Arbitrary Order Boundary Reconstruction Algorithm for Robin Boundary Conditions in Particle-Resolved Direct Numerical Simulations

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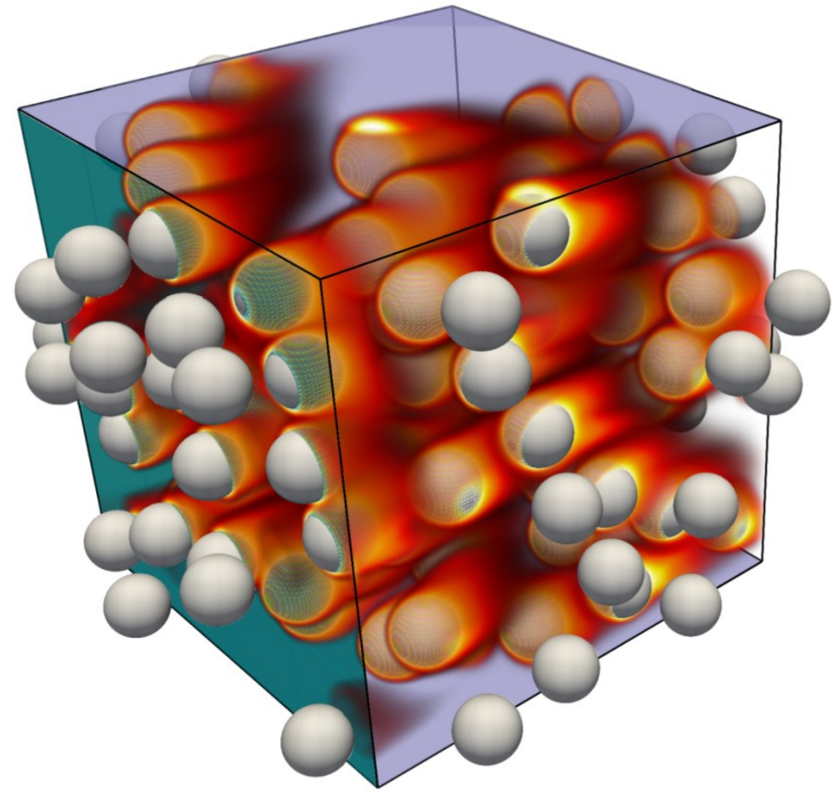
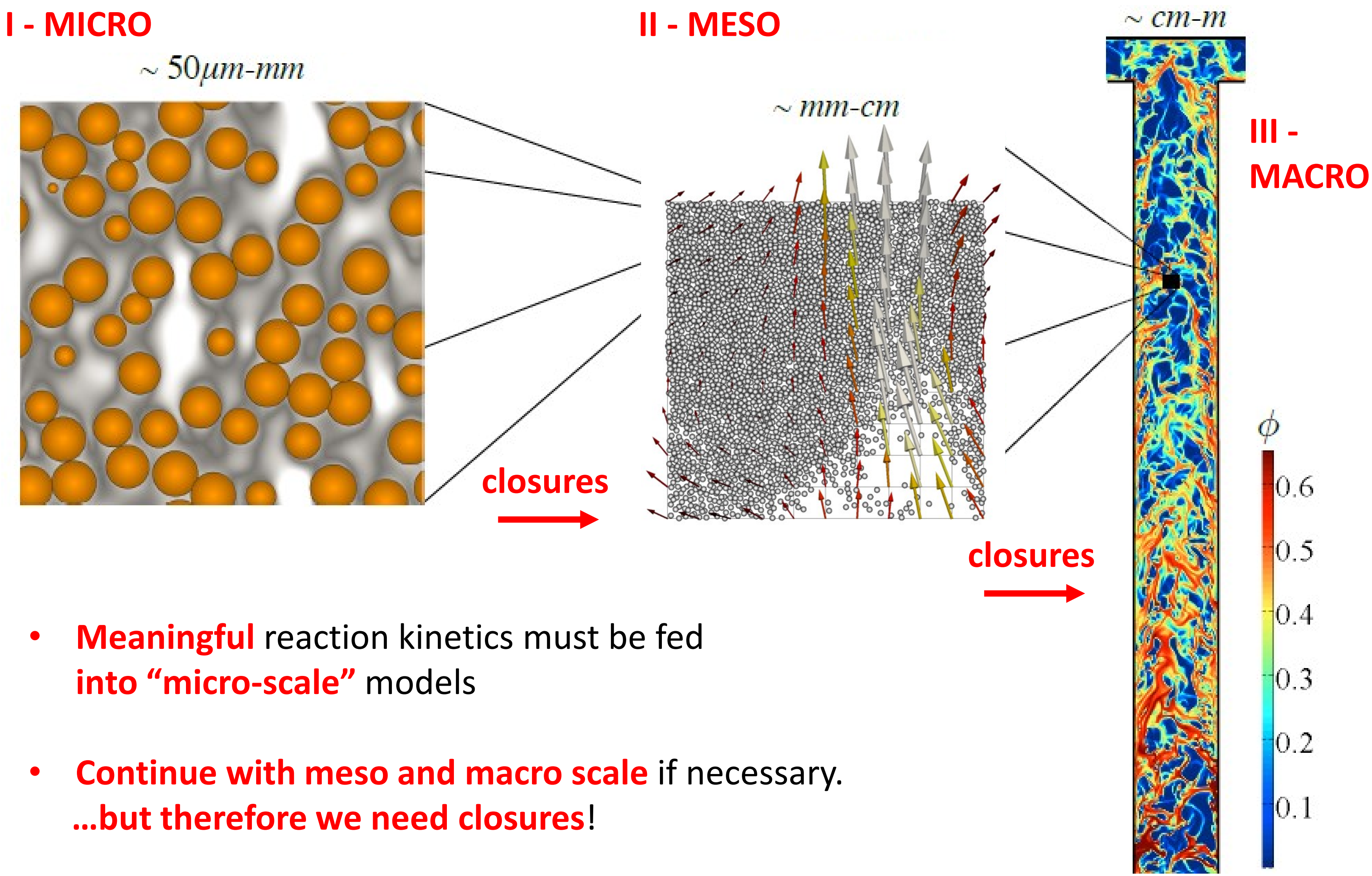
Particle-Resolved Direct Numerical Simulations

F. Municchi, S. Radl[1]

[1]Graz University of Technology



Example Application of CxD

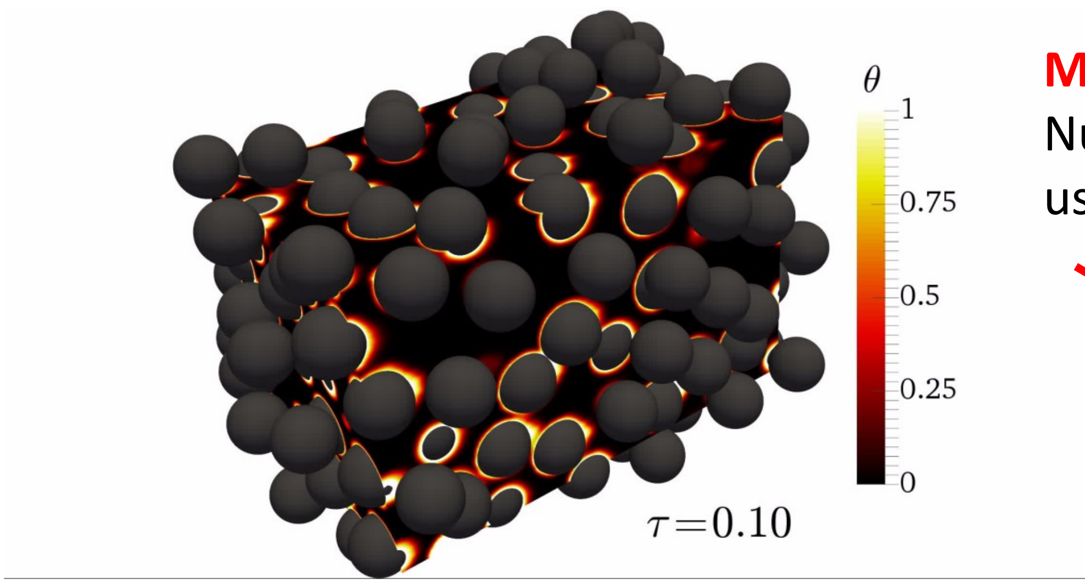


- **Meaningful** reaction kinetics must be fed **into "micro-scale"** models

- **Continue with meso and macro scale** if necessary. **…but therefore we need closures**!

