Closures for Meso-scale Models of Dense Suspensions

The Euler-Lagrange Perspective

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with contributions from

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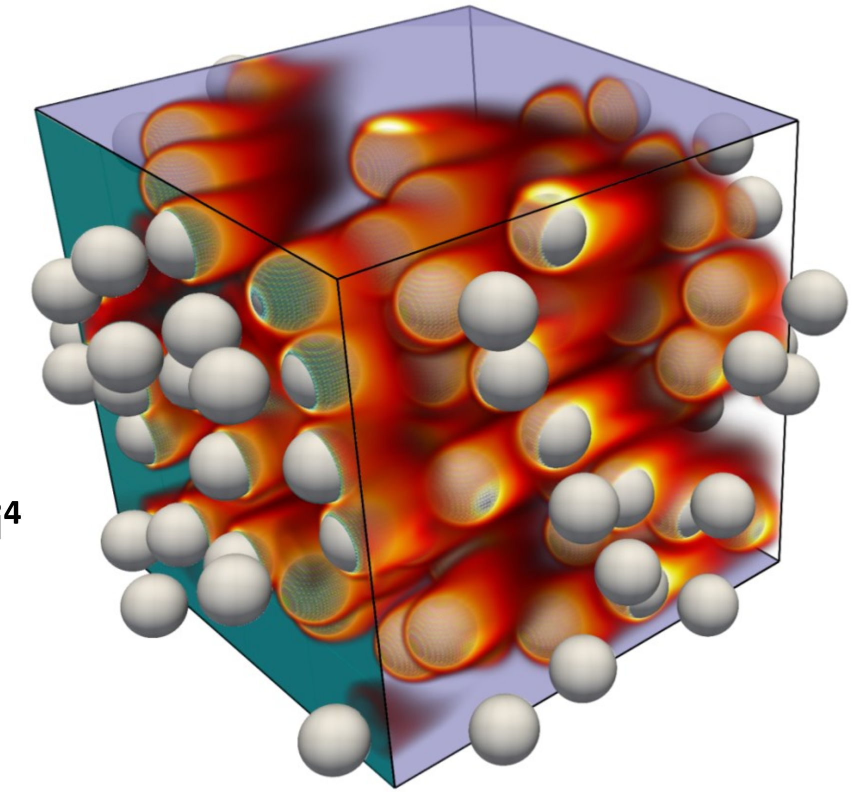


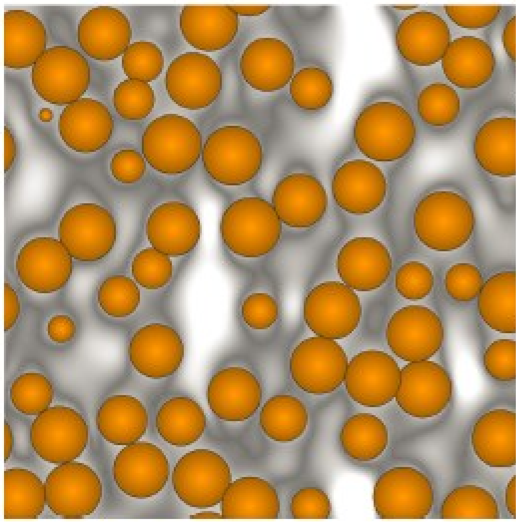
SEVENTH FRAMEWORK PROGRAMME

NanoSim

Example Application of CxD

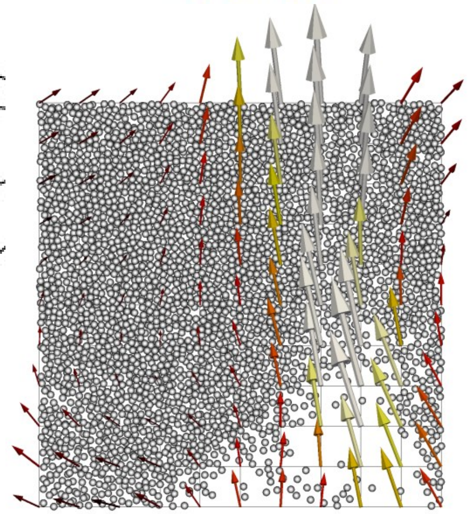
I – MICRO

~ 50μm-mm



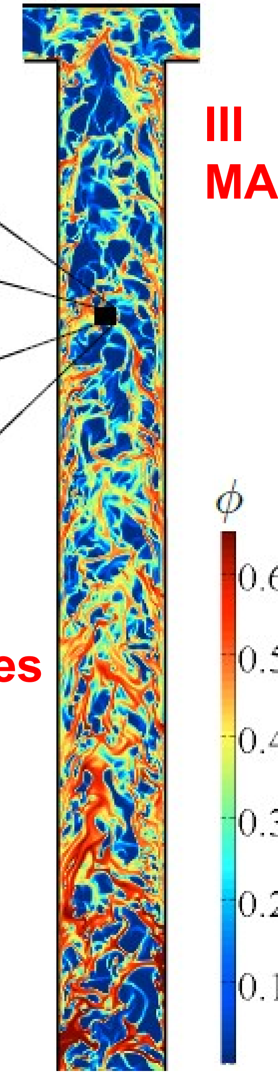
II – MESO

~ mm-cm



closures →

~ cm-m



III MACRO

closures →

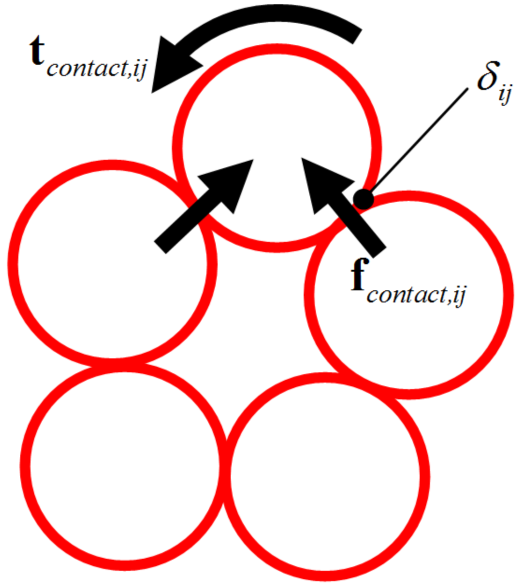
- **Meaningful** reaction kinetics must be fed **into "micro-scale"** models
- **Parameter Screening** at the micro scale to answer "*what matters*" (i.e., pore-scale diffusion, reaction, etc.)
- **Continue with meso and macro scale** if necessary.
- **Need closures**!

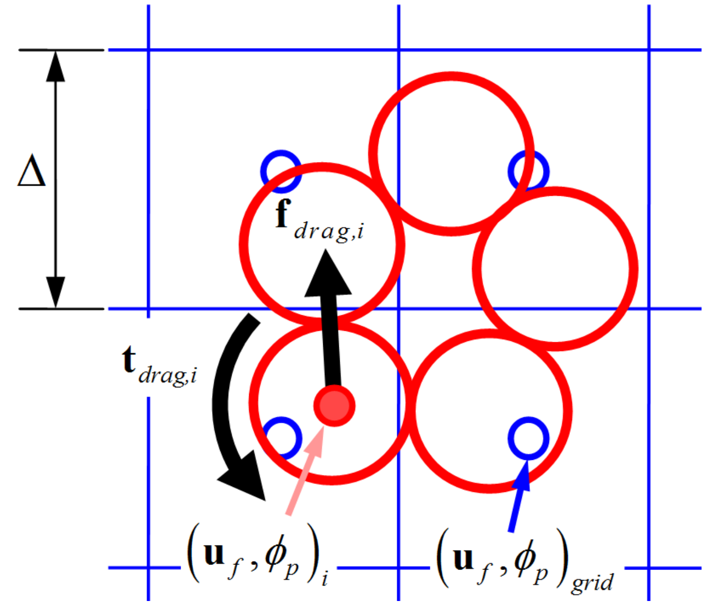
[1] W. Holloway, PhD Thesis, 2012.

Closures at the Meso Level

Flow

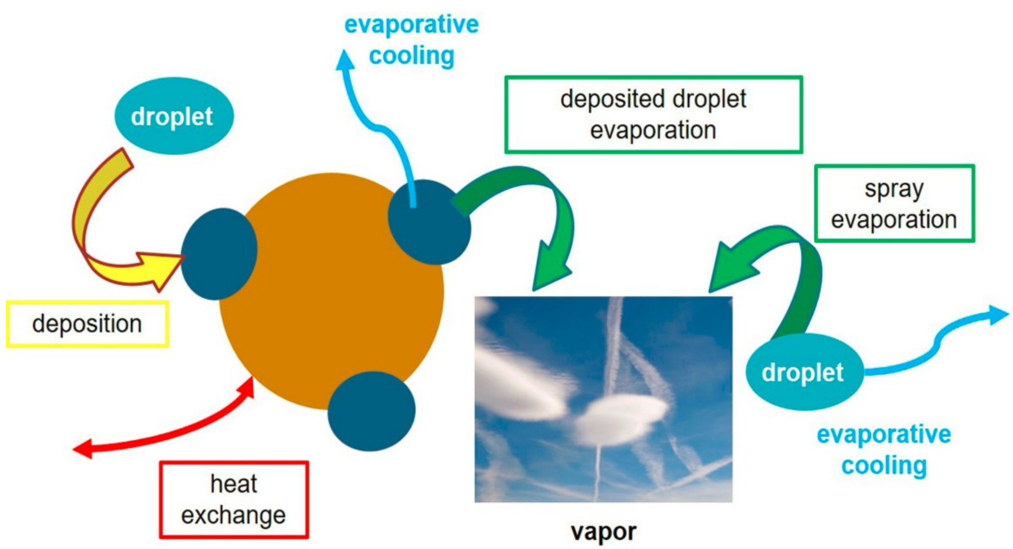
- Contact+cohesive forces and torques ***per contact***
- Fluid-Particle interaction (drag) forces and torques ***per particle***





