Beyond classical CFD-DEM

Forgotten Challenges and New Tools

S. RADL

with contributions from

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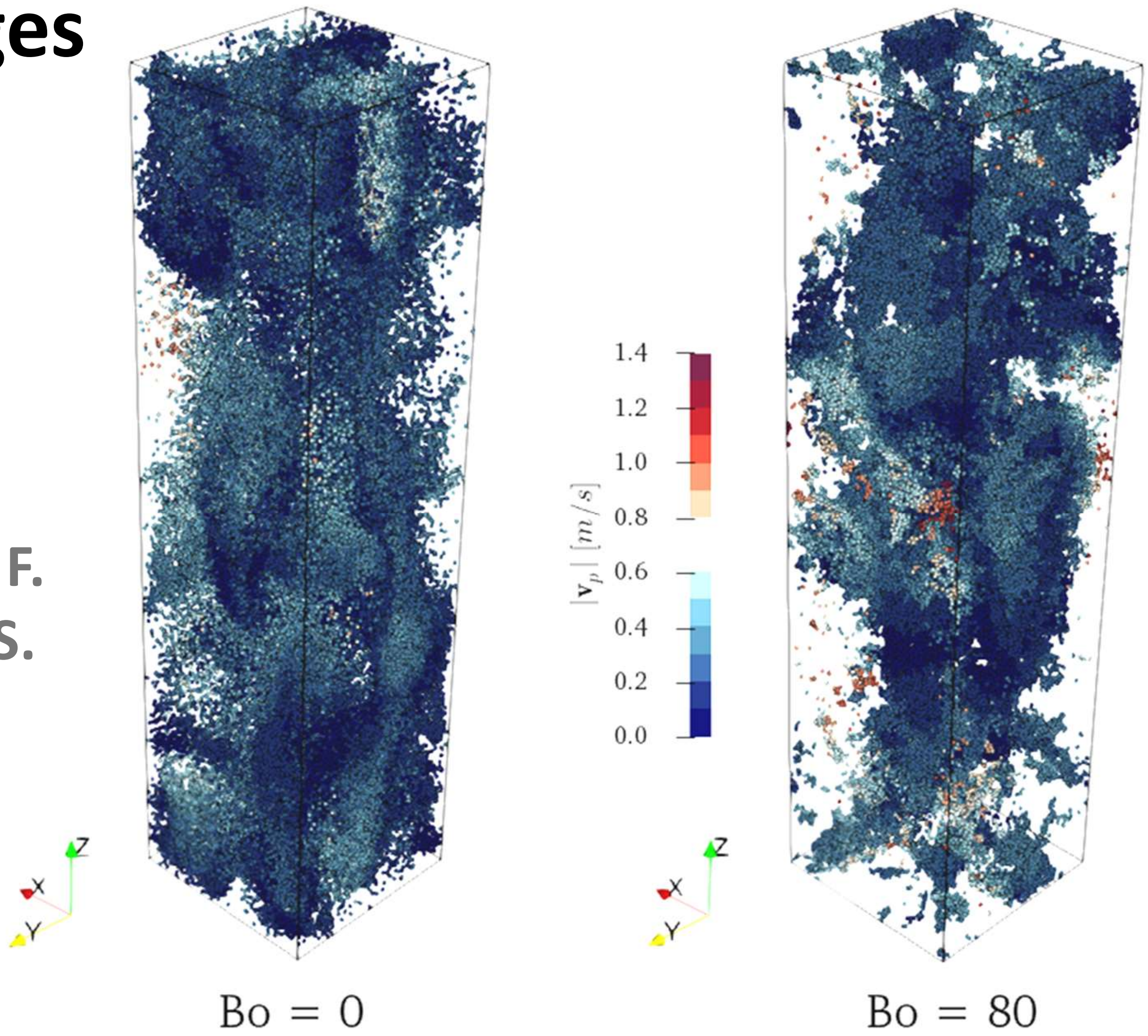
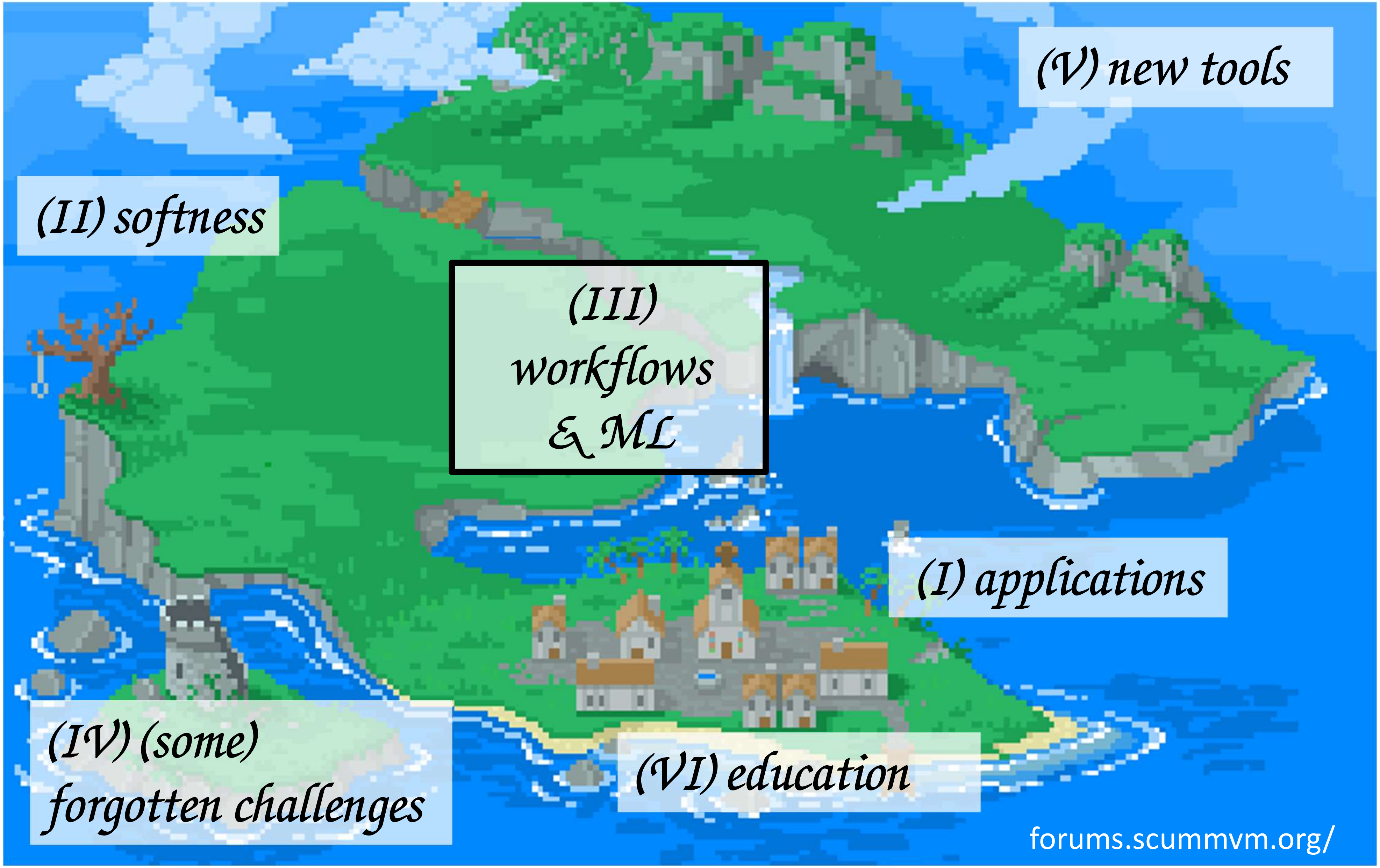