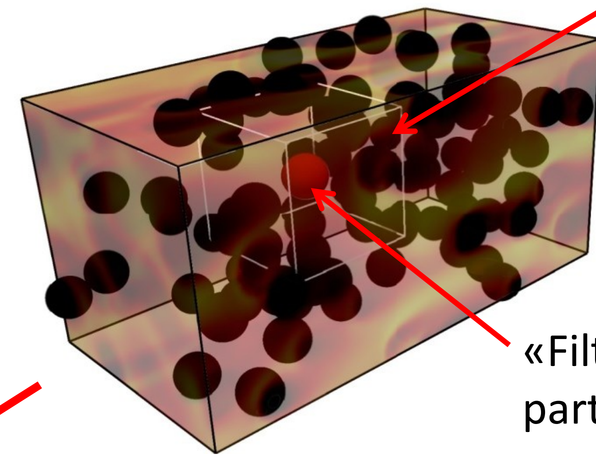
[1] W. Holloway, PhD Thesis, 2012.

Micro & Meso Level: Typical Results



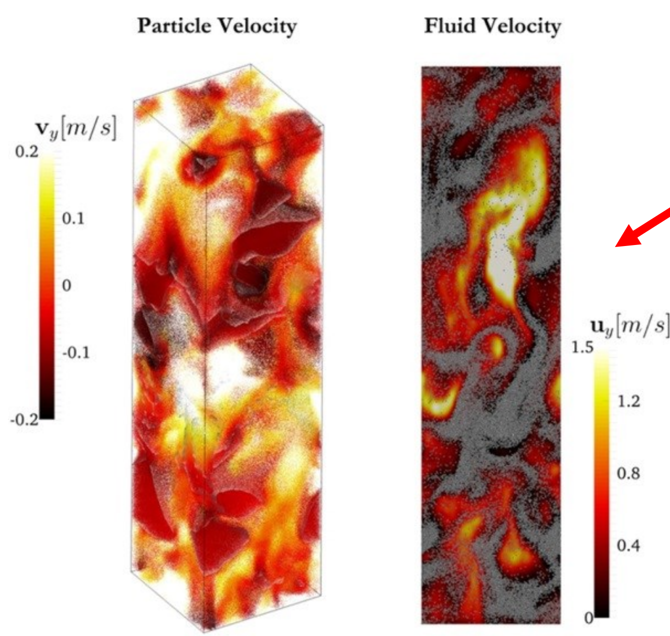
Micro Level: Particle-Resolved Direct Numerical Simulation (PR-DNS), e.g., using the tool CFDEM®

Filtering domain (i.e., coarse cell)



«Filtered particle»

Meso Level: Closures are used in Particle-Unresolved Euler-Lagrange models, e.g., using the tool CFDEM®

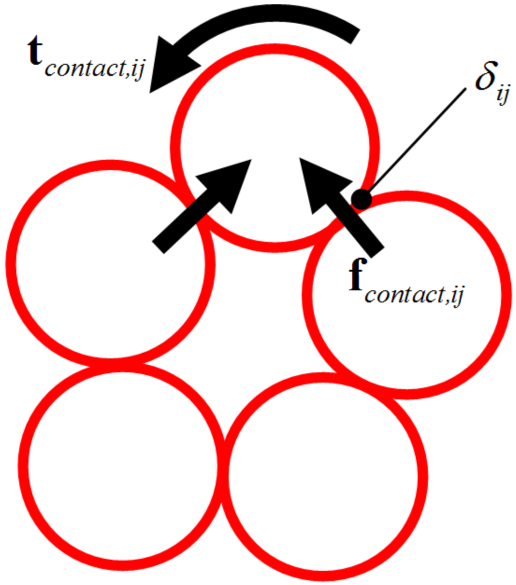


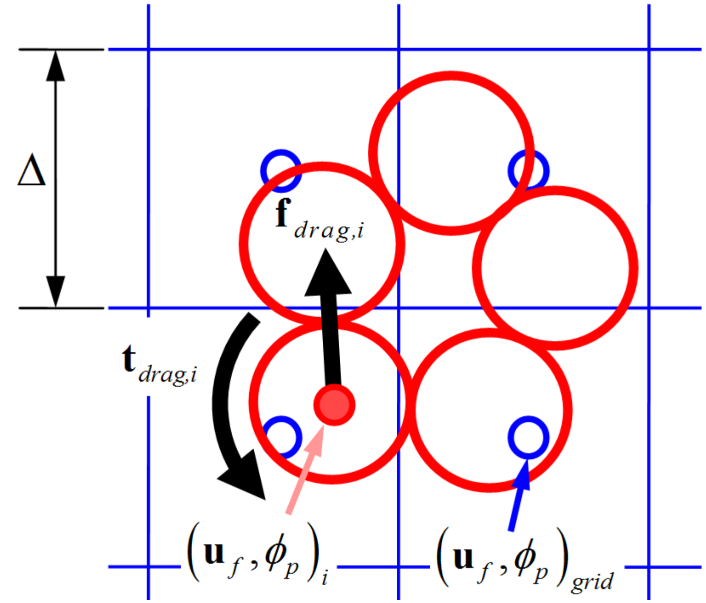
Micro-Meso Bridging: data filtering and statistical analysis (closure development) using the tool CPPPO

Closures at the Meso Level

Flow

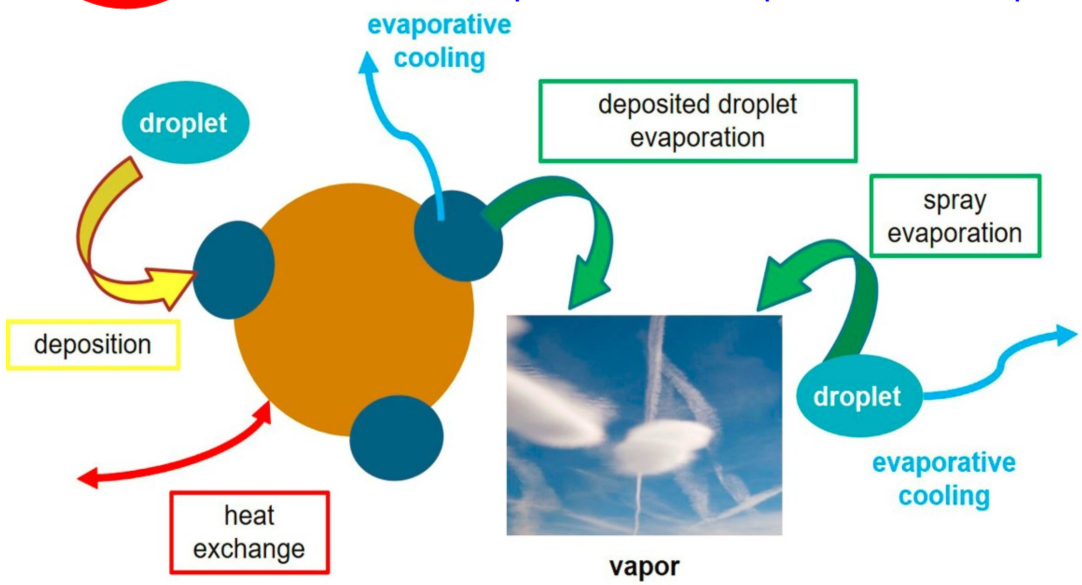
- Contact+cohesive forces and torques ***per contact***
- Fluid-Particle interaction (drag) forces and torques ***per particle***





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

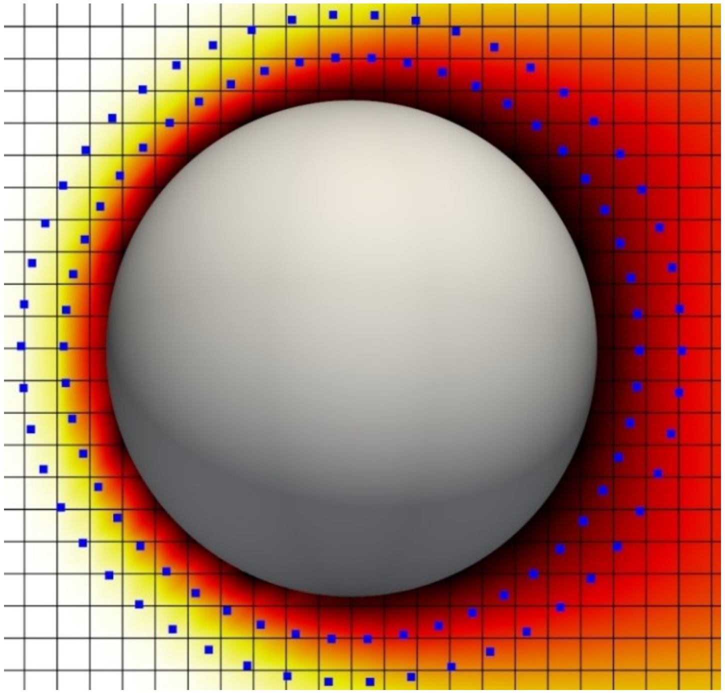
- Part I **The Method**
- Part II **Application to Bi-Disperse Flows**
- Part III **Application to Wall-Bounded Flows**