Scalar Transport

- Heat and mass transfer rates (Nusselt/Sherwood numbers) ***per particle***
- Dispersion rates ***(fluid phase)***
- Filtration rates ***per particle***
- Liquid transfer rates ***per contact***



[2] M. Askarhishahi et al., *AIChE J* (2017) 63:2569-2587

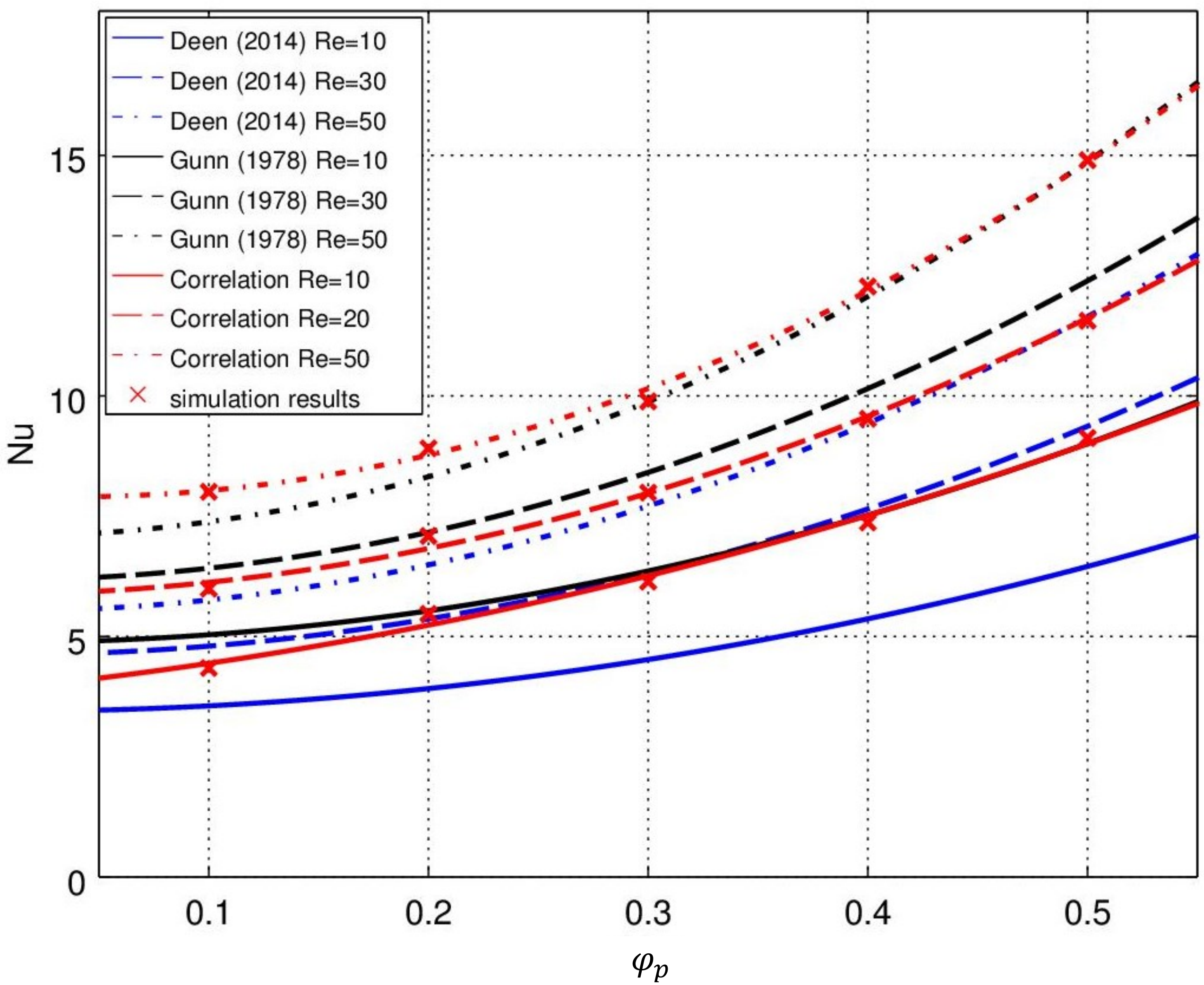
Overview

- Part I **The Bad**
  (…things done *incorrectly* in the past)
- Part II **The Hope (…present research)**
- Part III **The Future (…most likely ‘The Good’)**

5 + 10 + 10 = 25 mins

The Bad

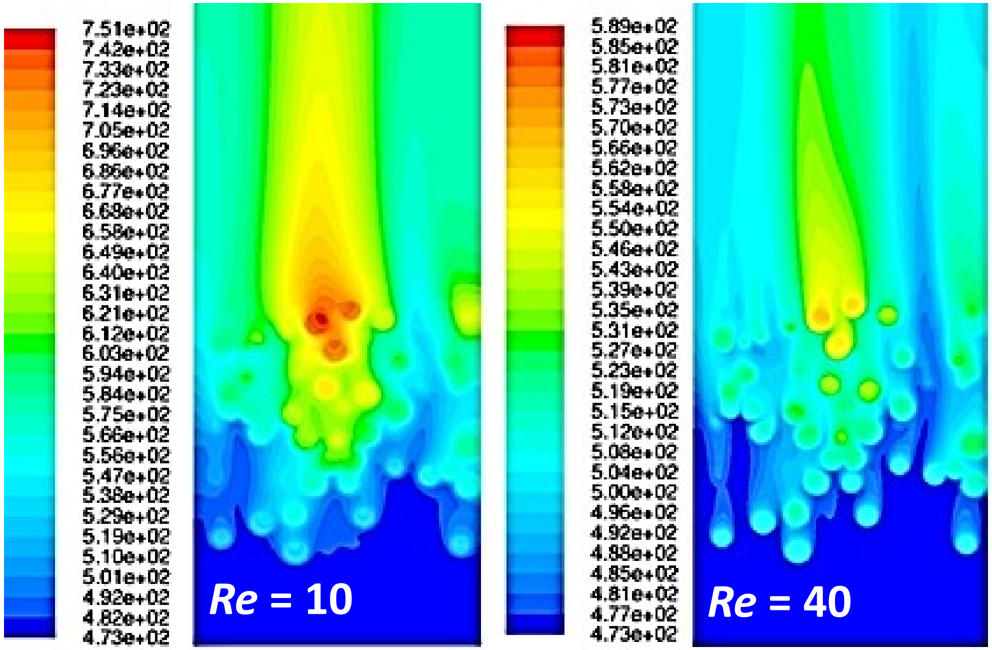
The Correlations



- Many exist for the **mean (i.e., an average over many particles)**
- The **fluid's cup-mixing** and **local mean temperature** are confused. Cup-mixing temp.: **okey for bed-average Nusselt numbers**, but in Euler-Lagrange models this quantity is **NOT known [3]**!
- **Correlations** are often **"over fitted"** in regimes where this is unnecessary (e.g., low Re, high ϕ_p)

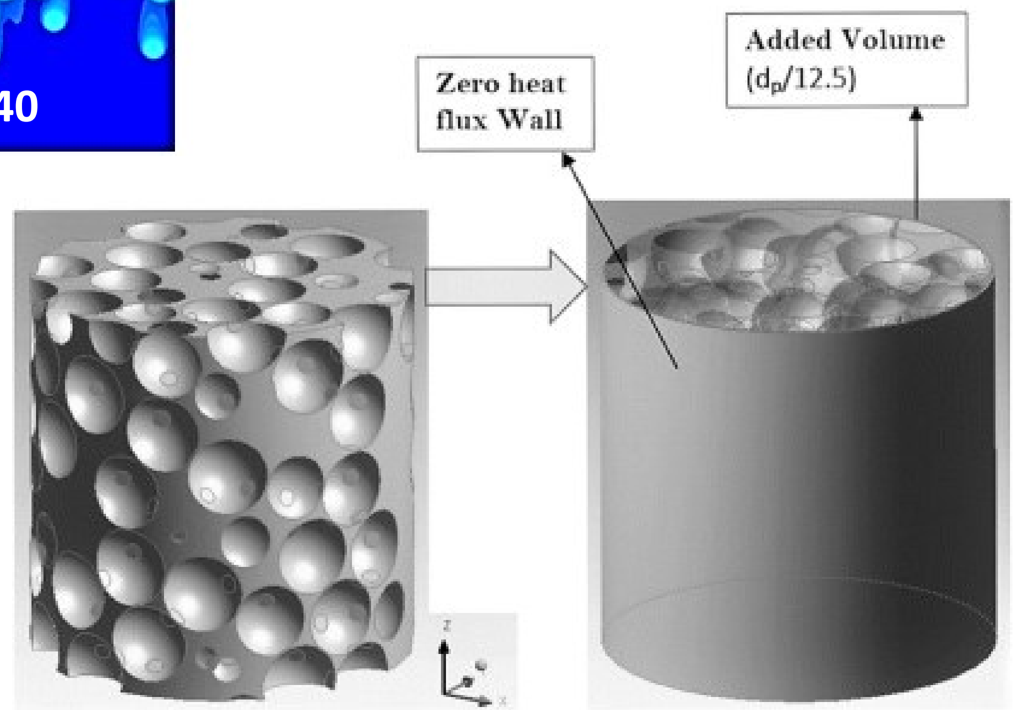
[3] B. Sun et al., *Int J Heat and Mass Transfer* (2015) 86:898–913

