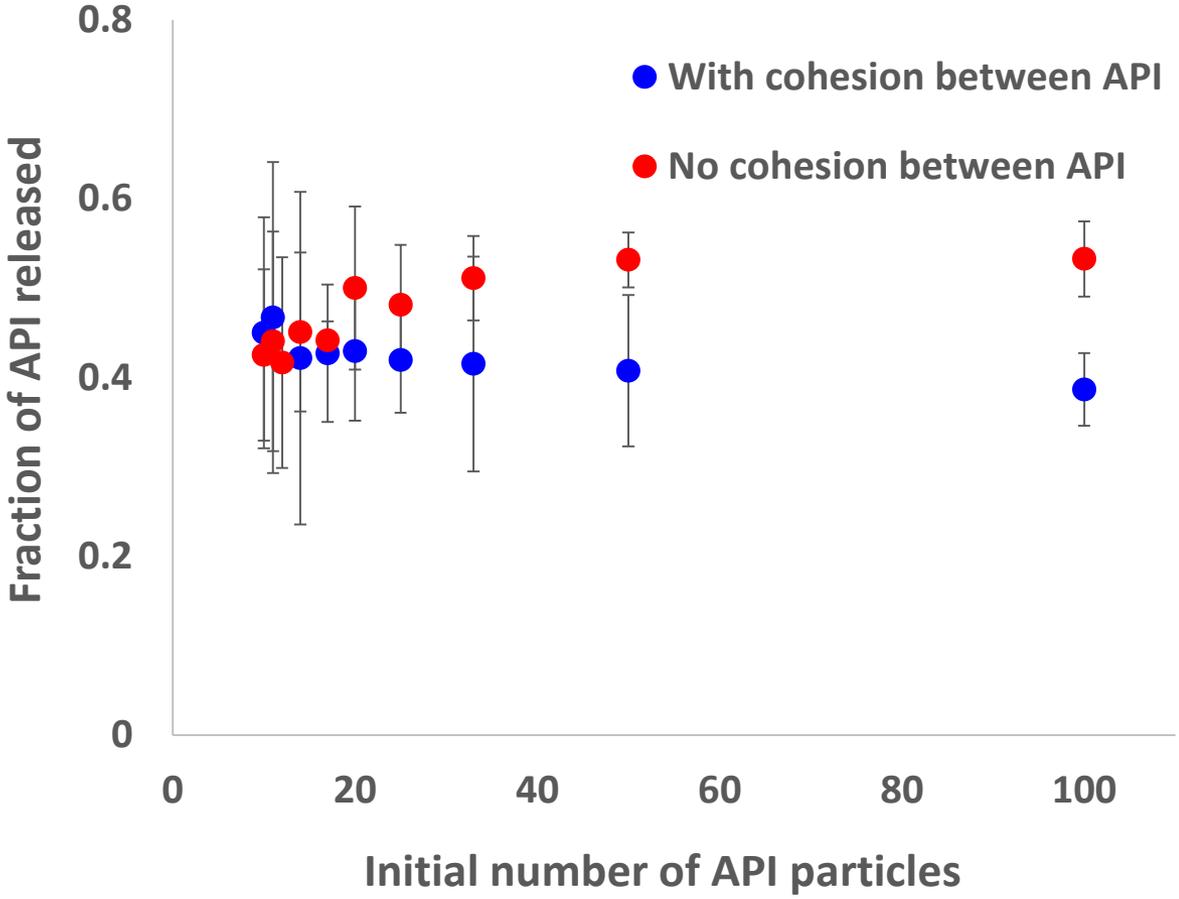
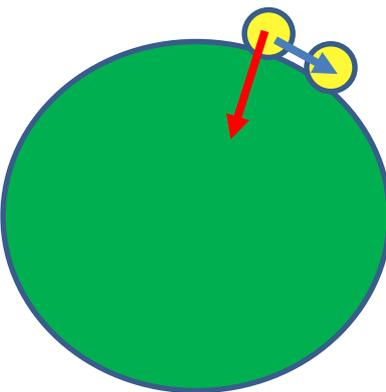
For a 3.5mg dosage case, there are 13k carrier particles (R = 35µm) and 1.7m API particles (r = 2.5µm)



*Fine particle fraction* =  $\frac{\text{weight of fragments smaller than } 5\mu\text{m}}{\text{total weight of API particles}}$  is used to measure quality of predictions

Coarsening Factor	CPU hours for 3.5mg dosage	Fine Particle Fraction
1 (No coarsening)	~ 15000 (Estimated)	Not simulated
3	5360	0.204
5	2570	0.227
10	1170	0.249

# Savings in computational cost and quality of predictions



What will happen if the API particle is positively charged and the carrier is negatively charged?



- Validation of interaction models with direct force measurements
- Ensuring that simplifications introduced to make computations affordable are faithful to the original interaction models:  
Particle softening, particle coarsening
- Fluidization/flow:
  - Non-cohesive particles form hydrodynamic clusters; lots of studies on filtering over them to deduce drag and stress correction models
  - Cohesive particles can also form agglomerates, but modern simulations have yet to lead to good models relating the agglomerate size and density to flow conditions





- Recap here

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Funding agencies get listed

Thank group members