SFB/CRC 287 Retreat

June 13, 2023

Hannover

Overview


(V) new tools
(II) softness
(III) workflows & ML
(I) applications
(IV) (some) forgotten challenges
(VI) education
forums.scummvm.org/

Applications

- **Batteries I: thermal runaway**

  …super fast, super hot and supersonic

  …tribocharging

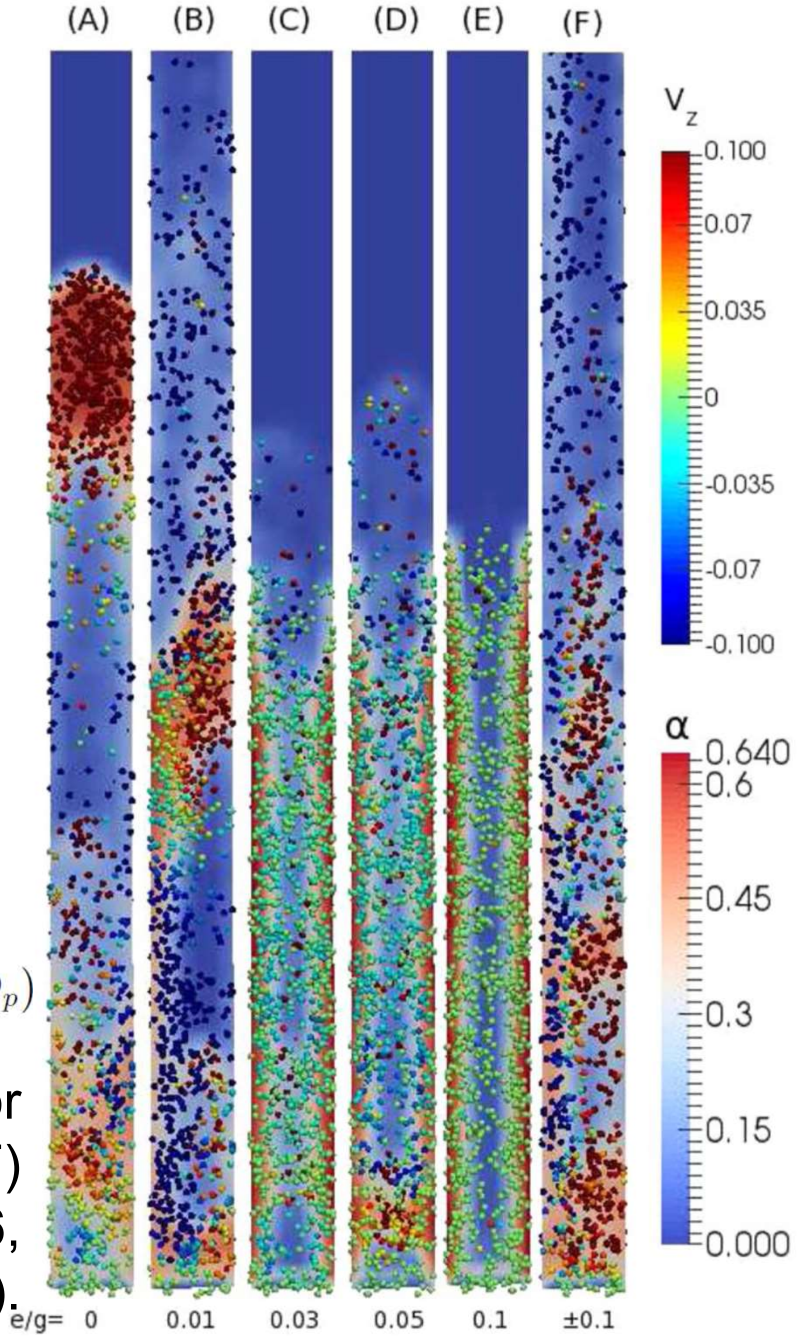
  …hydrolysis of water vapor

  …sparks and arcs

  …800V operating voltage

$$\frac{3}{2}\frac{\partial}{\partial t}(\alpha_p\rho_p\Theta_p)+\frac{3}{2}\nabla\cdot(\alpha_p\rho_p\Theta_p\mathbf{u}_p)=\nabla\cdot(\kappa_p\nabla\Theta_p)-\left(\Sigma_p^{\mathrm{kc}}+\Sigma_p^{\mathrm{fr}}\right):\nabla\mathbf{u}_p$$
$$-12\left(1-e_{c,p}^2\right)\frac{\alpha_p^2\rho_p g_{0,p}}{d_p\sqrt{\pi}}\Theta_p^{\frac{3}{2}}$$
$$-3\beta\Theta_p,$$

$$\frac{\partial}{\partial t}\left(\frac{\alpha_p}{V_p}Q_p\right)+\nabla\cdot\left(\frac{\alpha_p}{V_p}Q_p\mathbf{u}_p\right)=\nabla\cdot(\sigma_{q,p}\mathbf{E})+\nabla\cdot\left(\left(\kappa_{q,p}+\kappa_{q,p}^{*}\right)\nabla Q_p\right)$$



Behavior of a fluidized gas-particle system for uncharged (A), monopolar (B-E), and bi-polar (F) particle charging (Kolehmainen et al., 2016, AIChE J.).

Applications

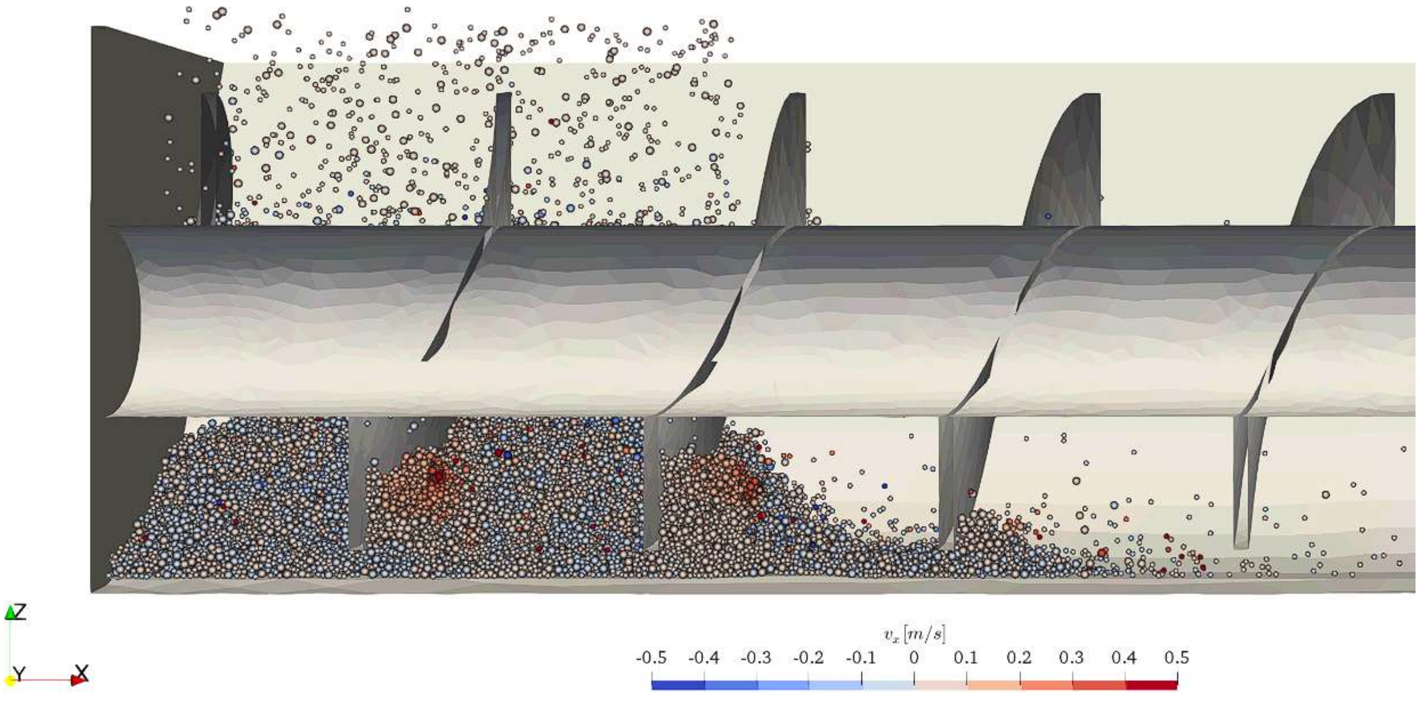
- **Batteries II: recycling**

  …keep cool! (because of reactions)