The Cylinder



- Correlations are valid for the **mean** and far away from **walls**
- **Confidence intervals** for parameters are not provided
- Computational domains are often **too small**

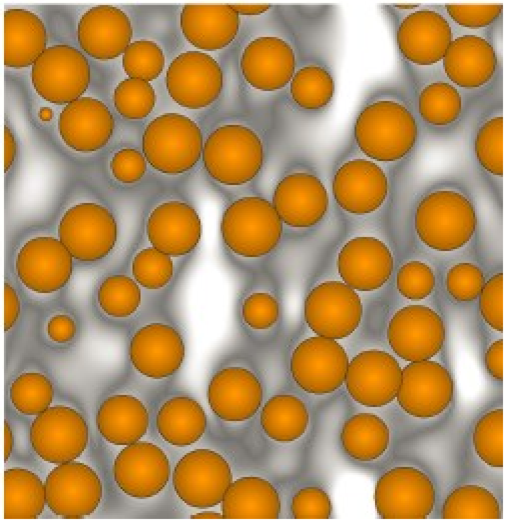
- Regions can be "cut out": this is **cumbersome (meshing!)**
- **Wall distance and wall curvature effects** are mixed up



[4] A. Singhal et al., *Chem Eng J* (2017) 314:27-37

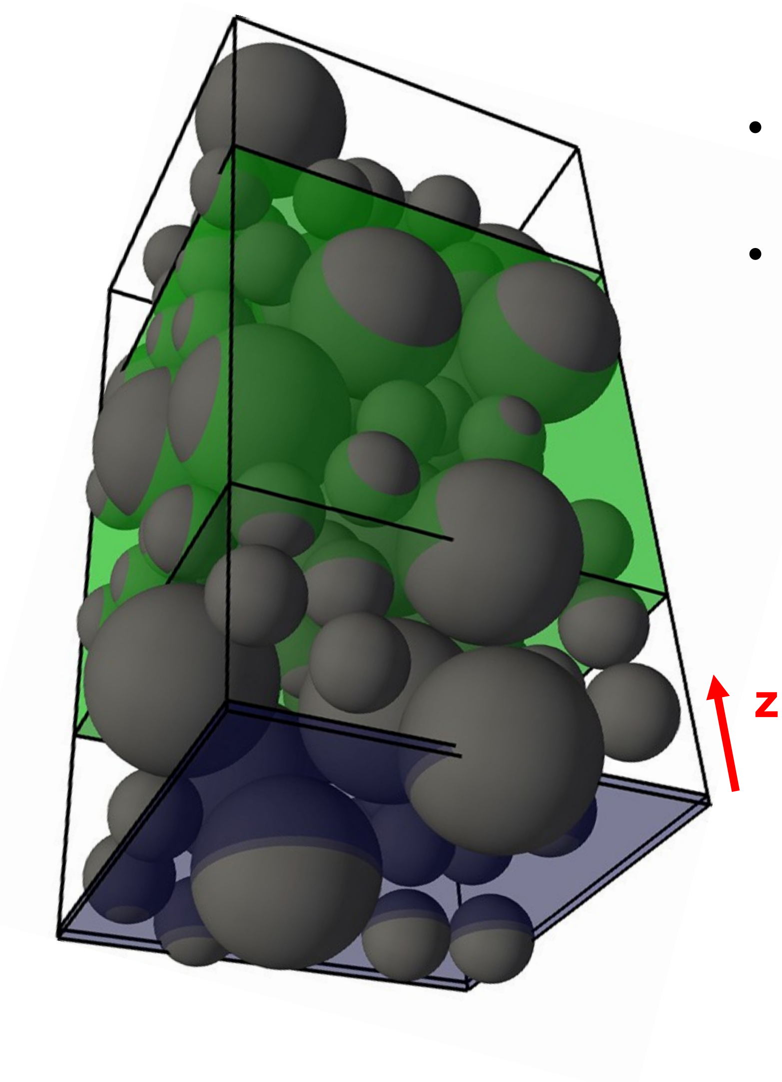
The Hope

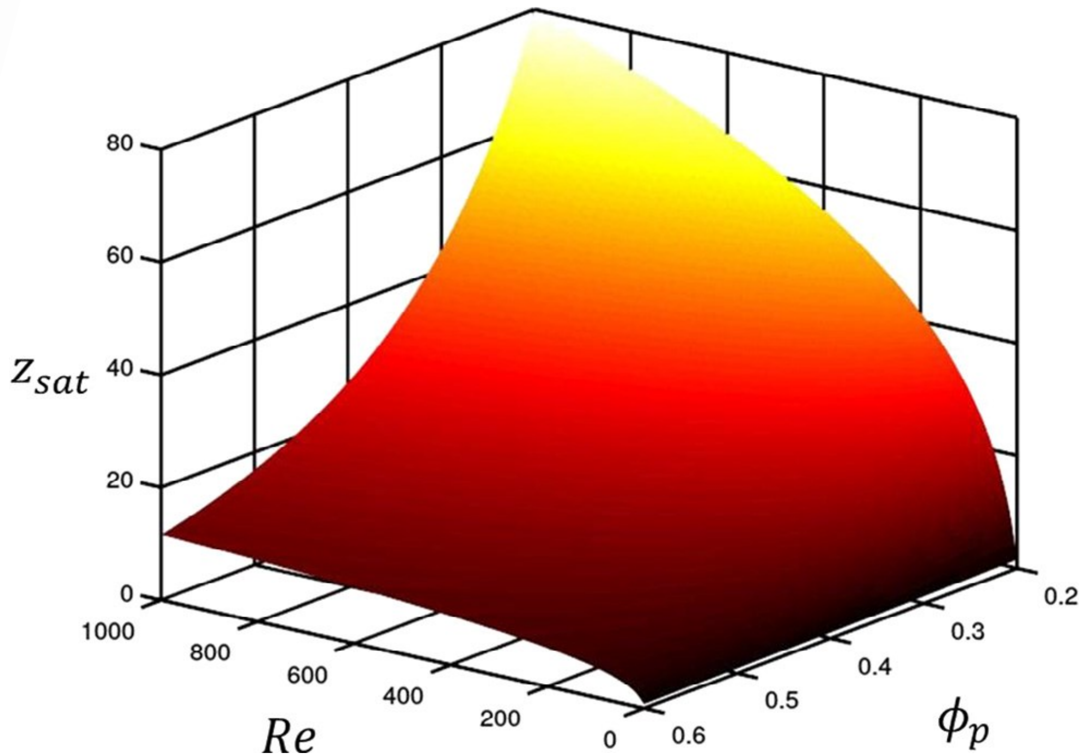
IIa – Towards Improved Closures



Saturation

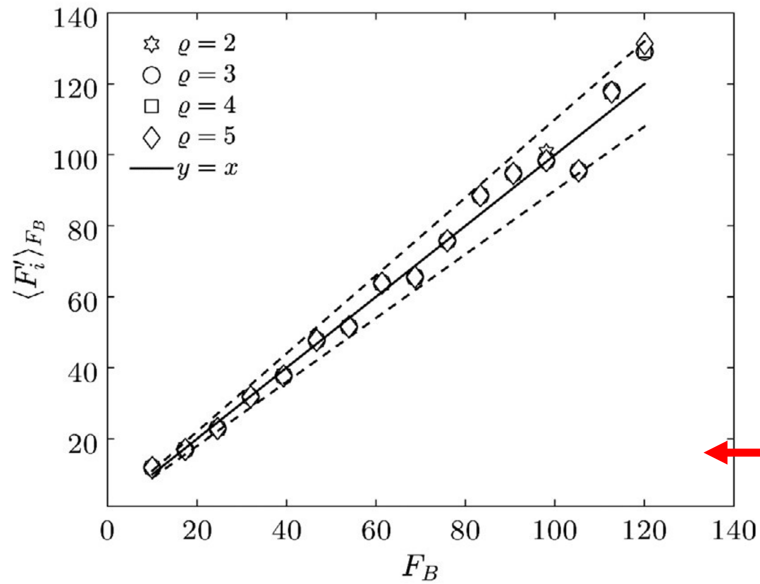
- For small Re and high ϕ_p → fluid phase is **quickly saturated** with the transferred quantity **(i.e., small z_{sat})**
- Fluid **field quickly relaxes** to equilibrium value provided at particle surface
- In a meso-scale simulation, ***Nu* would NOT matter**!