5 + 5 + 5 = 15 mins

The Method

The Idea

Hybrid Fictitious Domain / Immersed Boundary Method



- **Combine** Fictitious Domain and Immersed Boundary algorithm (HFD-IB, [3]).
- **Impose** the rigidity inside immersed bodies (in the spirit of the fictitious domain method)
- **Enforce** a (Dirichlet) boundary condition at the immersed surfaces: Specifically, we rely on a **reconstruction of the flow and concentration field** in the vicinity of the immersed surface using an interpolation technique
- **Advantage:** high order boundary treatment
- **Drawback:** interpolation points must be in domain to ensure highest order

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

The Idea

Hybrid Fictitious Domain / Immersed Boundary Method

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i^{IB,u}$$

$$\frac{\partial \theta}{\partial t} + \frac{\partial u_i \theta}{\partial x_i} = \frac{1}{Pe}\frac{\partial^2 \theta}{\partial x_i \partial x_i} + f^{IB,\theta}$$

Take into account the presence of rigid bodies inside the fluid domain

Fictitious Domain
The forcing term imposes a rigidity condition inside the immersed body [4].

Immersed Boundary
The forcing term forces the solution to a (Dirichlet) boundary condition at the immersed body surface [5].
It would be desirable to have a **single flexible formulation** that allows, e.g., Dirichlet and Neumann BCs.

[4] Smagulov S., *Preprint CS SO USSR, N 68* (1979)
[5] Peskin C., *Journal of computational physics* (1971)

Algorithmic Details

How to calculate the forcing terms near the surface?

$$\mathcal{P}^k\theta(t,\boldsymbol{x}) - \Phi(t,\boldsymbol{x}) = f^{IB,\theta}(t,\boldsymbol{x})$$

Rewrite the scalar transport equation: general partial differential equation of order k

$$\sum_{n=0}^{k-1}\alpha_n[\mathbf{n}(t,\boldsymbol{x})\cdot\boldsymbol{\nabla}]^n\theta\,(t,\boldsymbol{x}) = \gamma$$

General boundary condition at the particle surface expressed via a «boundary operator»

The forcing term is calculated from:

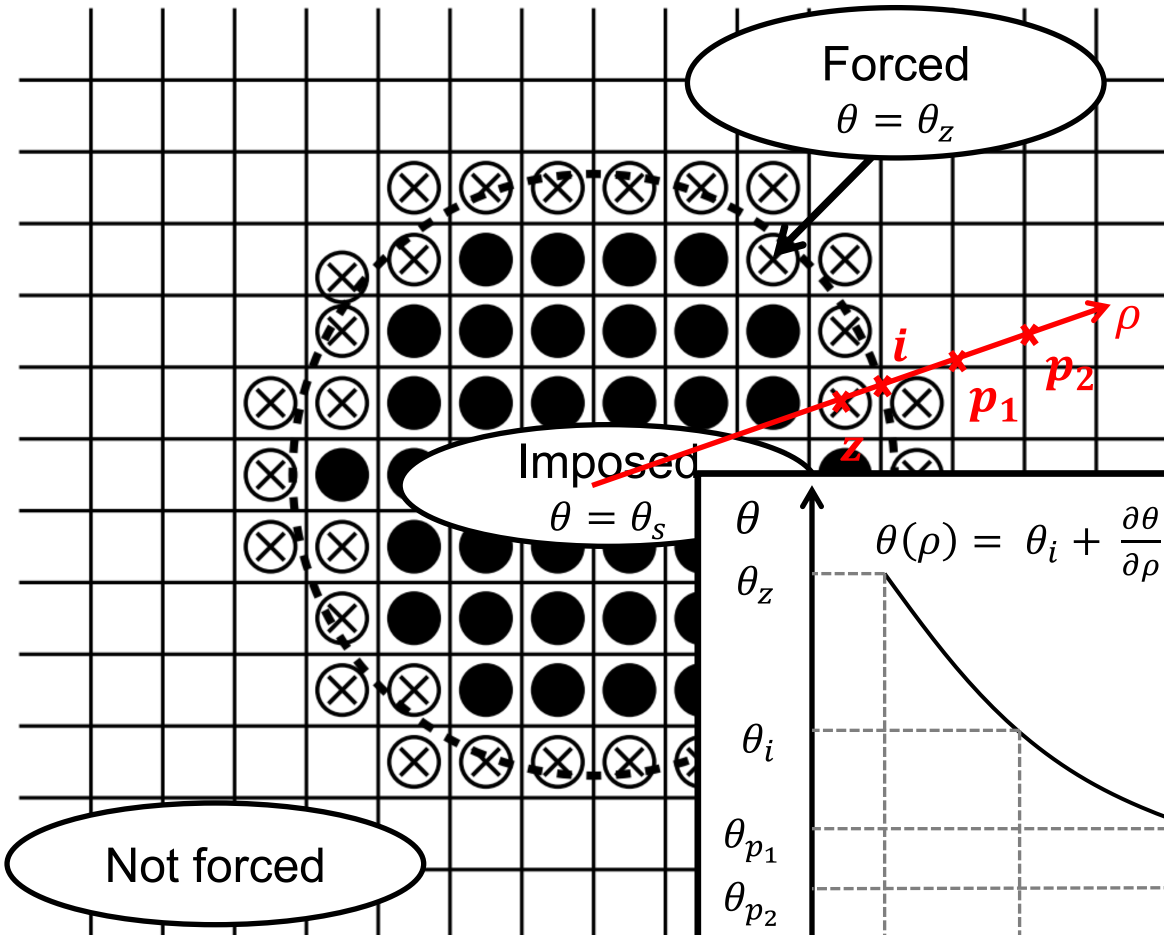
$$f^{IB,\theta}(t,\boldsymbol{x}) = \mathcal{P}^k\theta(t,\boldsymbol{x}) - \Phi(t,\boldsymbol{x}) + \left(\theta(t,\boldsymbol{x}) - \theta_i(t,\boldsymbol{x})\right)$$

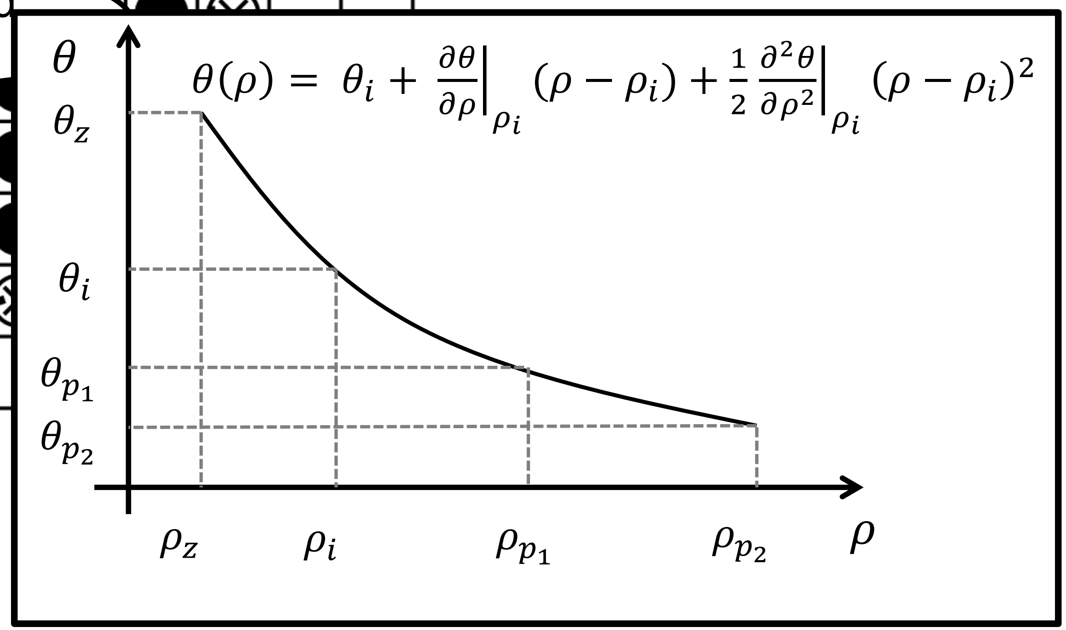
$$\theta_i(t,\boldsymbol{x}) = \left\{\sum_{n=0}^{k-1}\alpha_n[\mathbf{n}(t,\boldsymbol{x})\cdot\boldsymbol{\nabla}]^n\right\}^{-1}\gamma$$

The boundary operator needs to be inverted!
Remaining challenge: determine the values at the cell centers z from that at the interface point i.

