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Chemical and Biological Engineering

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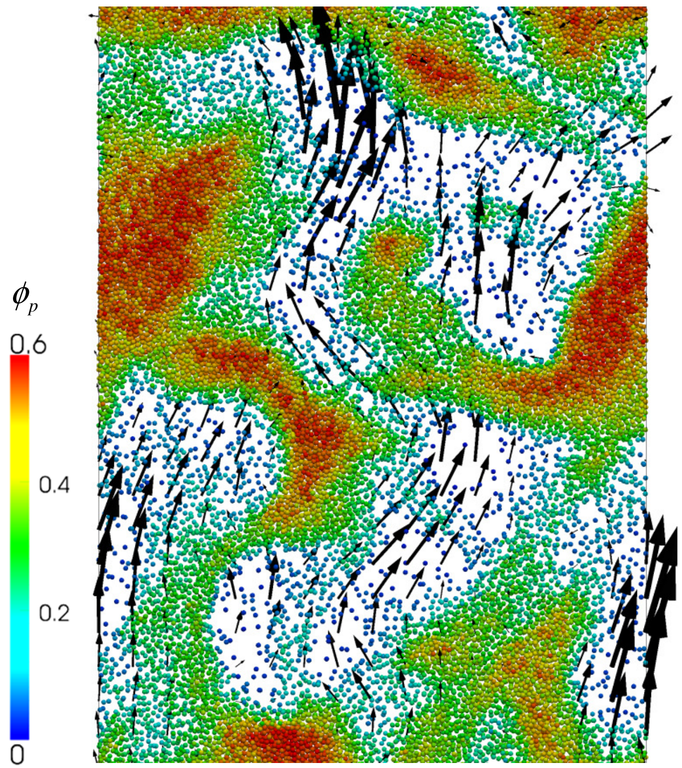
Effective Drag Law for Parcel-Based Approaches

What Can We Learn from CFD-DEM?

Stefan Radl, Matthew Girardi, Sankaran Sundaresan

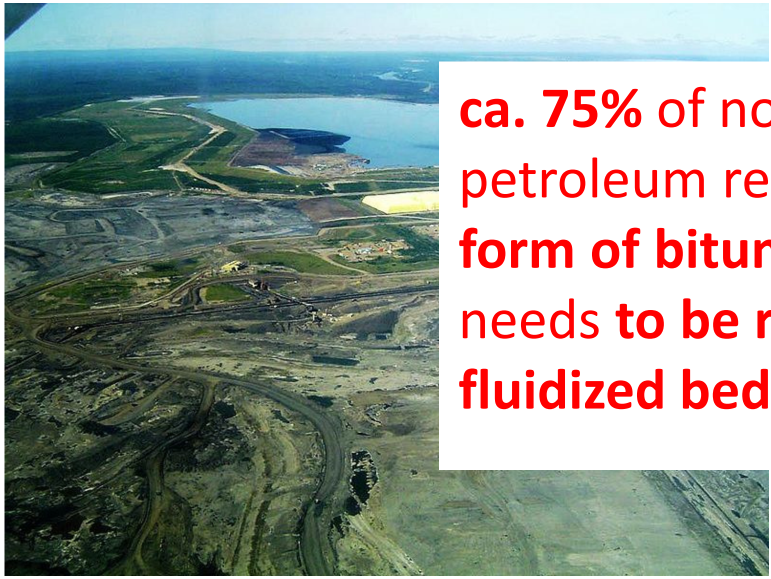


European Congress on Computational Methods in Applied Sciences and Engineering

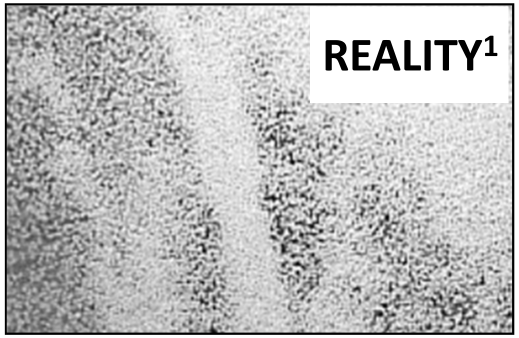
Vienna, September 11, 2012

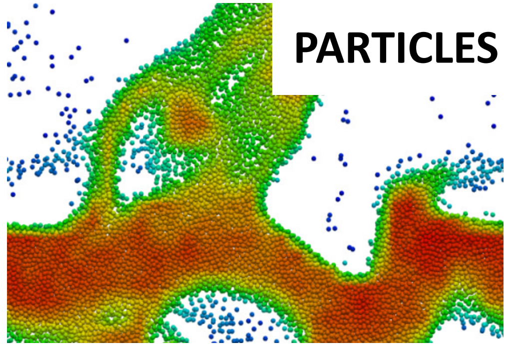
Outline

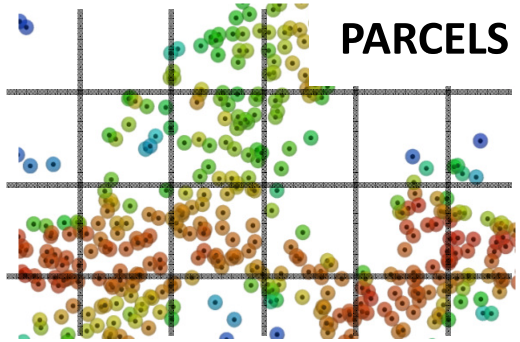
- **Motivation**
- **Computational Tools**
- **A Validation Study**
- **An Effective Drag Law**



ca. 75% of north america's petroleum reserves are in **form of bitumen**, which needs **to be refined in fluidized beds.**







[1]Courtesy: Franklin Shaffer, NETL, Morgantown, WV (2009).

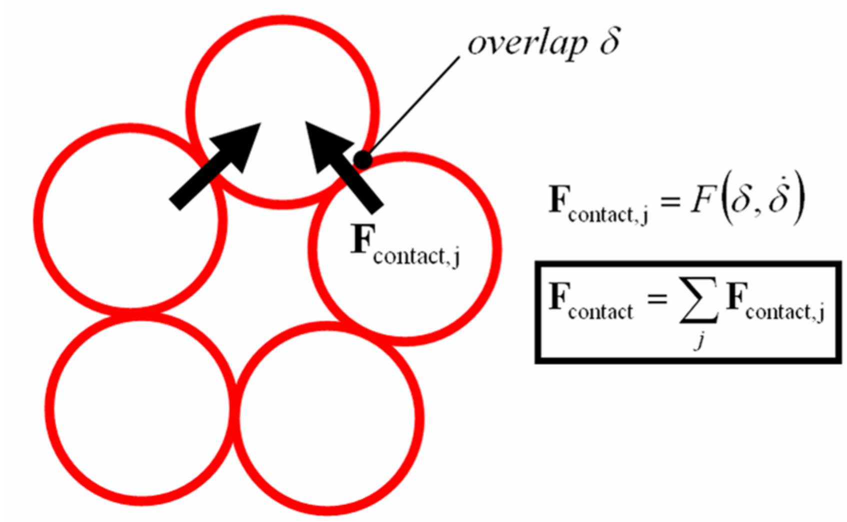
How? - Computational Tools

Handling of Dense Regions - Particles & Parcels

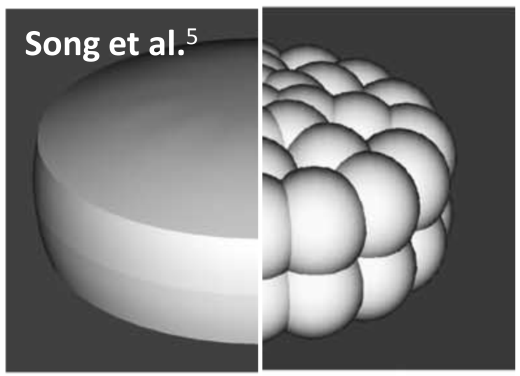
- The „standard“ Discrete Element Method (DEM) approach requires the **computation of all collisions** to calculate **contact forces and torques**.