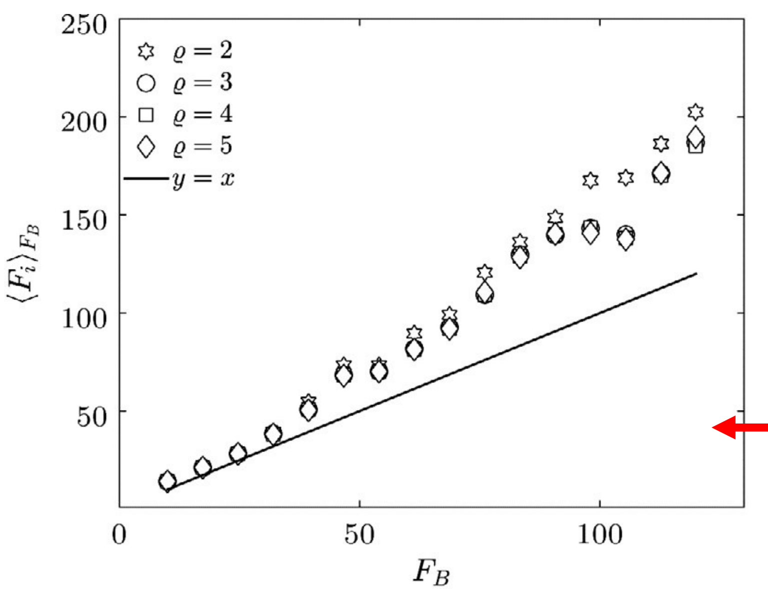
[5] F. Municchi and S. Radl, *Int J Heat Mass Transfer* (2017) 111:171–190

Bi-Disperse Systems: Drag Coefficient



- One **cannot simply re-scale** the fluid-particle interaction force (with 1-ϕ_p) to extract the drag force in bi- (and poly) disperse suspensions
- Fortunately, this can be **"repaired"**

Municchi and Radl (simple re-scaling) versus Beetstra et al. (simple re-scaling)



$$\mathbf{f}_{drag,i} \equiv \mathbf{f}_i - \mathbf{f}_i^{\nabla p^{\varrho}}$$

$\mathbf{f}_i$: Total force acting on particle i

$\mathbf{f}_i^d$: Drag force acting on particle i

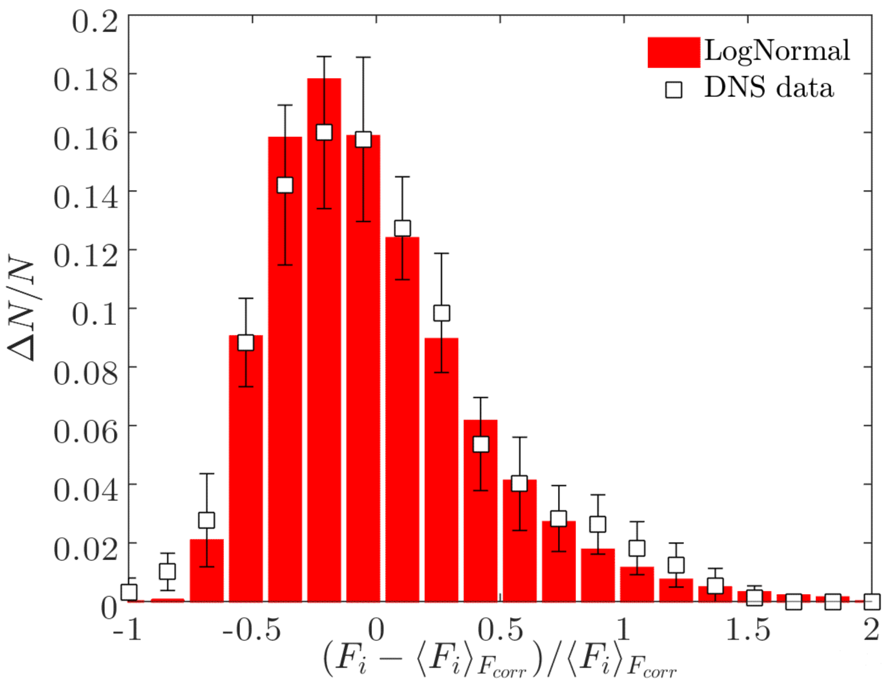
$\mathbf{f}_i^{\nabla p^{\varrho}}$: Force due to mean pressure gradient

Municchi and Radl (correct pressure gradient handling) versus Beetstra et al. (simple re-scaling)

[5] F. Municchi and S. Radl, *Int J Heat Mass Transfer* (2017), 111:171–190.

Bi-Disperse Systems: Mean versus Per-Particle

Drag Coefficient

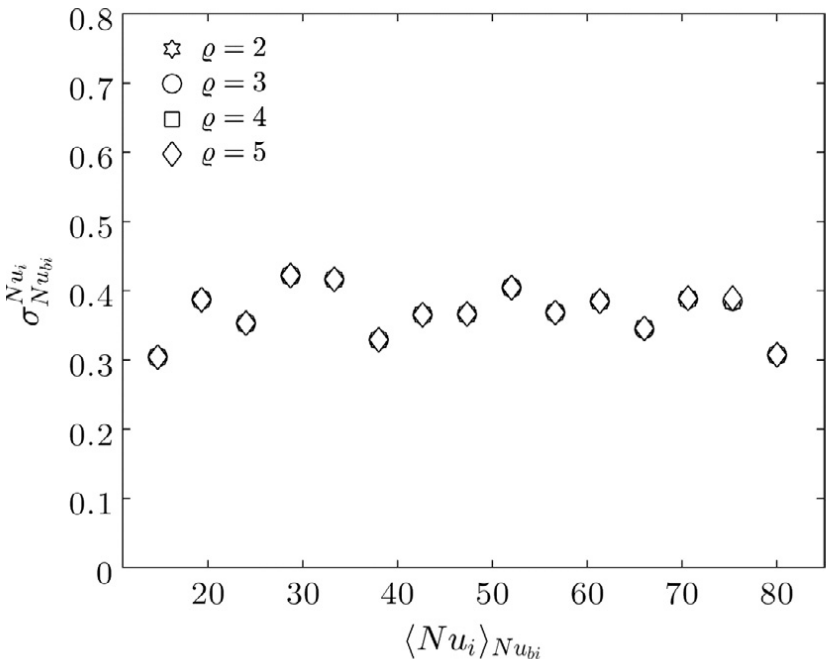


- Previous work [6] on per-particle drag variation attempted to model the **total fluid-particle force** (with moderate success)
- However, when using a correctly-defined drag coefficient: the **scaled variance for the drag coefficient** is approximately constant: **simple closure possible!**
- Particle-individual deviations can be approximated using a **Log-Normal distribution**

[6] S. Kriebitzsch et al., AIChE J 59:316–324, 2012.

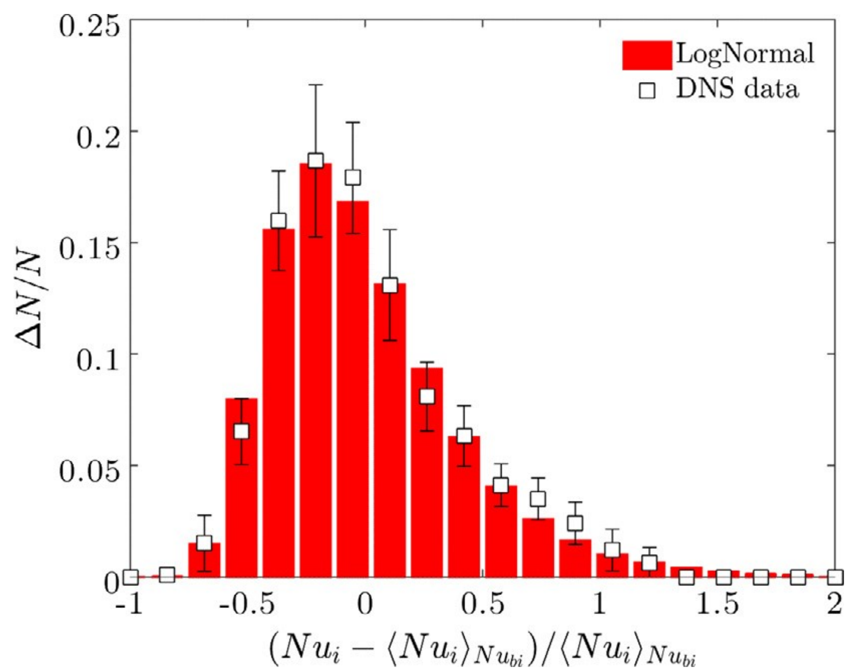
Bi-Disperse Systems: Mean versus Per-Particle

Nusselt Number



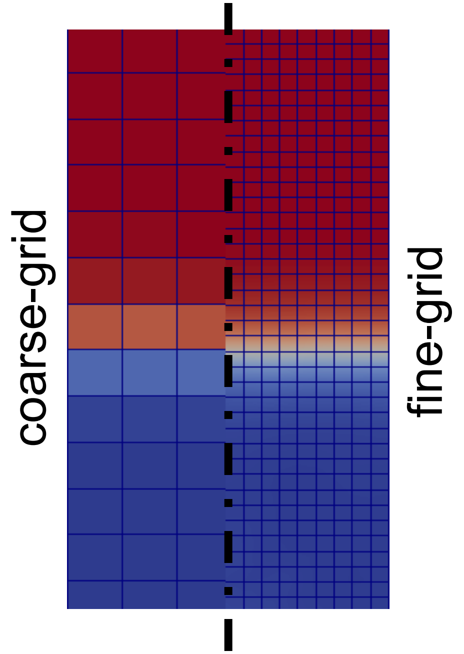
- Same as for the drag coefficient: **scaled variance for the Nusselt number** is approximately constant: **simple closure possible!**

- Particle-individual deviations again follow a **Log-Normal distribution,** which is a bit more peaked.



[5] F. Municchi and S. Radl, *Int J Heat Mass Transfer* (2017), 111:171–190.