Algorithmic Details

How to calculate the forcing terms near the surface?





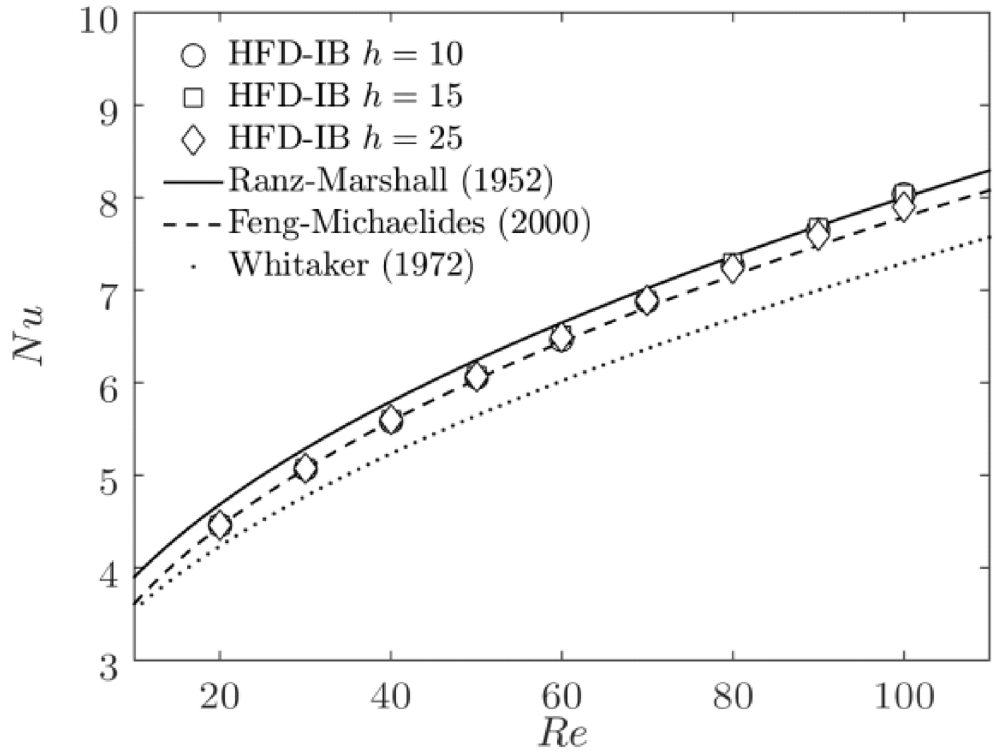
use a **Taylor expansion** to construct a system of equations to calculate $\theta_i(t, \boldsymbol{x})$ and its derivatives

θ_z is calculated from $\theta_i(t, \boldsymbol{x})$ and its derivatives

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

Algorithmic Details

Verification - Forced convection around a sphere



Excellent agreement with existing correlations

Weak mesh dependence

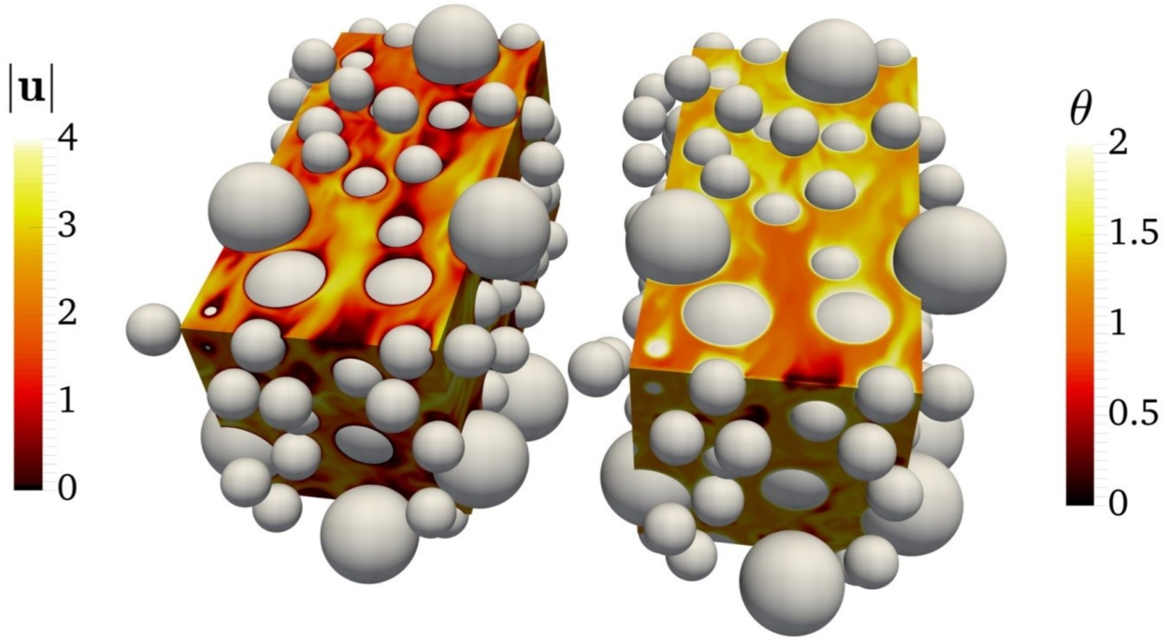
Accurate even on coarse grids

Boundary operator

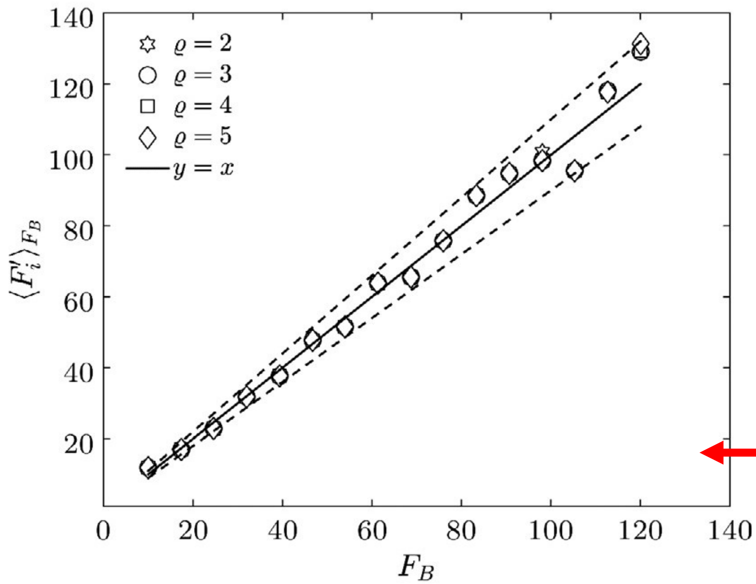
$\theta(t, \boldsymbol{x}) = \gamma$

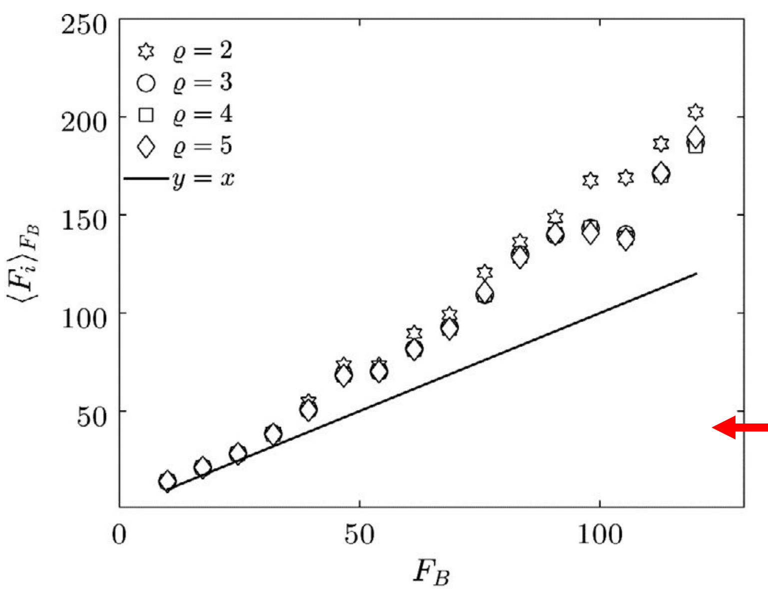
[3] F. Municchi and S. Radl, *Int J Heat Mass Transfer* (2017) 111:171–190