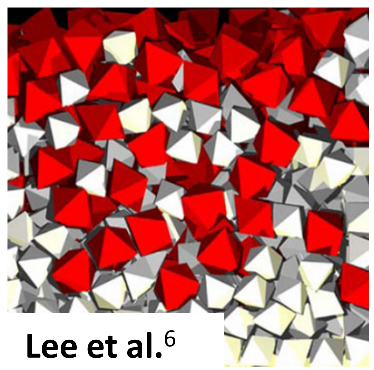
DEM

(Cundall and Strack,[2] Luding[3])



- Particle shape considered via **glued-sphere approach**, **super-quadrics**,[4] or other „smart“ approaches.[5,6]





[2]Cundall and Strack, ***Geotechnique*** 29 (1979). [3]Luding, ***Granular Matter*** 10 (2008).
[4]Hilton et al., ***CES*** 65 (2010). [5]Song et al., ***Powder Tech*** 161 (2006). [6]Lee et al., ***Granular Matter*** 11 (2009).

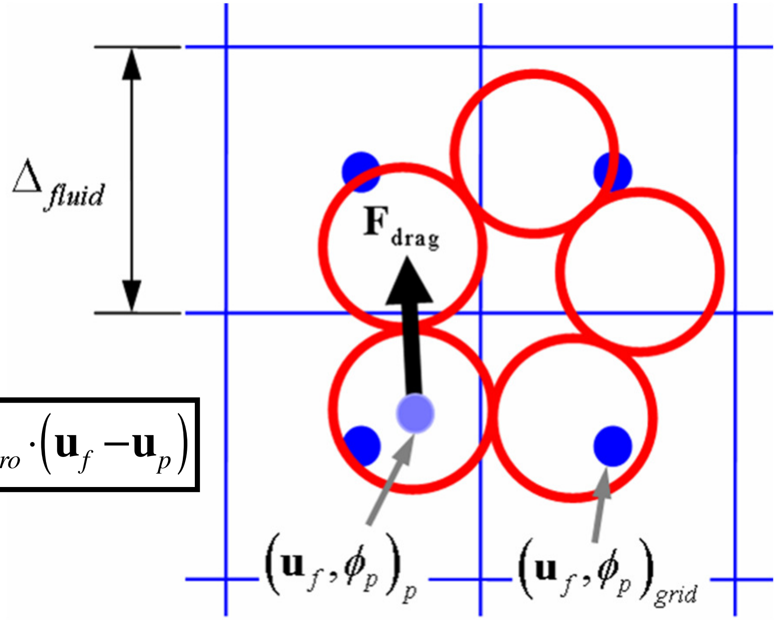
How? - Computational Tools

- In the CFD-DEM[7,8] the fluid flow is calculated on a **computational grid that is larger than the particles** - **„microscopic“ drag law**.
- In the CFD-DPM one computes **virtual „contact“ forces** via a DEM-like tracking of **parcel collisions.**[9] **Scaling of interaction parameters**.

CFD-DEM

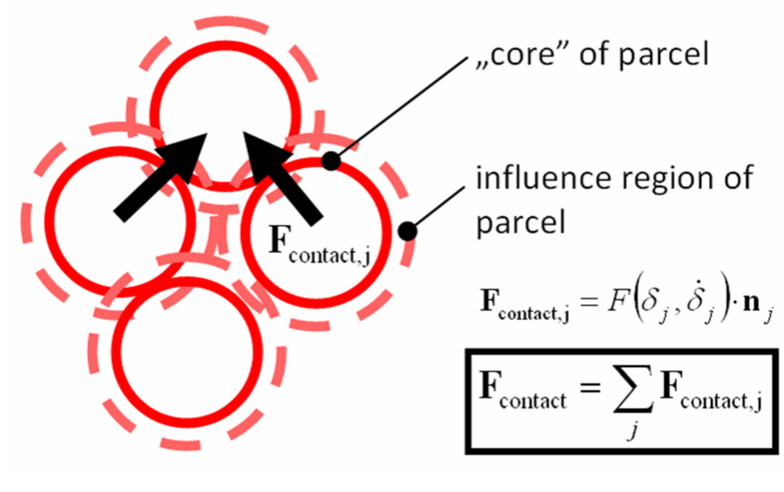
(Zhou et al.,[7] Link et al.[8])

$$\mathbf{F}_{\mathrm{drag}} = \beta_{p,micro} \cdot \left(\mathbf{u}_f - \mathbf{u}_p\right)$$



(CFD-)DPM

(Patankar and Joseph[9])



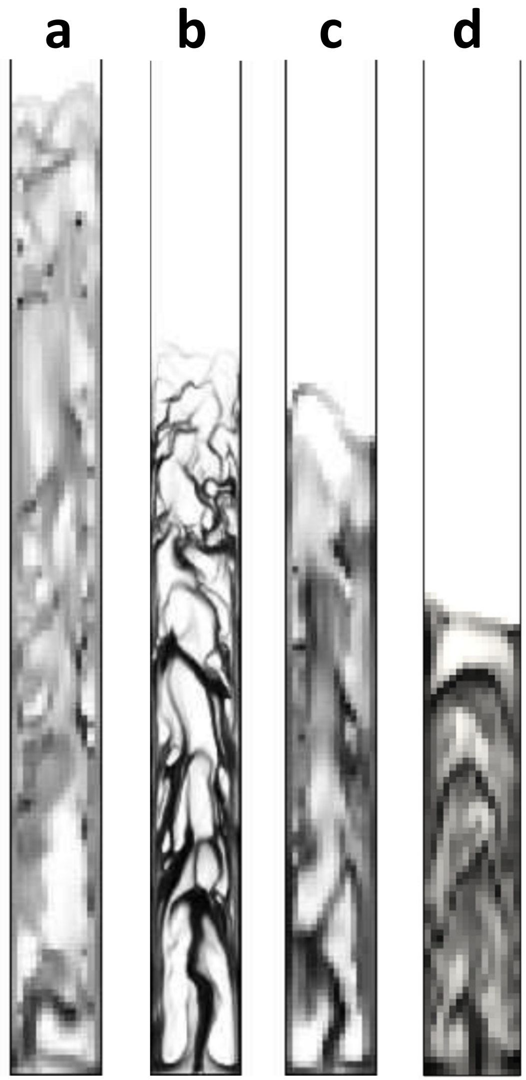
SOFT-SPHERE APPROACH BECAUSE WE WANT TO BE ABLE TO MODEL STICKY PARTICLES!

[7]Zhou et al., ***JFM*** 661 (2010) , [8]Link et al., ***Powder Tech*** 189 (2009), [9]Patankar and Joseph, ***IJMF*** 27 (2001).

Why a New Drag Model?

Well Accepted Facts

- The 'uniformly fluidized state' **is unstable.**[10] A rough estimate for the characteristic cluster size is $L_{ref} = u_t^2 / g$ (ca. **5 mm** for 75 µm particles in air at ambient conditions).
- Instability reflected by **a strong grid-dependency** of simulation results (e.g., slip velocity).
- **Previous work**[11,12] **was based on two-fluid models** (**TFM**s), supplemented with closures from **kinetic theory (KT)** for the particle-phase stress.