IIa – Towards Improved Voidage Reconstruction



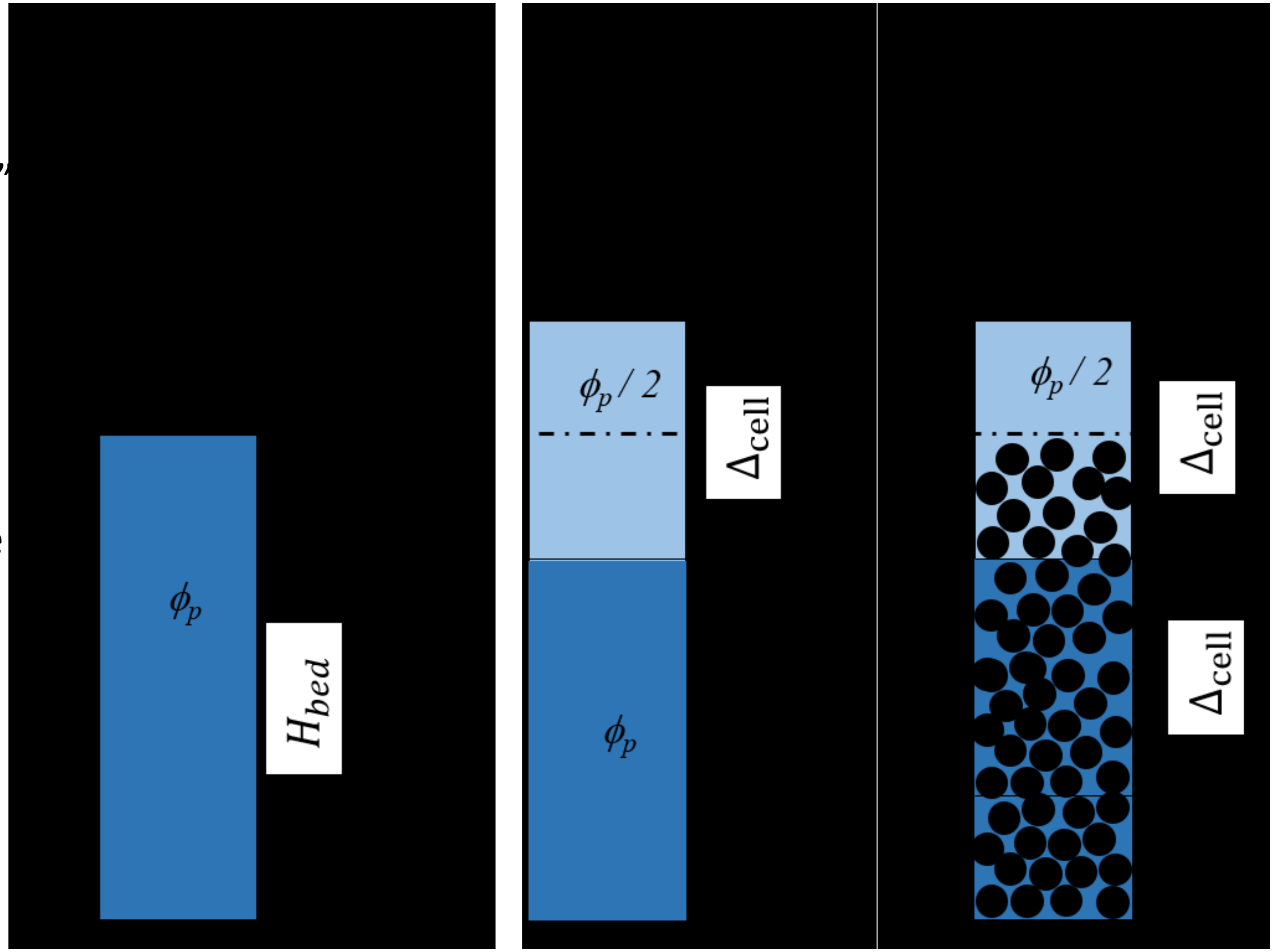
Eulerian versus Lagrangian

Base case:
fine grid

grid aligned with the jump in the voidage profile ("perfect" solution)

Case 1:
"coarse Eulerian grid"
the jump in voidage profile at the centre of the interface cell

Case 2:
"coarse Lagrangian grid"
the voidage is linearly interpolated at each particle position



Eulerian versus Lagrangian

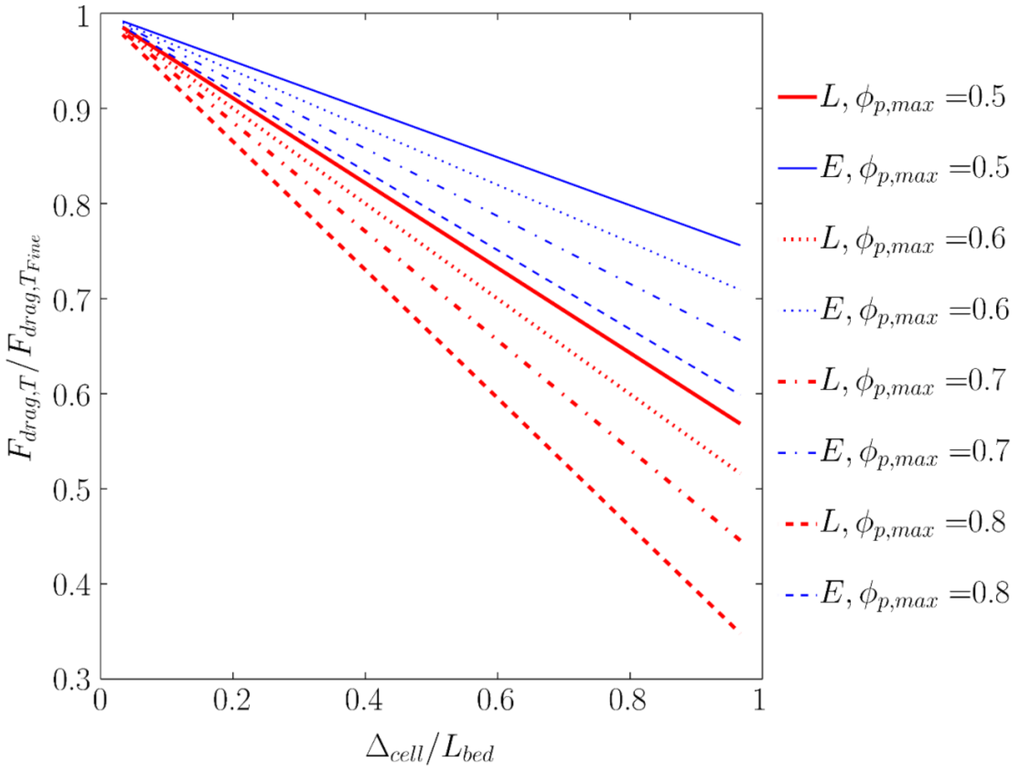
Local voidage is ***overpredicted on average***

↓

Underprediction of exchange coefficients

↓

Voidage correction is needed!



Lagrangian approach results in a **larger error** compared to Eulerian approach!

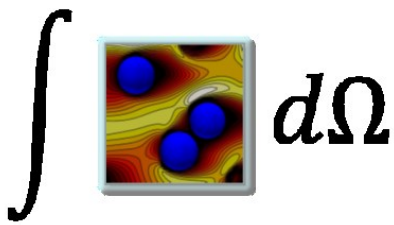
More on this later today (1.40 p.m.) from Maryam

The Future

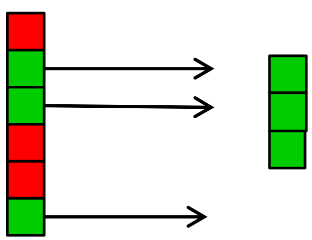
Coherent Toolsets

Post-Processing Utilities (e.g., CPPPO)

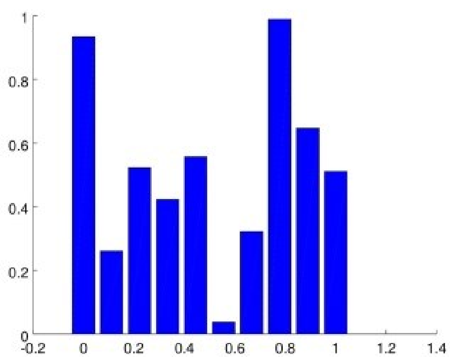
A Typical Set of Operations



Filtering of fluid and particle data, including **variance calculation**



Sampling of filtered data (**defined at runtime**) and their derivatives with statistical **biasing** (e.g., limiters)

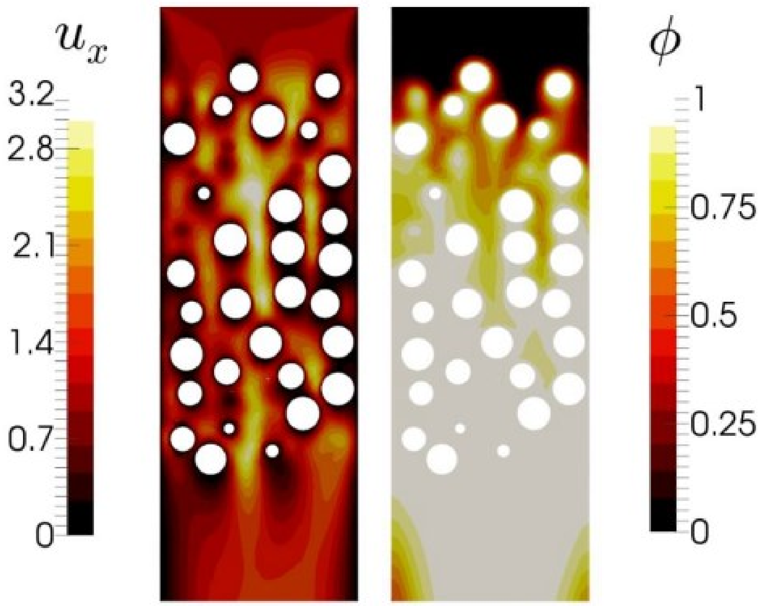


Binning of sampled data using running **statistics**

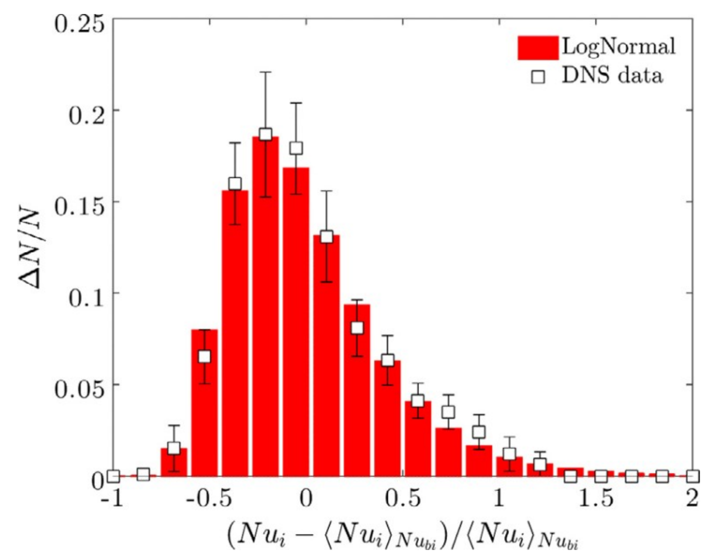
[7] Municchi et al., Comp Phys Comm (2016), 207:400–414.

