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Dos and Don’ts

Coarse-Grained Models for Gas-Particle Flow

S. Radl[a]

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with contributions from

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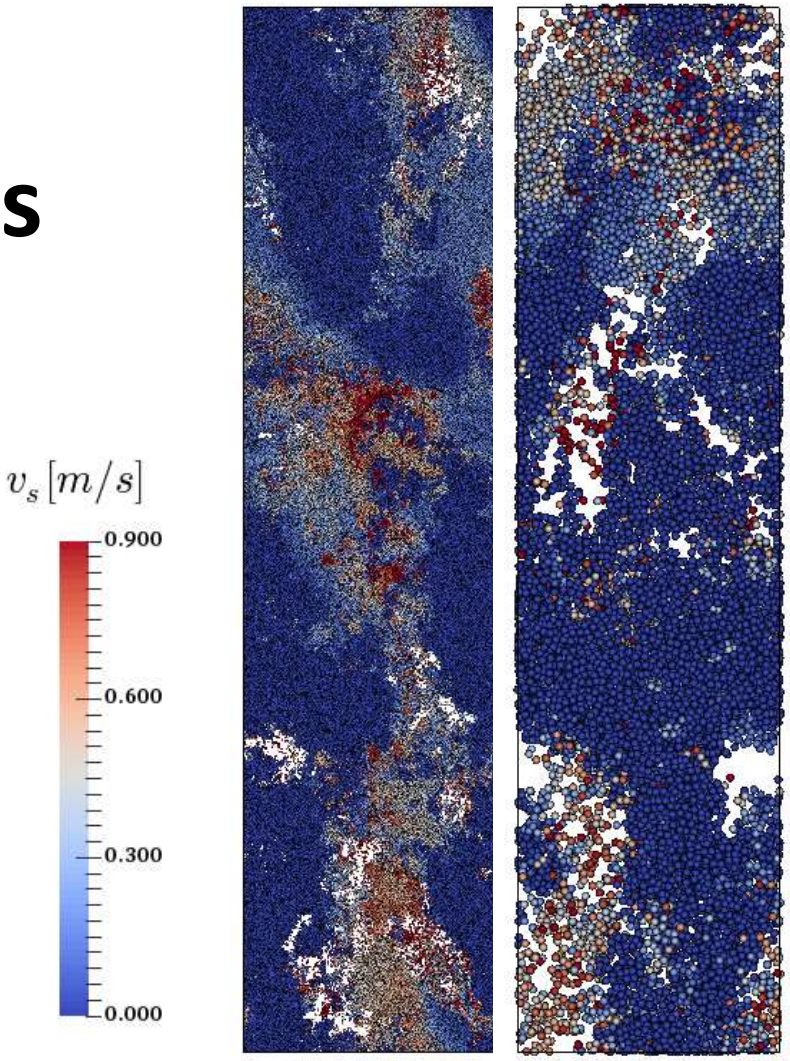
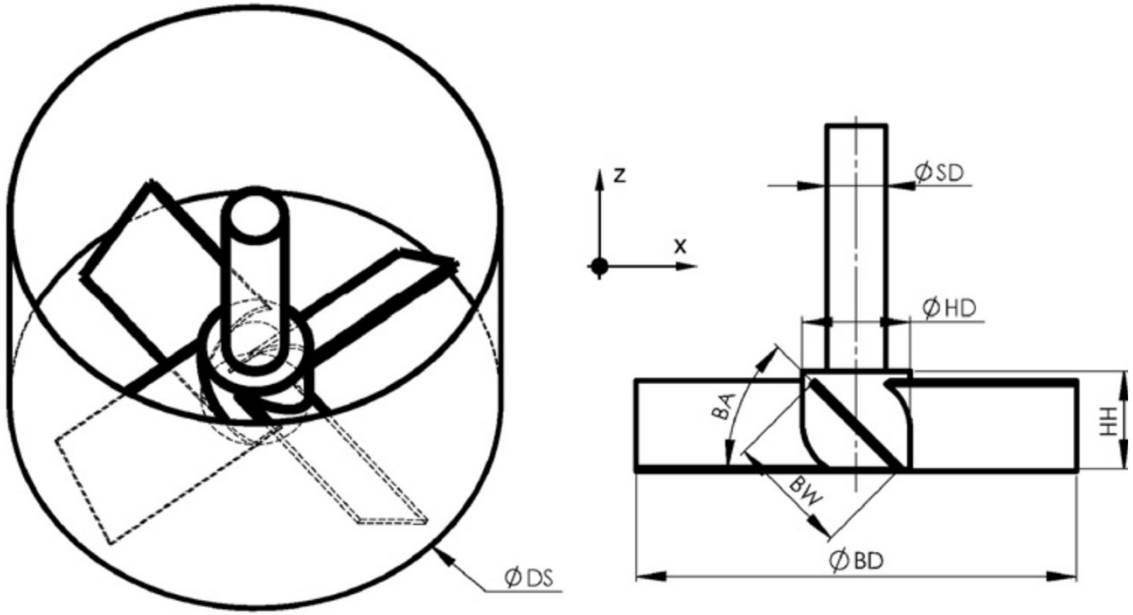
[b]SINTEF (NOR)

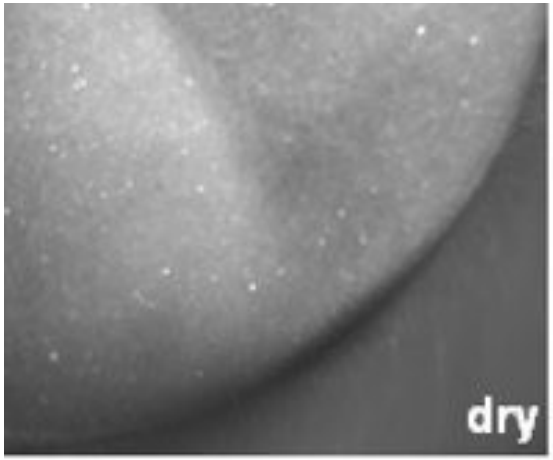


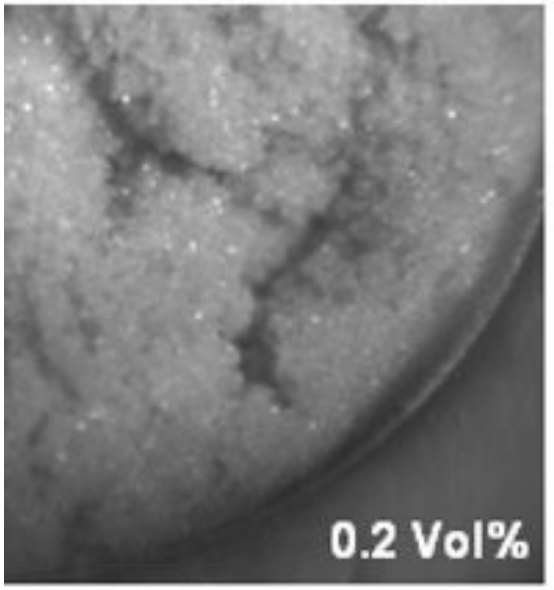
Direct and parcel-based simulation of a cohesive gas-particle mixture

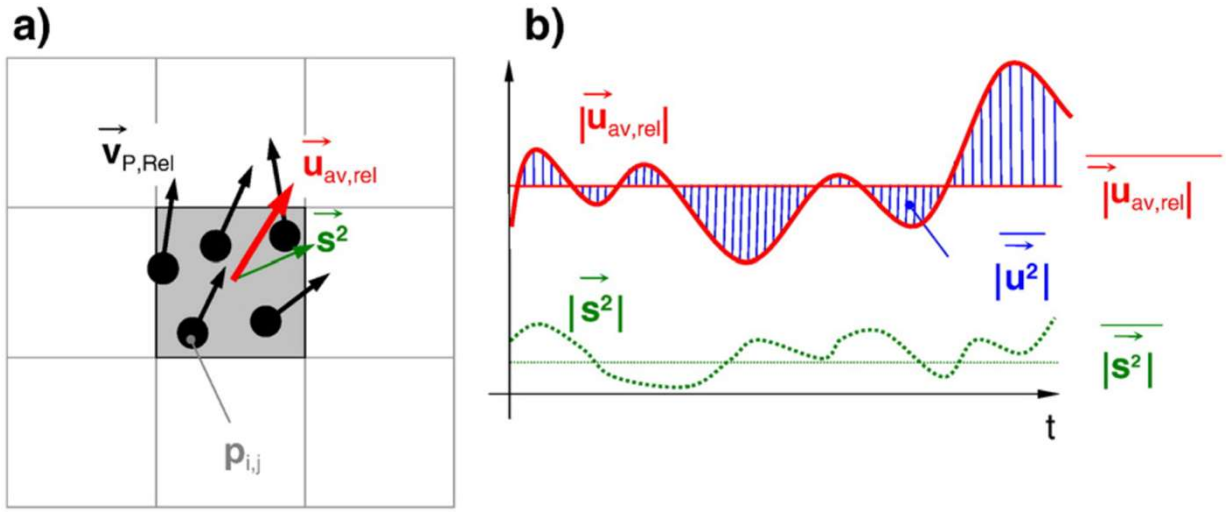
25 minutes speaking time

Why Particles?









Radl et al., Powder Technology 200 (2010) 171–189

Why Particles?

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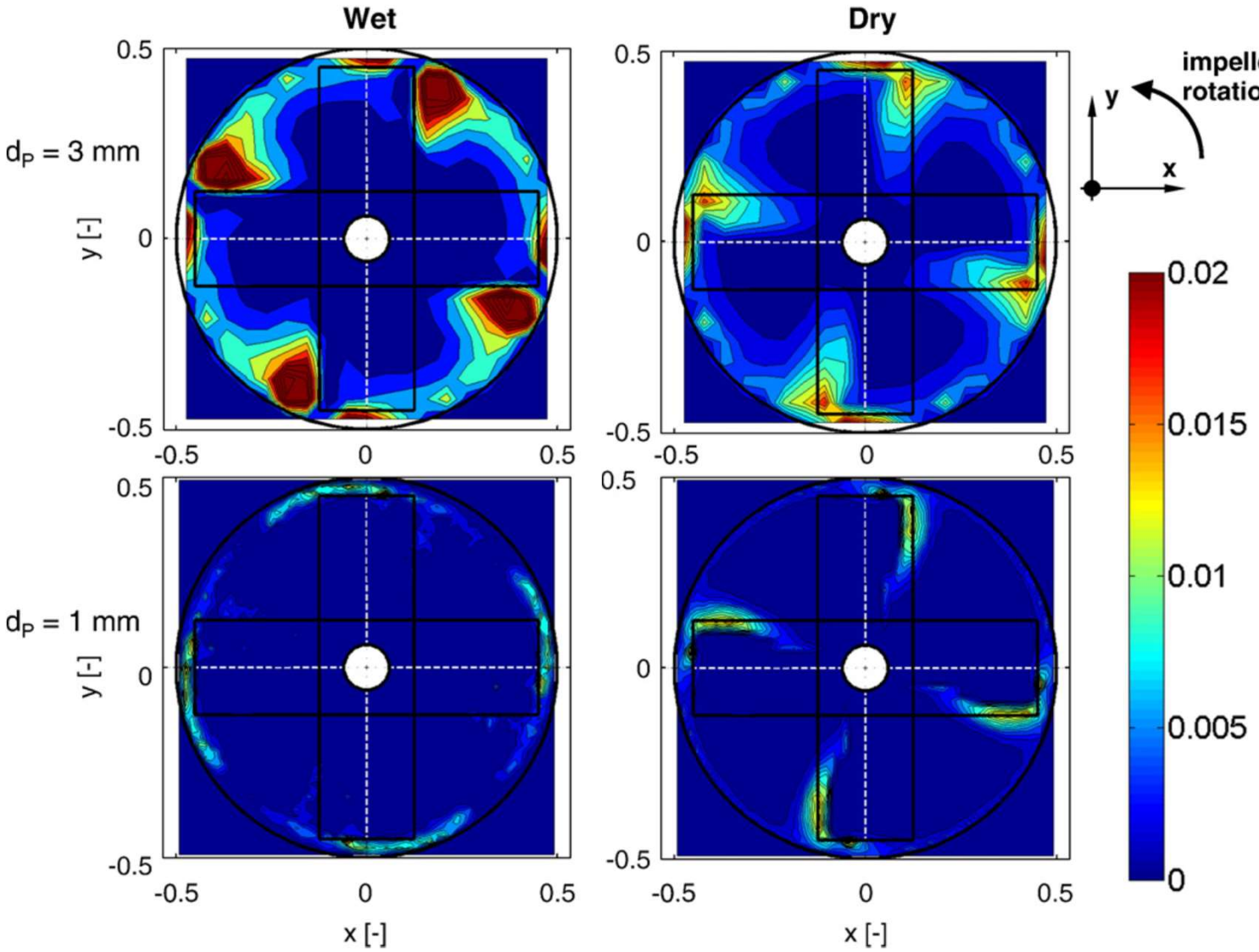
Granular temperature "s^2" for dry and wet granular matter



„wet" means Bo = 11.9

…cohesive force

versus

gravity force

Why Particles?