Application: Bi-Disperse Flows



Bi-Disperse Systems: Mean 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"** [3]

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

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

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

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

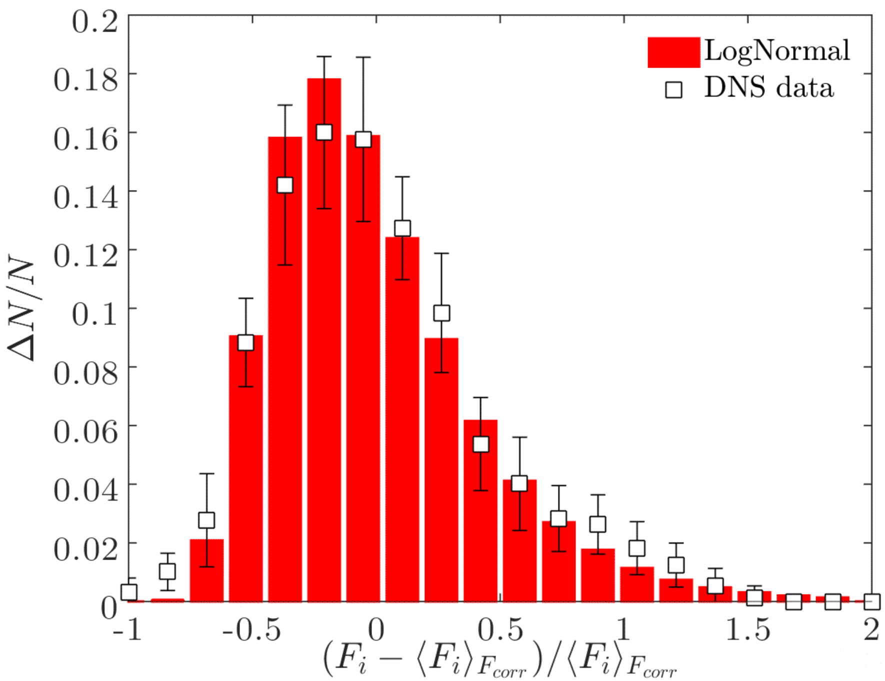
$\mathbf{f}_i^{\nabla p^{\varrho}}$: Force due to mean pressure gradient

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

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

Bi-Disperse Systems: Mean versus Per-Particle

Drag Coefficient

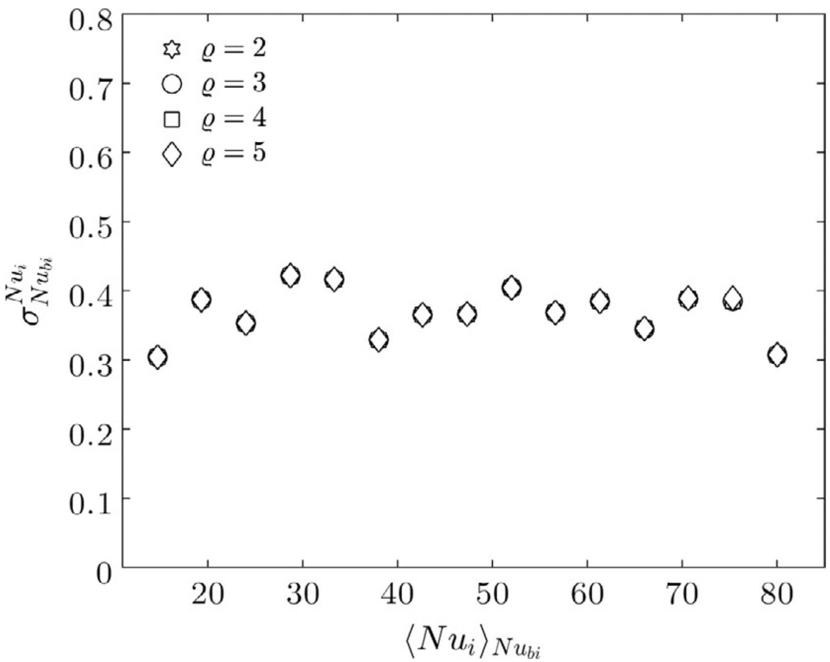


- Previous work [6] on per-particle drag variation attempted to model the **total fluid-particle force** (with moderate success)
- However, when using a correctly-defined drag coefficient: the **scaled variance for the drag coefficient** is approximately constant: **simple closure possible!**
- Particle-individual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

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

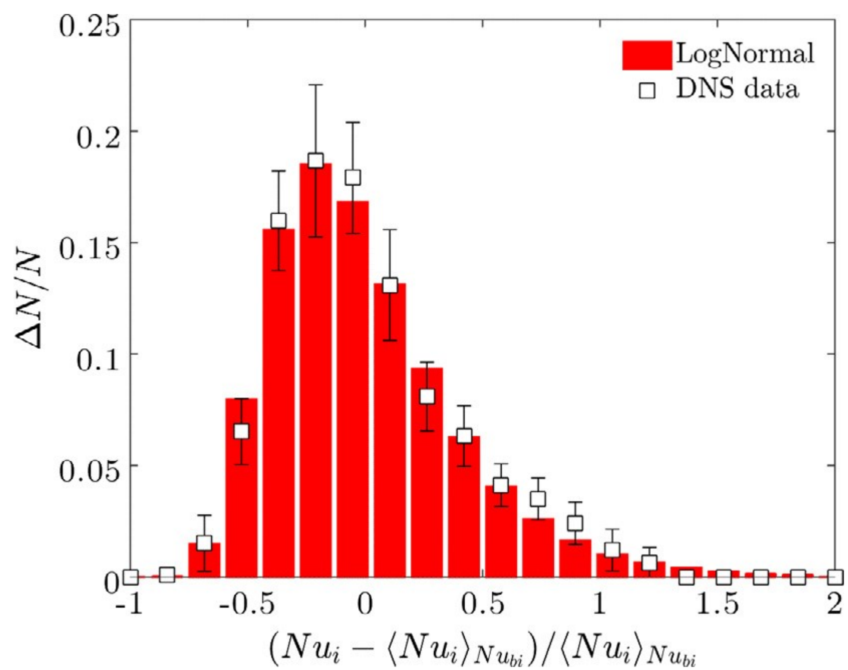
Bi-Disperse Systems: Mean versus Per-Particle

Nusselt Number



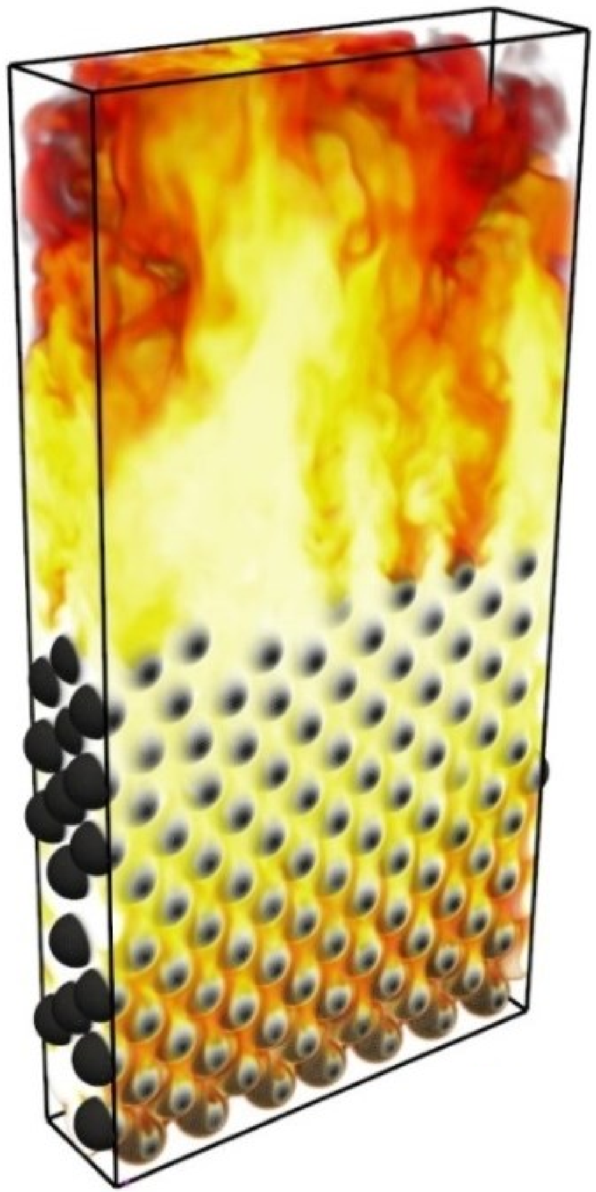
- Same as for the drag coefficient: **scaled variance for the Nusselt number** is approximately constant: **simple closure possible!**