Coherent Toolsets

Post-Processing Utilities (e.g., CPPPO)



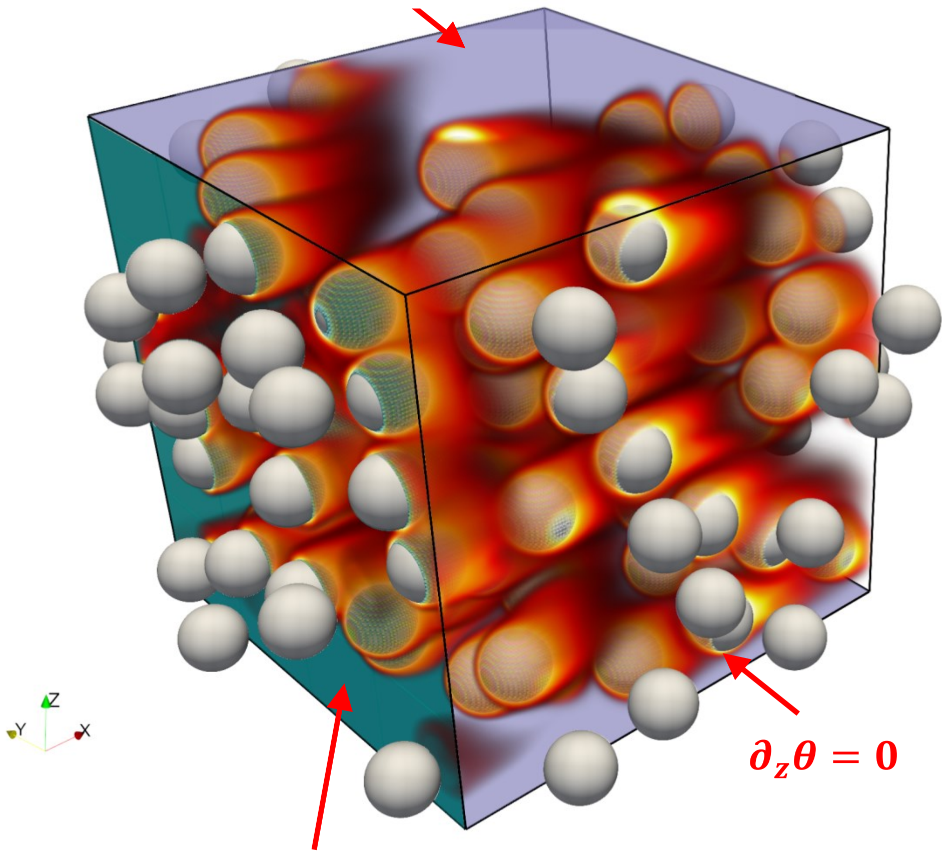
- **Support theory** (NOT mindless parameter fitting!): test hypothesis, supply data to establish closure, etc..
- Faster evaluation of filtered quantities desirable **(differential filtering)**.
- Exploration of a wider array of raw data sources (“**embedded** DNS boxes”, “**forcing**”) desireable → **database of filtered statistics**



Walls

Particle-Resolved DNS to identify Modeling Needs

Boundary conditions: temperature field



artificial **heat sink to** sustain fluid-particle temperature gradient

- Particle bed generated via bi-axial **compaction** in the *xy* plane using LIGGGHTS®
- Flow and temperature fields are solved in a *xy* **periodic domain**. **Particles are isothermal.**
- **CFDEM®Coupling** to solve the governing equations for the continuum phase
- Particles are represented by forcing terms in the governing equations, **Hybrid Fictitious Domain-Immersed Boundary** method

[8] Municchi et al., *Int J Heat and Mass Transfer* (2017), submitted

Walls

Particle-Resolved DNS to identify Modeling Needs

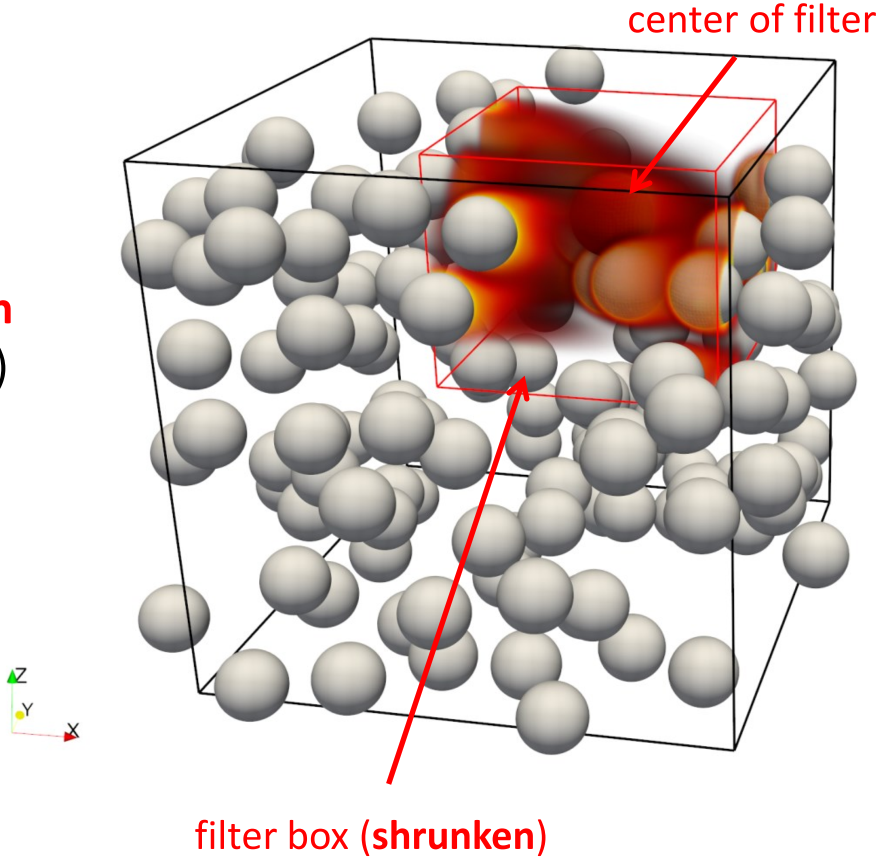
- We make use of the filtering toolbox **CPPPO** to spatially average ("filter") the continuum phase properties around **each particle**

$$\varrho = \frac{L_{filter}}{d_p}$$ Dimensionless filter size

- CPPPO is also employed to draw more "conventional" statistics (e.g., **profiles in wall-normal direction, "pancake filter"**)

- Filter boxes are **shrunk in the vicinity of wall boundaries**, same as done for wall bounded single phase turbulent flow