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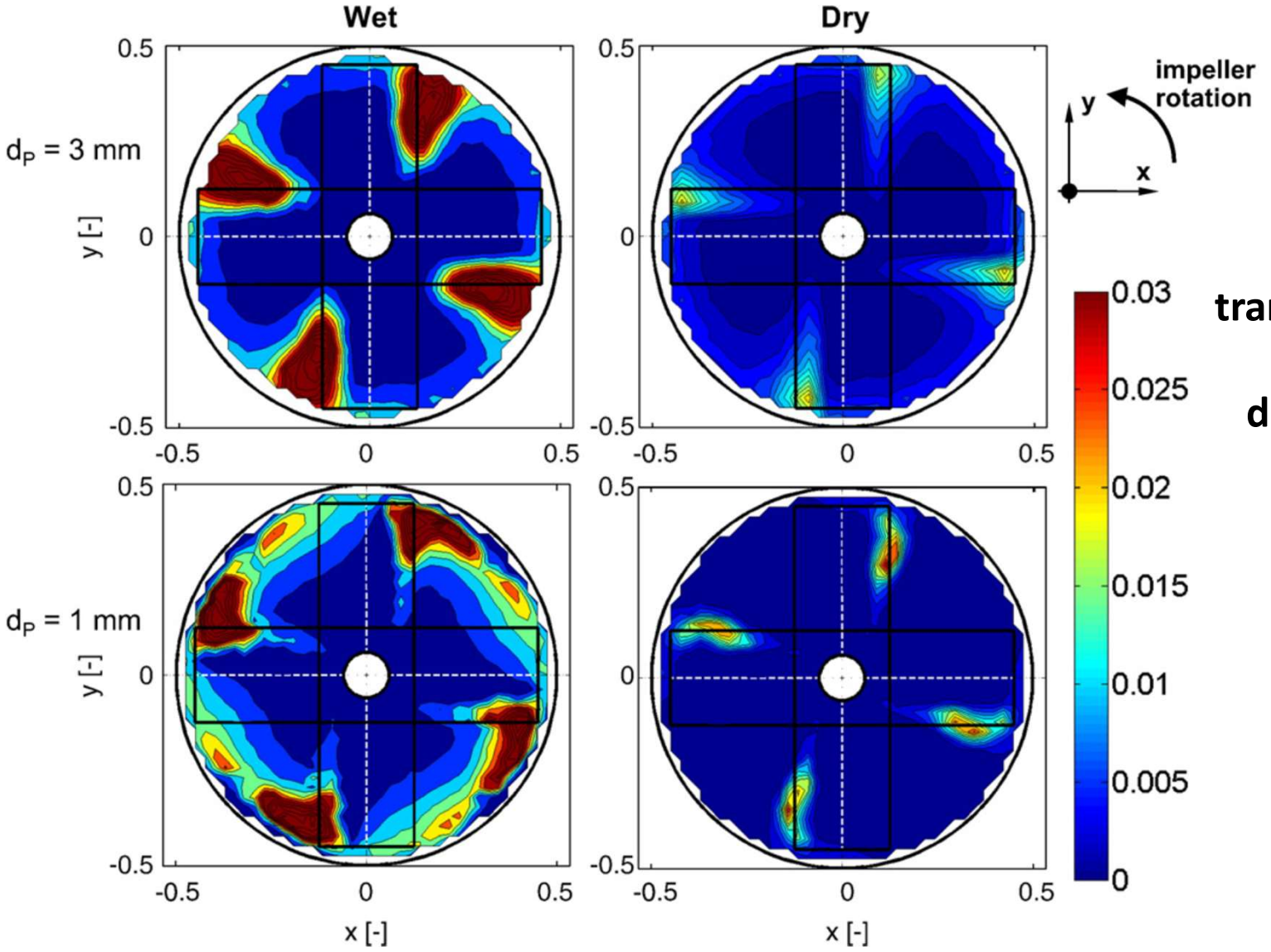
Mean velocity fluctuations "u^2" for dry and wet granular matter



Cohesion INCREASES "meso" transport rates quite dramatically!

Can we develop "meso models" to account for such effects?

Content of this Presentation

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1 - Coarse Graining: A Review

Why do we need parcels?

What is a parcel? What is NOT a parcel?

What is a „filtered model“?

…particle coarsening

…fluid coarsening

2 - Choosing Coarse Graining Parameters

How shall we perform the particle-to-fluid mapping?

The maximum permissible parcel size and cohesion

What happens if the fluid cell size is increased?

3 - Future Improvement of Models & Closures

How shall we account for anisotropy?

What about reactions?

1 - Coarse Graining: A Review

Phenomena to be modelled

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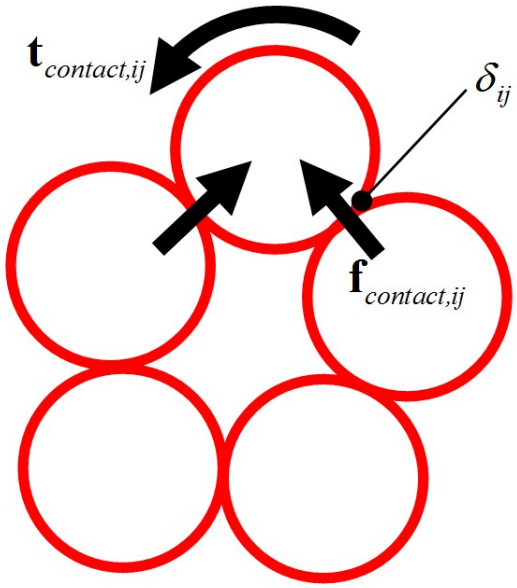
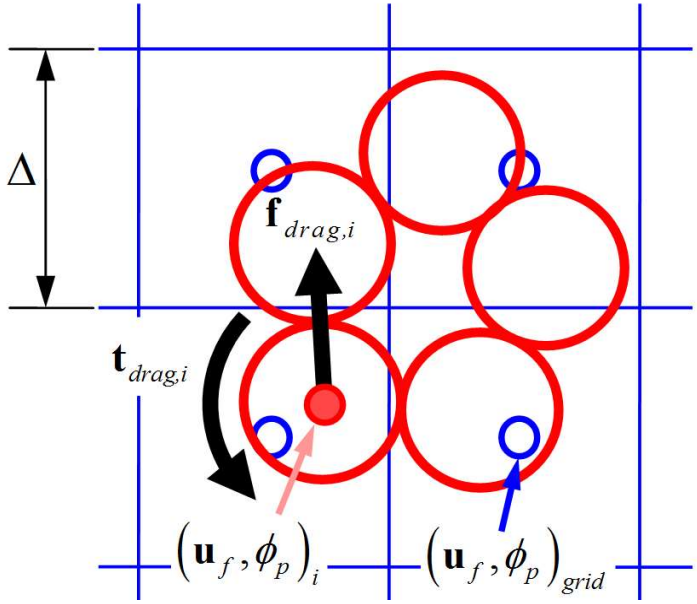
Flow

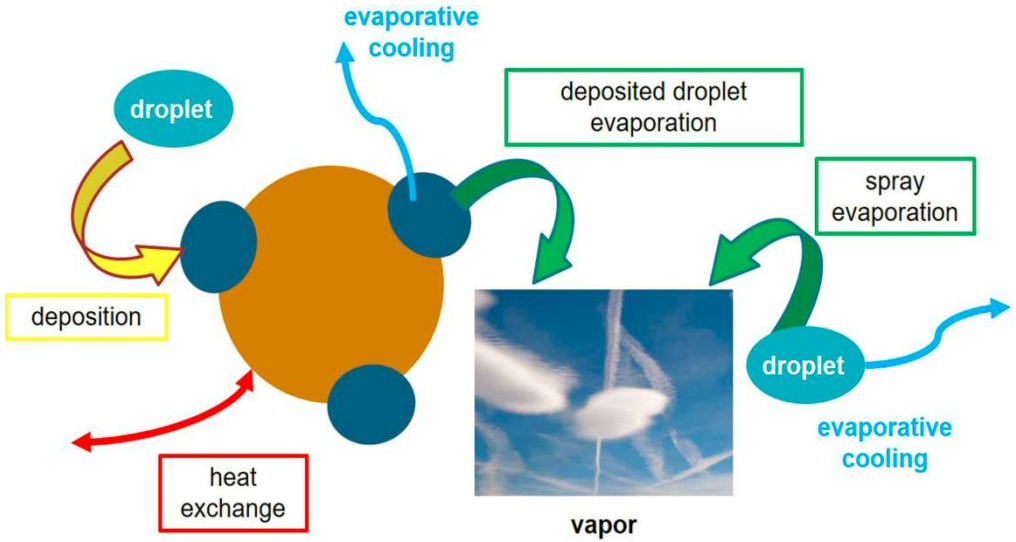
- **Particles**: Contact + cohesive forces and torques
- **Fluid & Fluid-Particle interaction**: (drag) forces and torques





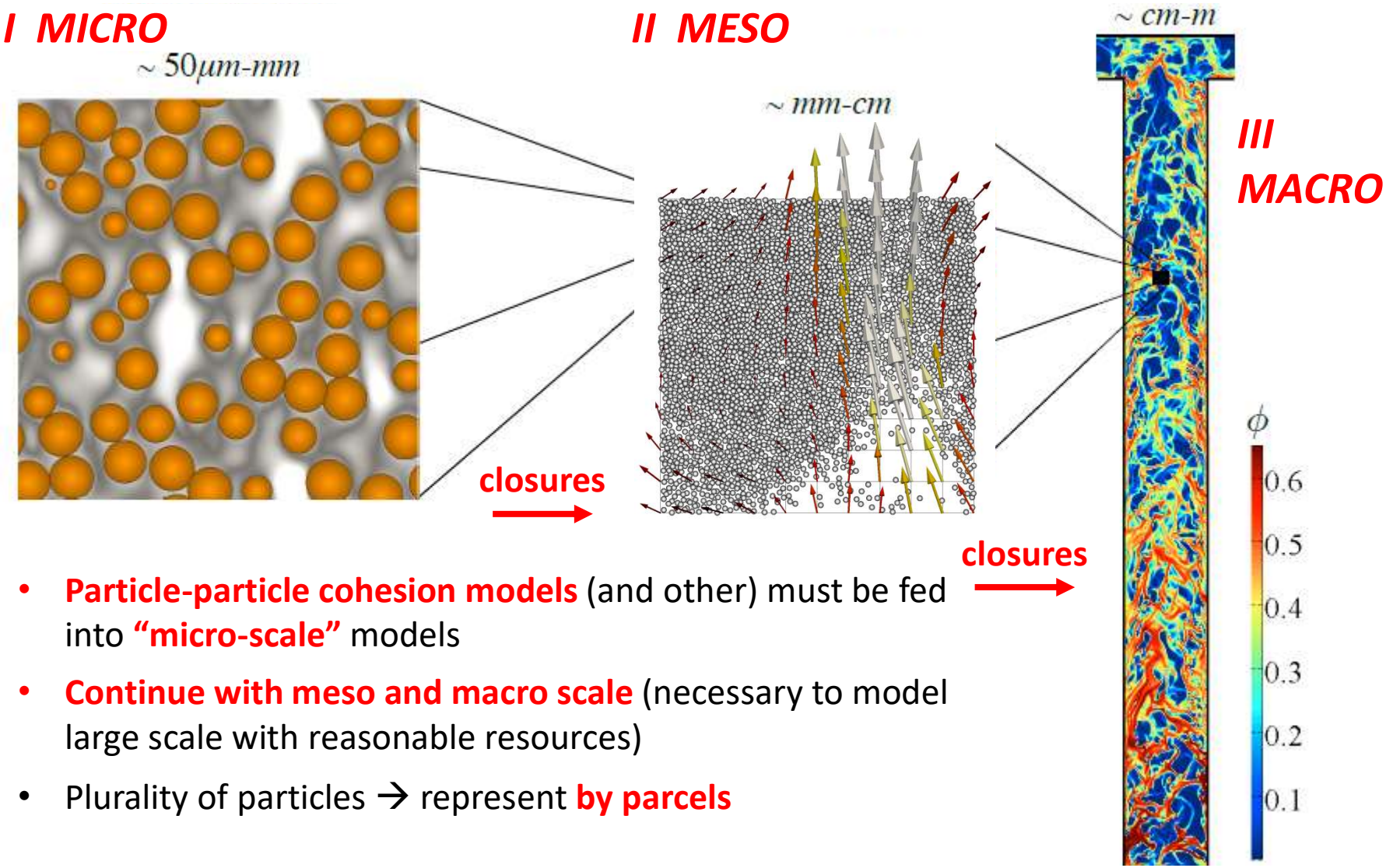
Scalar Transport

- Heat and mass transfer rates ***(fluid and particle phase)***
- Filtration rates
- Dispersion rates ***(fluid and particle phase)***
- ***Reactions***