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



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

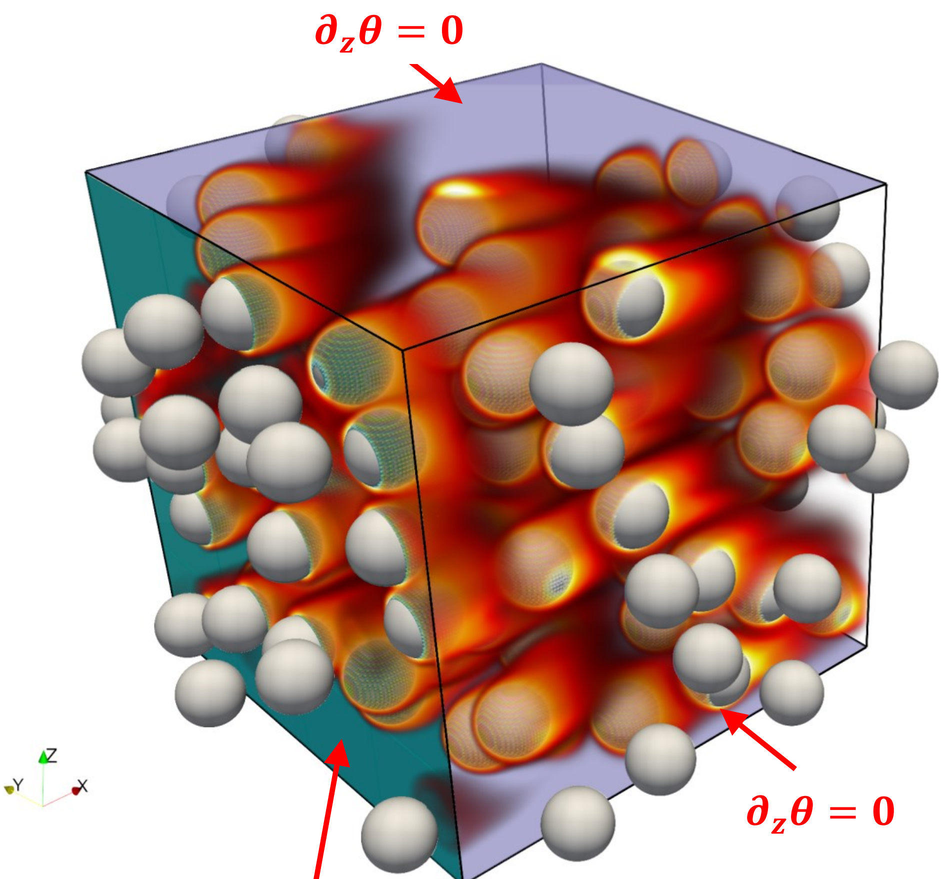
Application: Wall-Bounded Flows



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

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

Walls

Particle-Resolved DNS to identify Modeling Needs

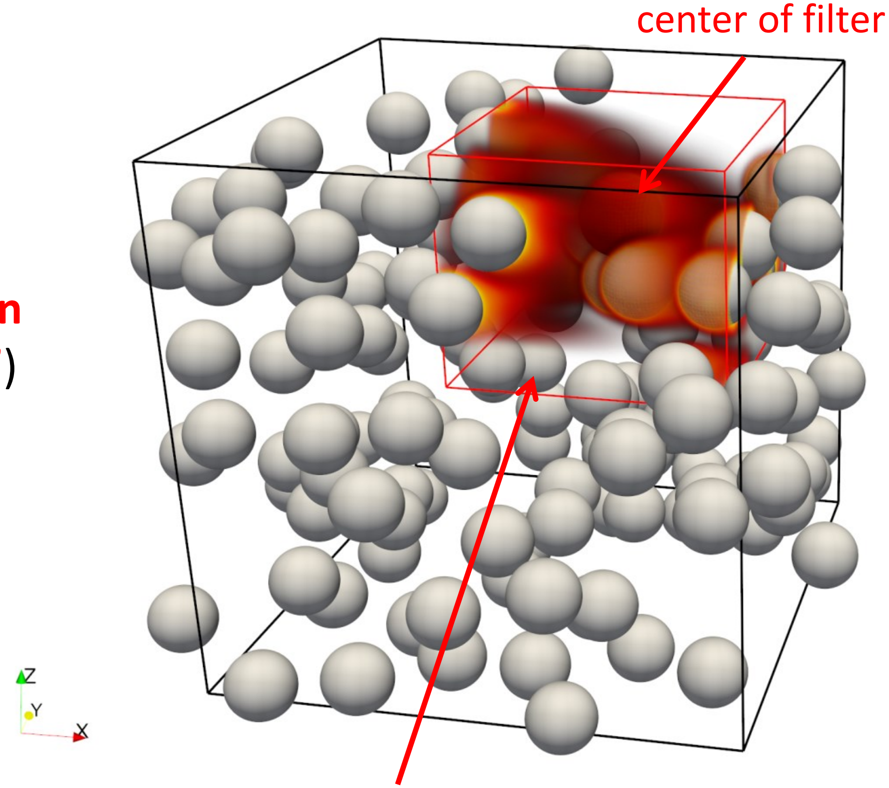
- We make use of the filtering toolbox **CPPPO** to spatially average ("filter") the continuum phase properties around **each particle**

