Modeling Cohesive Gas-Particle Flows

with a Parcel-Based Lagrangian Approach

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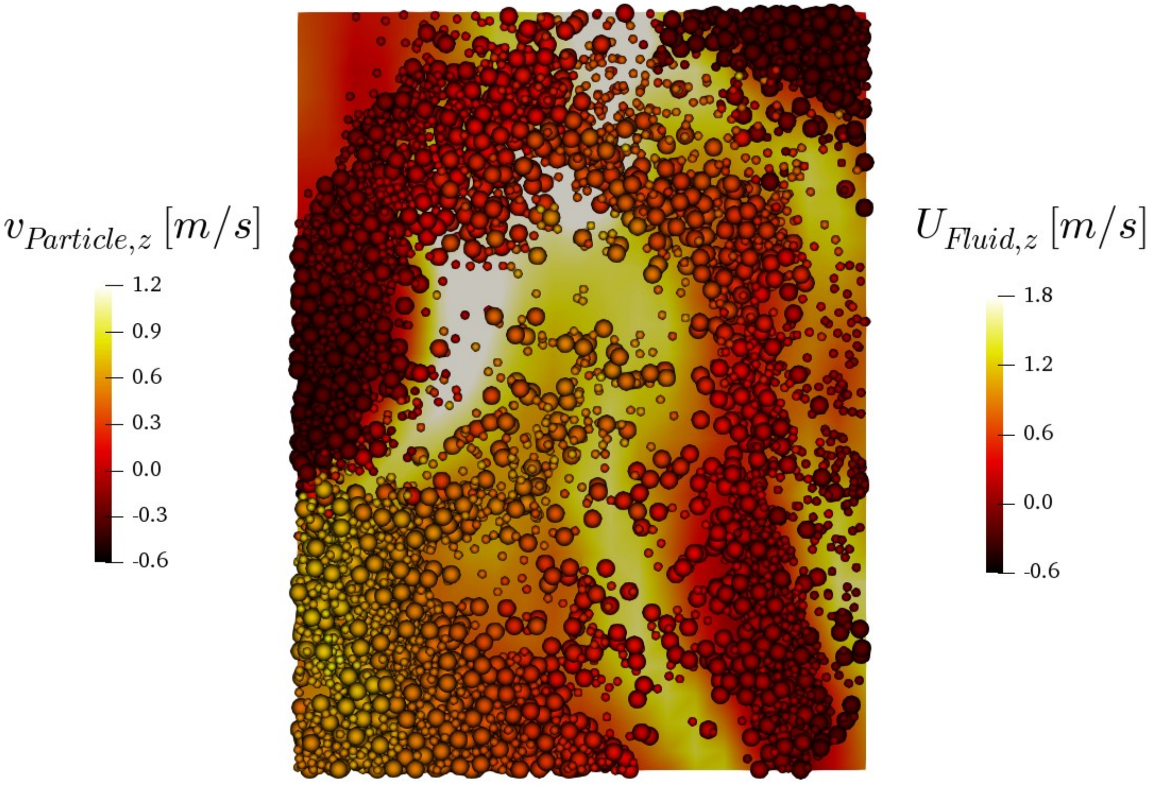
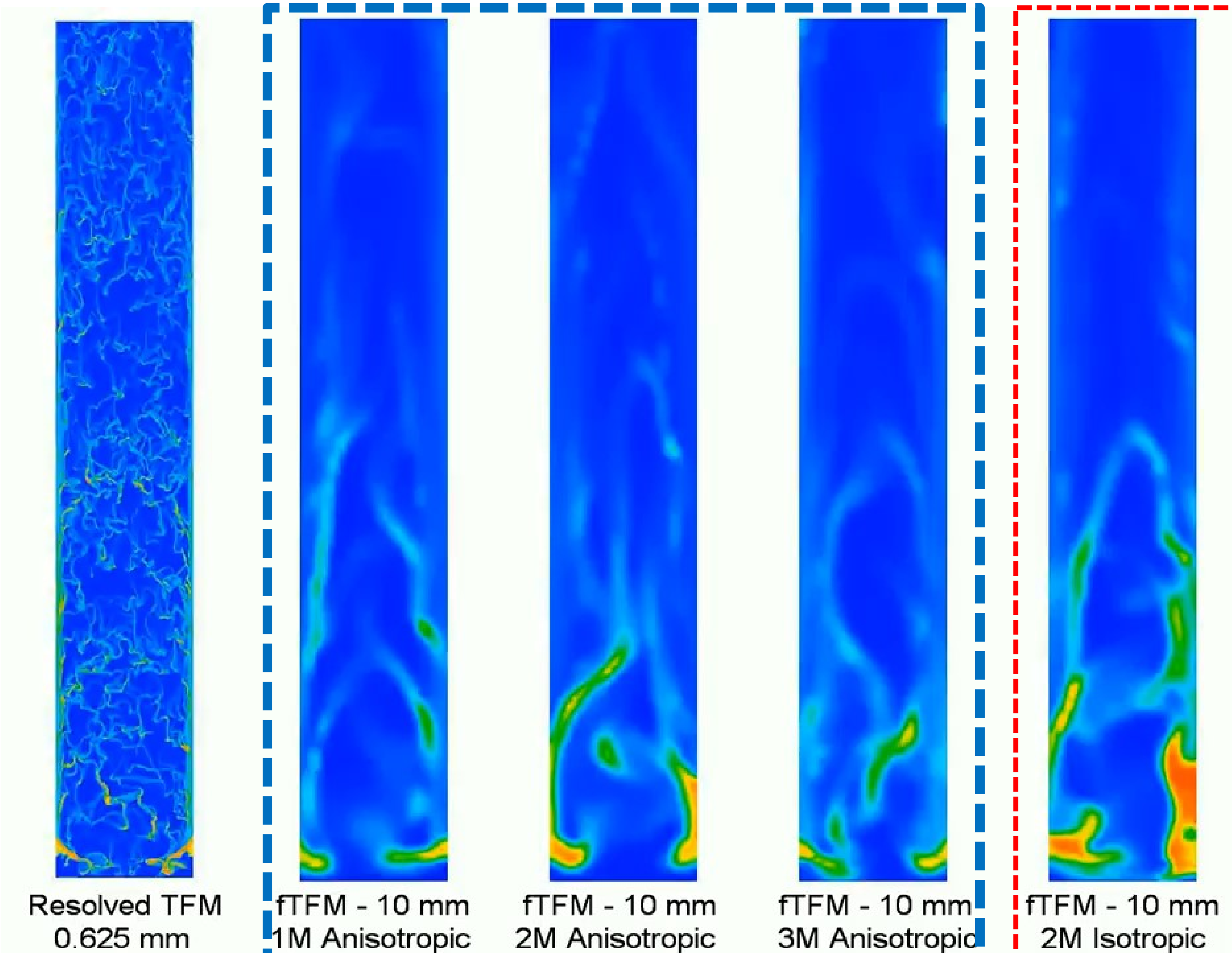
AIChE Annual Meeting 2019

17+3 mins



Motivation



New approach: correction depends on direction

Classical approach: correction identical in each direction

On the large scale: a **filtered model** is needed (e.g., filtered TFM)