  …really complex rheology (wet fibres mixed with small particles) → calibration

  …spontaneous carbonation in air (changing rheology)

Cohesive battery recyclate flow in a screw conveyor (Hadie Benabchiasli)



screw conveyor simulation - cohesive particles

Applications

- **Wet Granulation**

  ...fluidization of cohesive powders

  ... spraying & drying

  ... binders with complex rheology

Askarishahi et al., Processes, 2023

Askarishahi et al., Ind. Eng. Chem. Res. 61, 2022

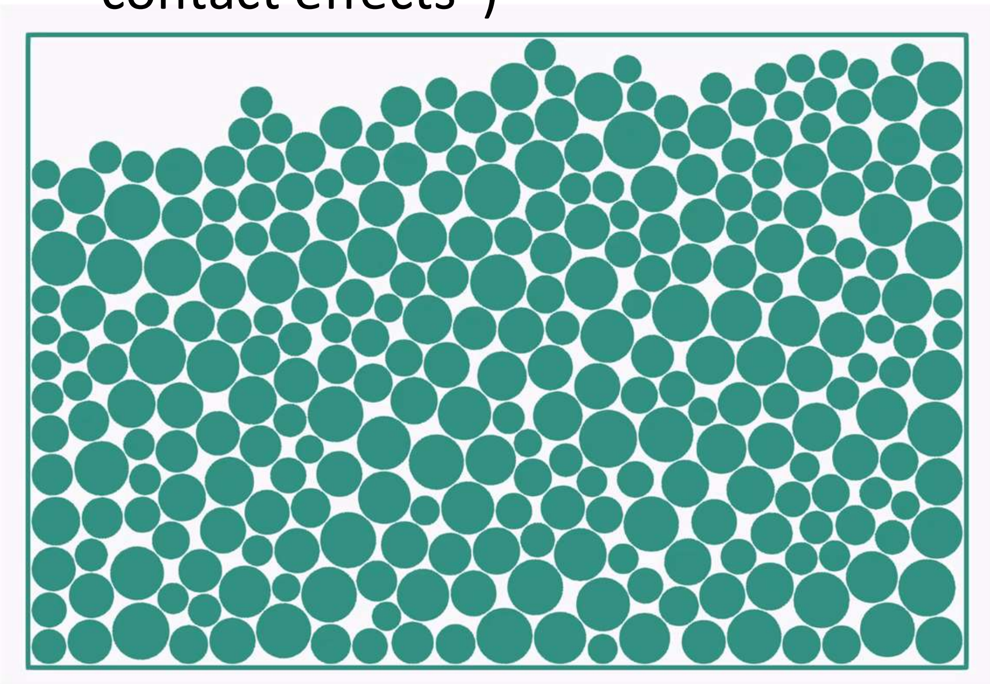
Applications

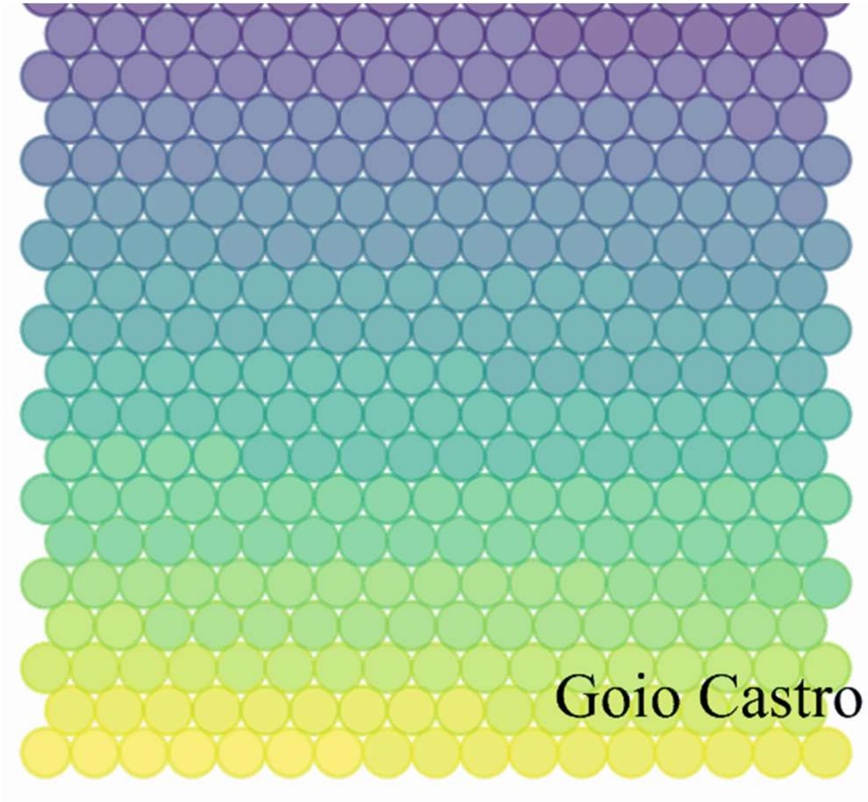
- **Compaction and discharge**

  …unsteady gas-particle at extreme speed (bag filling time < 1 s)

  …effect of (relative) softness

  …multi-contact DEM model ("neighbor contact effects")