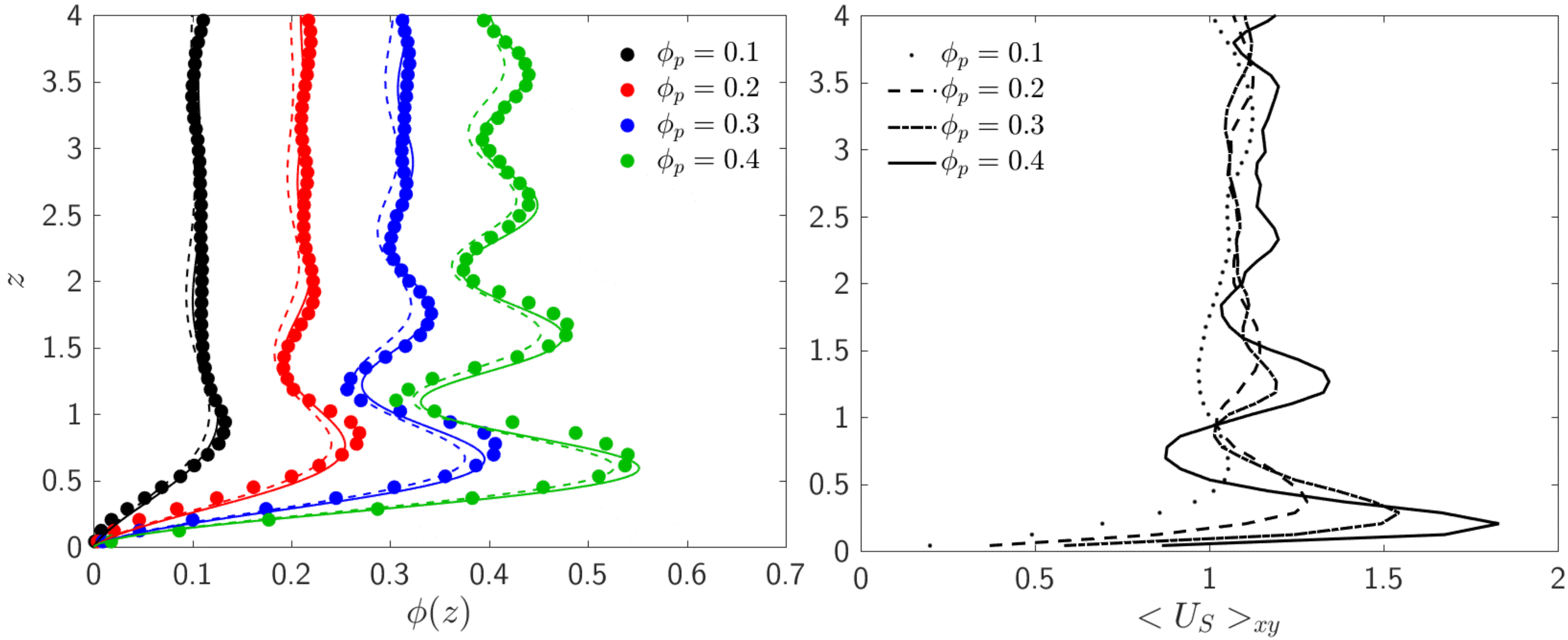
Lagrangian filtering: wall particles



Walls

Particle-Resolved DNS to identify Modeling Needs

Local Voidage and Speed

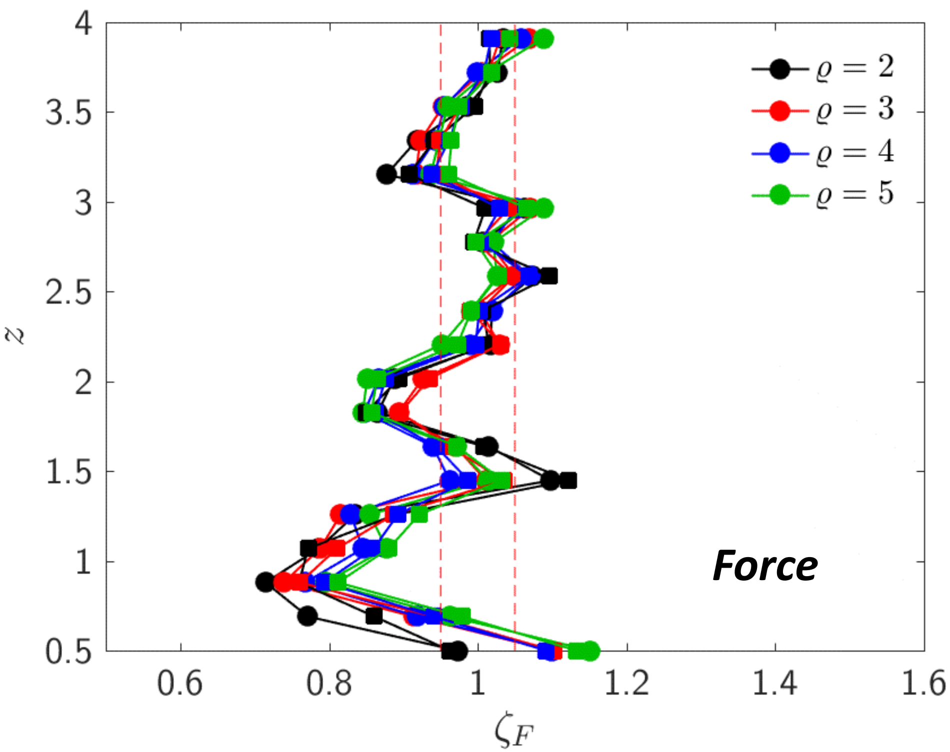


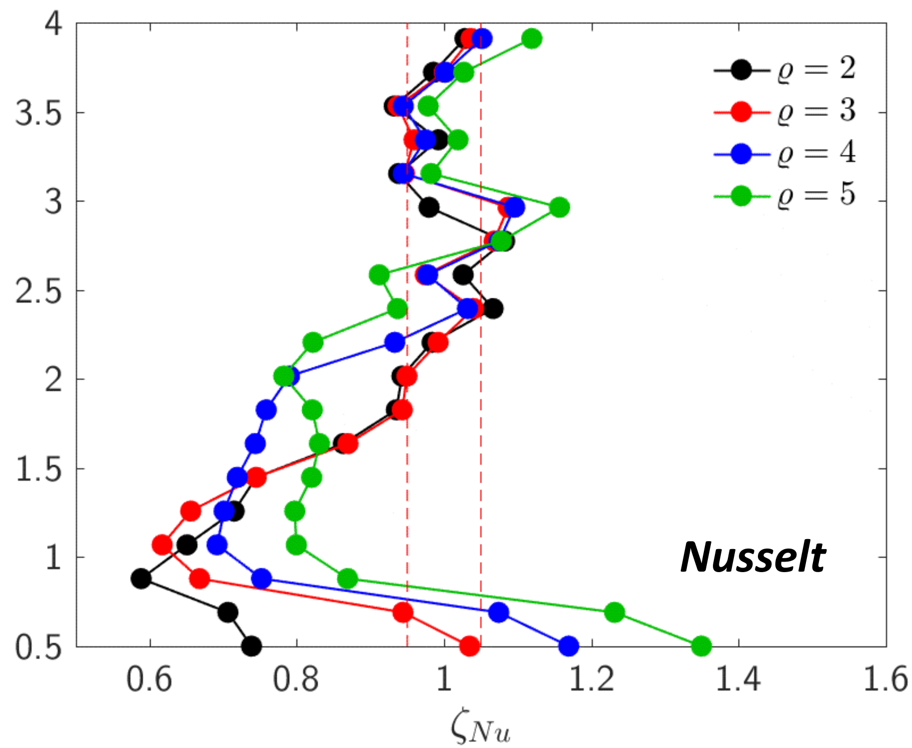
- General **correlation proposed for $\phi(z)$**
- Fluid speed **fluctuates strongly**, but with **small wavelength →** we expect a **filter-size independent near-wall correction**

Walls

Particle-Resolved DNS to identify Modeling Needs

Local Drag Correction and Nusselt Number

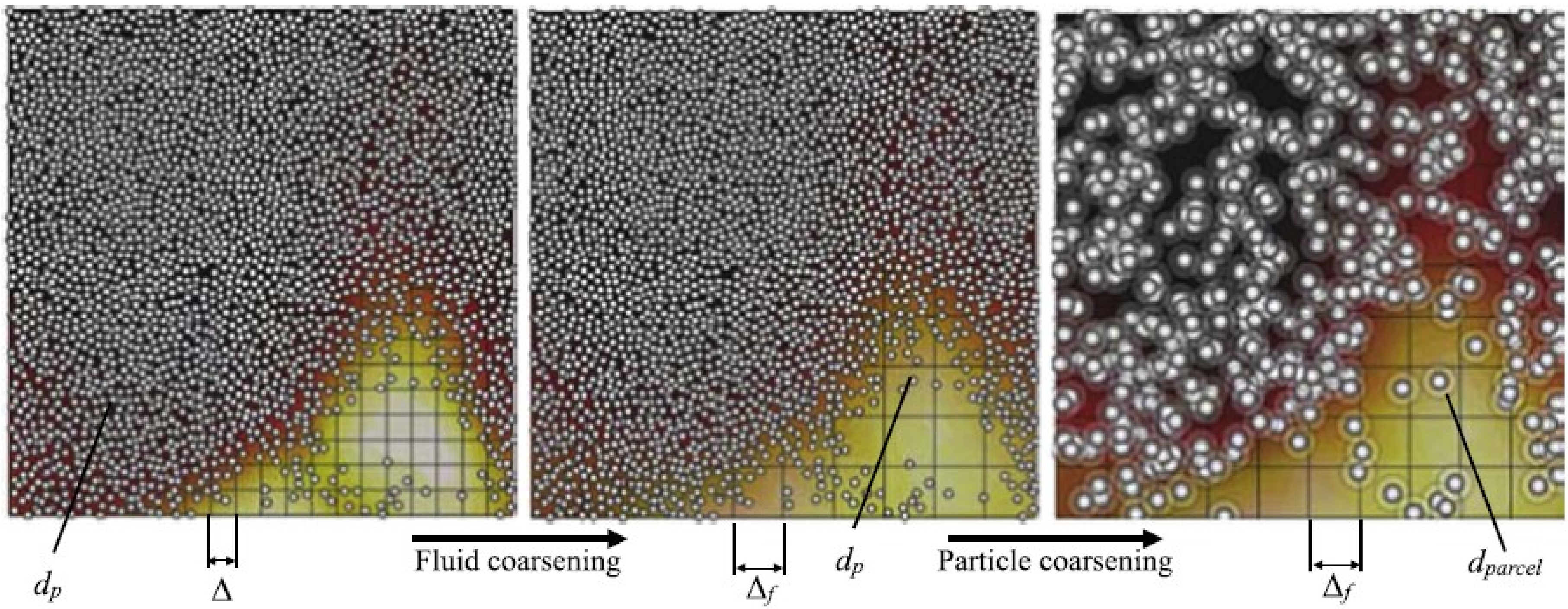




- $<\phi_p>$ = 0.4: substantial **negative drag correction for "2nd layer" particles**
- For the Nusselt number, the situation is **more complex (due to temperature profile!)**, and even higher **(mixed) heat flux corrections** are necessary