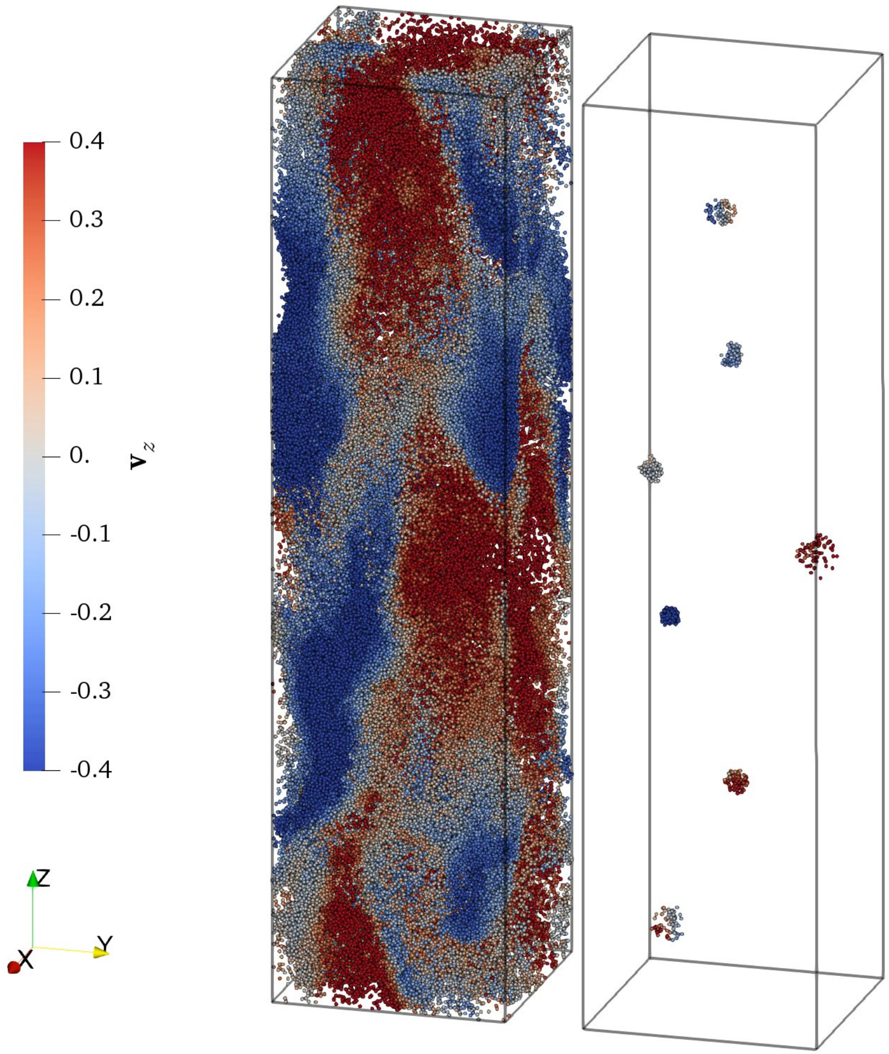
Improved „meso scale" closures (drag, stress) are needed

Q1: How do these closures look like for **cohesive & polydisperse** powders?

Q2: Is a **filtered „CFD-parcel" (Lagrangian)** approach feasible?

Cloete et al., *Chem Eng Sci* 207 (2019) 379–396

Coarse-Graining Basics



$Bo = 0$

A parcel is…

- approximation of a **particle ensemble**
- representation of a **fixed number of particles**, but not a fixed set
- **cannot directly predict particle-particle** collisions → approximate "**parcel collisions**"

Coarse-Graining Basics

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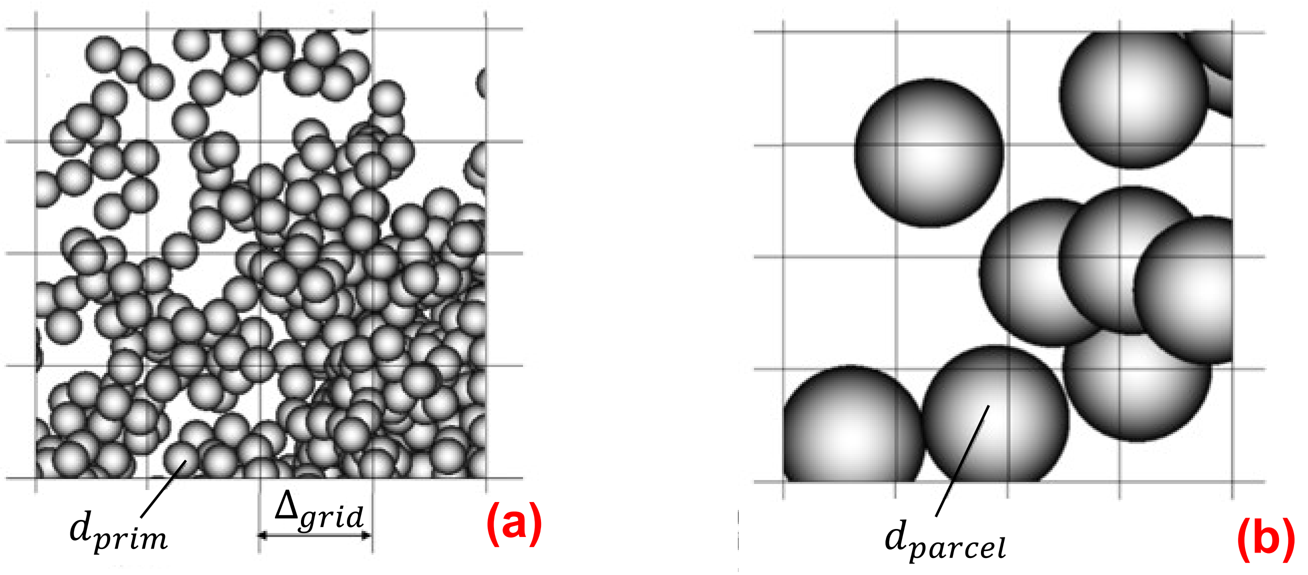
- **Coarse Graining of the Particles:**
  $d_{parcel} = \alpha \cdot d_{prim}$ => one parcel consists of α^3 primary particles



- **With a fixed CFD grid size, parcels can become bigger than a CFD cell!**
  => typically, CFD cell size is increased for $\alpha > 1$

Coarse-Graining Basics

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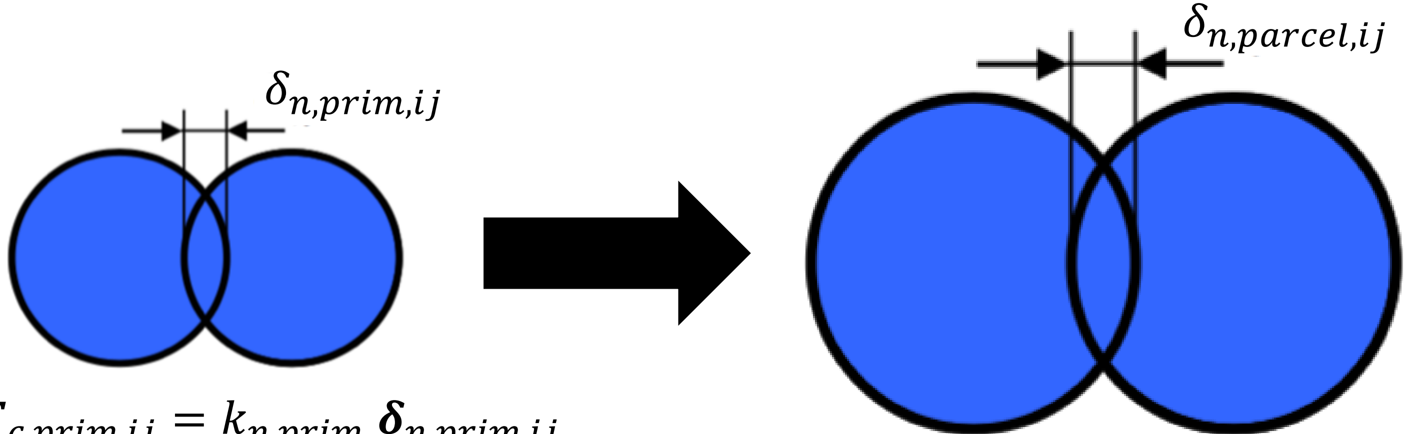


$$\boldsymbol{F}_{c,prim,ij} = k_{n,prim}\, \boldsymbol{\delta}_{n,prim,ij} + c_{n,prim}\dot{\boldsymbol{\delta}}_{n,prim,ij}$$

$$F_{c,parcel,ij} = k_{n,parcel}\, \boldsymbol{\delta}_{n,parcel,ij} + c_{n,parcel}\, \dot{\boldsymbol{\delta}}_{n,parcel,ij}$$

- we suggest a scaling of contact and cohesive forces based on **constant stress:**

Force/R^2 = const., leads to

$$\begin{cases} \gamma_{prim} \cdot \alpha = \gamma_{parcel} \\ \mu_{liq,prim} \cdot \alpha = \mu_{liq,parcel} \\ k_{n,prim} \cdot \alpha = k_{n,parcel} \\ c_{n,prim} \cdot \alpha^2 = c_{n,parcel} \\ A_{prim} \cdot \alpha^3 = A_{parcel} \end{cases}$$

k_n = Particle Stiffness

c_n = Normal Damping coeff.