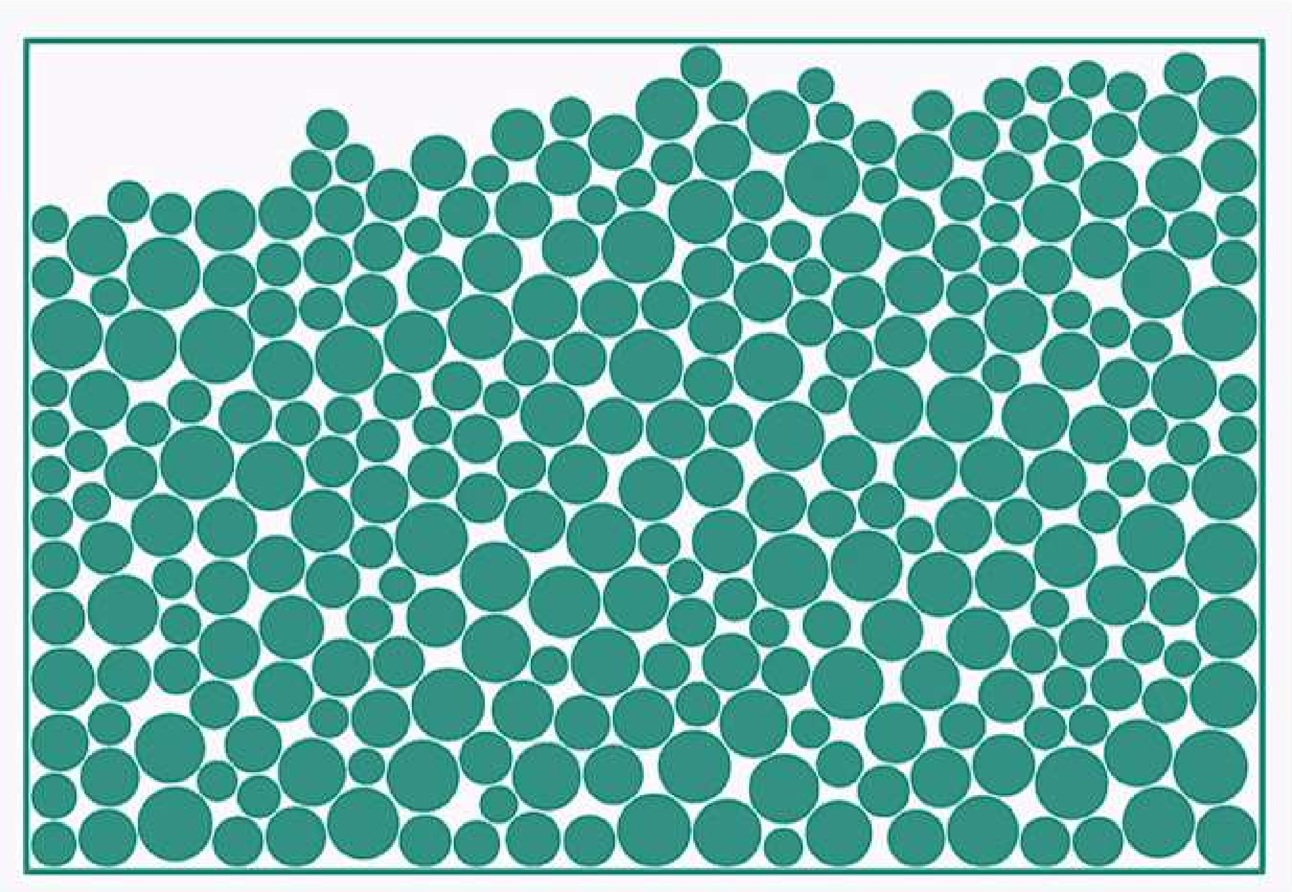


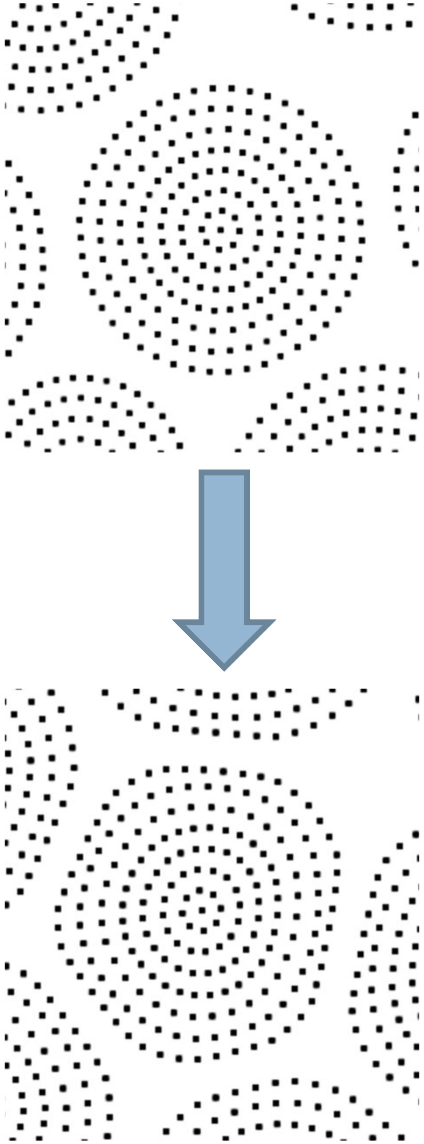


SPH-DEM simulation of compaction (left) and silo discharge (right; 2D Francisco Goio Castro)

Softness

- **Approach I: Resolved Particles with SPH-DEM**





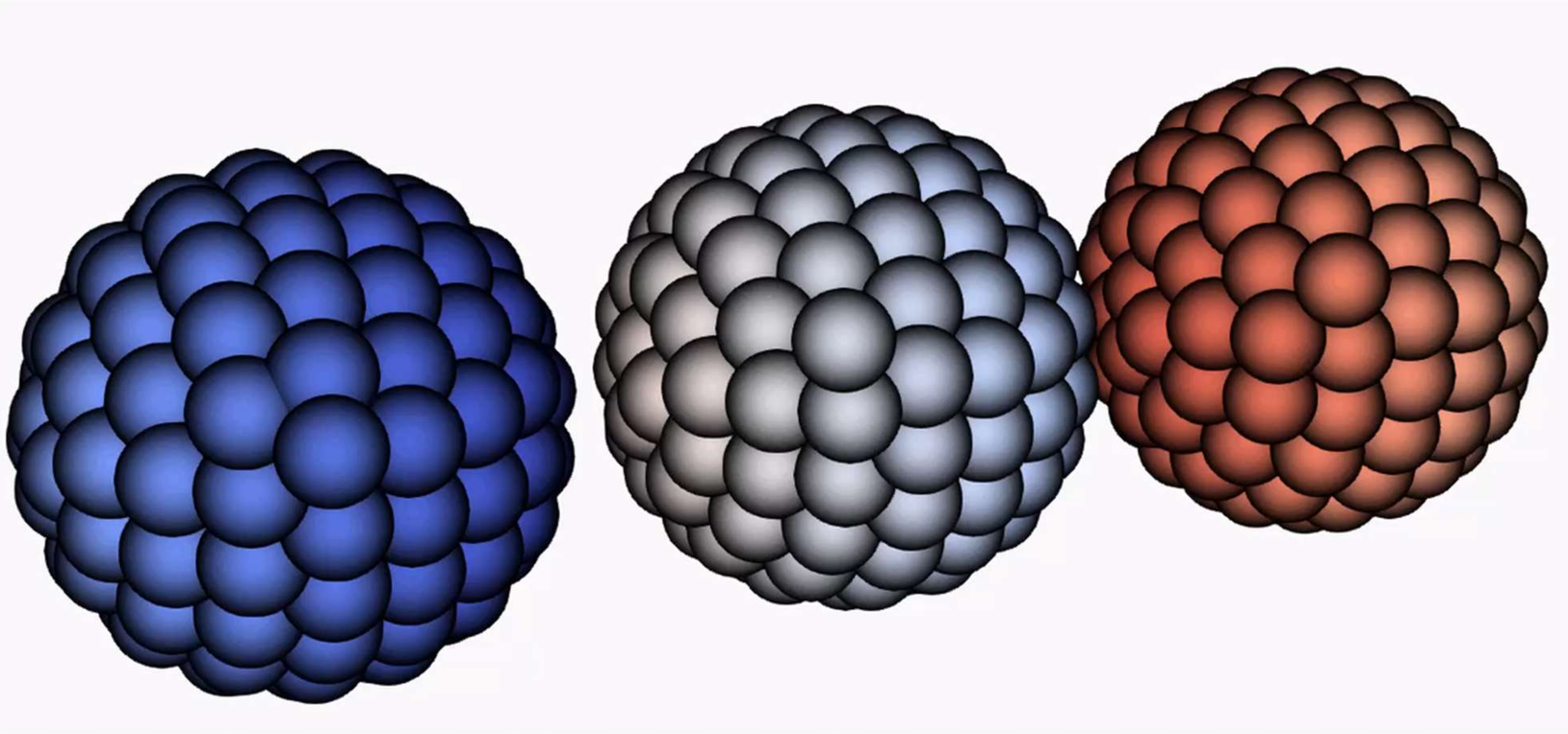
Goio Castro & Radl, Comput Part Mech (accepted)

Softness

- **Approach I: Resolved Particles with SPH-DEM**

  …SPH for intra-particle deformation

  …DEM-type model for inter-particle interactions (penalty approach)



Goio Castro & Radl, Comput Part Mech (accepted)