Askarishahi et al., *AIChE J* (2017) 63:2569-2587

Phenomena to be modelled

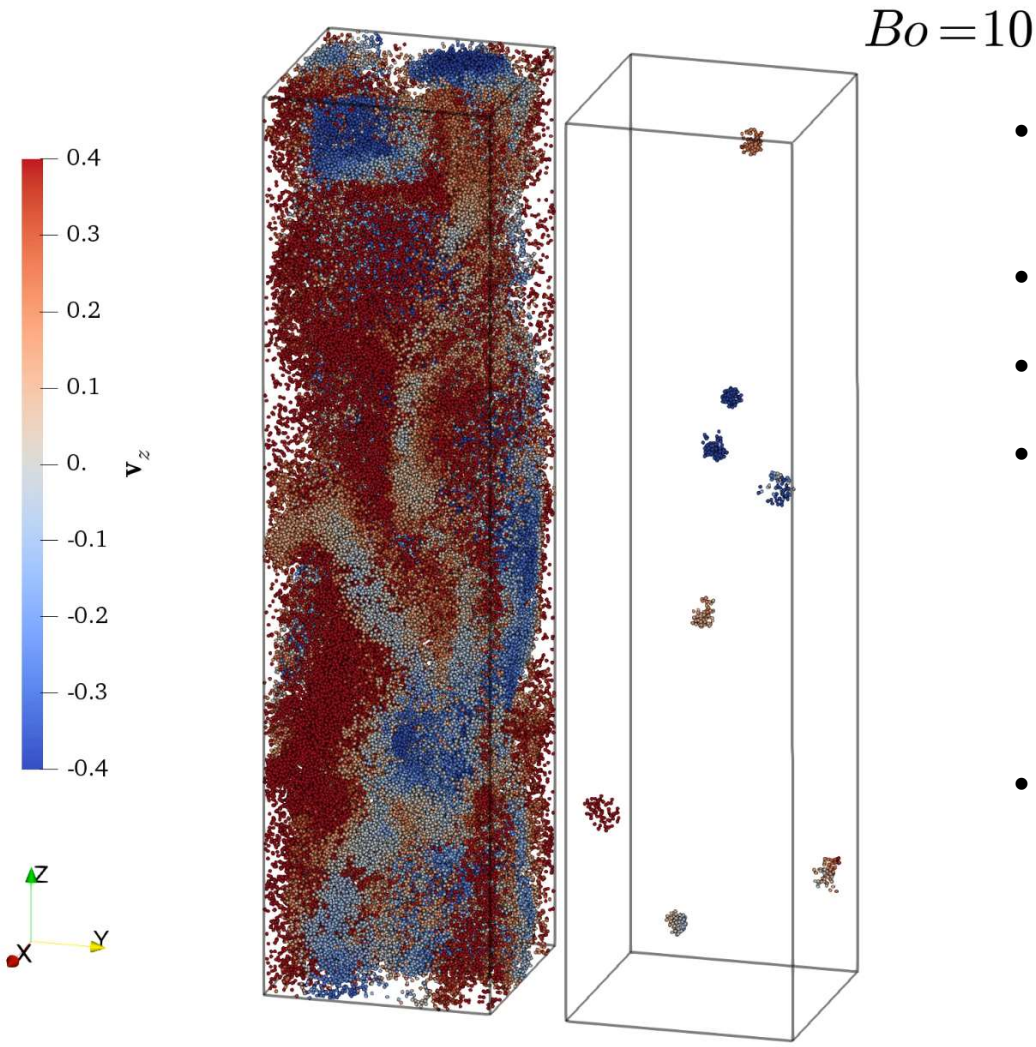


- **Particle-particle cohesion models** (and other) must be fed into **"micro-scale"** models
- **Continue with meso and macro scale** (necessary to model large scale with reasonable resources)
- Plurality of particles → represent **by parcels**

Holloway, PhD Thesis, 2012.

The Parcel

Visualization of what can be interpreted as a "parcel"



- „Particle filtering" considering a particle oarse graining ratio **CG = 4**
- Parcels **expand and contract**
- Parcels **"collide gently"**
- Particles have a different speed, i.e., an **"intra-parcel" fluctuation $v''_{p,i}$ of particle speeds exists**:

$$v''_p = v_p - \widetilde{v_p}$$

- Thus, parcels develop a **kinetic stress (pressure):**

$$\Sigma_{p,meso} = \rho_p \overline{\alpha_p \vec{v}_p'' \vec{v}_p''}$$

The Parcel

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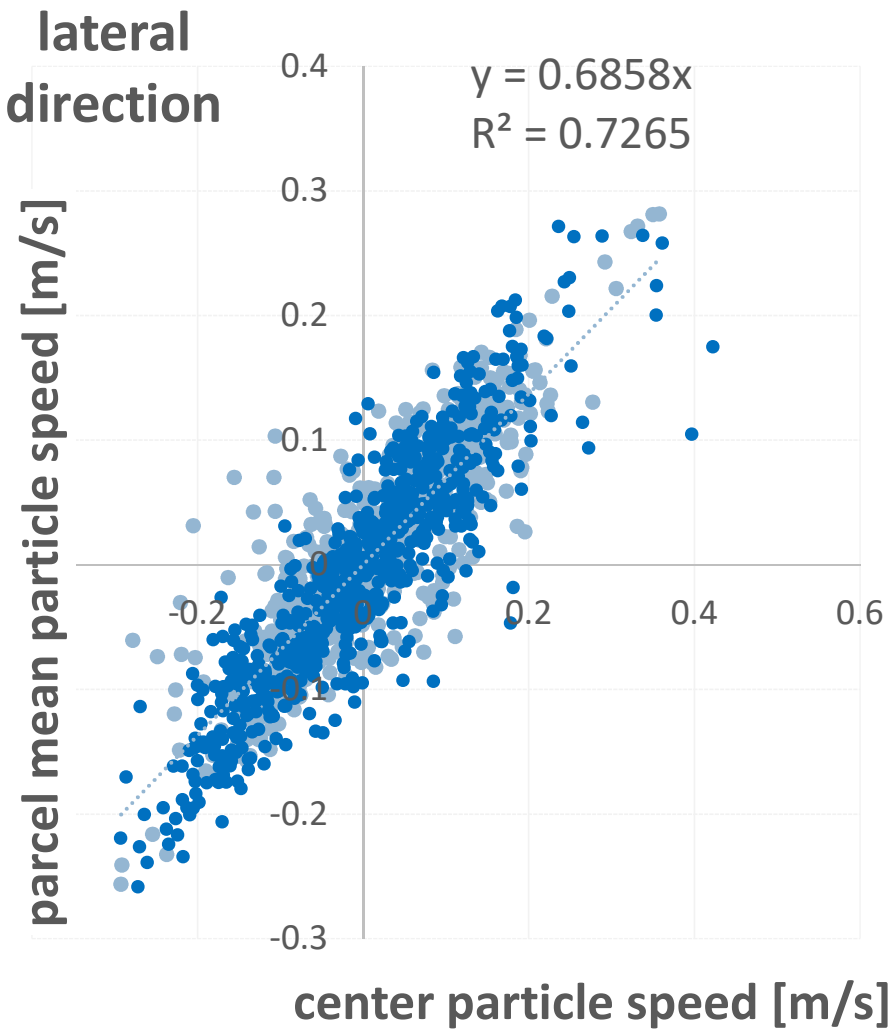
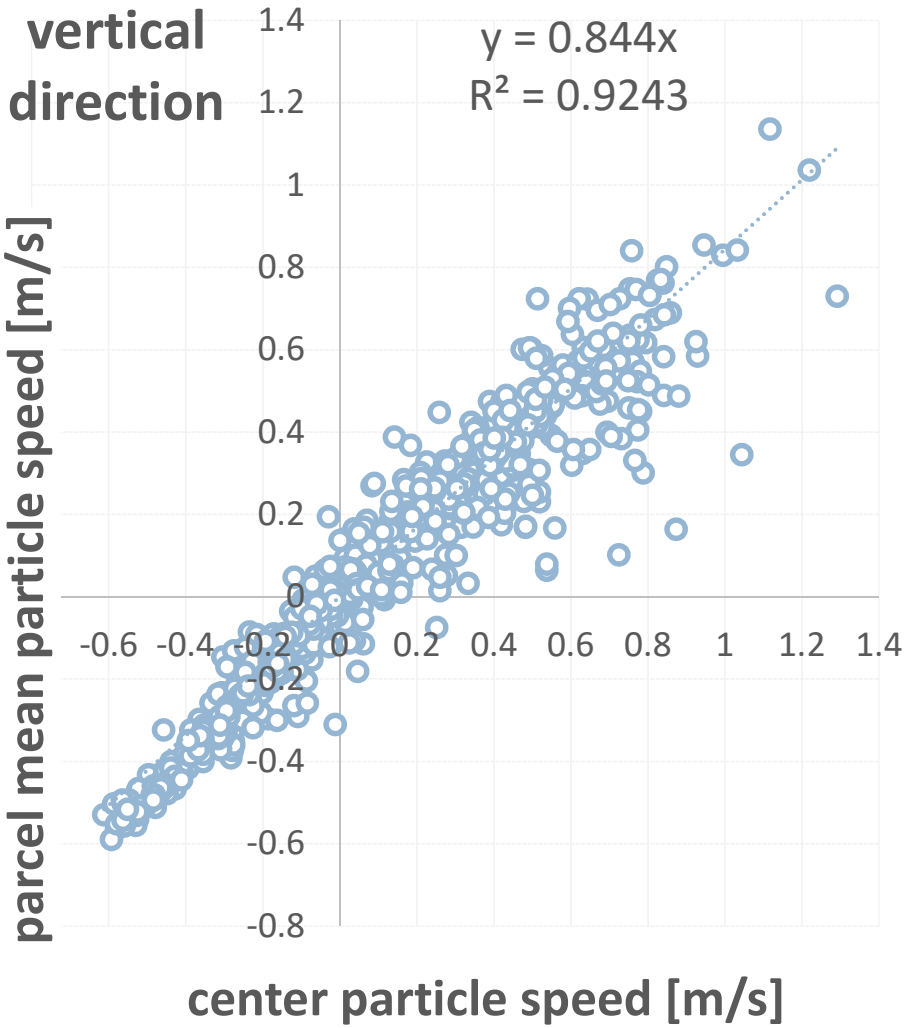
Key observation: strong anisotropy of “intra parcel” velocity fluctuations

Non-cohesive (Bo = 0, CG = 4)