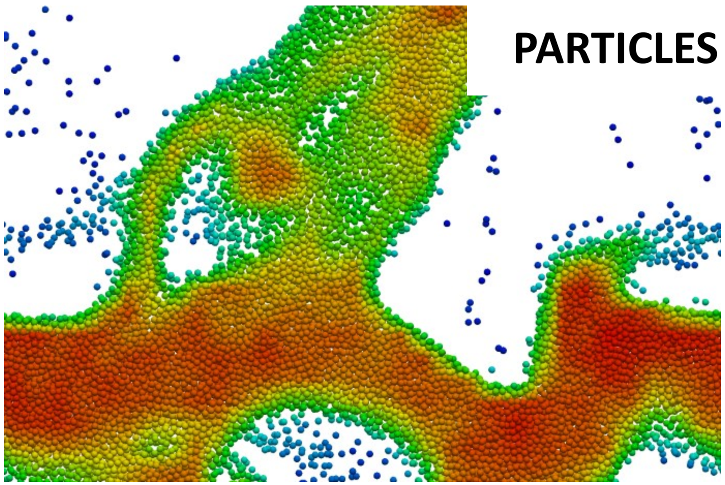
γ = Surface Tension

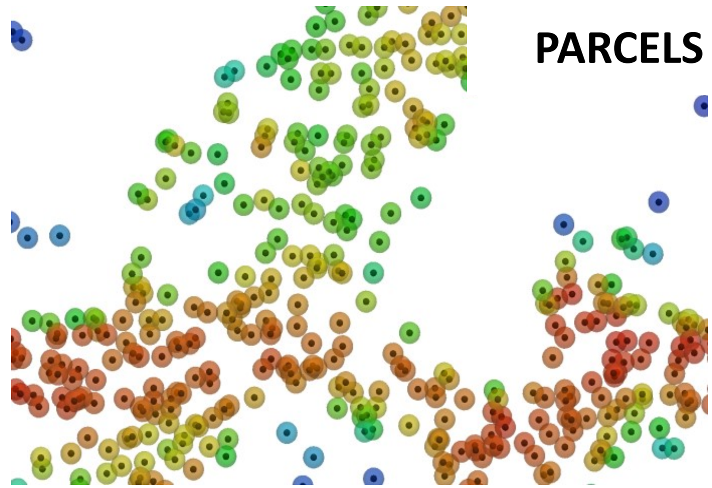
μ_l = Liquid Viscosity

A = Hamaker const.

Tausendschön et al., *submitted manuscript*

Can we predict Stress?





$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{cont} + \boldsymbol{\sigma}^{kin} = \boldsymbol{\sigma}\left(\mathbf{u}_p, \phi_p, T, d_{prim}, e_p, \mathbf{f}_{coh}\right)$$

$$\boldsymbol{\sigma}^{cont} = \frac{1}{V} \sum_{p \in p_V} \sum_{j \in C_p} \frac{1}{2} \mathbf{r}_{pj} \mathbf{F}_{pj}$$

$$\boldsymbol{\sigma}^{kin} = \frac{1}{V} \sum_{p \in p_V} m_p \left(\mathbf{v}_p - \overline{\mathbf{v}}_p\right)\left(\mathbf{v}_p - \overline{\mathbf{v}}_p\right)$$

Stress Prediction

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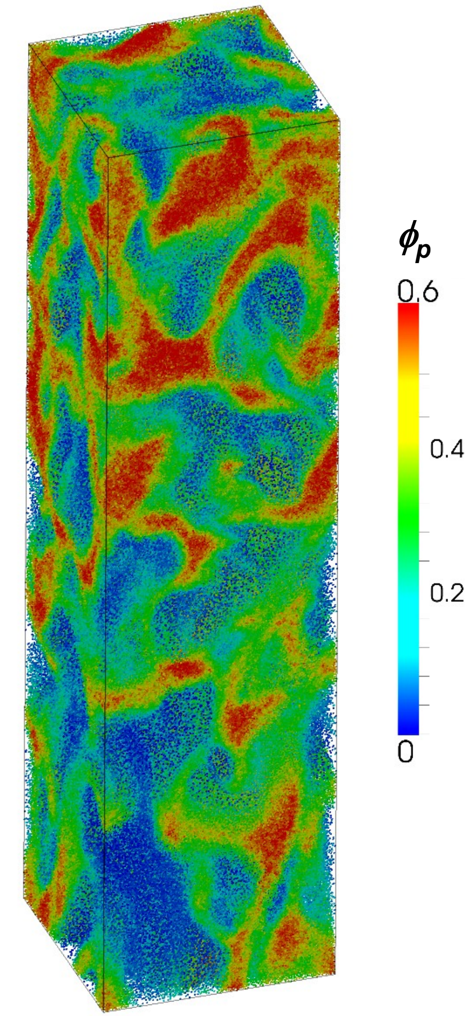
- **Setup**

  - Gas-particle system ($\rho_p/\rho_f \approx 1000$), freely sedimenting.
  - Low Re system (u_t = 0.22 m/s, $Re_p \approx 1$).
  - 3D, size: **8x32 mm** & 4x16 mm, **periodic.**