Faster Simulations

Deriving Closures for Large(r) Scale-Models



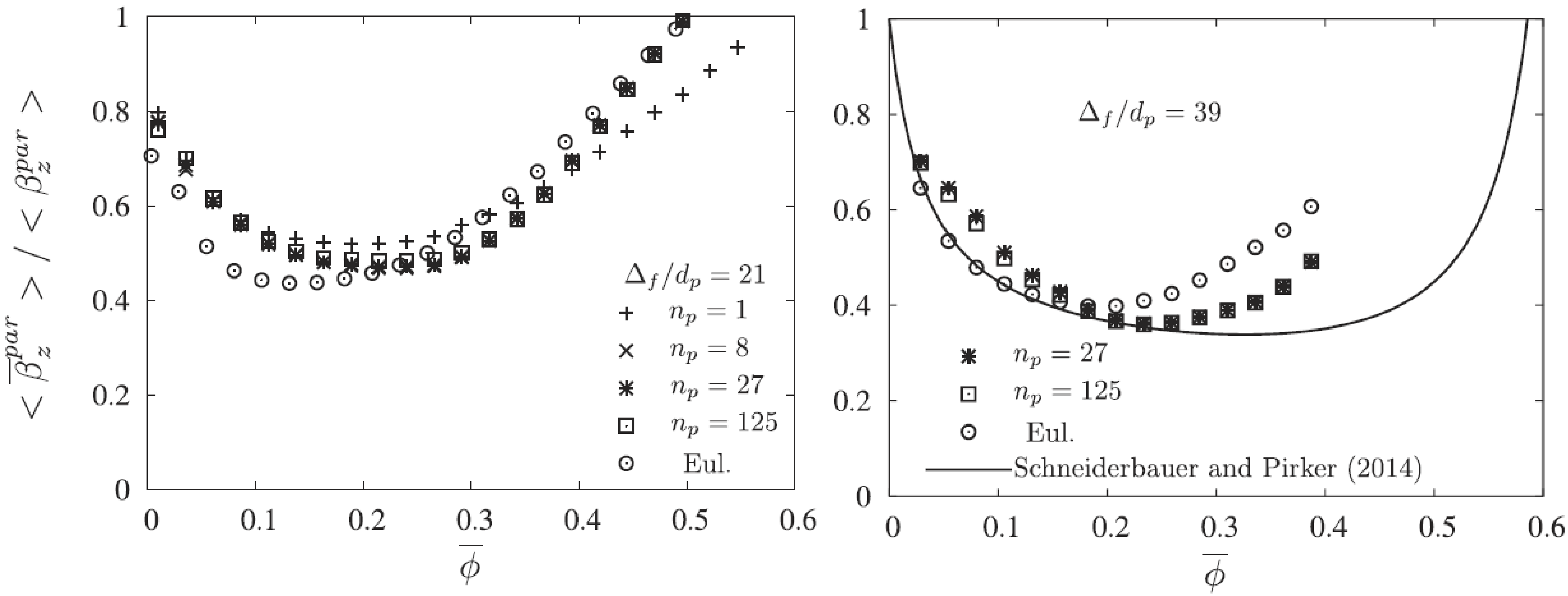
- CFD-DEM **allows two-step coarsening approach**
- In addition: use **projected (mean) particle speed**, which is approximating data from a Two-Fluid-Model (TFM).
- **3 choices of "filtered" coefficients**!

Q: What are the differences?

[9] Ozel et al., *Chem Eng Sci* (2016), 155:258–267

Faster Simulations

Deriving Closures for Large(r) Scale-Models



- **Fluid-coarsening** causes *the* dominant reduction in the effective drag coefficient
- **Only small difference** when going from coarse-grid CFD-DEM (n_p = 1) to parcel-based coarse-grid CFD-DEM
- Even **differences to TFM** are small!

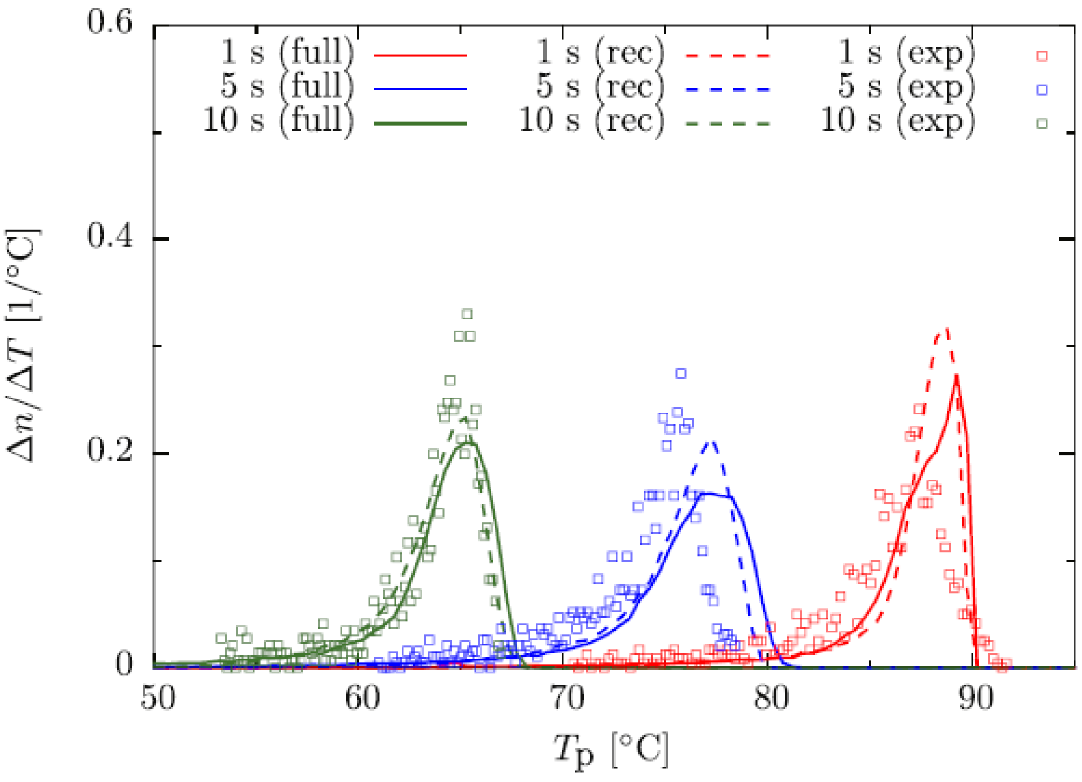
A: only resolving the gradients in the voidage field is important (in line with theory [10])!

[10] Schneiderbauer, *AIChE J* (2017), in press.

Even Faster Simulations

The long-standing Problem: How to put "Particles in the Loop"

- **Return to our starting point: 'Meaningful** reaction kinetics must be fed into **"micro-scale"** models'
- **Option 1**: Direct approach: necessitates full simulation of all involved particles for long times (can be hours real-time!). **Not feasible for "closure screening"**
- **Option 2: "Record and Playback"** as suggested by Lichtenegger et al. [11] appears to be attractive! Currently demonstrated for **heat transfer (i.e., particle temperature distributions)**, but this could be extended.



[11] Lichtenegger et al., *Chem Eng Sci* (2017), 172:310–322

Conclusions

Conclusions

- Closures for drag and heat/mass transfer are still **poor on a *per-particle* level** (and we even have not started looking at non-spherical or irregular particles!). **Particle (thermal) inertia "irons out" this problem**. But it persists for low particle-to-fluid density ratios, heat-sensitive reactions, etc.!
- **A first set of near wall corrections** ready to use! …but there are still many improvements necessary near walls (e.g., wall-fluid heat transfer rates, polydispersity)
- A large number of closures need potential improvement. **Which one to attack first (experiments, DNS, calibration)**? Sensitivity analysis using fast meso-scale models appears essential.

Thank you for your Attention!

TU Graz

Closures for Meso-scale Models of Dense Suspensions

The Euler-Lagrange Perspective

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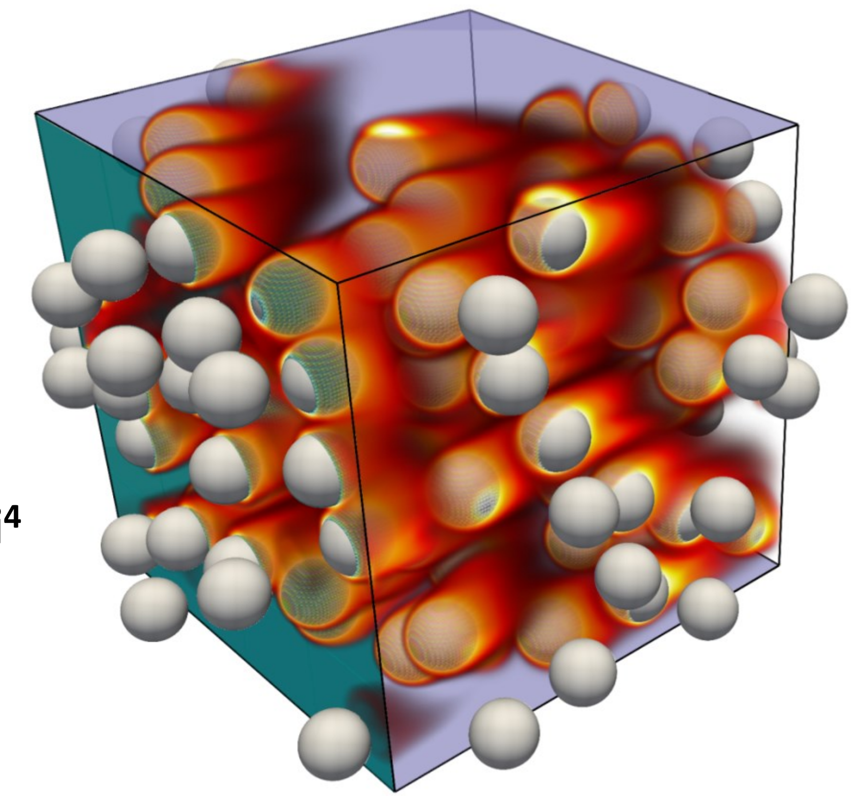

SEVENTH FRAMEWORK PROGRAMME

NanoSim

escape _ 28

Graz | AUSTRIA

June 10th to 13th | 2018

EFCE

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Acknowledgement and Disclaimer

Parts of the "CPPPO" code were developed in the frame of the "NanoSim" project funded by the European Commission through FP7 Grant agreement no. 604656.
http://www.sintef.no/projectweb/nanosim/

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NanoSim