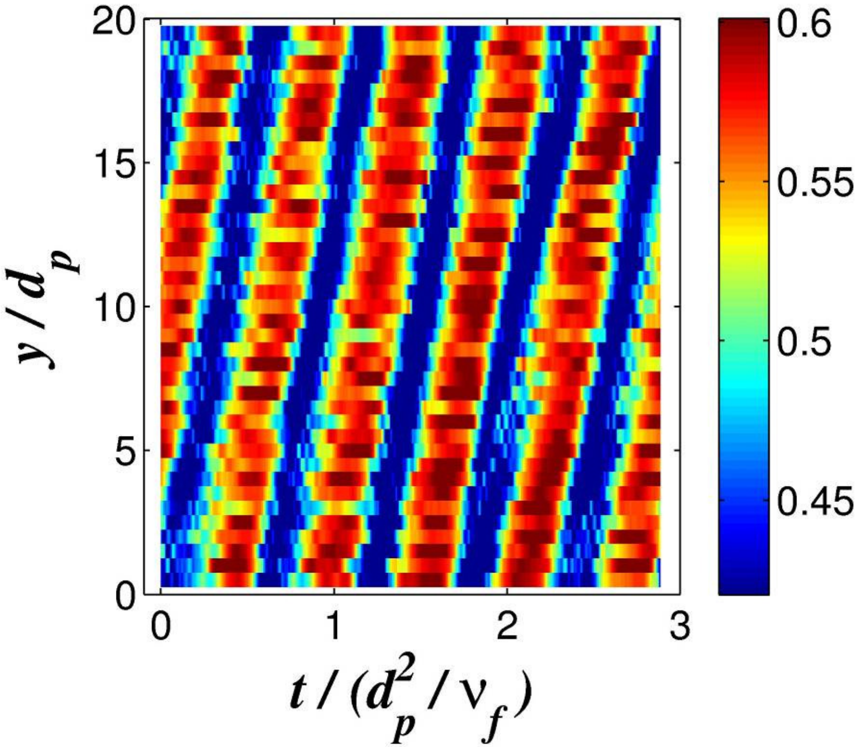


Particle volume fraction distribution in a 3 [cm] wide riser.
a: standard drag model;[12] b: fully resolved;[12] c: Parmentier drag model;[12]
d: Igci drag model,[11] no stress model.

[10]Jackson, ***Trans Inst Chem Eng*** 41 (1963). [11]Igci and Sundaresan, ***I&EC Res*** 50 (2011). [12]Parmentier et al., ***AIChE J*** 58 (2012).

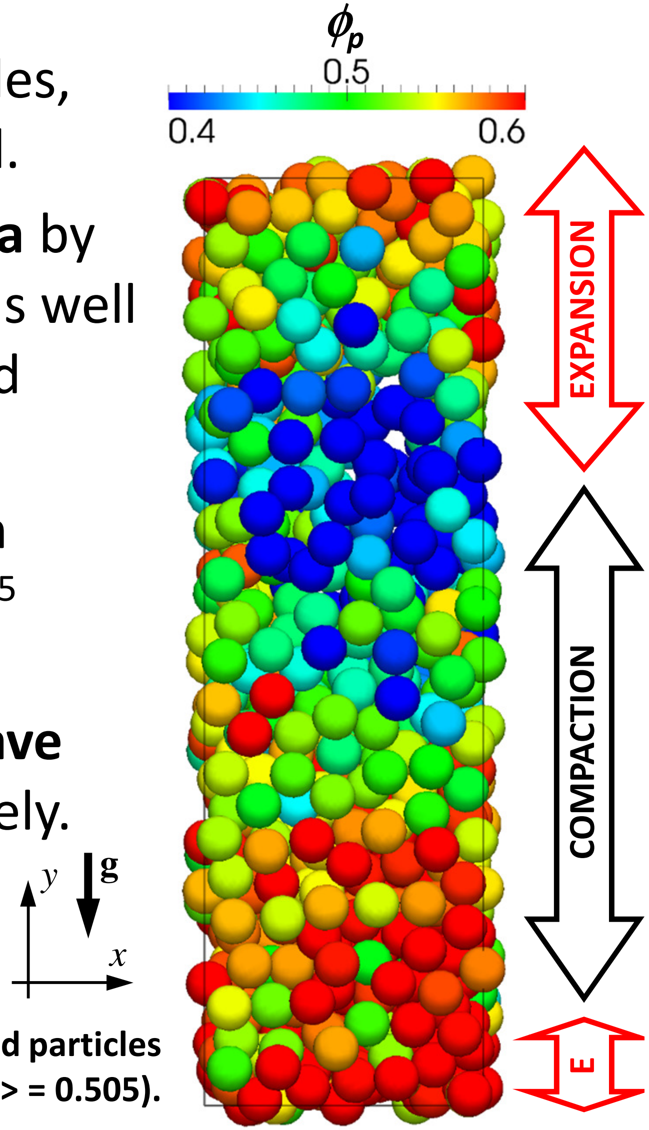
CFD-DEM Validation

- Setup



Space-time plot of the particle volume fraction in a liquid-fluidized bed.

- **685 μm** particles, liquid fluidized.
- **Reference data** by Duru et al.,[13] as well as Derksen and Sundaresan.[14]
- **CFD-DEM** with Beetstra drag[15] predicts **wave profile** and **wave speed** accurately.



Liquid-fluidized particles ($\langle\phi_p\rangle$ = 0.505).

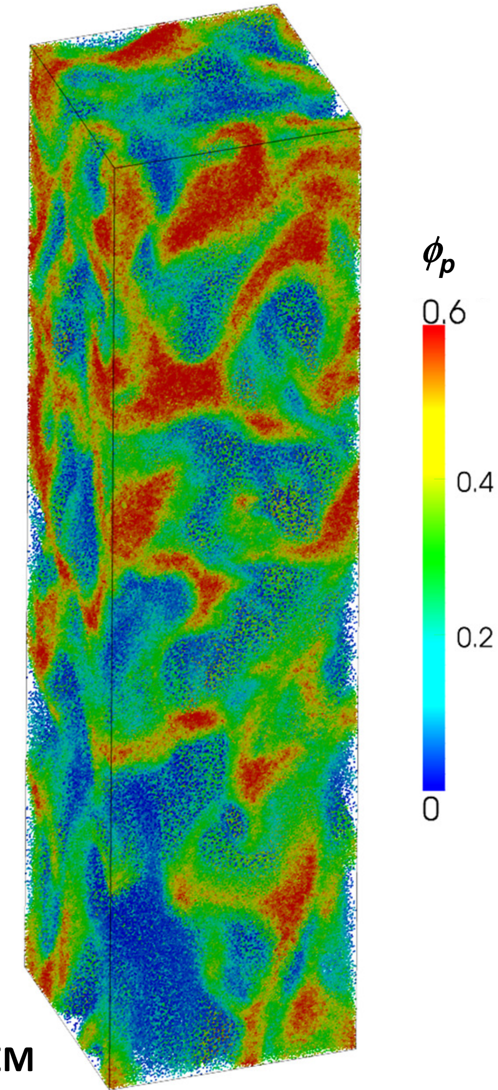
[13]Duru et al., ***JFM*** 453 (2002), [14]Derksen and Sundaresan, ***JFM*** 587 (2007), [15]Beetstra et al., ***AIChE J*** 53 (2007).