- **Fluid Grid & Coarse Graining Sensitivity**

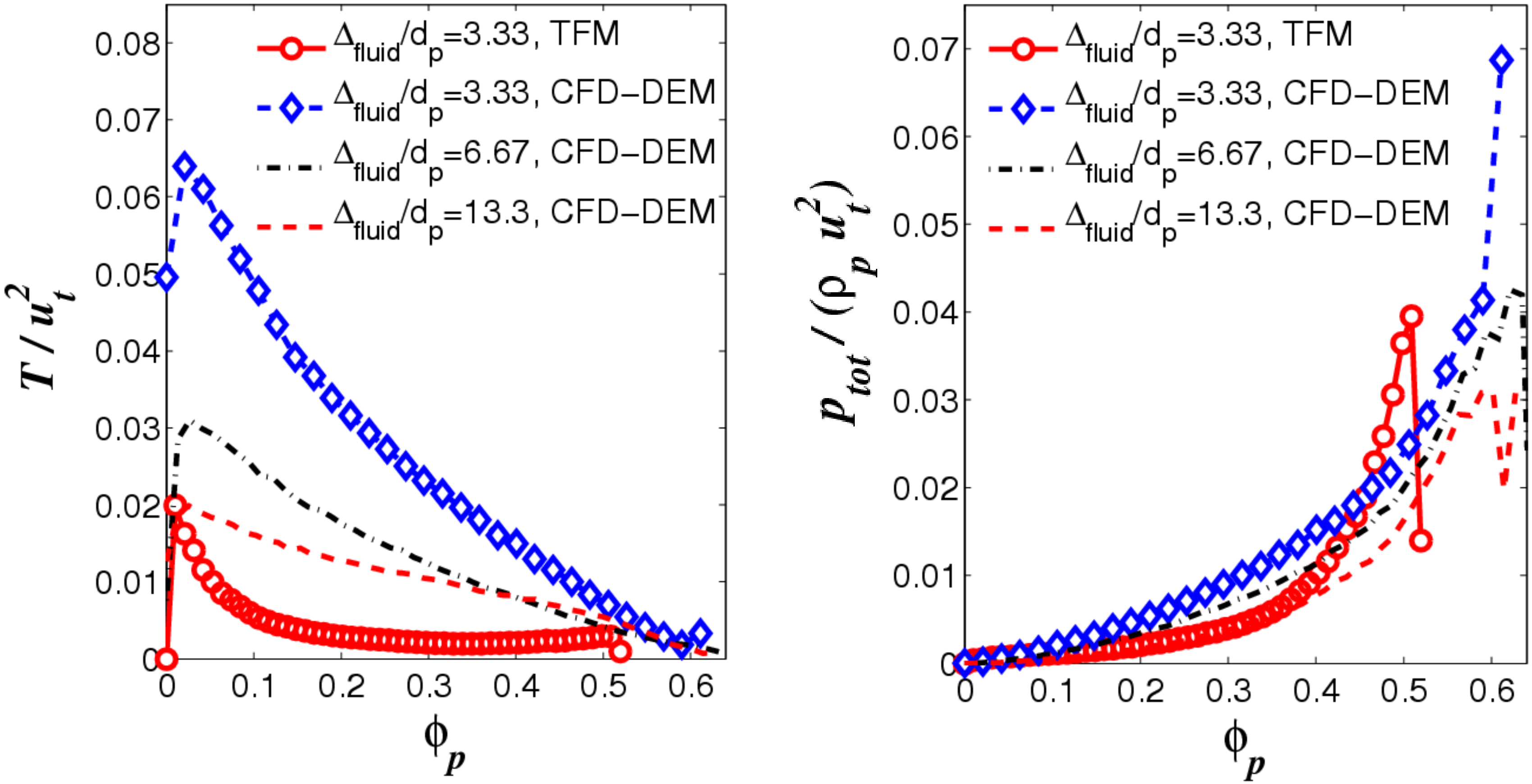
  - Analyze distribution of granular **temperature and pressure** to illustrate effect of grid resolution
  - Investigate effect of **coarse graining** (on **coarse grids**!)



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

Stress Prediction

- Gran. Temperature and Particle-Phase Pressure



- ***T*** and **stress** quantitatively sensitive to grid resolution
- **TFM** significantly off

Stress Prediction

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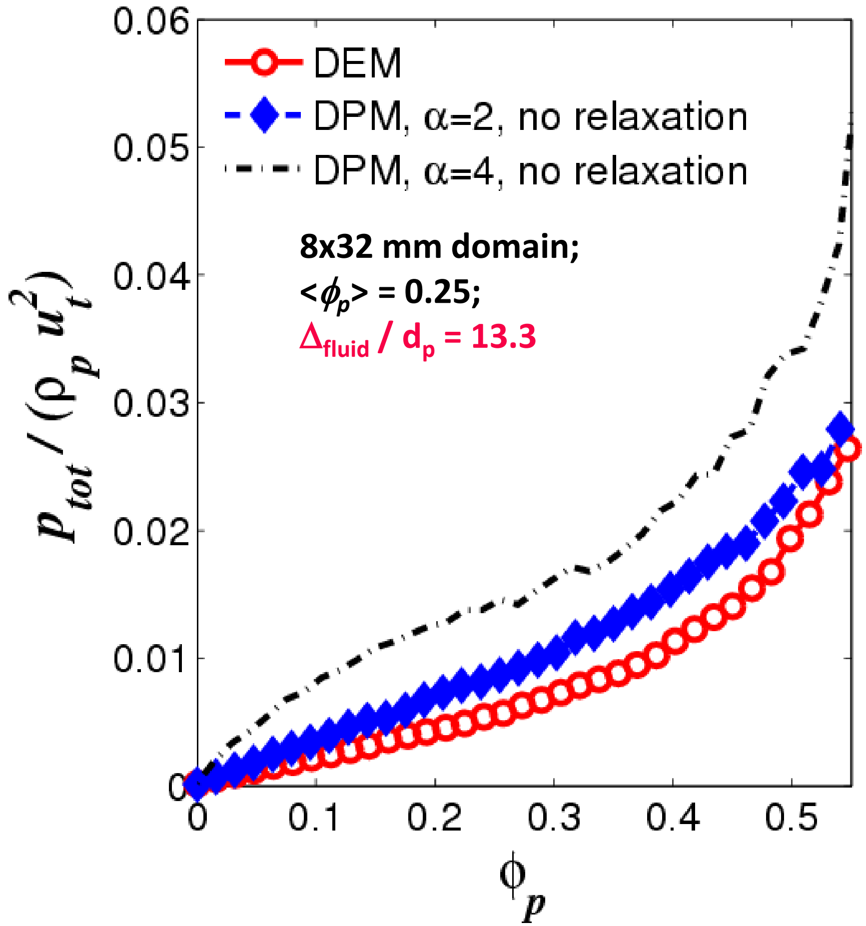
- Comparison DEM and Coarse Grained DEM

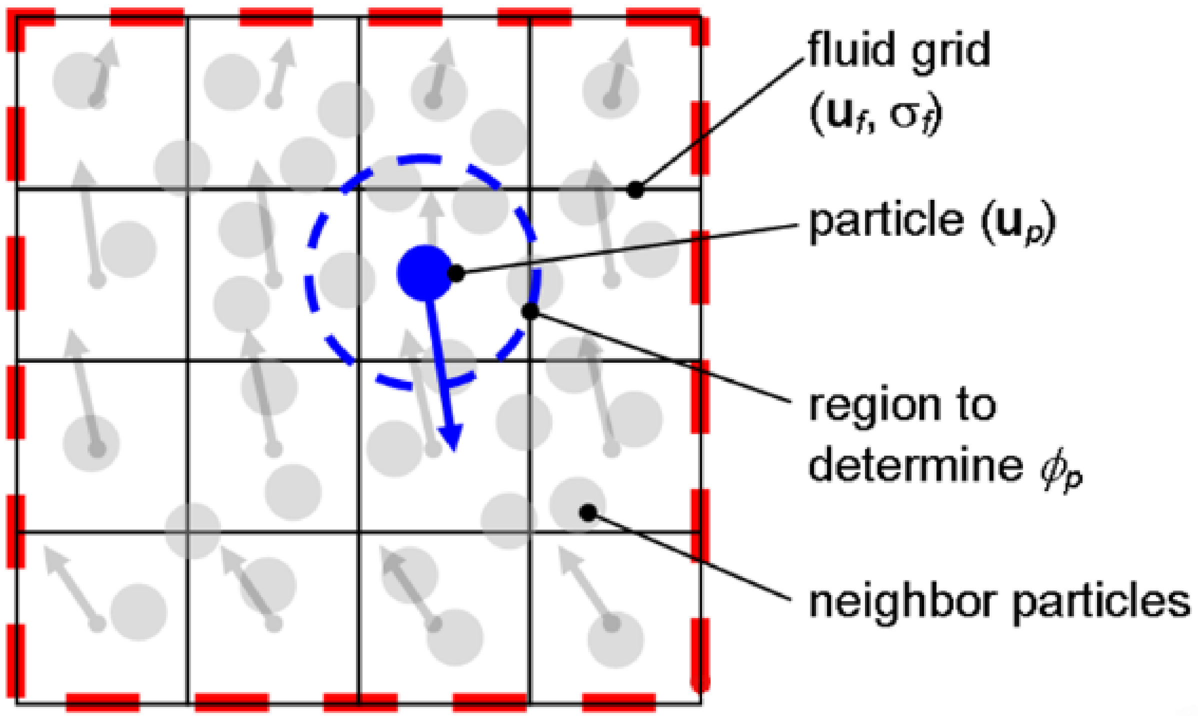


- **Particle-phase Pressure**
  - **stress increases with increasing parcel size** as expected from shear-flow simulations