The Parcel

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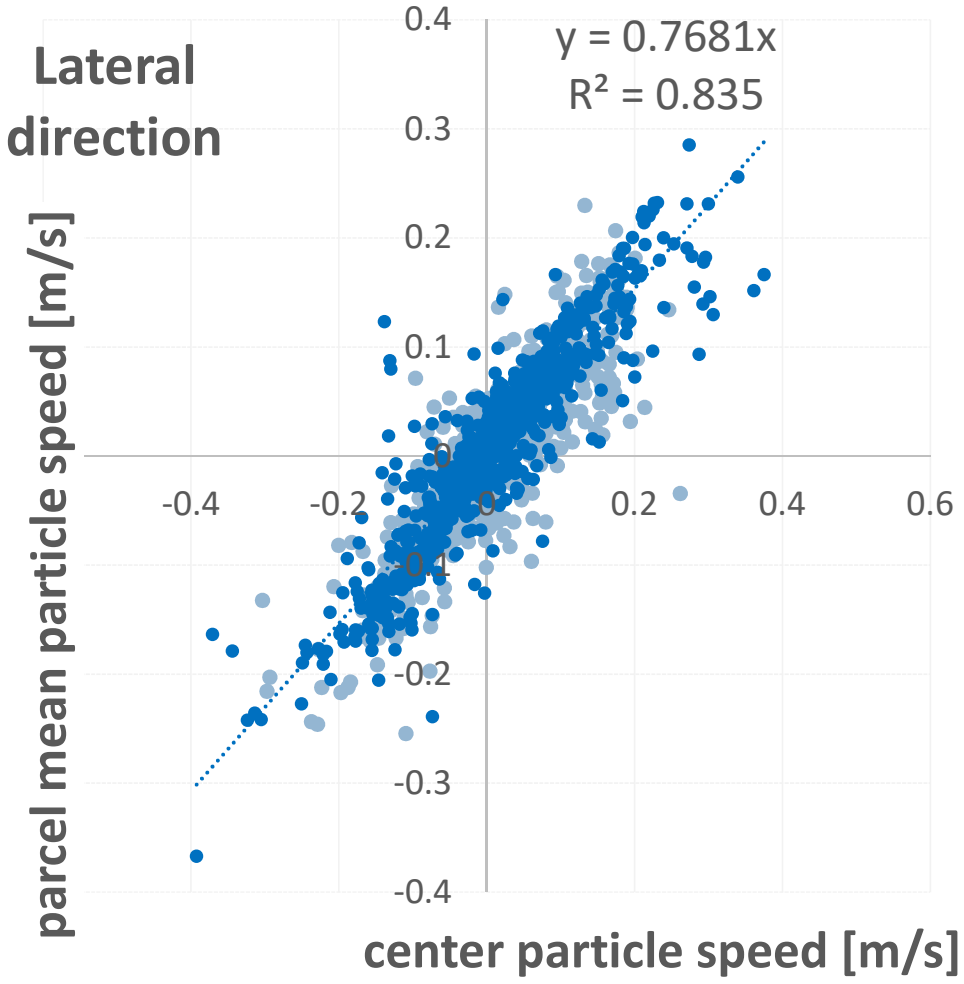
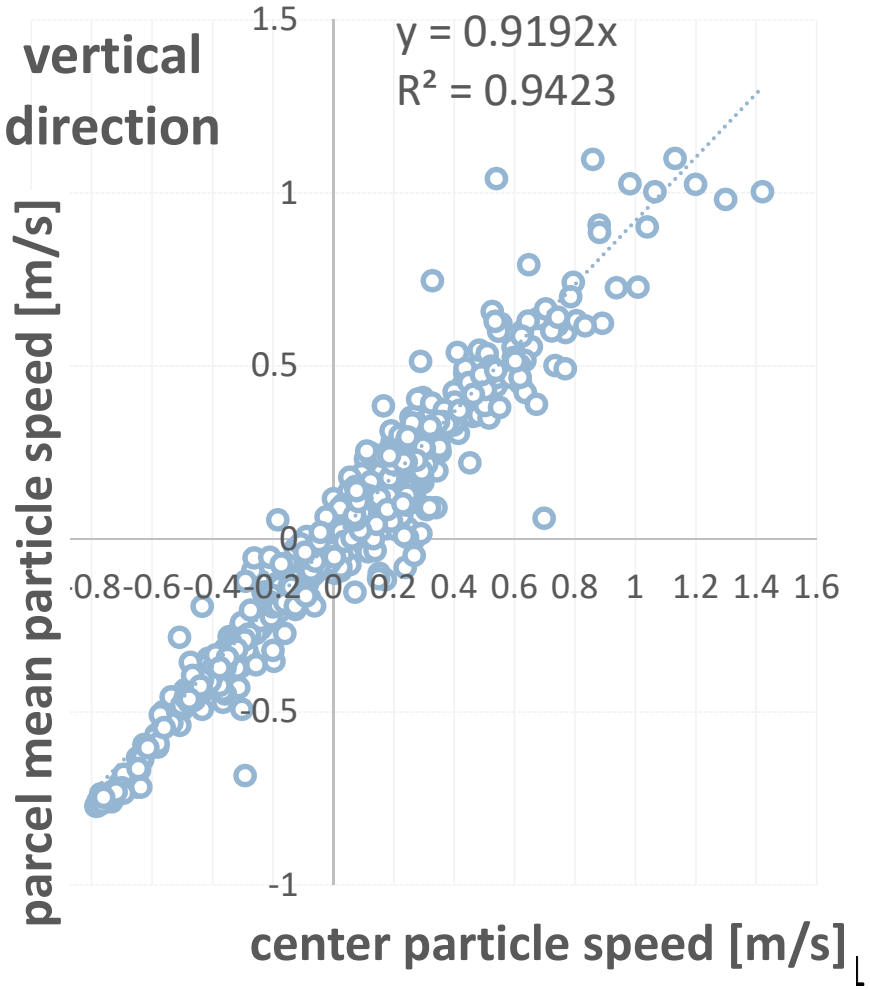
Key observation: cohesive flow shows higher coherence in particle speeds

Bo = 10, CG = 4





The Parcel

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A parcel:

- *is a way to* ***approximate an ensemble*** *of particles*
- *represents a* ***fixed number of particles*** *(the „statistical weight“ is fixed)*
- *approximates the* ***average particle motion*** *at a certain point in space*

A parcel CANNOT:

- *represent a fixed SET of particles, since* ***particles „move into and out“ of a parcel***
- *be used* ***directly prediction particle-particle collisions***
- *be assumed to be of* ***fixed size*** *(spatial extension)*

The Parcel

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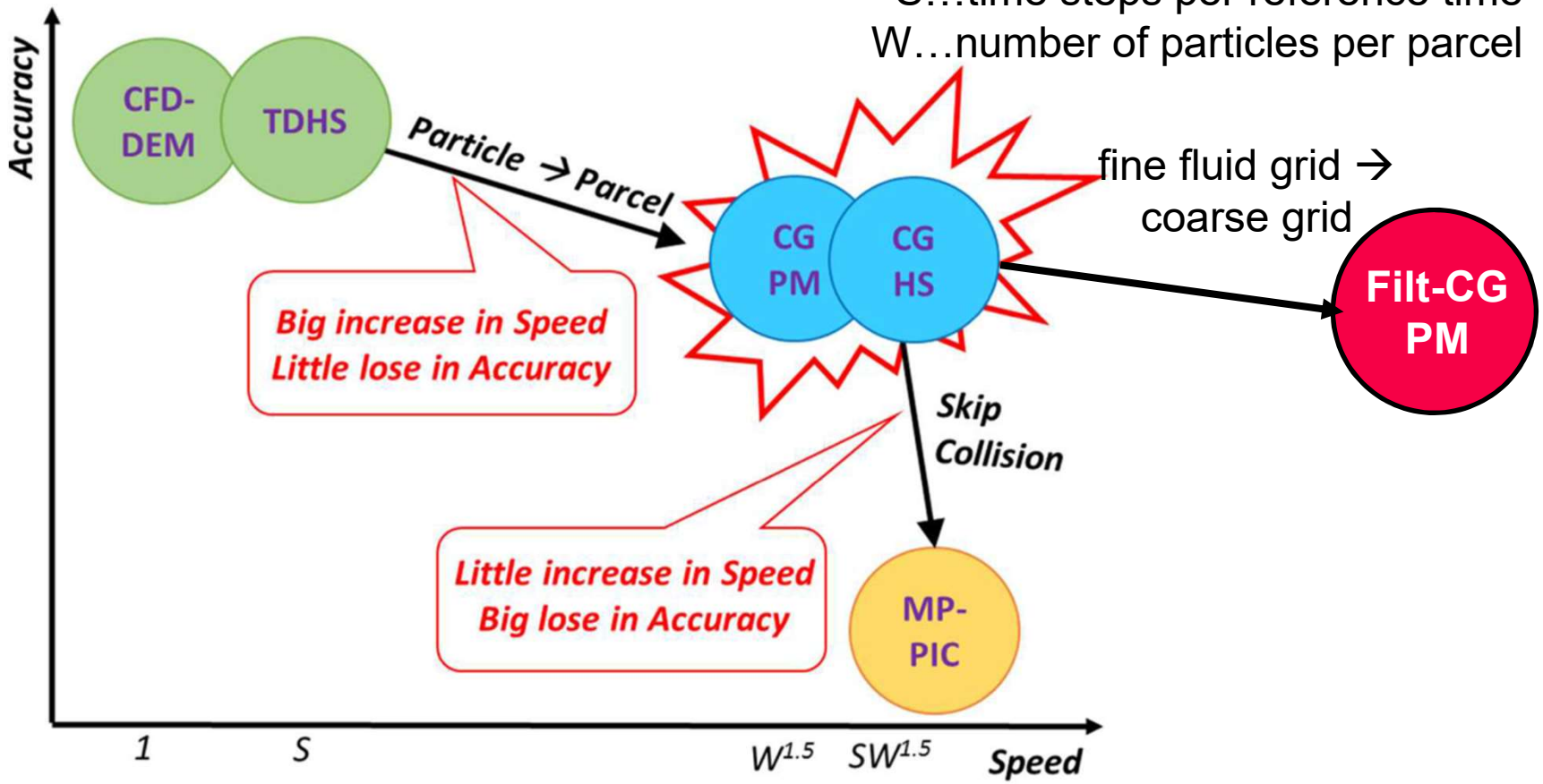
What people made out of it: the map of parcel modeling approaches

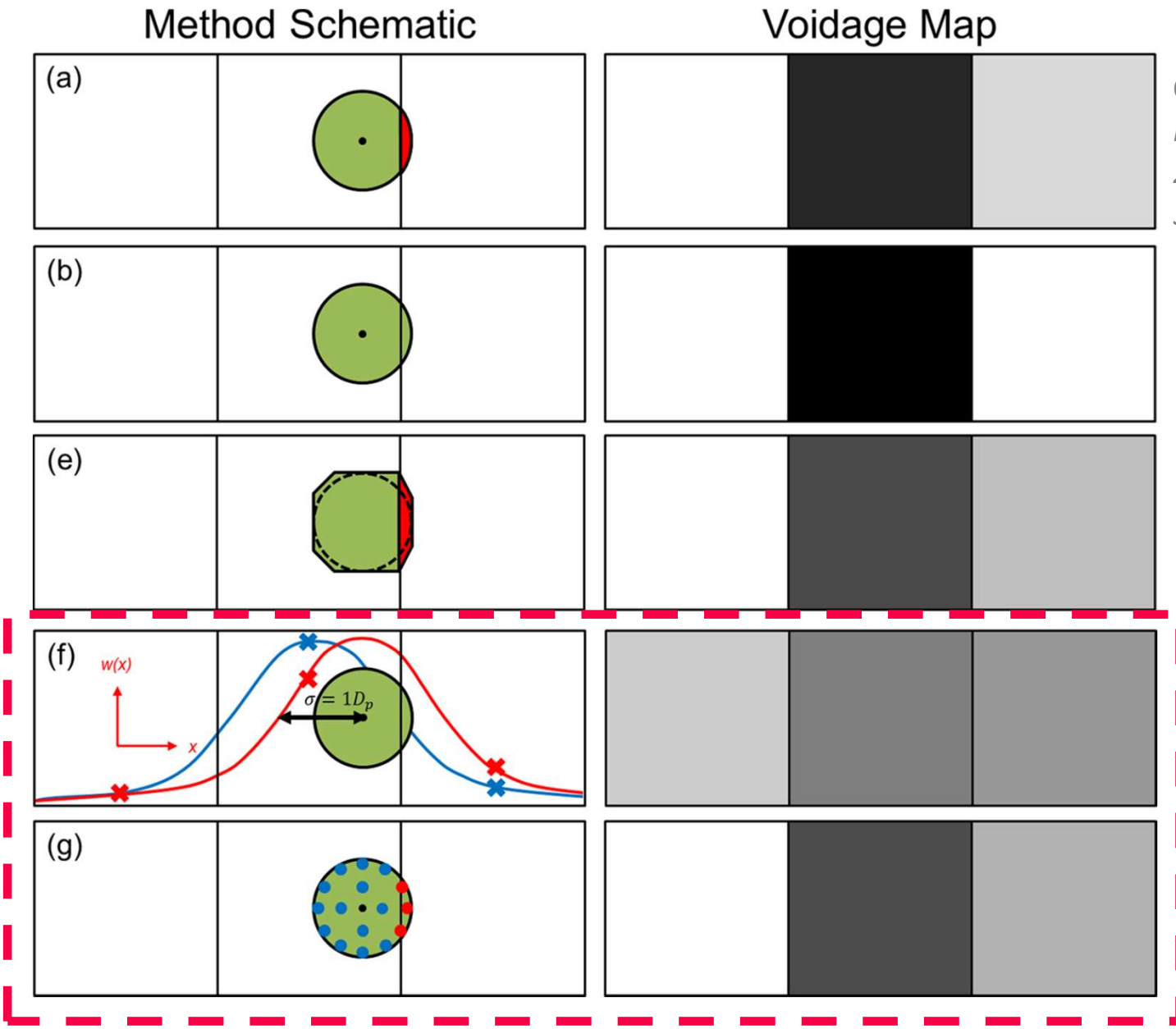
TDHS = time-driven hard sphere
CGPM = coarse-grained particle method
Filt-CGPM…Fluid-filtered CGPM
MP-PIC = multiphase particle-in-cell
S…time steps per reference time
W…number of particles per parcel