Gas-Particle System

- Setup
  - Sedimentation in a **periodic box** (8x32x8 mm)
  - Gas-particle system ($\rho_p/\rho_f \approx 1000$).
  - Low Re system (75 µm; u_t = 0.22 m/s, Re ≈ 1).

- Sensitivity Studies
  - Microscopic drag model (Wen-Yu, Beetstra; stochastic drag model; hydrodynamic torque) — **Small, if normalized**
  - Mapping and interpolation
  - Domain size — **Relevant for overall slip**
  - Fluid grid resolution

Key factor!



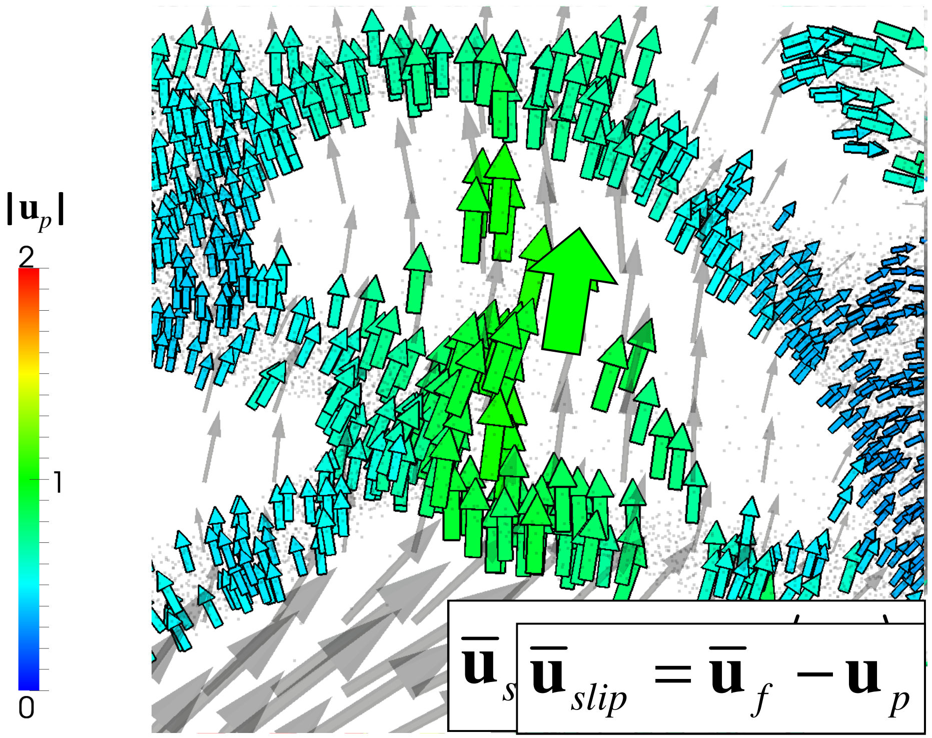
Clustering predicted by CFD-DEM (2.3 · 10^6 particles, <ϕ_p> = 0.25).

Filtered Drag Model

- How do we filter?

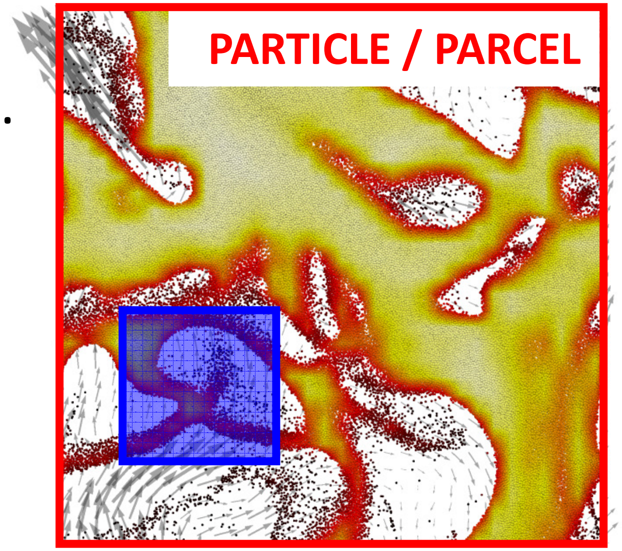
  1 - We define a filtered velocity for the fluid phase.

  2 - We *can* define a filtered velocity for the particle phase (results are based on **CFD-DEM**).



$$\overline{\mathbf{u}}_{slip} = \overline{\mathbf{u}}_f - \mathbf{u}_p$$

Δ_{filter}



$$\overline{\mathbf{u}}_f = \frac{\overline{\mathbf{u}_f \cdot (1-\phi_p)}}{1-\overline{\phi}_p}$$ **fluid**

$$\langle \mathbf{u}_p \rangle = \frac{\sum_{N_p} \mathbf{u}_{p,i} \cdot m_{p,i}}{\sum_{N_p} m_{p,i}}$$ **particles**

Filtered Drag Model

- The Idea Behind "Filtered" Drag

- "Filter-Out" fluid velocity seen by the particle, and compute a **filtered drag coefficient for a single particle.**

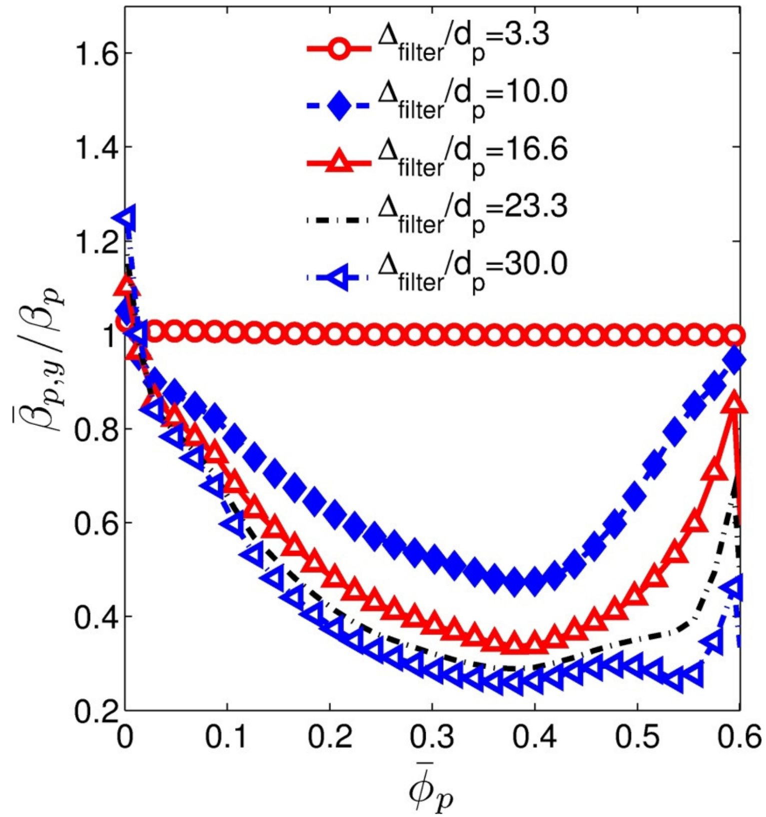
$$\bar{\beta}_{p,i} = \frac{1}{\left.\bar{\mathbf{u}}_{f,i}\right|_{\mathbf{x}_p} - \mathbf{u}_{p,i}} \cdot \left[-\left(\nabla \cdot \left.\boldsymbol{\sigma}_f\right|_{\mathbf{x}_p}\right)_i + \left(\nabla \cdot \left.\bar{\boldsymbol{\sigma}}_f\right|_{\mathbf{x}_p}\right)_i + \beta_p \left(\left.\mathbf{u}_{f,i}\right|_{\mathbf{x}_p} - \mathbf{u}_{p,i}\right) \right]$$