However,

→ **...this is for a coarse grid!** We need **smoothing** for a fair comparison

Smoothing Strategy



Smoothing Basics

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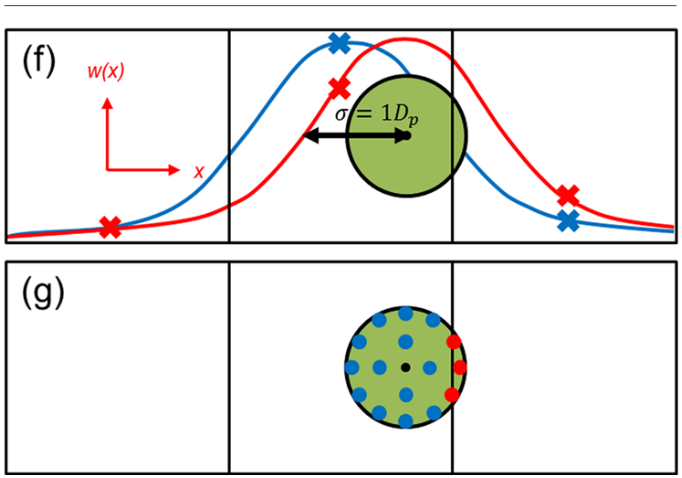
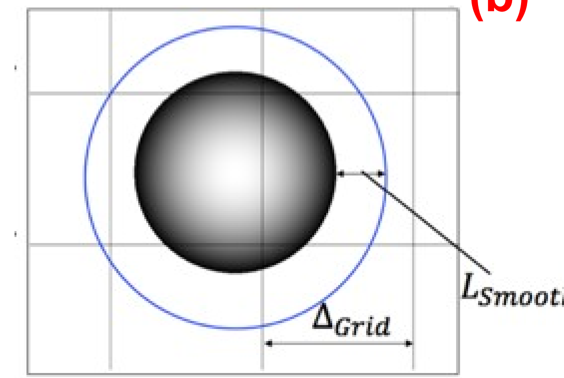
(a)[3]



Combination of these two schemes

Diffusive Smoothing

(b)



- **Smoothing operation is performed via (an implicit) solution of a diffusion equation for each transferred quantity ψ:**

$$\frac{\partial \psi}{\partial t} = D\nabla^2\psi \quad , \qquad D = {L_{Smooth}}^2/\Delta t$$

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

Optimal Smoothing Length

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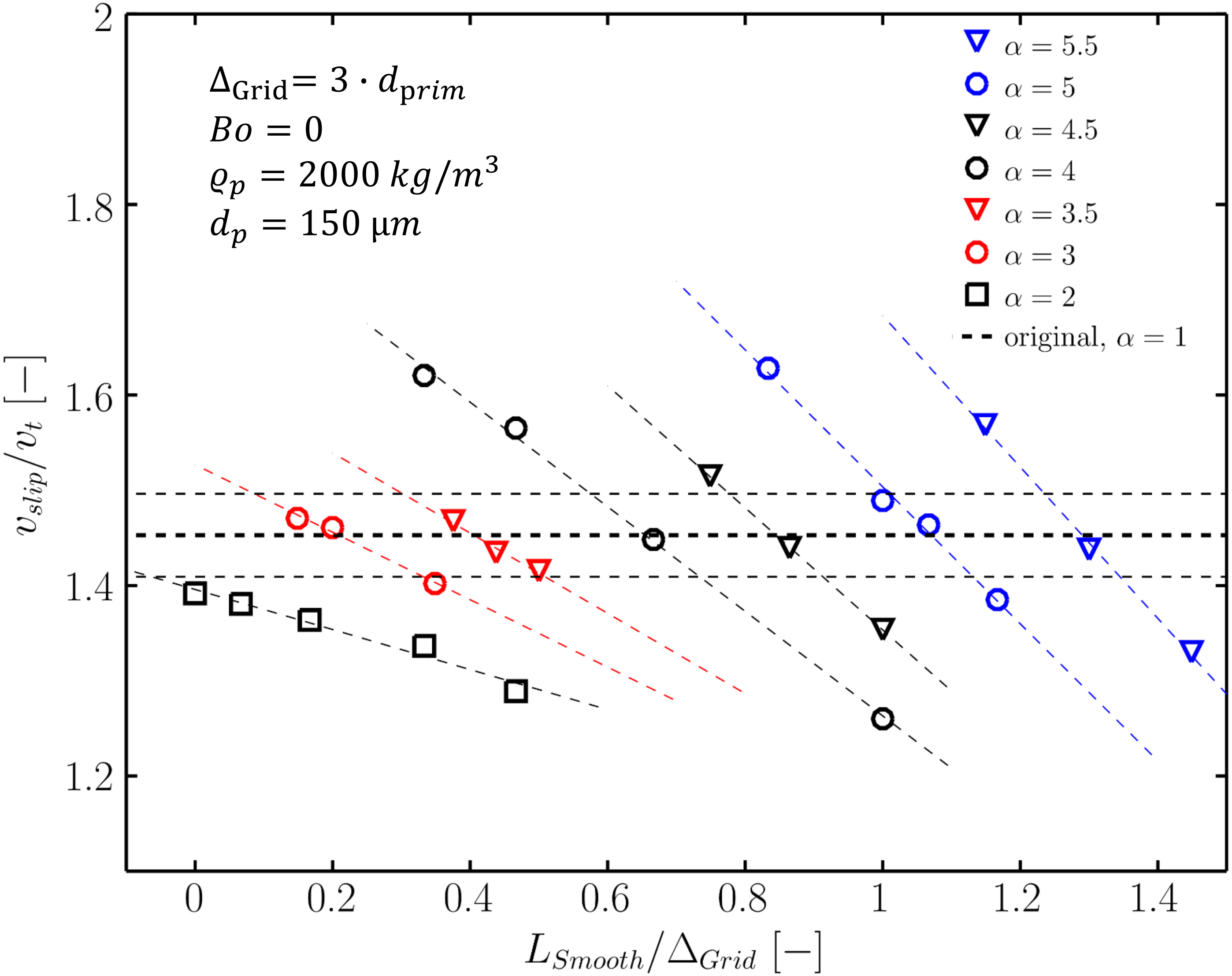