Adopted from Lu et al., Ind. Eng. Chem. Res. 2017, 56, 7865−7876

2 - Choosing Coarse Graining Parameters

Fluid-To-Particle Mapping



Clarke et al., *Ind. Eng. Chem. Res. 2018, 57, 3002−3013*

We use a combination of this schemes with a „diffusion length“ L_{smooth}

Fluid-To-Particle Mapping

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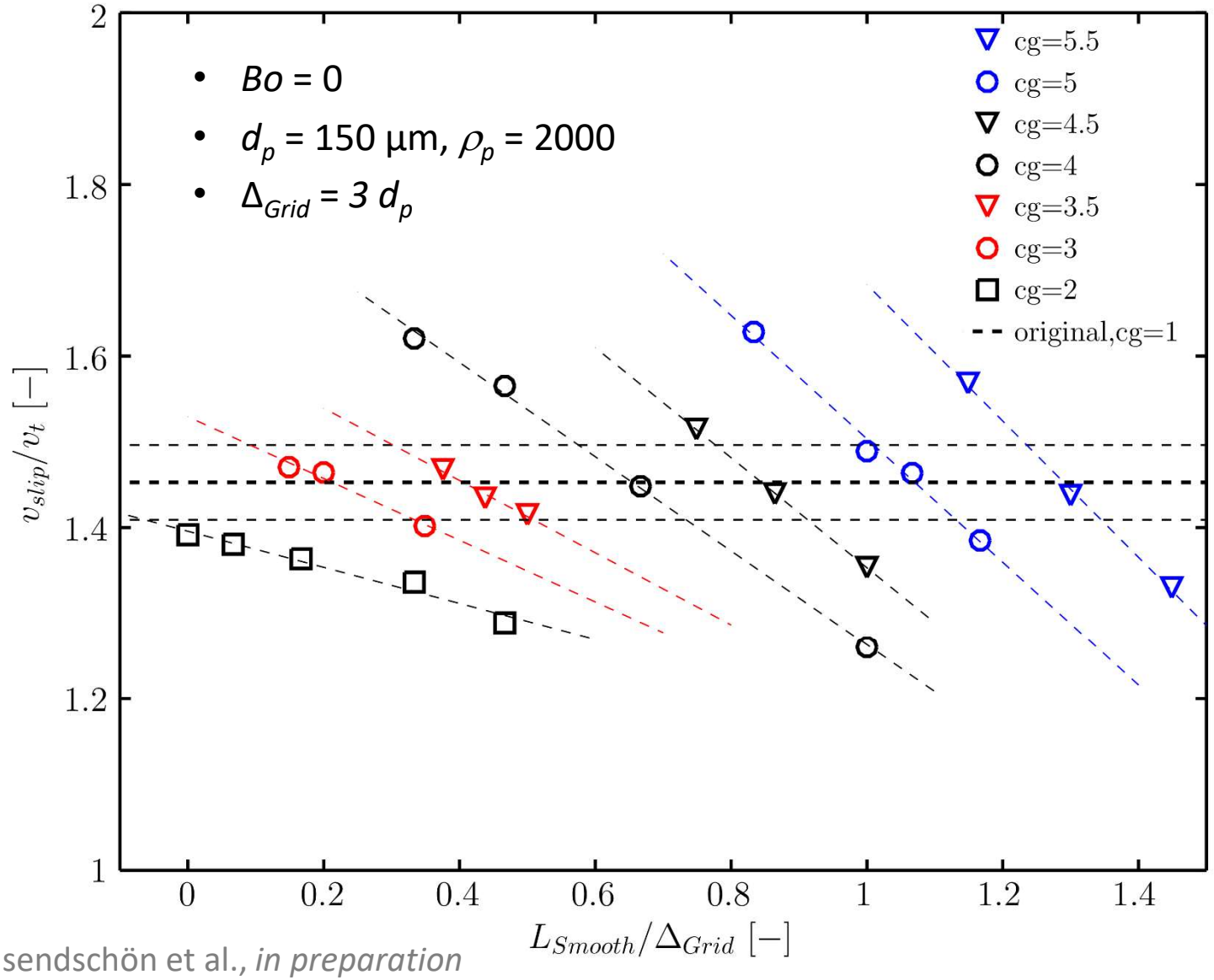

Non-cohesive

Tausendschön et al., *in preparation*

Fluid-To-Particle Mapping

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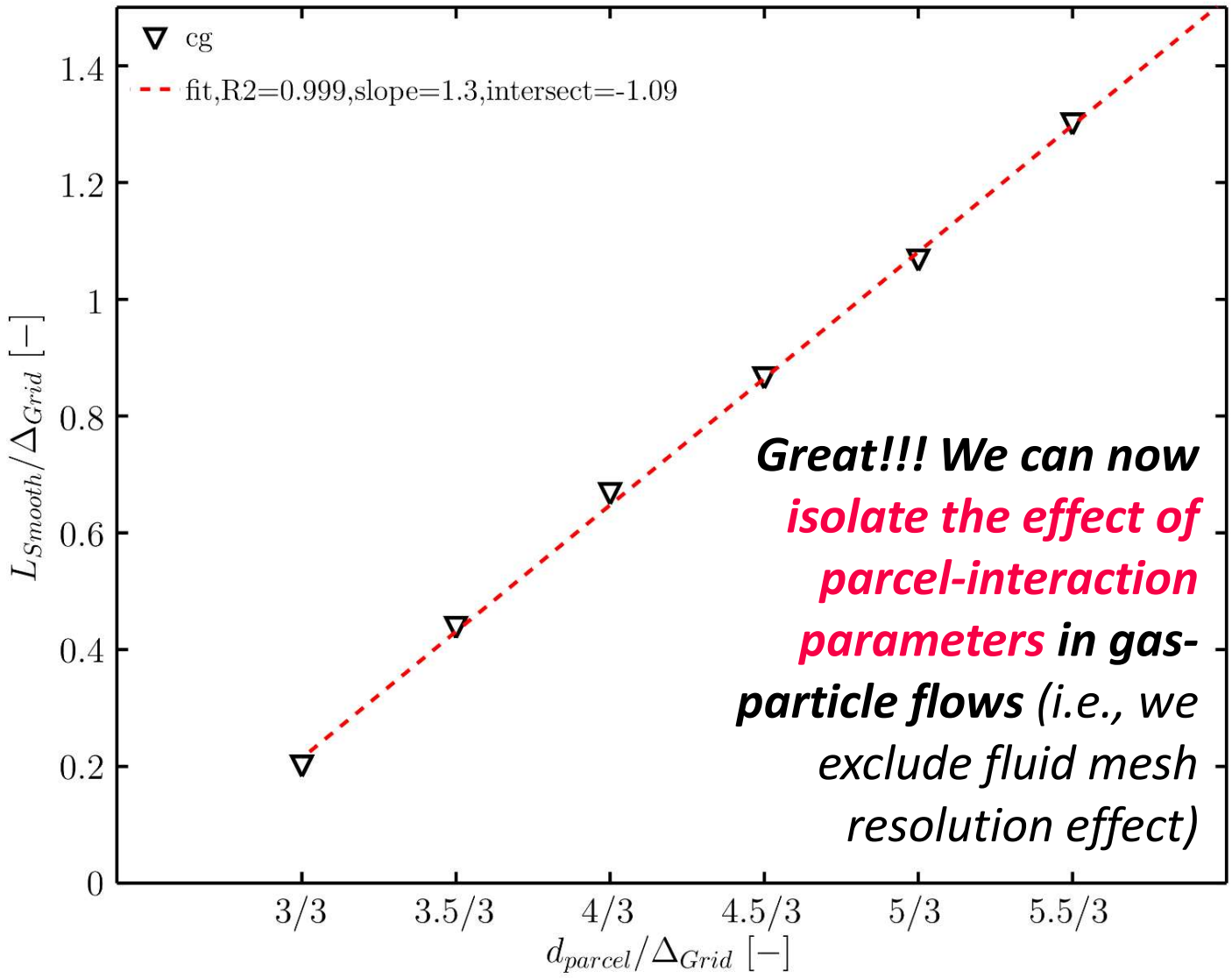

Non-cohesive

Great!!! We can now isolate the effect of parcel-interaction parameters in gas-particle flows *(i.e., we exclude fluid mesh resolution effect)*

Tausendschön et al., *in preparation*

Scaling of Cohesion Parameters

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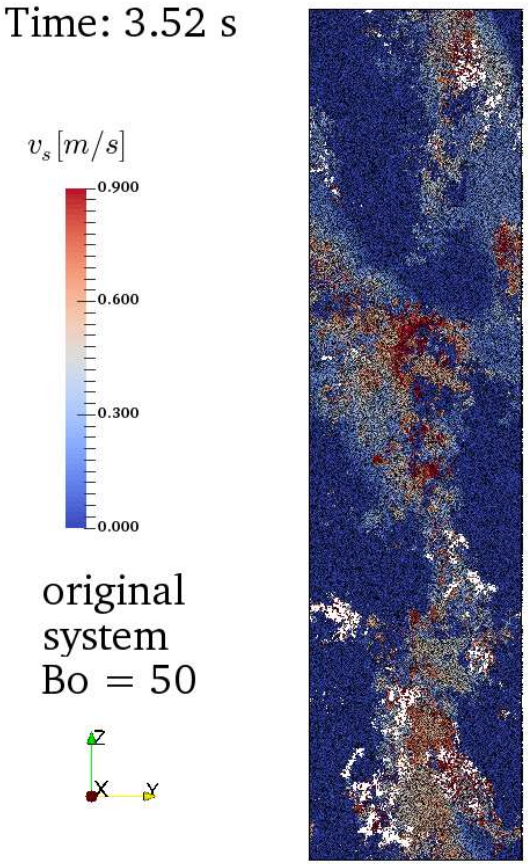
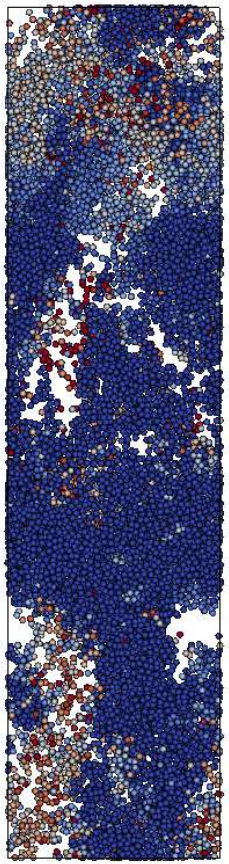
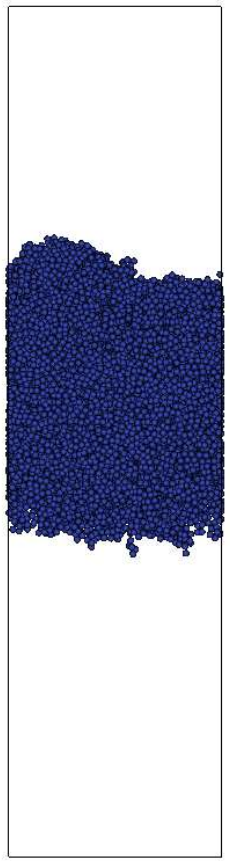
Next question: how shall we scale the cohesive strength?