Softness

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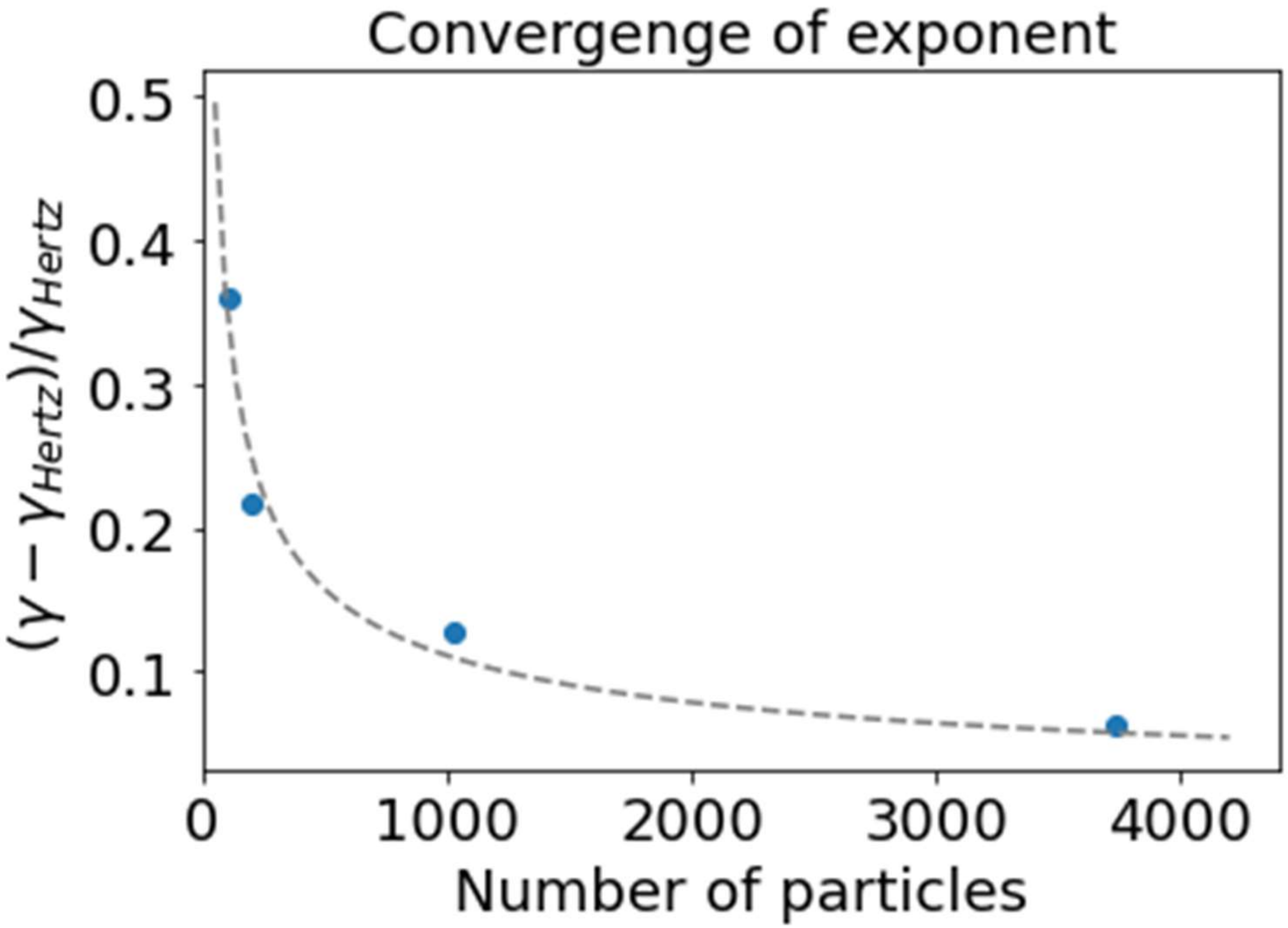
- **Approach I: Resolved Particles with SPH-DEM**

Resolution Requirements: force Exponent in overlap relation: $F_{cont} \propto \cdot\, \delta^{\gamma}$



Goio Castro & Radl, Comput Part Mech (accepted)

Softness

- **Approach II: Multi-Contact (MC) Force Closure**

Basics and Benchmarking (Compaction)

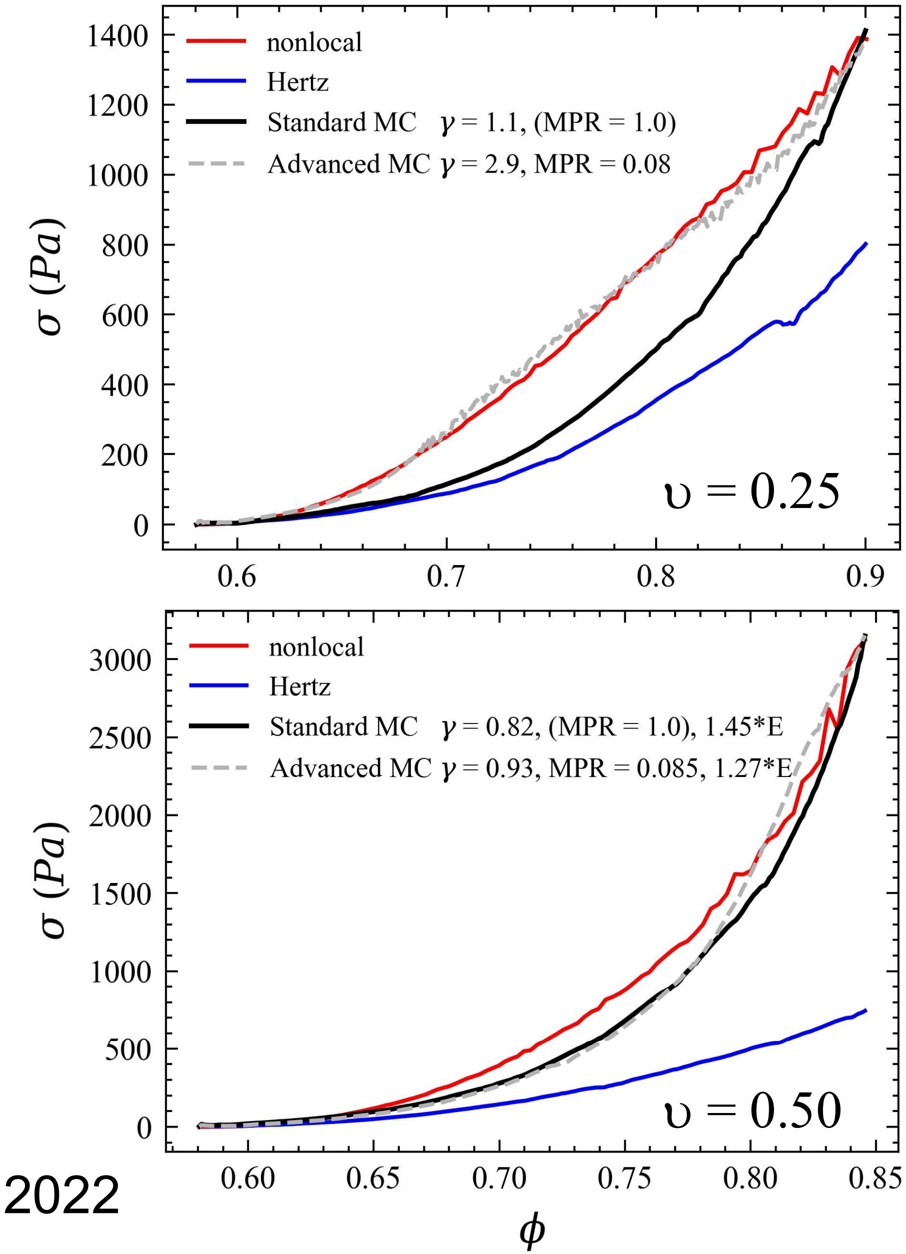
$$\delta_c = (r_i + r_j) - (\mathbf{x}_i - \mathbf{x}_j) \cdot \mathbf{n}$$

$$\delta_{k\to c}$$

$$= -\gamma \frac{(1+\upsilon)F_k}{2\pi E d_{kc}} \Big\{ (\mathbf{n}_k \cdot \mathbf{u}_{kc})(\mathbf{n}_c \cdot \mathbf{u}_{kc}) + (3$$

$$- 4\upsilon)\mathbf{n}_k \cdot \mathbf{n}_c - (1 - 2\upsilon) \frac{(\mathbf{n}_k + \mathbf{u}_{kc}) \cdot \mathbf{n}_c}{1 + \mathbf{n}_k \cdot \mathbf{u}_{kc}} \Big\}$$