"Fully-resolved" quantities at particle location

Filtered quantities at particle location

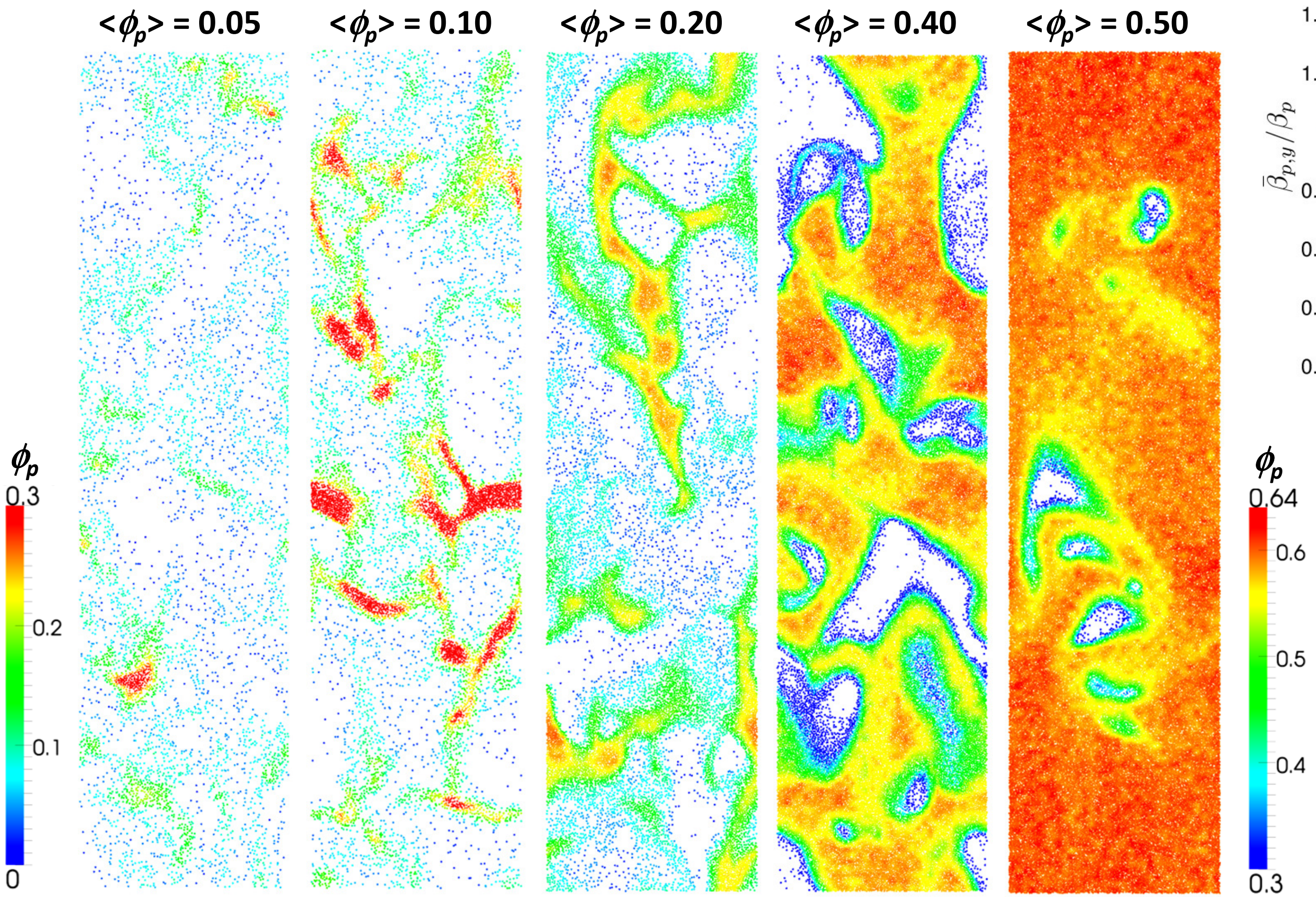
- Filtered Drag - Results

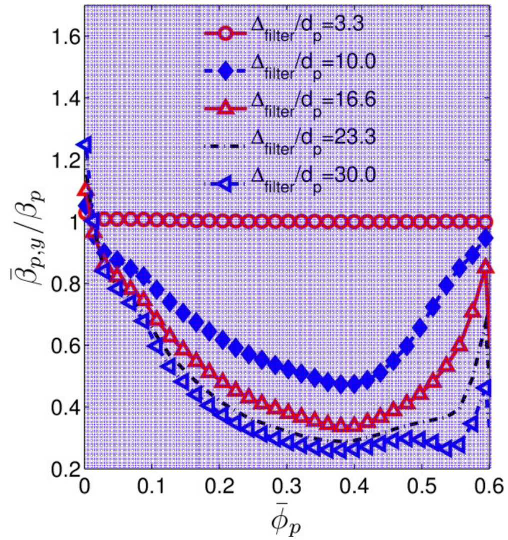
- Clustering leads to a **drag reduction** for $\phi_p > 0.02$.
- The correction is huge (**-75%**).