CG = 4
Stress
Bo = 50

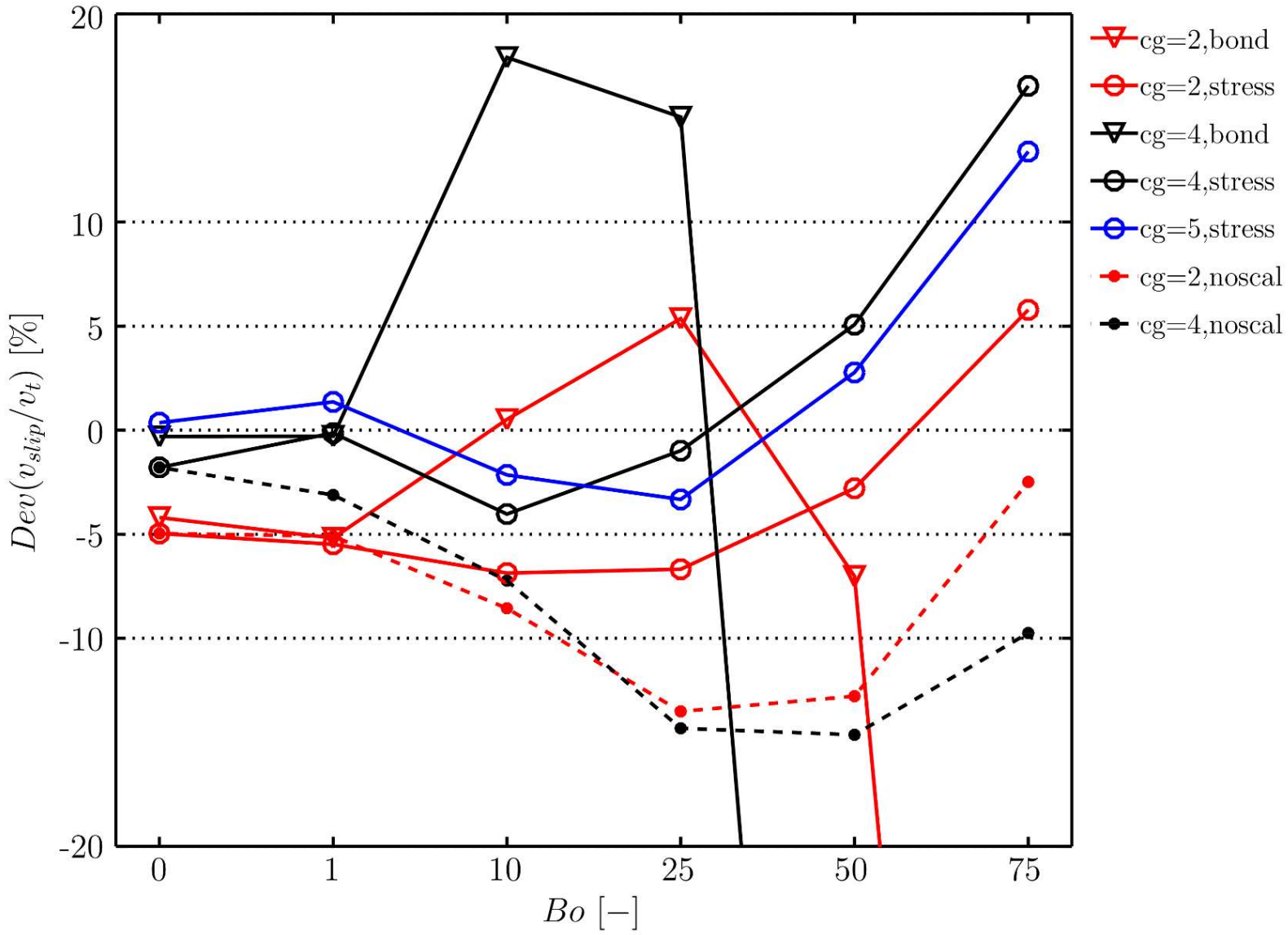


CG = 4
Bond
Bo = 50



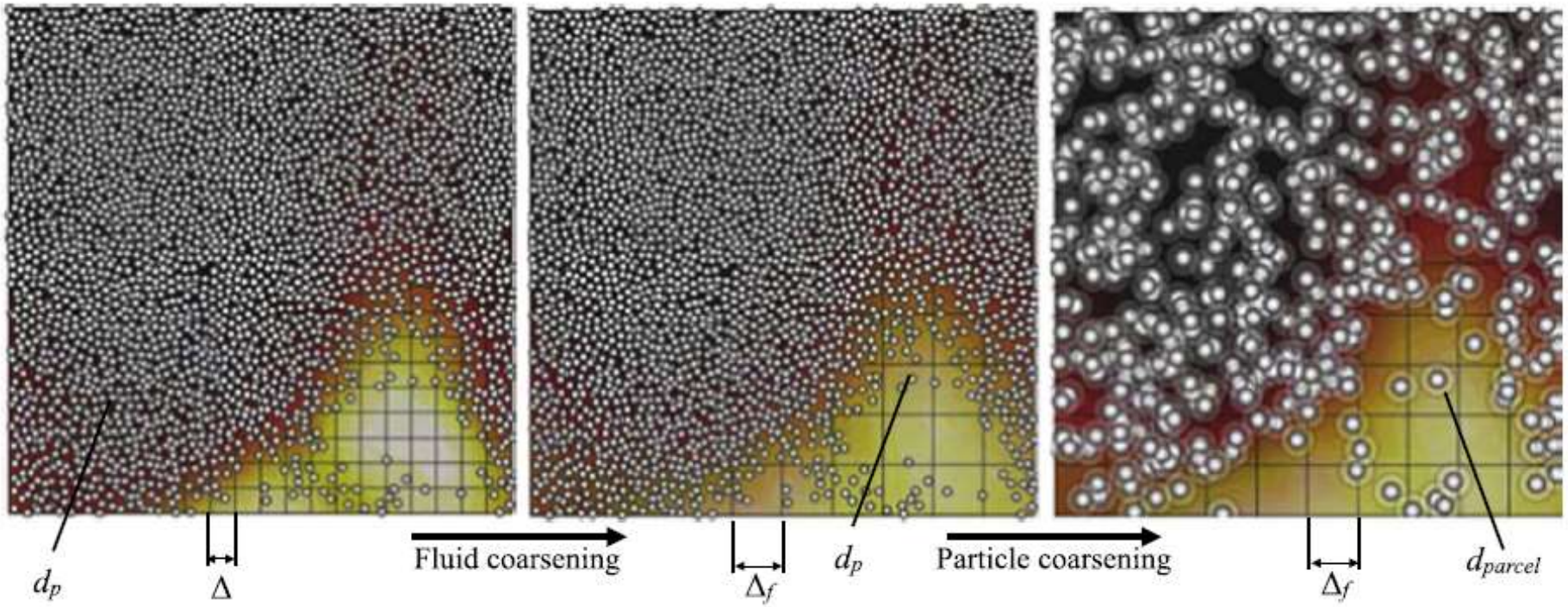
Tausendschön et al., *in preparation*

Scaling of Cohesion Parameters



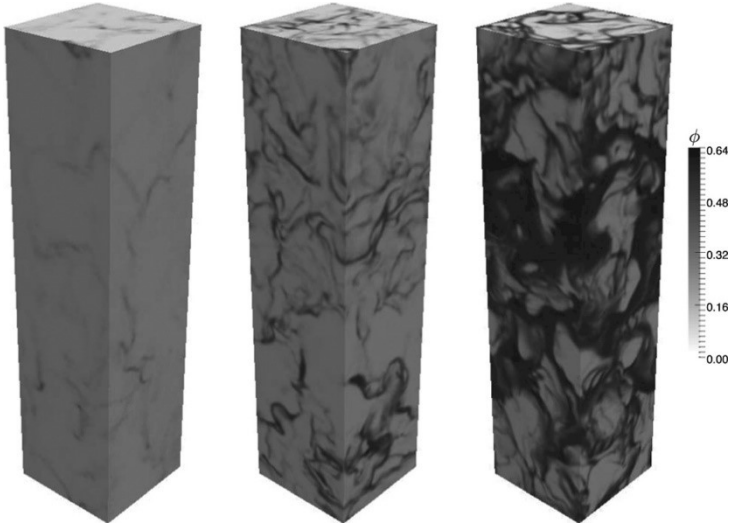
Tausendschön et al., *in preparation*

Large Fluid Cell Size



- $Bo = 0$
- d_p = 75 … 300 µm, ρ_p = 1500 kg/m³
- $\Delta_{Grid} = 3\ d_p$

Non-cohesive



Ozel et al., Chem Eng Sci 155 (2016), 258-267

Large Fluid Cell Size

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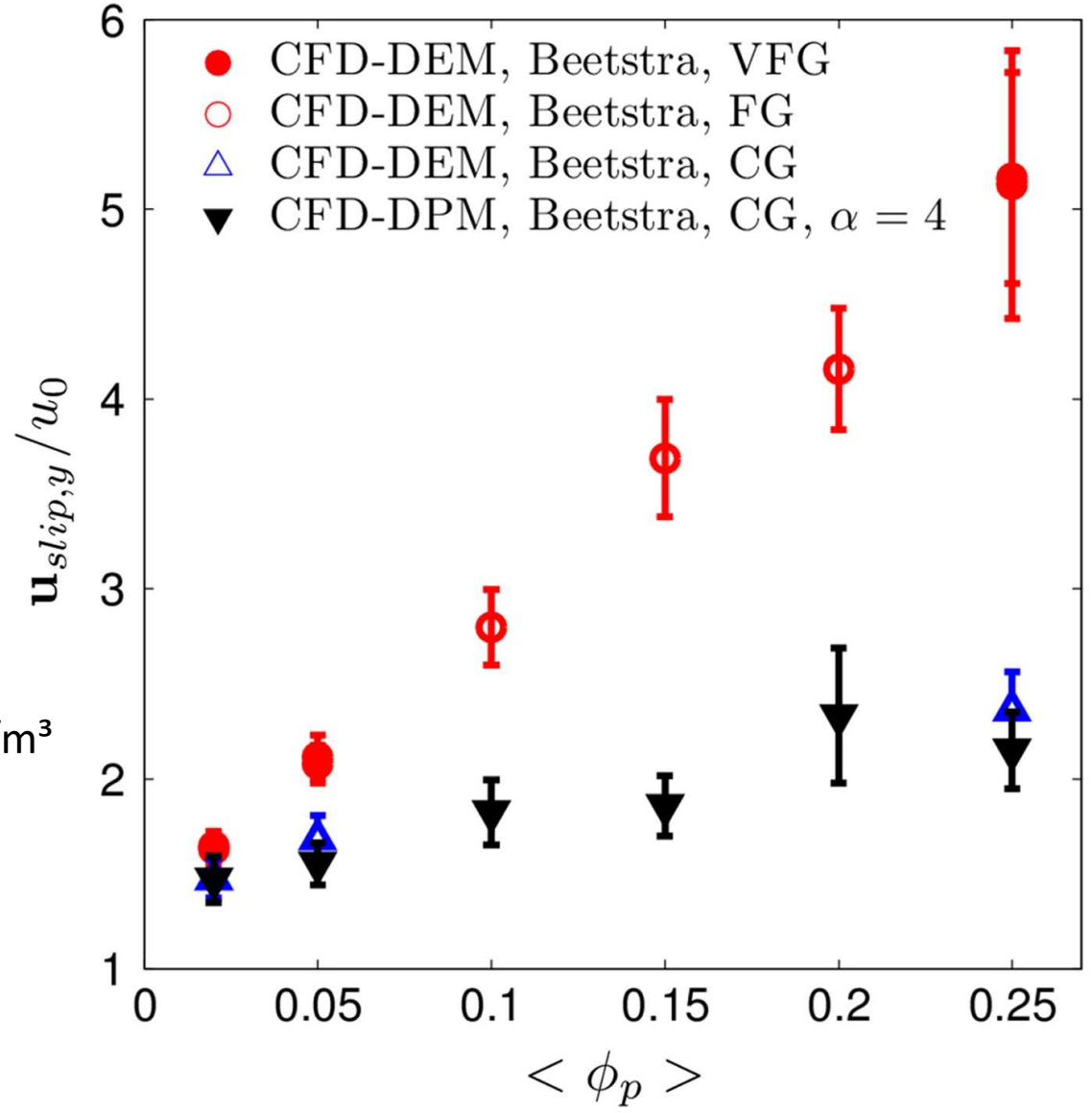
Non-cohesive

- $Bo = 0$
- d_p = 75 µm, ρ_p = 1500 kg/m³
- VFG: $\Delta_{Grid} = 1.67\ d_p$
- FG: $\Delta_{Grid} = 3\ d_p$
- CG: $\Delta_{Grid} = 26.7\ d_p$