+limiter

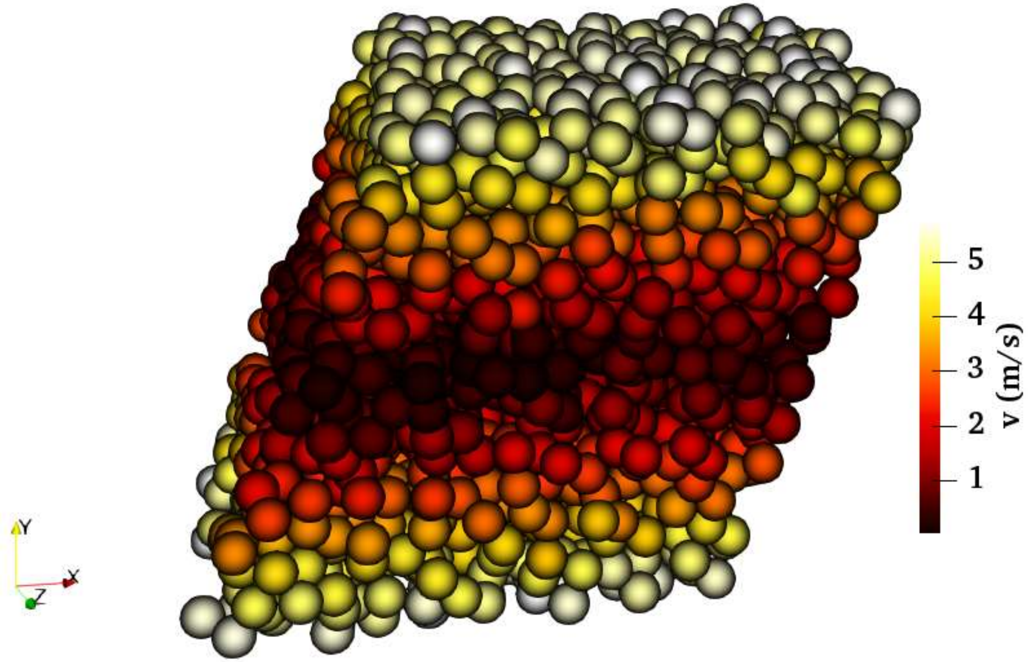


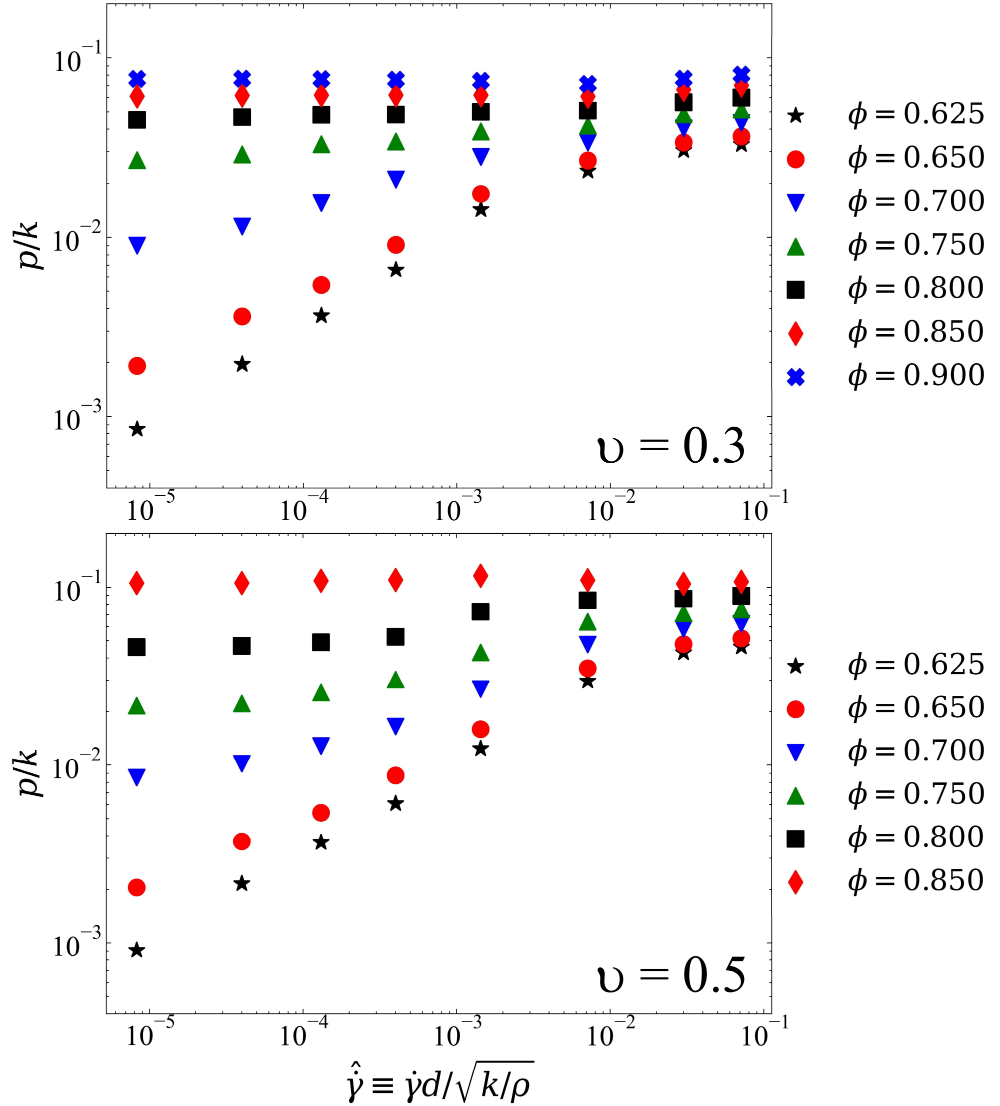
Ghods et al., Powder Technol., 2022

Softness

- **Approach II: Multi-Contact (MC) Force Closure**

Application case: dense shear flow (Lees-Edwards BCs)