Filtered Drag Model

- Clustering and its Effect on Drag

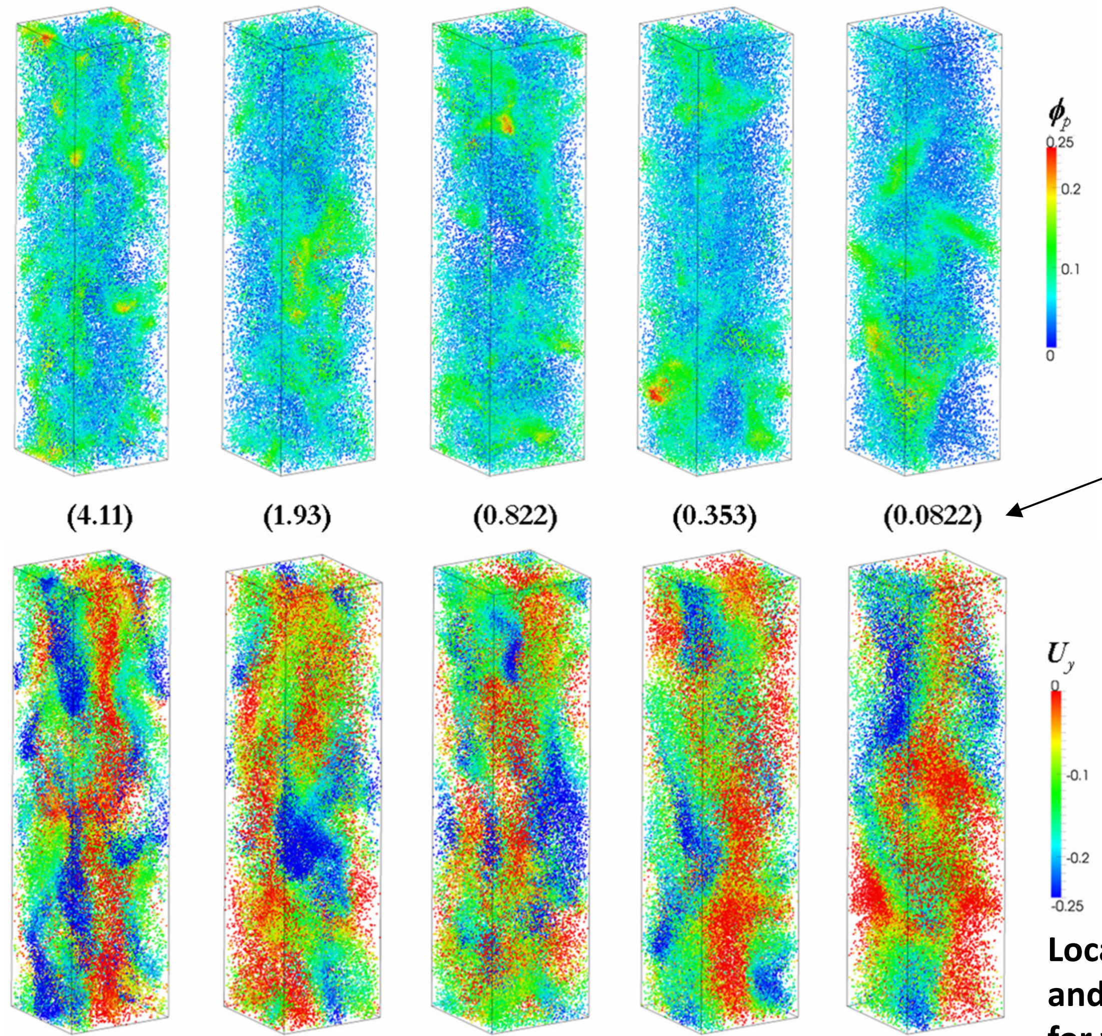




Cross sections showing ca. 1/80th of tracked particles.

Filtered Drag Model

- Reference Length Scale Justification



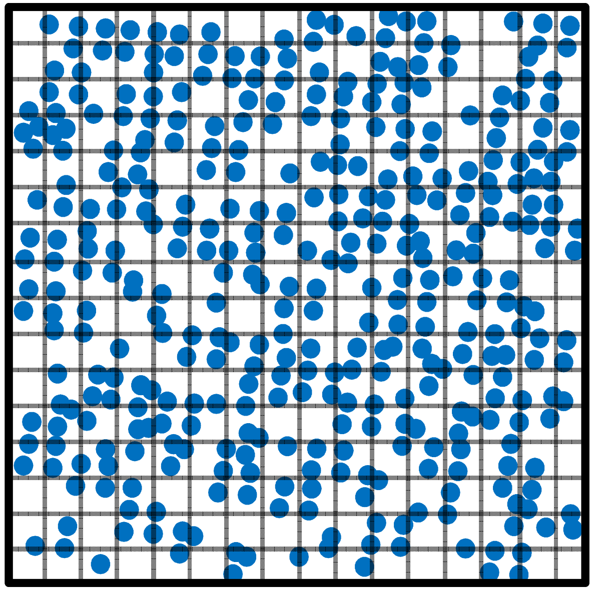
Local particle volume fraction (top row) and vertical particle velocity (bottom row) for various dimensionless domain sizes.

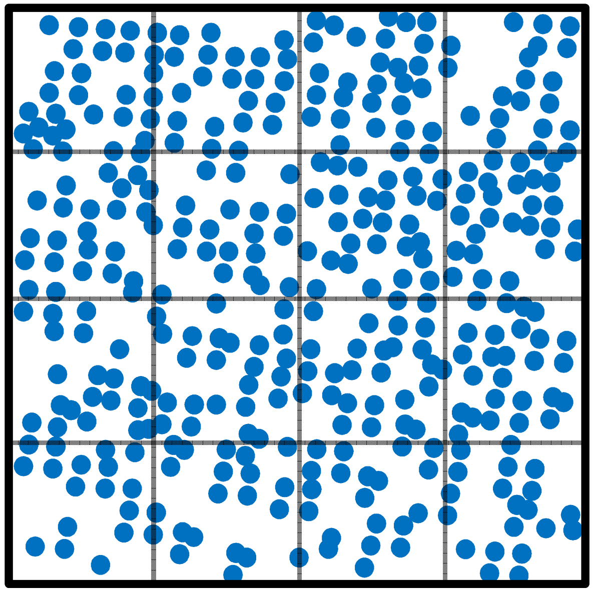
Q: *Does our model also work for systems* ***other than*** d_p ***= 75 μm and Re ≈ 1****?*

…obviously, we should take $L_{ref} = u_t^2 / g$ into account when using a filtered model!

Coarse Grid Simulations

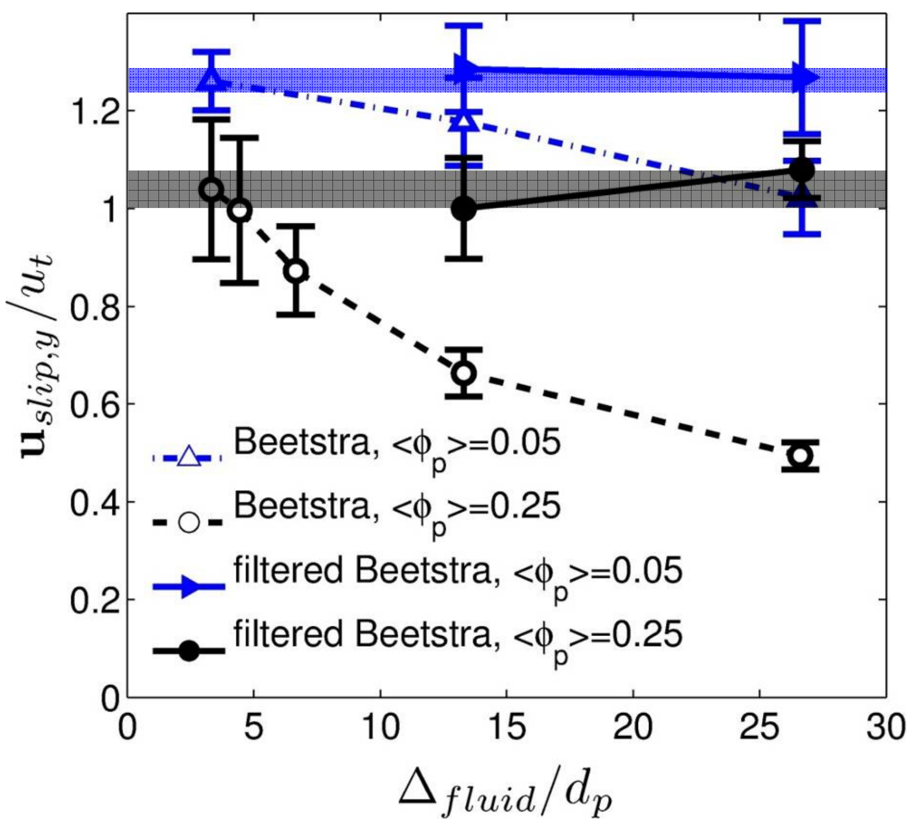
1. **CFD-DEM**
   - Micro-scale drag law
   - **Fine fluid grid**
   - Track **all the particles**
   - Obtain filtered drag law #1
2. **Coarse Grid CFD-DEM**
   - Use filtered drag law #1
   - **Coarse fluid grid**
   - Track **all the particles**