Non-cohesive & Monodisperse

Tausendschön et al., *submitted manuscript*

Optimal Smoothing Length

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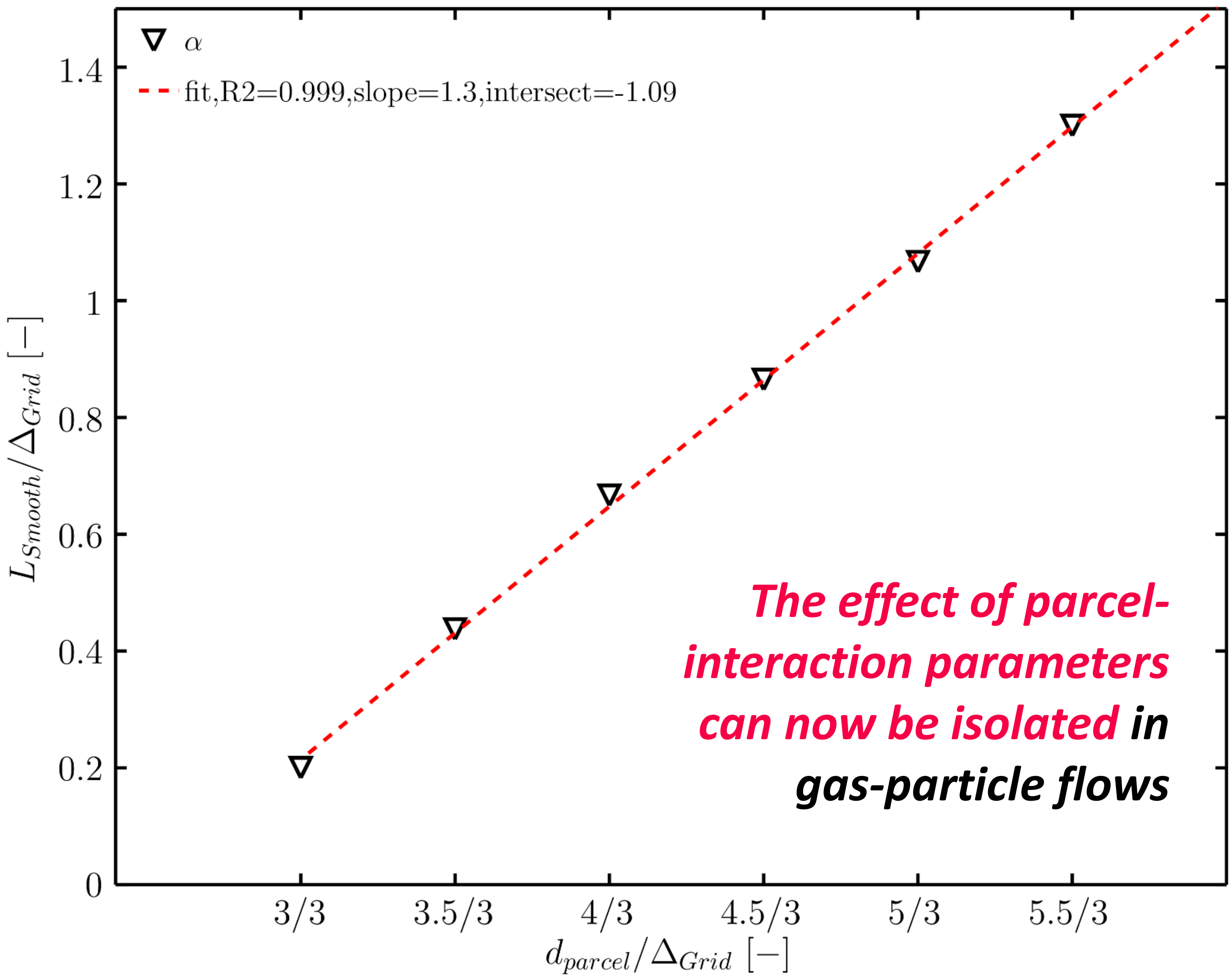
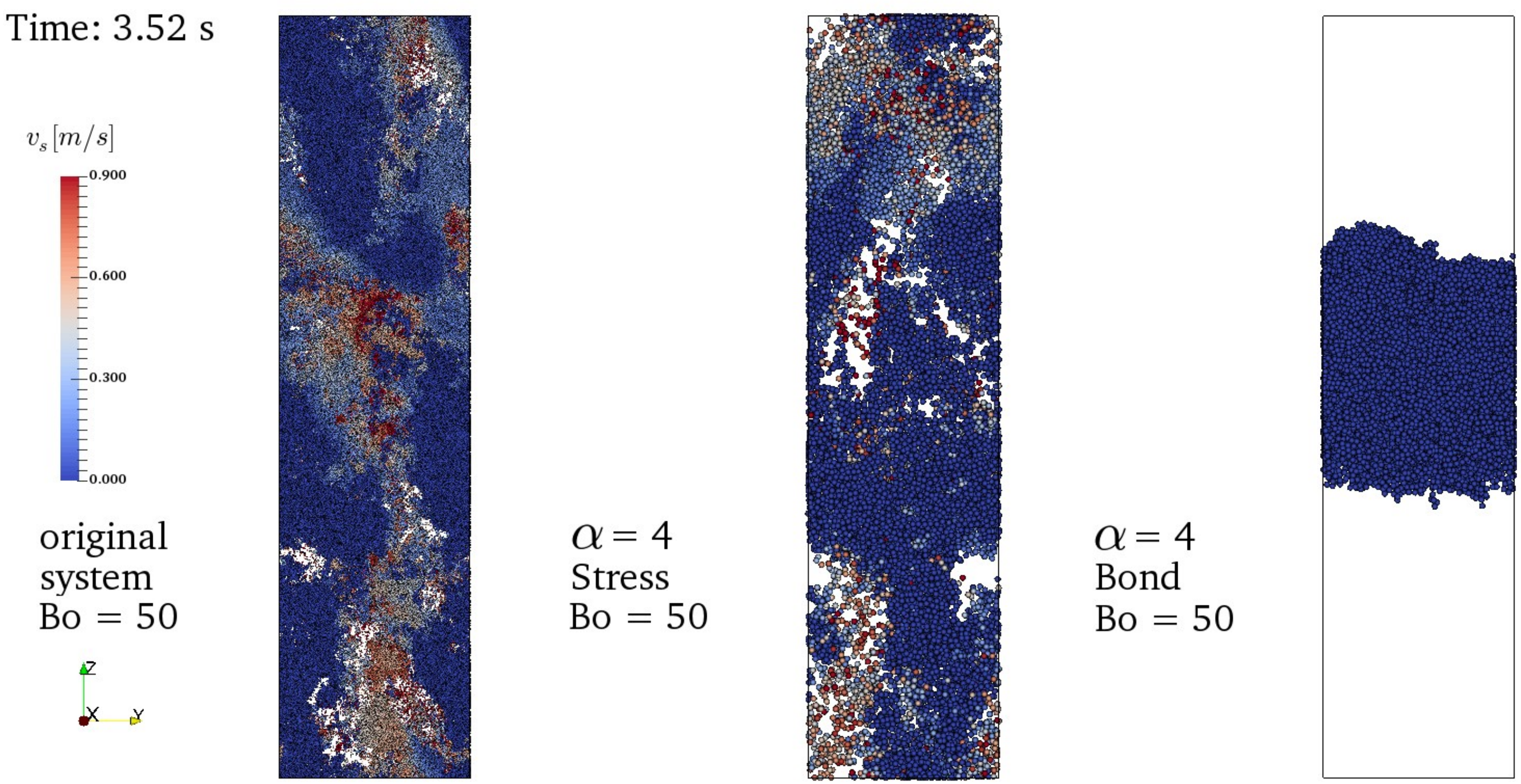


Non-cohesive & Monodisperse

The effect of parcel-interaction parameters can now be isolated in gas-particle flows