Ghods et al., Powder Technol., 2022

Overview

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Workflows & ML

- **From the past…**

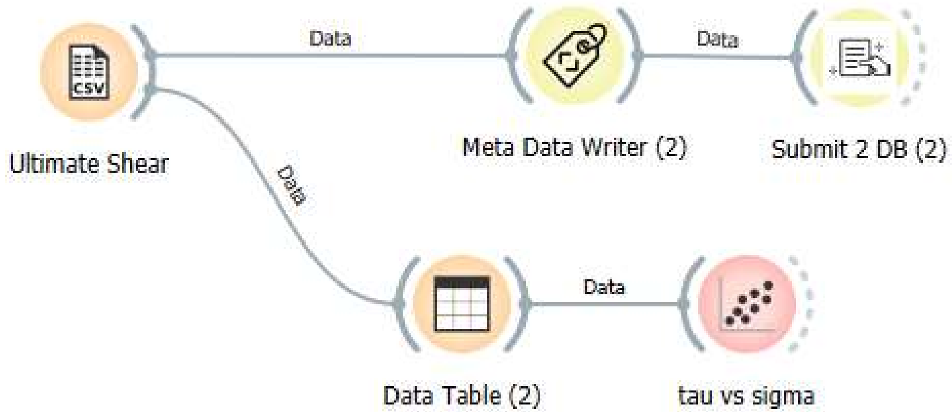
  …“New” NNs

  …via coarse graining

  …to anisotropic drag corrections

- **…via the Need 4 Speed…**

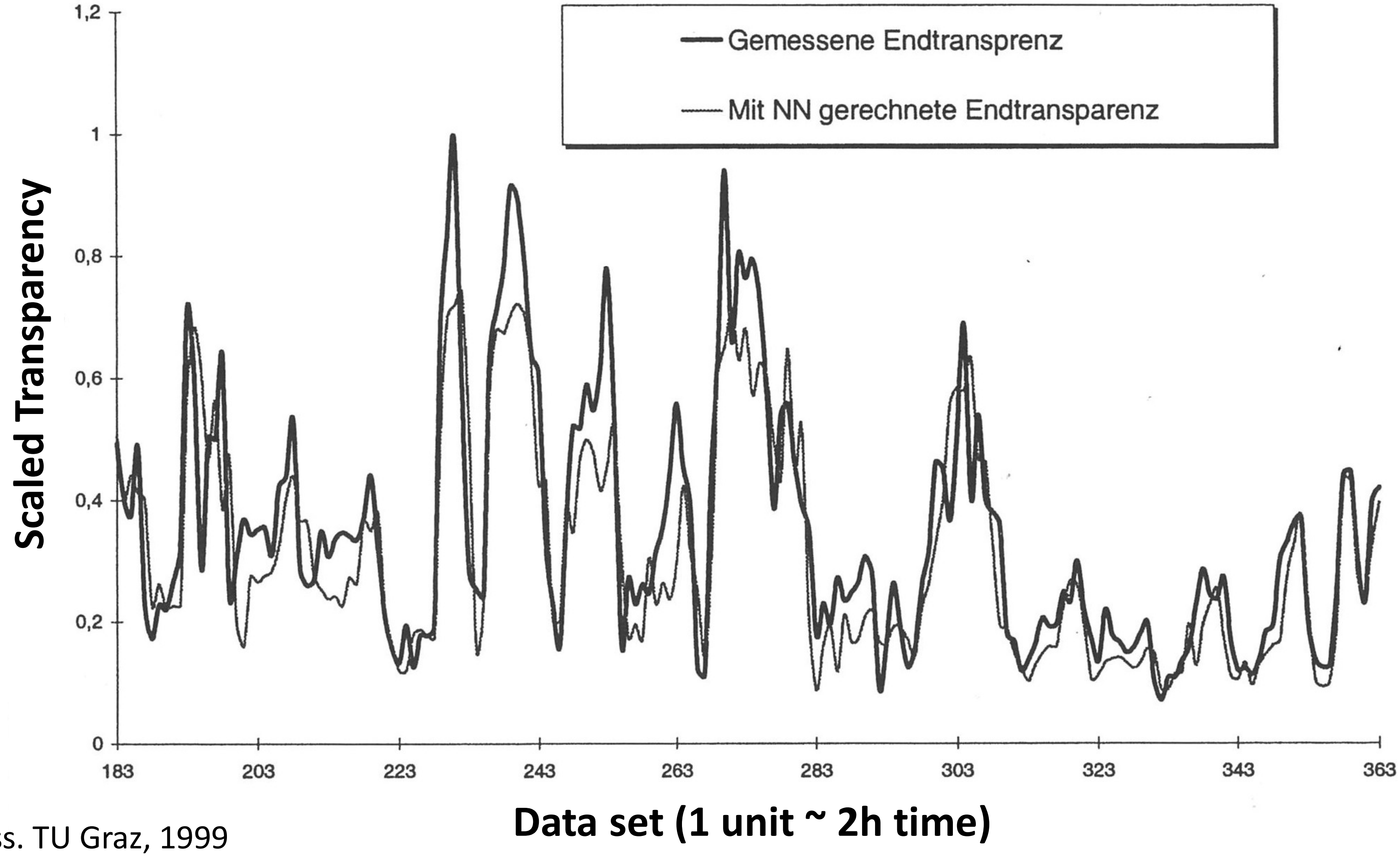
- **…to new perspectives**



Workflows & ML::The Past

- "**SNNS**" is created in 90's as a tool to make predictions
- Fuchs uses SNNS to predict sedimentation performance of sludge based on training with **182 (!) data points**

"Smart" (ML-based) predictors



Fuchs, Diss. TU Graz, 1999

Workflows & ML::The Past

- The **need for coarse graining** when simulating suspensions is demonstrated (Agrawal et al, 2001; Radl & Sundaresan, 2014)
- **Refinement of E-L and E-E simulators** and post-processing tools (Capecelatro & Desjardins, 2013)

Euler-Euler, and Euler-Lagrange simulators

Askarishahi et al., Ind. Eng. Chem. Res., 61, 2022.

Workflows & ML::The Past

- **Dedicated tools** for spatial averaging were developed (Municchi et al., 2016)