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

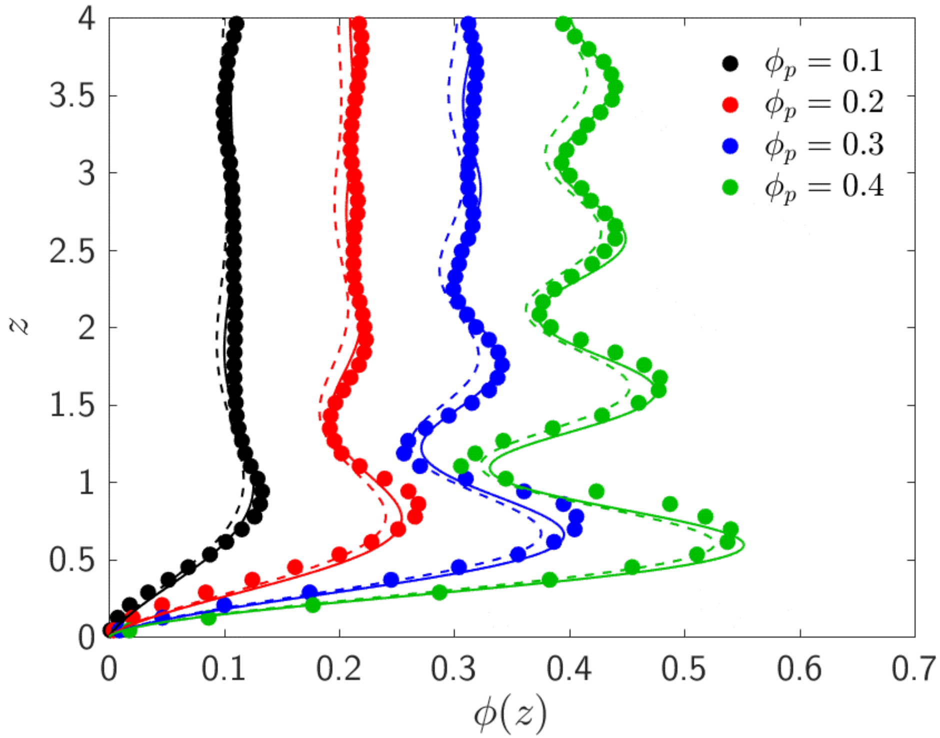
Lagrangian filtering: wall particles

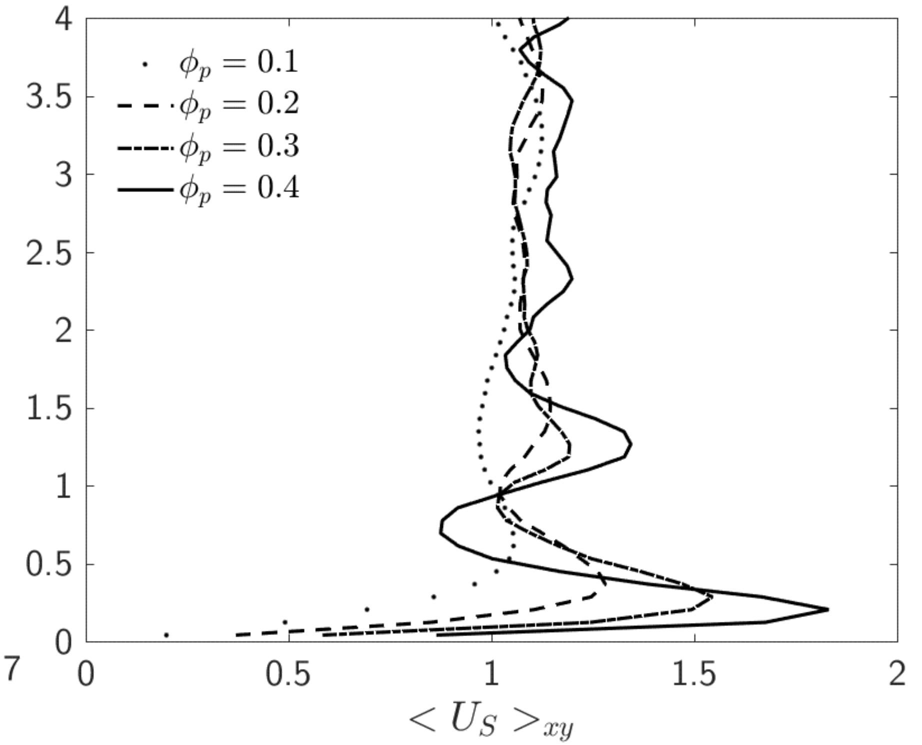


Walls

Particle-Resolved DNS to identify Modeling Needs

Local Voidage and Speed



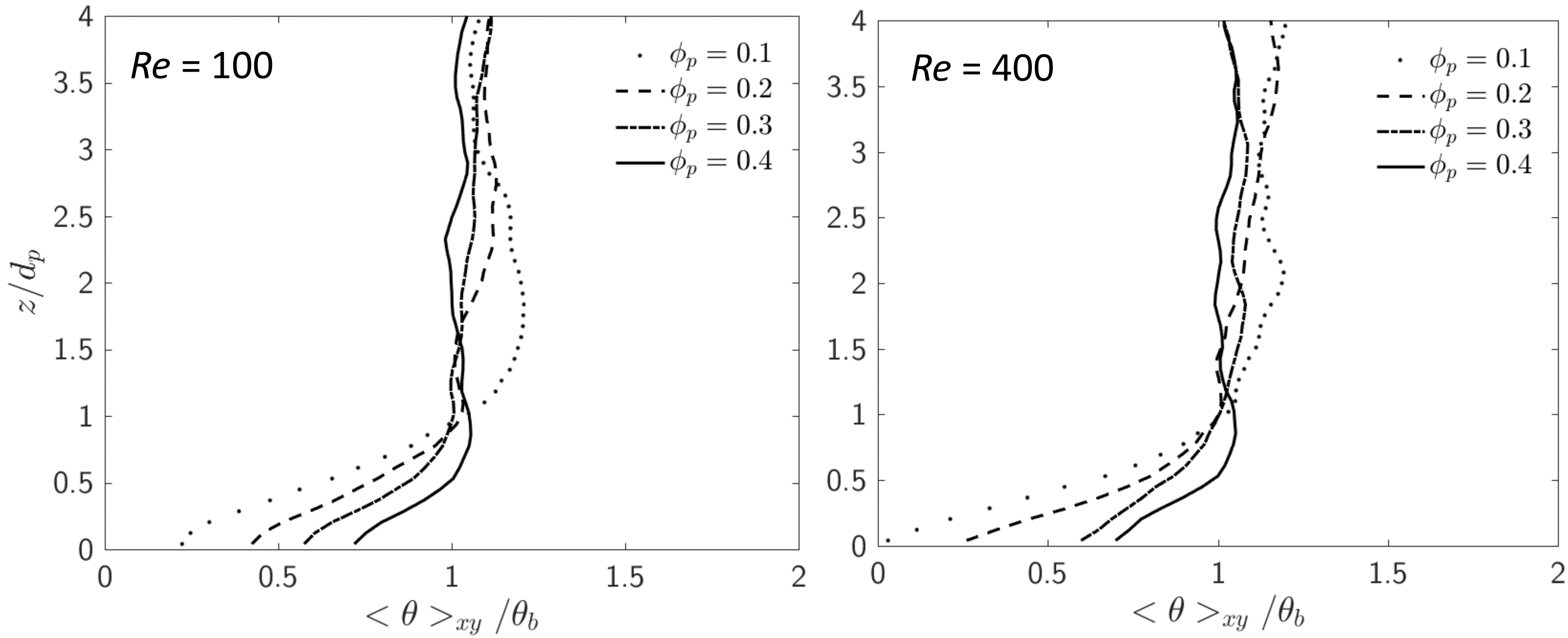


- General **correlation proposed for $\phi(z)$**
- Fluid speed **fluctuates strongly**, but with **small wavelength →** we expect a **filter-size independent near-wall correction**

Walls

Particle-Resolved DNS to identify Modeling Needs

Local Temperature

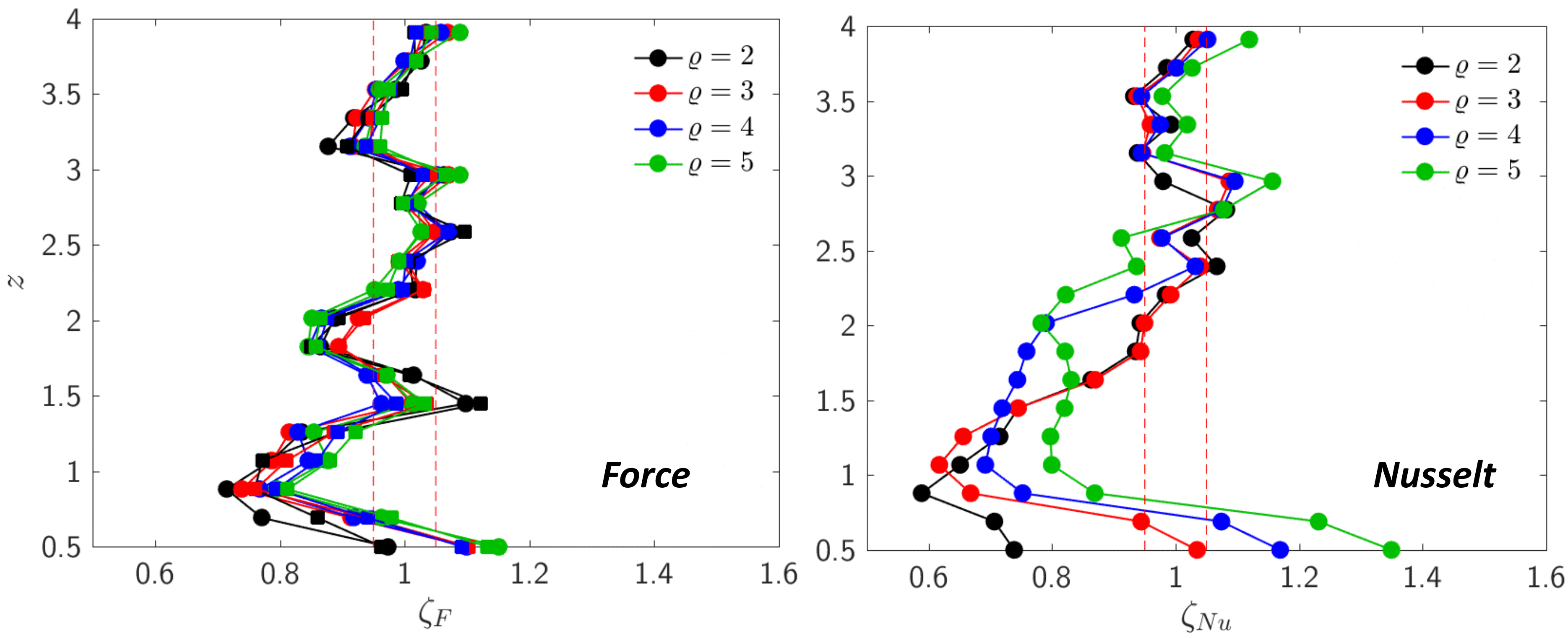


- Fluid temperature **shows a "boundary layer" behavior** due to "near-wall convection"
- Significant and systematic **decrease of temperature when approaching the (adiabatic!) wall →** we expect a **filter-size dependent near-wall correction**

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

Conclusions

Conclusions

- Adopting the **boundary operator concept** allows one to implement **flexible BCs**. Order of boundary treatment depends on number of **reconstruction points**

- **Mean drag coefficient and Nusselt number** in bi-disperse systems: worth to **recheck** existing closures

- Closures for drag and heat/mass transfer are still **poor on a *per-particle* level**. **Particle (thermal) inertia "irons out" this problem**.