Coarse Grid Simulations

Q4: *Do **CFD-DEM** and **Coarse Grid CFD-DEM** yield the same results?*



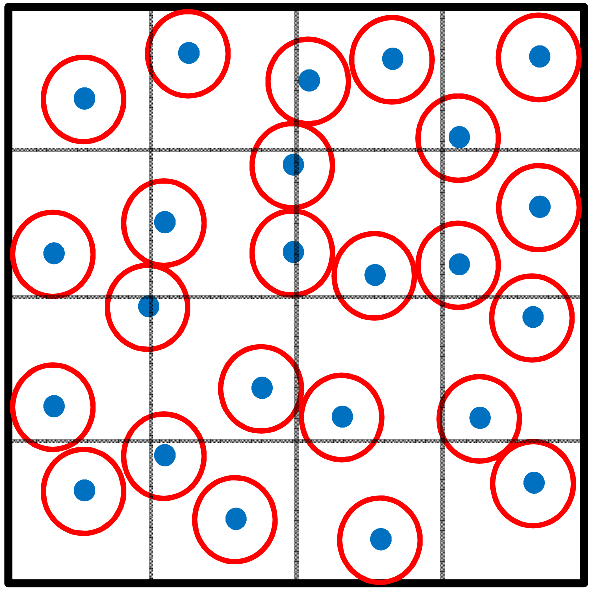
- Large decrease of slip velocity if using **"standard" Beetstra** drag law **(-53% for <ϕ_p>=0.25)**.
- Coarse Grid CFD-DEM with **filtered drag law** is within **+2% (<ϕ_p>=0.05)** and **±3.8% (<ϕ_p>=0.25)** of well-resolved CFD-DEM!

75 µm particles, 8 x 32 x 8 mm domain, 0.46M - 2.32M particles.

Coarse Grid Simulations

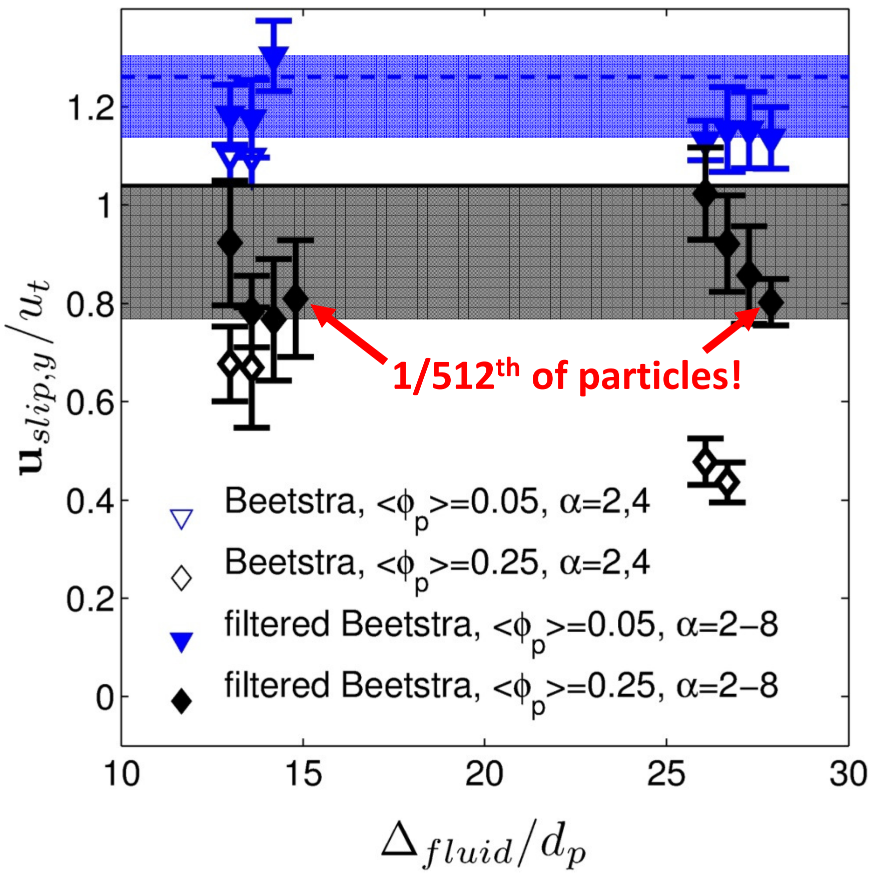
3. CFD-DPM

- Use filtered drag law #1
- **Coarse fluid grids**
- Track **parcels**
- Obtain filtered drag law #2 (future work)



Coarse Grid Simulations

Q5: Do **CFD-DEM** and **CFD-DPM** yield the same results?



- CFD-DPM with **"standard" drag law** significantly under-predicts slip **(-58% for <ϕ_p>=0.25)**.
- **Filtered drag law** improves results, but still significant under prediction: **-22% (<ϕ_p>=0.25)**
- Now, we introduce a correction to **account for parcel size**:

$$c_{corr} = \exp\left[-k\left(\alpha - 1\right)\right]$$

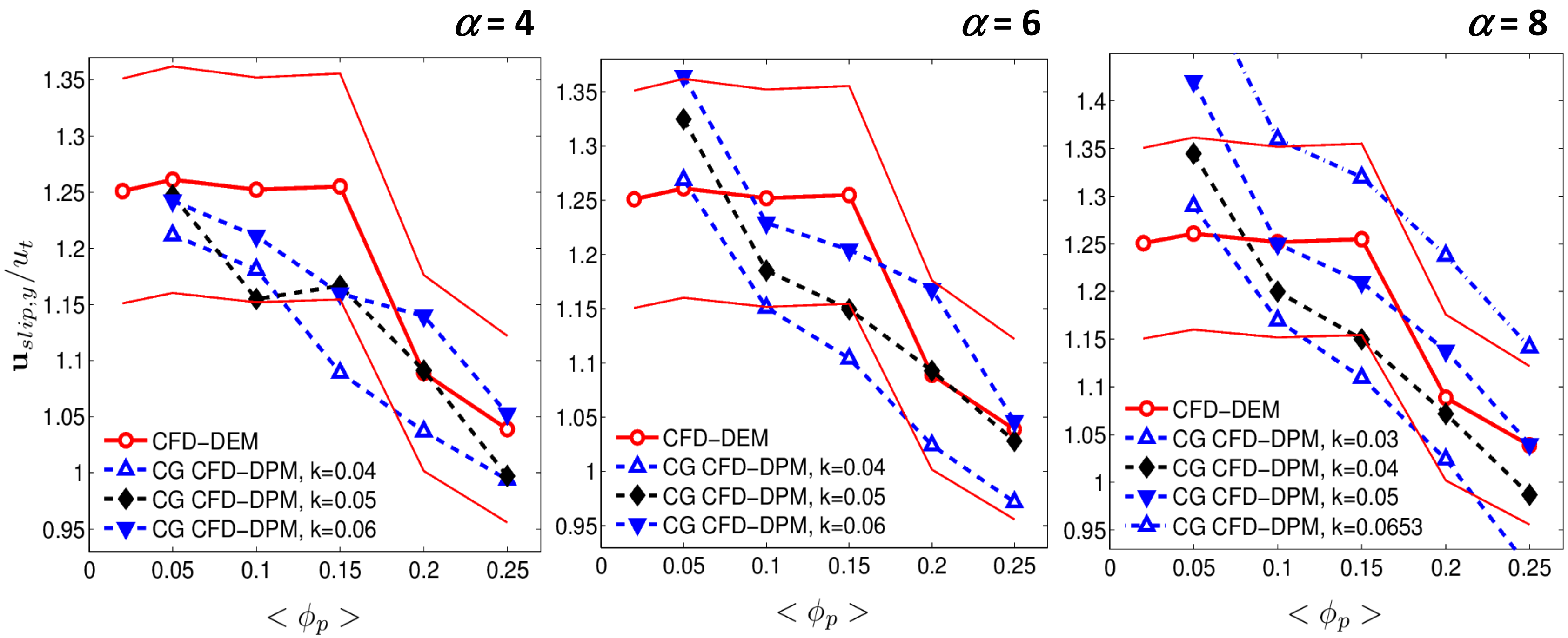
k … model constant.