Radl and Sundaresan, Chem Eng Sci 117 (2014), 416-425

Large Fluid Cell Size

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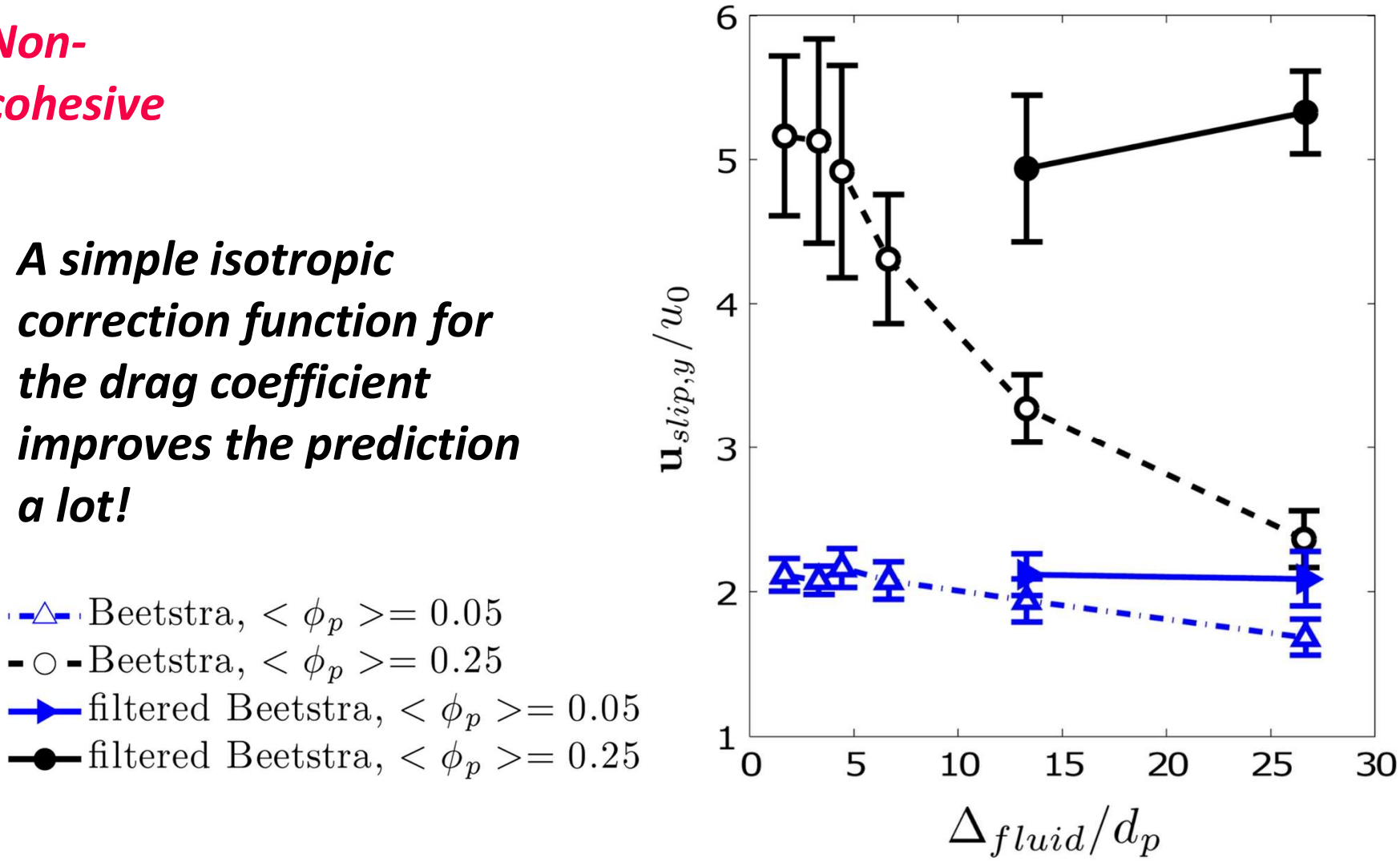
Non-cohesive

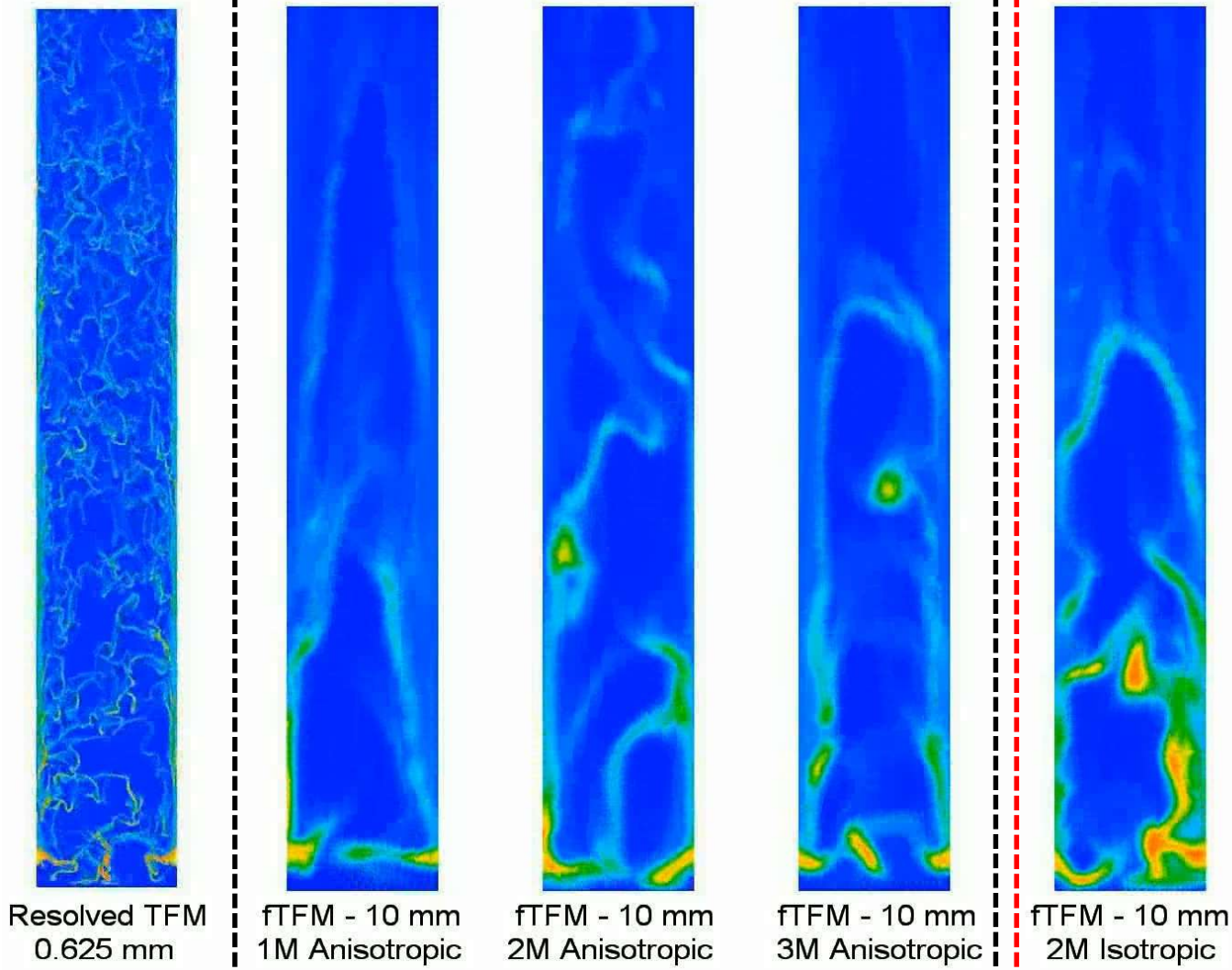
A simple isotropic correction function for the drag coefficient improves the prediction a lot!



Radl and Sundaresan, Chem Eng Sci 117 (2014), 416-425

3 - Future Improvement of Models & Closures

Anisotropy



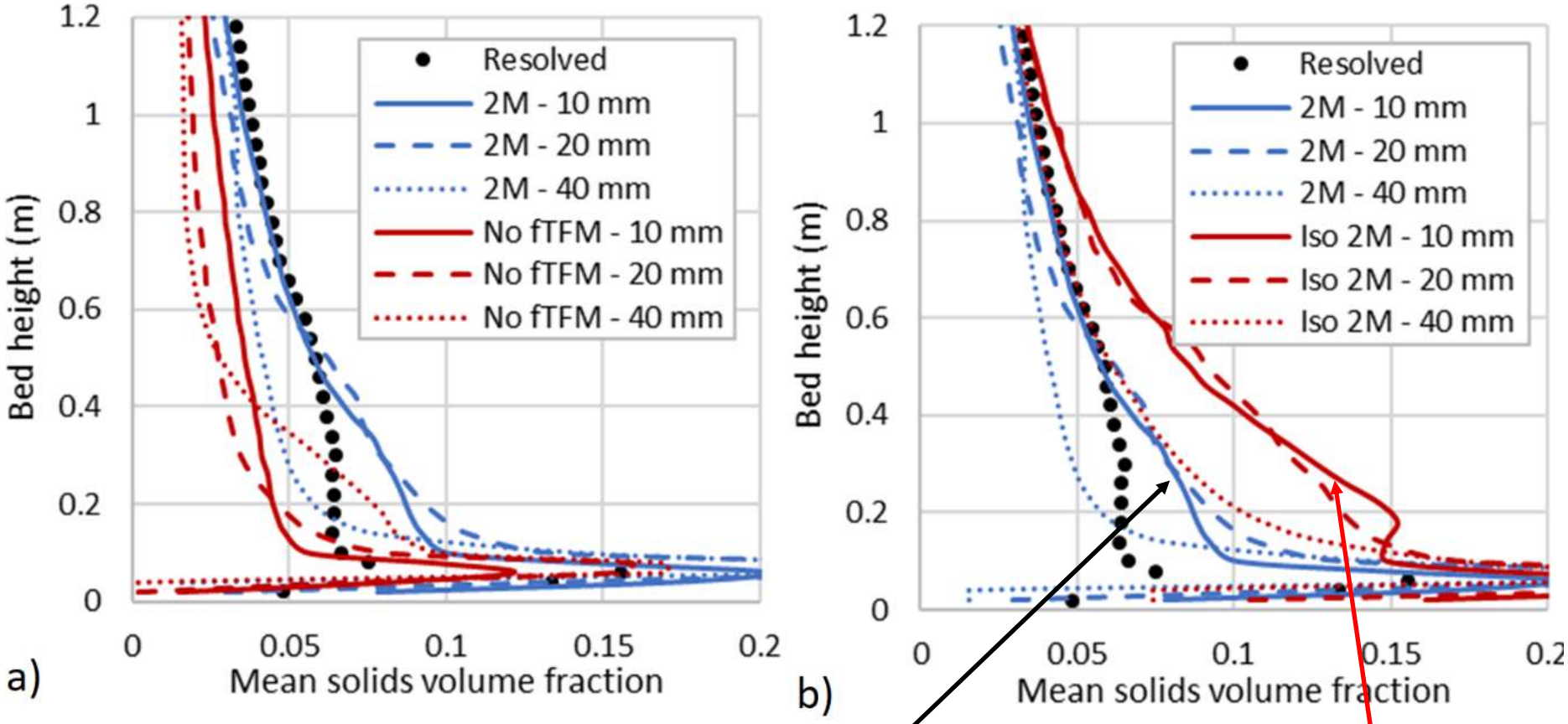
- **Euler-Euler simulations indicate some room for improvement with respect to drag force closures**

Cloete et al., *submitted*

New approach: correction depends on direction

Classical approach: correction identical in each direction

Anisotropy

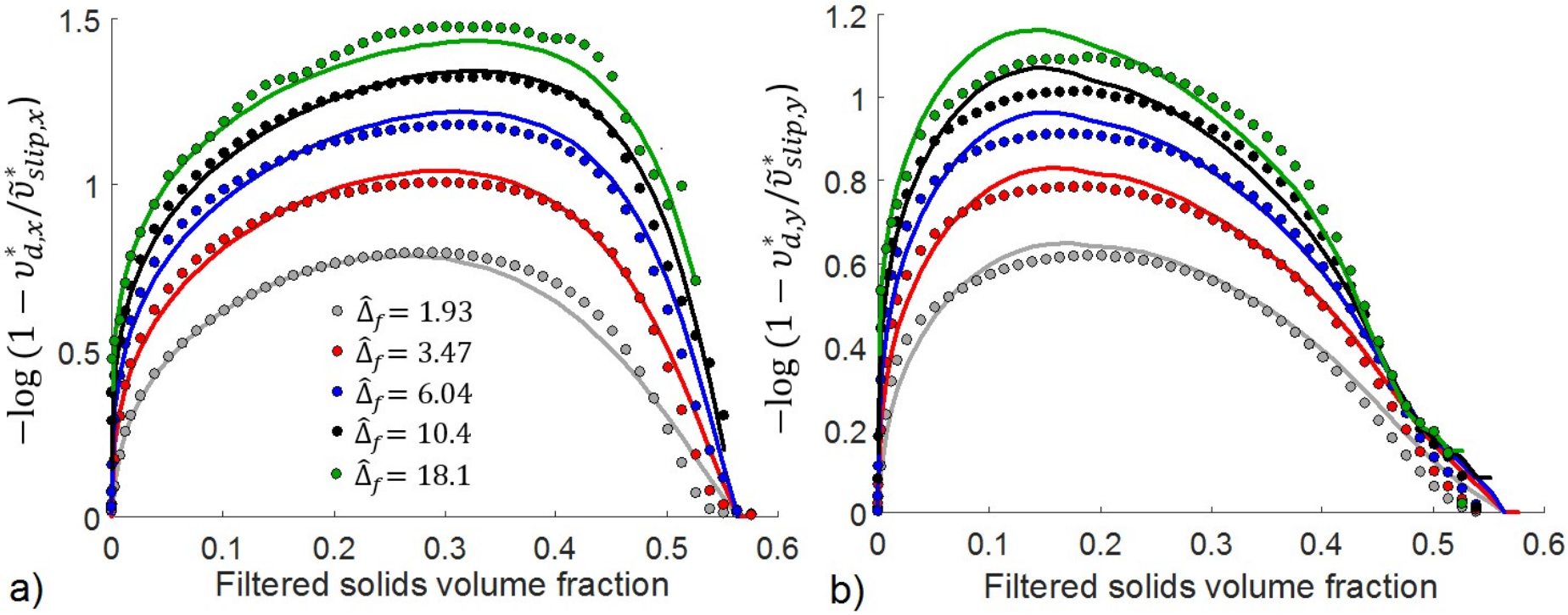


New approach: correction depends on direction

Classical approach: correction identical in each direction

Cloete et al., *submitted*

Anisotropy



lateral direction ***vertical direction***

- **Correction of drag force depends on direction**
- **The same is true for the meso-scale stress**
- **Can we increase performance of CG Euler-Lagrange models by including these effects?**