- **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)

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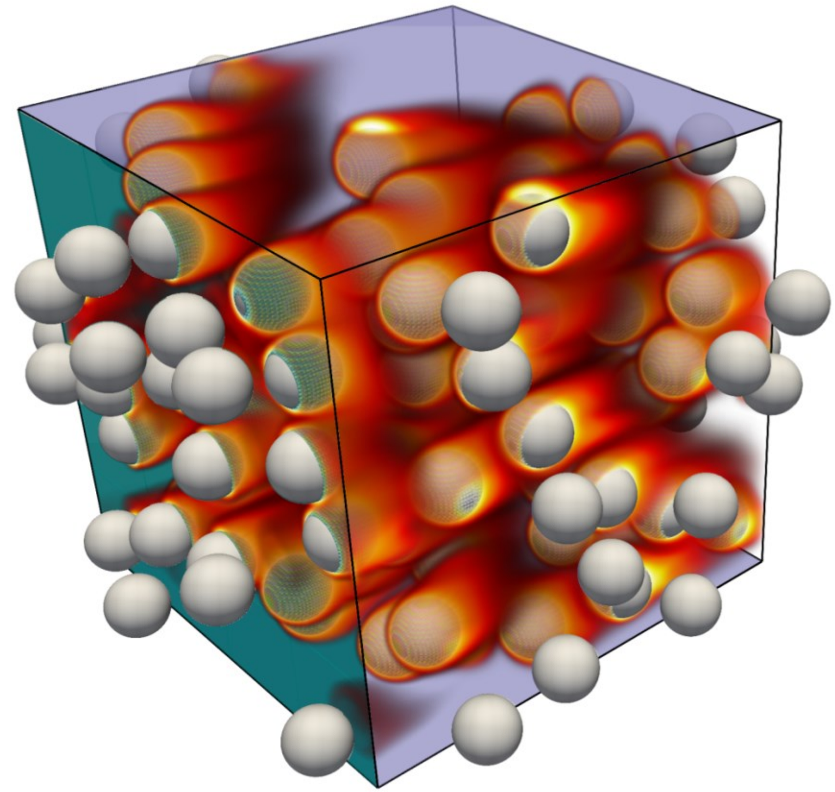

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NanoSim

SEVENTH FRAMEWORK PROGRAMME

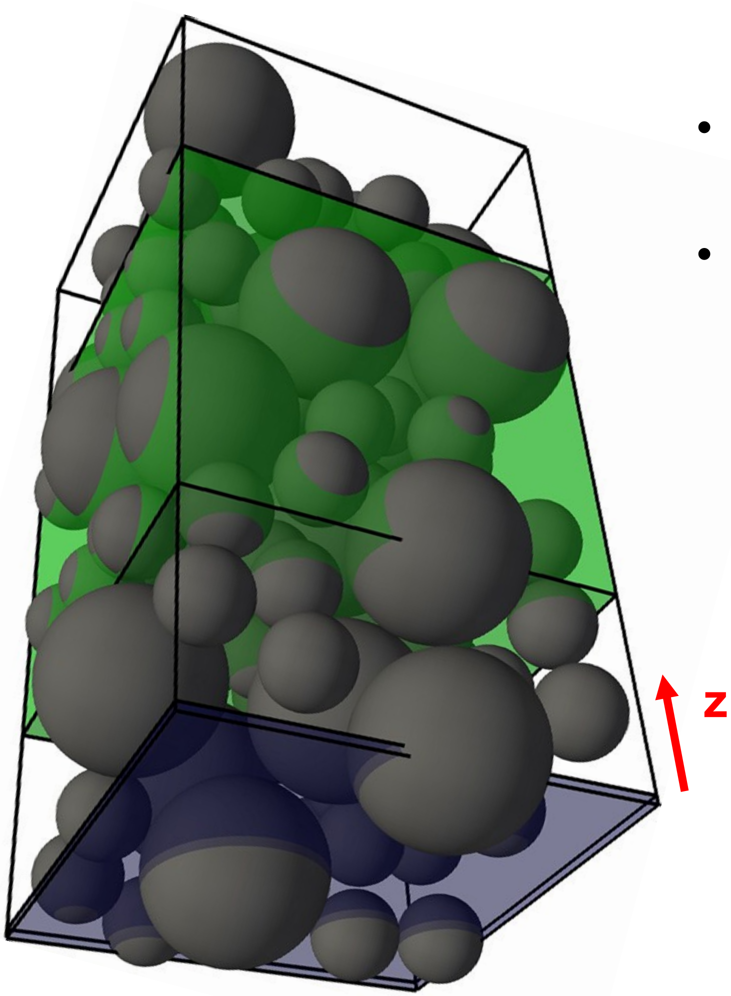
Acknowledgement and Disclaimer

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/

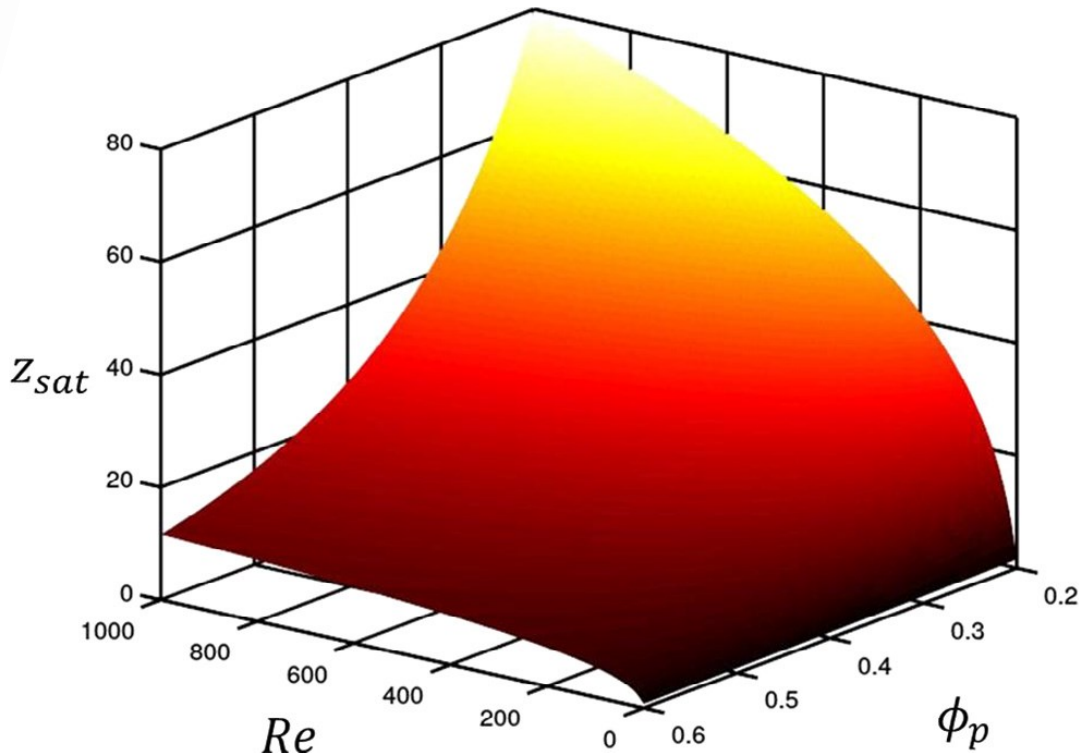
SEVENTH FRAMEWORK PROGRAMME

NanoSim

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