Tausendschön et al., *submitted manuscript*

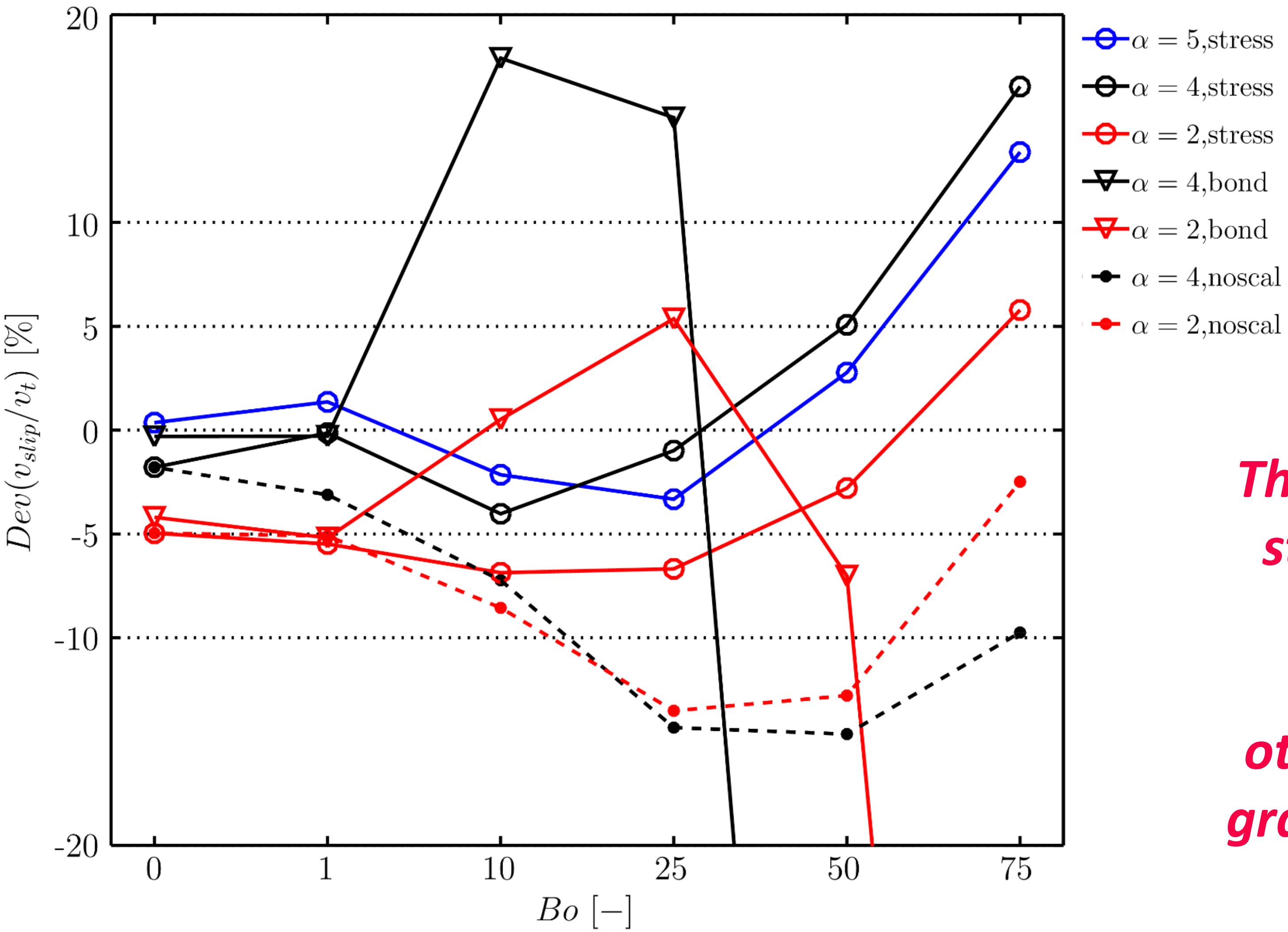
Cohesion & Coarse Graining



$$Bo = \frac{6\,\gamma}{d_p^2\;g\;\rho_p}$$

Cohesion

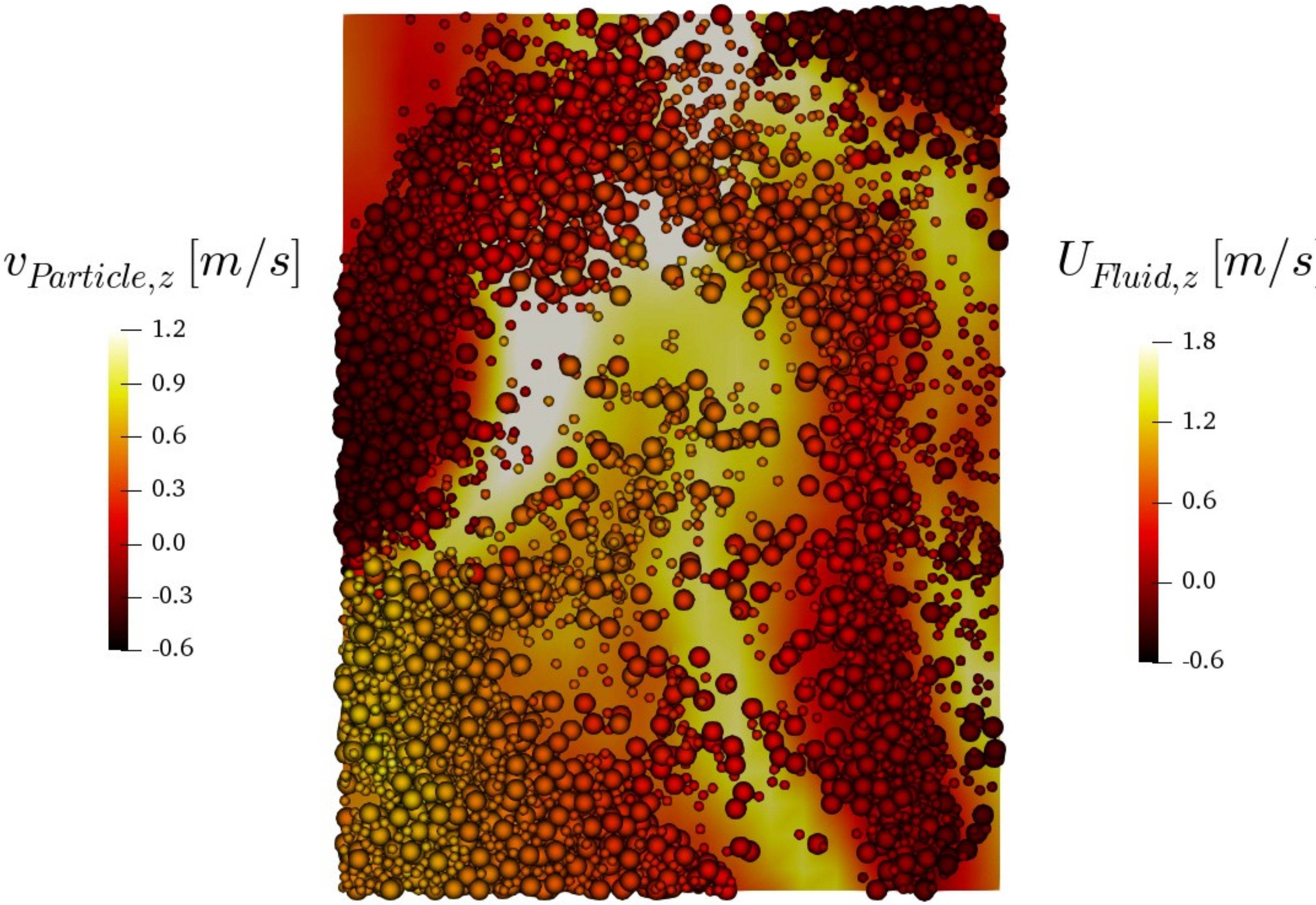
wet particles



The proposed stress-based scaling is superior to other coarse-graining force models

Tausendschön et al., *submitted manuscript*

Outlook & Conclusion



Polydispersity

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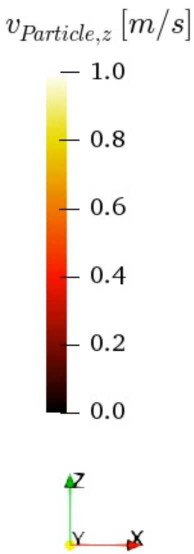
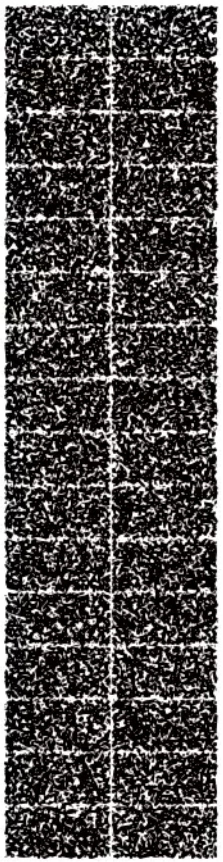
Primary Particle System