Cloete et al., *submitted*

Chemical Reactions

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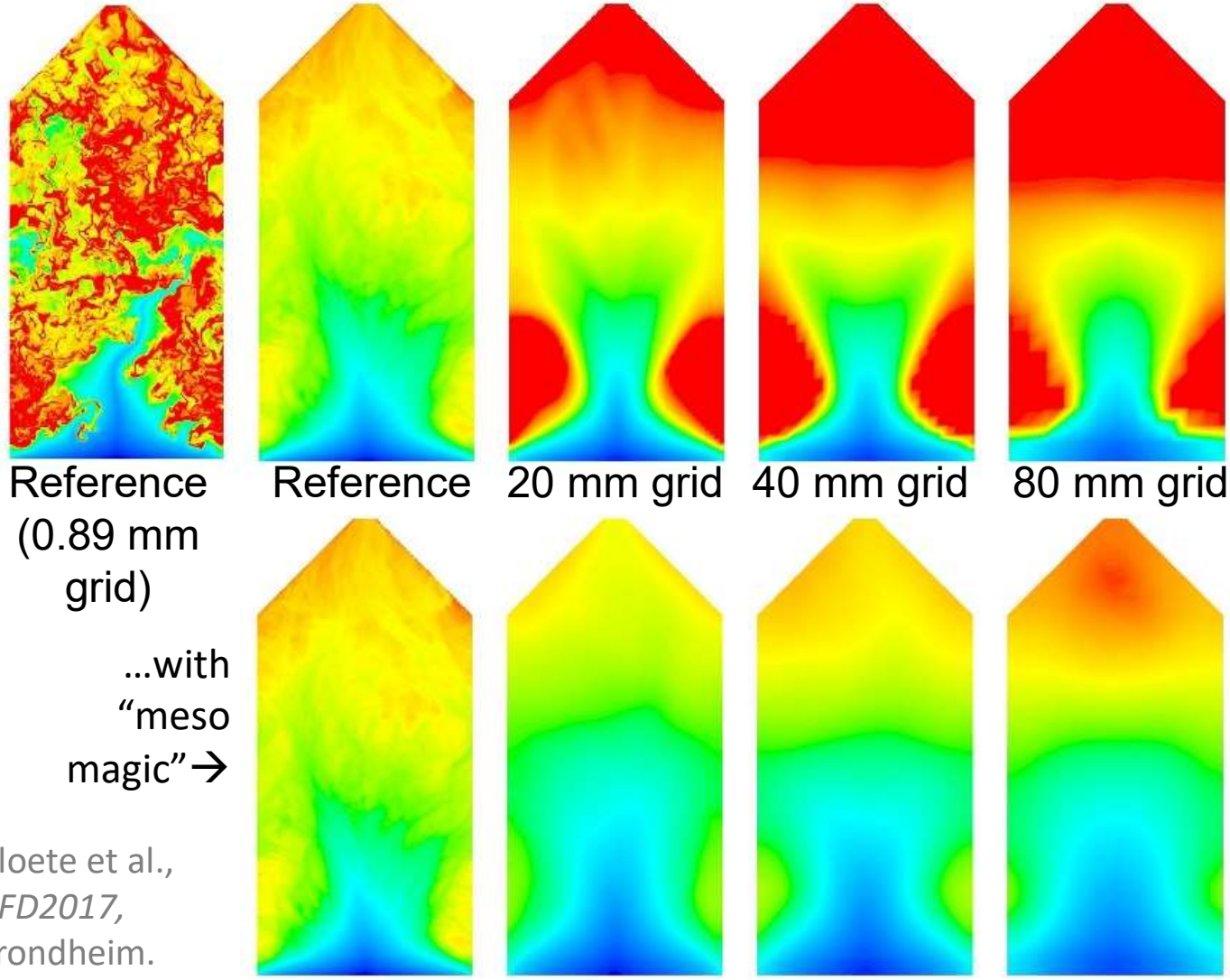
Is the outcome of heterogeneous reactions affected as well? Let us consider the conversion of a solids-catalyzed reaction in an FB…



- **Yes!** If we **do not** account for meso-scale structures, we typically **overpredict conversion A LOT** (figures use a log scaling)!

$$\eta_{meso} = \frac{\overline{\alpha_p X_i}}{\overline{\alpha_p}\,\overline{X_i}}$$

- However, if we **consider a meso-scale effectiveness factor**, we can **substantially improve predictions!**

Cloete et al., *CFD2017,* Trondheim.

Chemical Reactions

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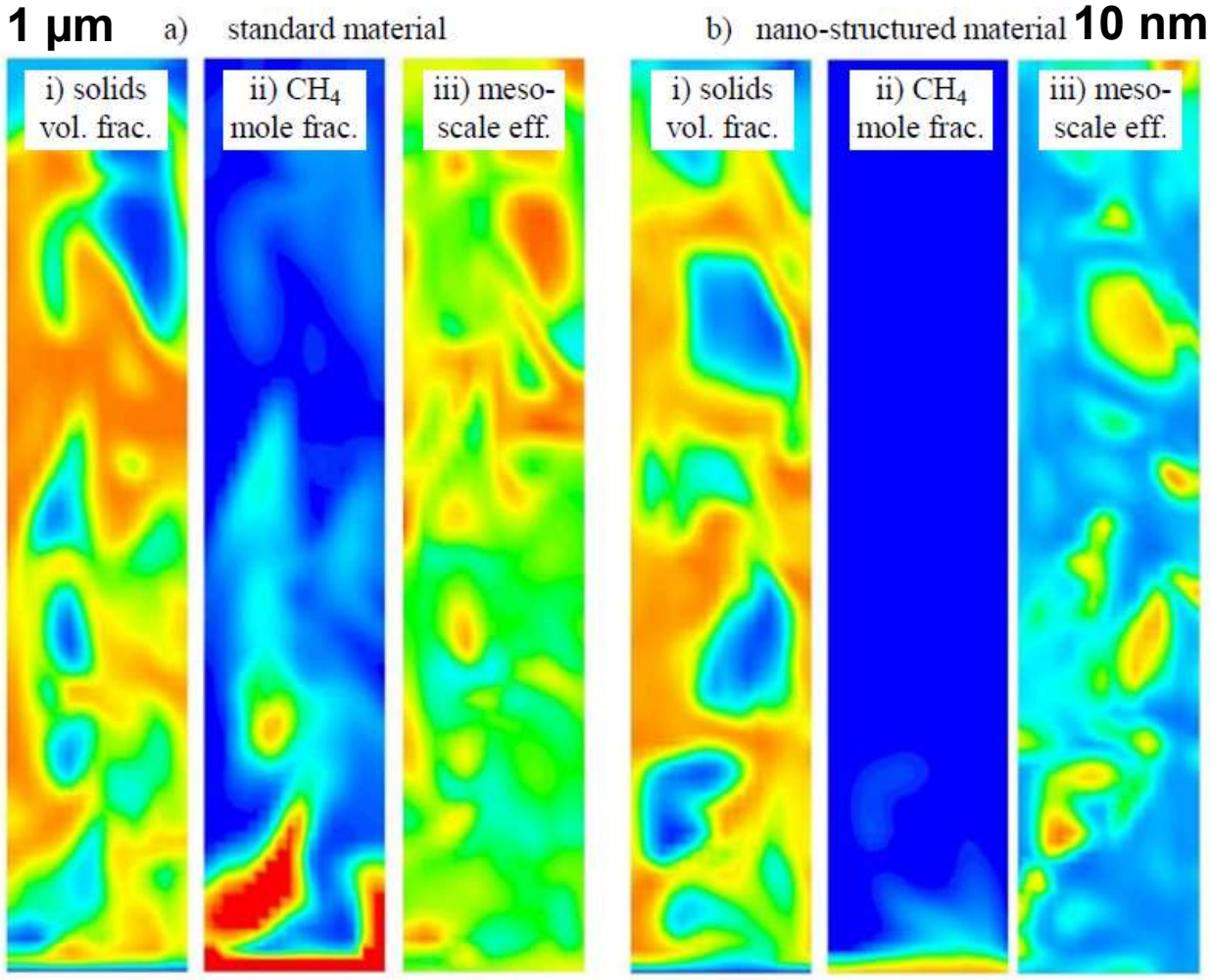
How does that impact the design of a reactor? Let us consider a multi-scale process intensification study…



- At the same methane feed rate (0.6 kg/s), the **nano-structured material achieves much higher conversion**
- **High particle and CH_4 concentration → low effectiveness factor** (more solid reactant→ more gas consumption)
- **Lower effectiveness factors for nano-structured** material (faster reaction → "meso-scale" mass transfer limitation)

Radl et al., *ESCAPE28,* Graz.

Conclusions

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- We still have no clear explanation for the correct strength of smoothing. But it is clearly needed…
- Scaling of cohesion parameters up to CG = 5 helps a lot!
  - 1 / 125 of particles need to be tracked
  - Study cohesive fluidization with (almost) no simulation time penalty due to particle tracking
- Adoption of Euler-Euler closures in CG EL simulators suggested
- Polydispersity: does the stress-based scaling law for cohesion also hold for these systems?

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Dos and Don'ts

Coarse-Grained Models for Gas-Particle Flow

S. Radl[a]

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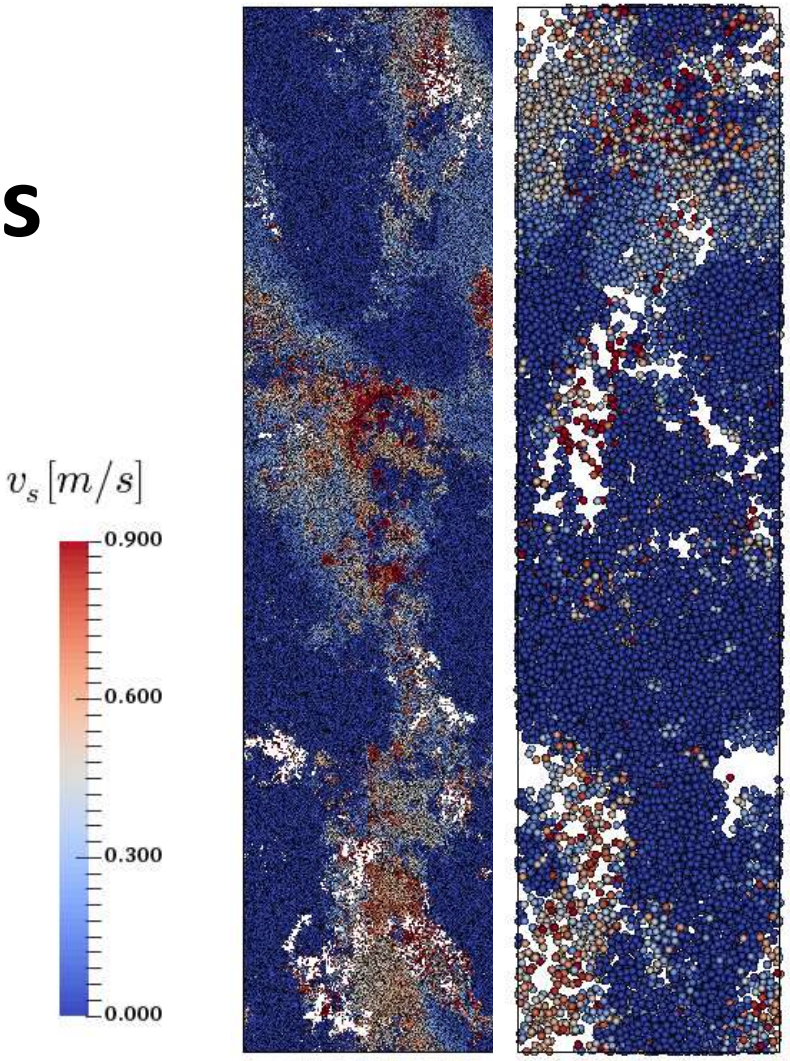
with contributions from

Josef Tausendschön,[a] **Schalk Cloete,**[b] **Henri Cloete,**[b] **Shahriar Amini**[b]

[b]SINTEF (NOR)

THANK YOU



Direct and parcel-based simulation of a cohesive gas-particle mixture