75 µm particles, 8 x 32 x 8 mm domain, 0.46M - 2.32M particles, pairs of symbols represent result for α=2 (left) and α=4(8) (right), horizontal lines are results for well-resolved CFD-DEM.

Coarse Grid Simulations

Q5: Do **CFD-DEM** and **CFD-DPM** yield the same results?

- Final form of the effective drag model: $$\frac{\bar{\beta}_p}{\beta_{p,micro}} = c_{corr}(\alpha)\left[1 - f\left(F_f, \bar{\phi}_p\right) h\left(\bar{\phi}_p\right)\right]$$
- **Error now within 8% of resolved CFD-DEM:**



Time-averaged slip velocities (filtered drag model) for various parcel sizes and domain-averaged particle volume fractions <ϕ_p> (CG…coarse-grid; thin red line indicate a 8% error corridor around the resolved CFD-DEM data).

Summary

Slip Velocity, Wave Speed and Stress

- **Excellent agreement** of CFD-DEM with **fully-resolved simulation** when looking at **clustering and wave speed**.
- Stress (and particle velocity fluctuations / granular temperature) prediction by CFD-DEM **is more challenging for very dense flows of liquid fluidized beds**. A simple fix (i.e., fluctuating drag coefficient[16]) did not help – artificially **high friction coefficient yielded acceptable results**.

Filtered Drag Model

- **Grid resolution is essential** for intermediate ϕ_p.
- This applies to **particles (DEM) and parcels (DPM)**!
- **CFD-DPM (1/512th of particles tracked!) within 8%** of resolved CFD-DEM.

[16]Kriebitzsch et al., ***AIChE J*** (in press).

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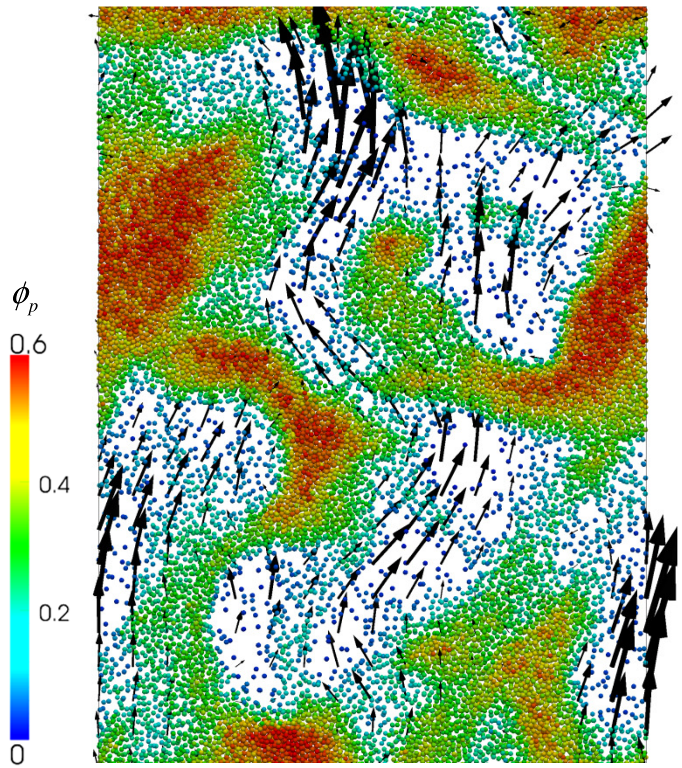
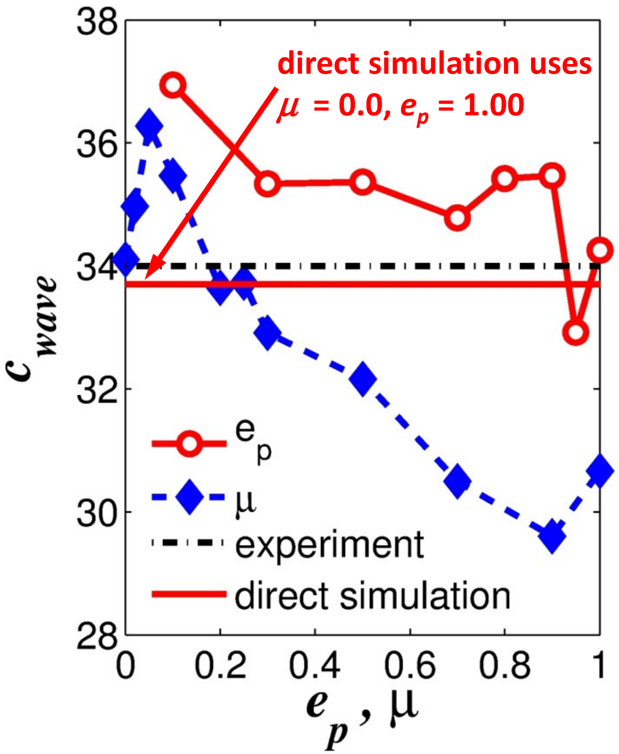


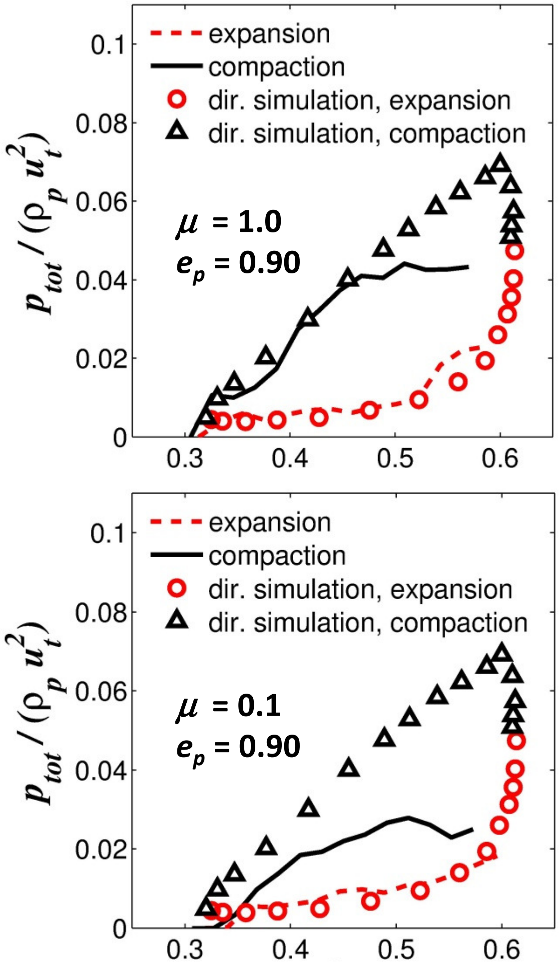
CFD-DEM Validation

- Results



Dimensionless wave speed for various particle interaction parameters (base case: μ = 0.1, e_p = 0.90).

- **Excellent agreement** for the **wave speed.**
- **Stress more challenging.** Good agreement for expansion, however, significant **differences for compaction**.
- CFD-DEM **problematic for extremely dense regions (ϕ_p>0.50)** in liquid-fluidized beds.



Particle-phase pressure for extremely frictional (top) and slightly frictional particles (bottom).

Open Positions

1 PhD Researcher

- Computational Modeling of Gas-Liquid-Solid Processes

5 Master Thesis Students

- Experimental Investigation Wet Powder Processes
- Computational Modeling of Gas-Solid Processes