Time: 0.01 s





$\alpha = 2$
const.Diff.
smoothing

$\alpha = 2$
local P.size
smoothing

Polydispersity

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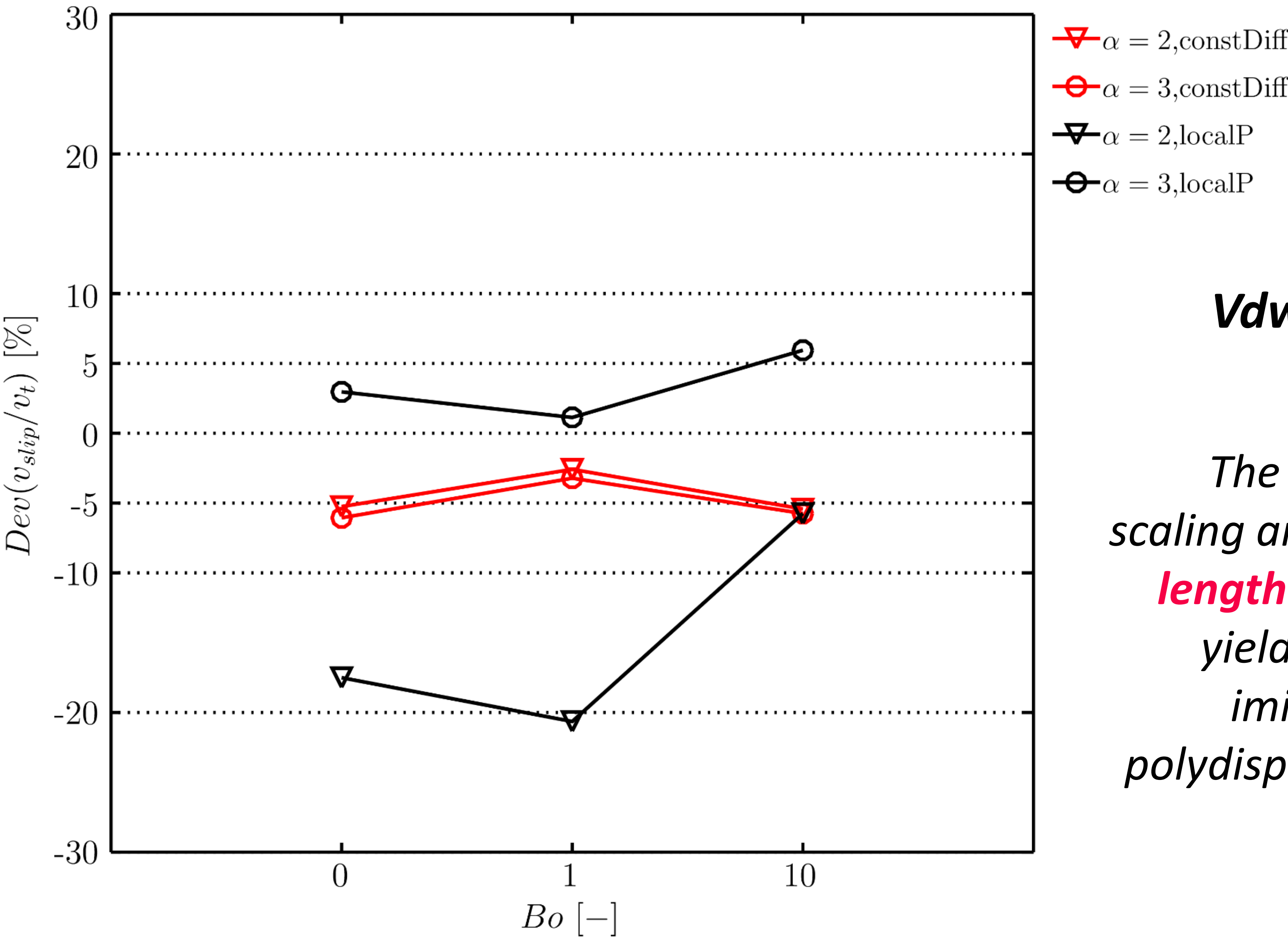

Vdw-cohesion

The stress-based scaling and ***"constant length" smoothing*** *yield an accurate imitation of the polydisperse primary system*

Conclusion & Outlook

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- With smoothing operation and optimal smoothing lengths: **effect of parcel-interaction parameters can be isolated**

- **Stress-based scaling** led to a very accurate imitation (of sedimentation speed!) of the original system in the monodisperse setup

- **Bo = 50 and α = 5** maximum permissible parameters to guarantee acceptable deviation from original system

- Stress-based scaling and **smoothing** appears suitable for **polydisperse systems** as well

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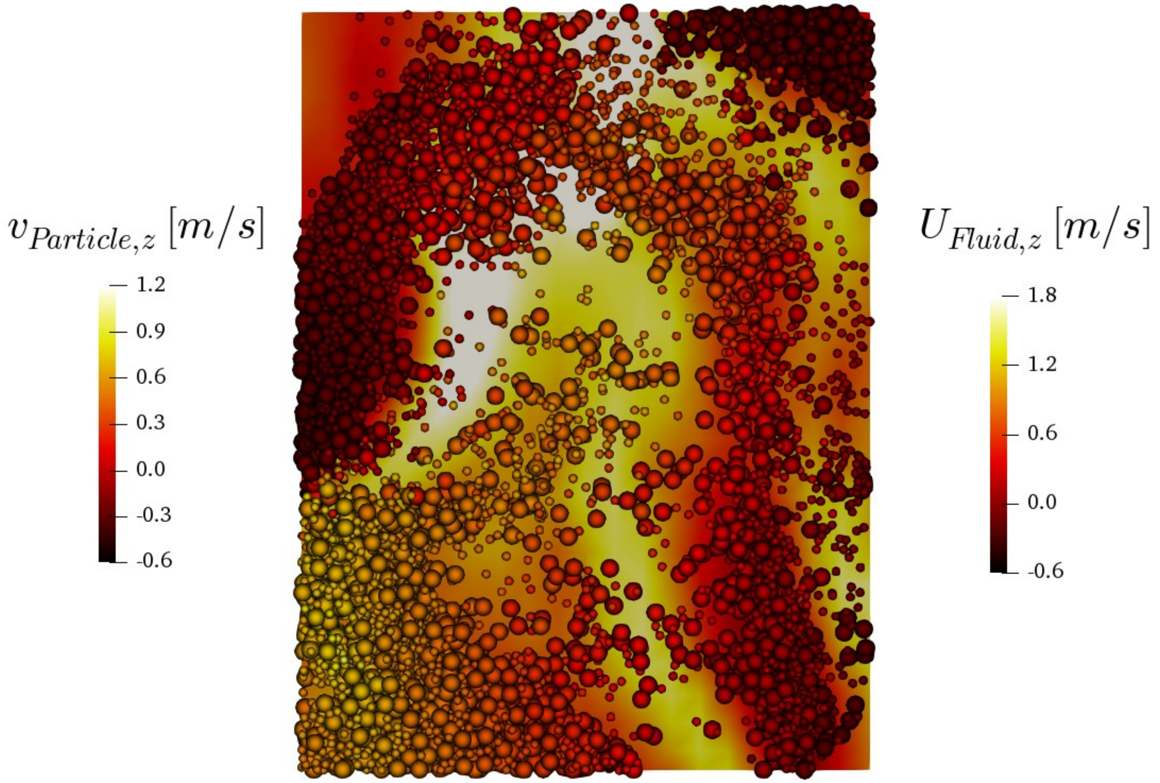

Thank you!

**Special thanks to
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