"Filtering" (averaging) Tools

for $A = 0 \rightarrow \mathrm{N_{cells}}$

do $\overline{\varphi_A} = \frac{\sum_{n=0}^{n=Nf} \varphi_n}{Nf}$

endfor

No final step required

φ: field to be filtered

A: current filtered cell

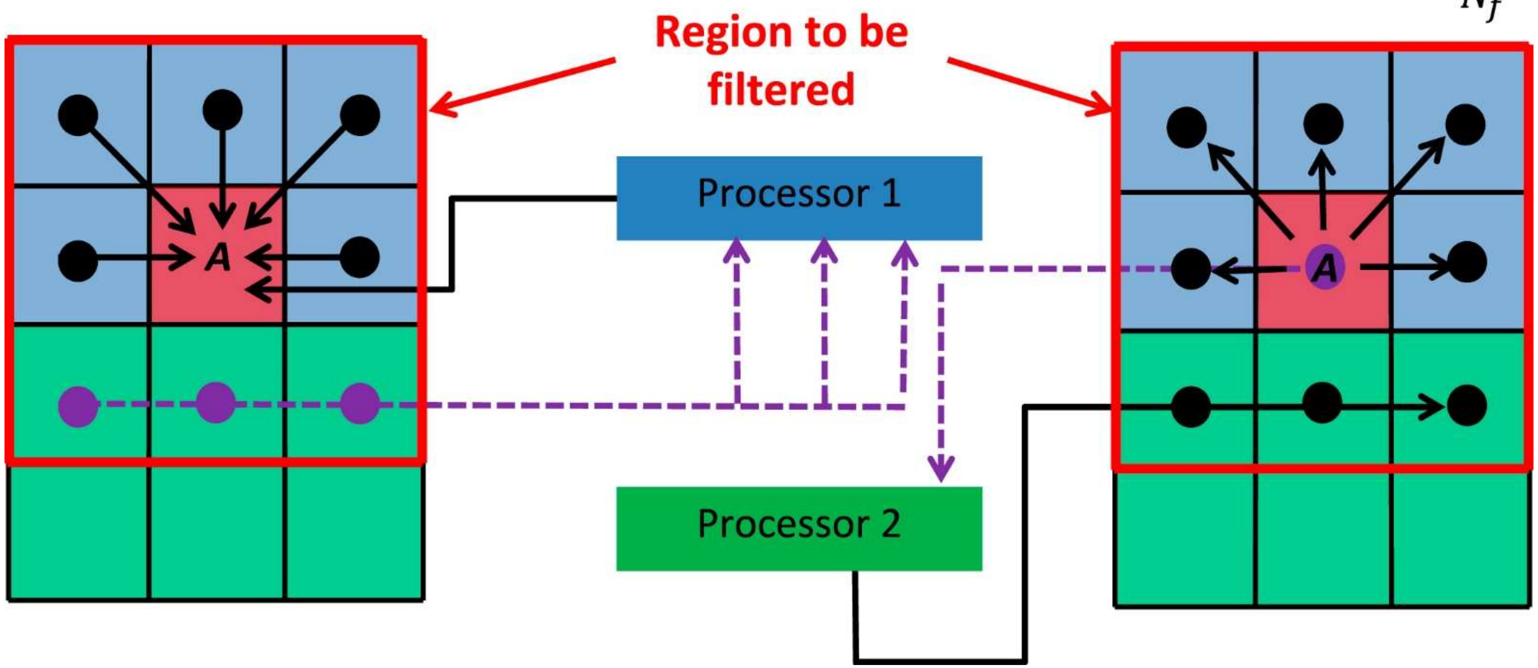
n: neighboring cells

for $A = 0 \rightarrow \mathrm{N_{cells}}$

do $\varphi_n \mathrel{+}= \varphi_A$

endfor

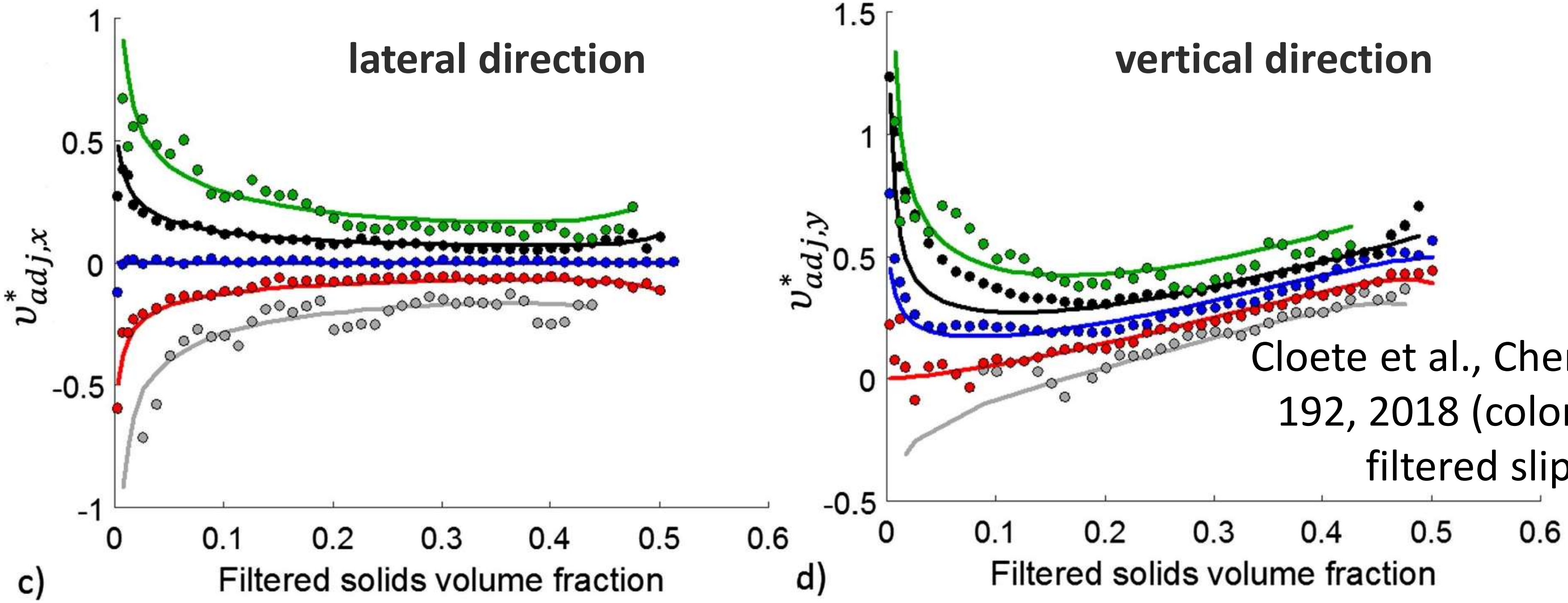
Final step: $\overline{\varphi_n} = \frac{\varphi_n}{N_f}$



Workflows & ML::The Past

- New families of closure strategies were developed ("**refiltering**" idea of Schneiderbauer and Saeedipour, PoF, 30, 2018)
- …or modeling is entirely **data-driven** ("**rCFD play back**" approach of Lichtenegger and Pirker, Chem Eng Sci, 153, 2016).
- **Anisotropy** of corrections is (not surprisingly!) identified as a **key need.** This is relevant for **stress and drag** terms!

filtered TFM, "fast" CFD, novel closures



Cloete et al., Chem Eng Sci, 192, 2018 (colors indicate filtered slip velocity).

Workflows & ML::Need4Speed

- Particles which are fine or with **cohesive interactions** (e.g., liquid bridge force) are widely used

Pharmaceuticals

Chemicals

Food

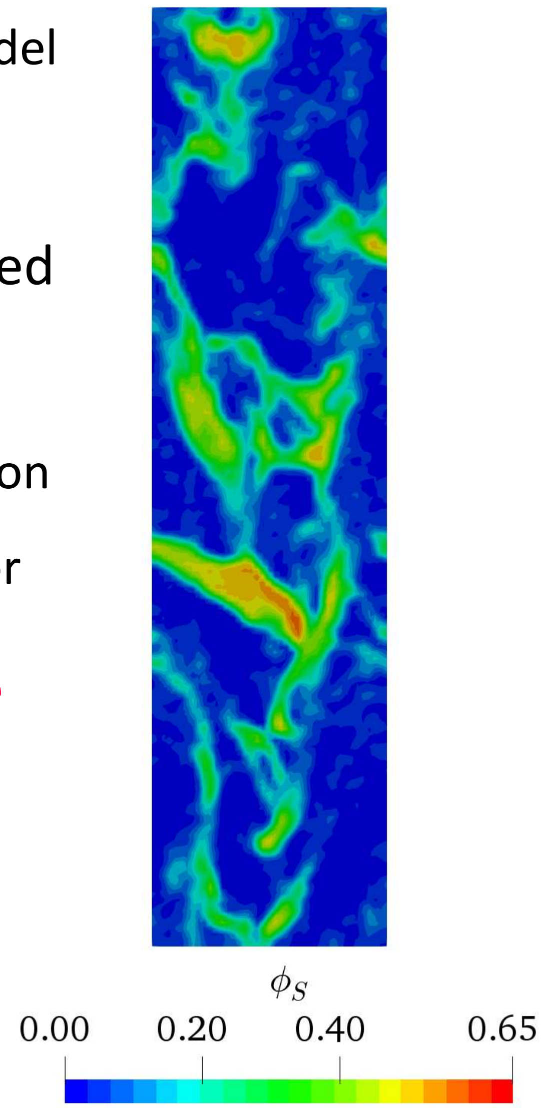
- **Challenges**
  - agglomeration and segregation
  - blockage & depositions
  - inefficient mixing
  - Equipment performance <20%

- **Experimental route**
  - Expensive, difficult & dirty
  - indirect & noisy data from the plant

https://www.gea.com/en/
https://burnertec.com/fcc-equipments/
https://www.industrialmeeting.club/food-processing-industry-plant-for-dry-mixed-products/

Workflows & ML::Need4Speed

- Modeling of gas-particle flows in **industrial-sized fluidized beds**
  - Typically, coarse-grid simulations using a “filtered” two-fluid model (fTFM)
- **fTFMs need sub-grid closure models** to approximate unresolved physical phenomena
  - Account for the effects of the inhomogeneous particle distribution
  - The drag force is essential for reliable prediction of flow behavior
- **Complexity increases** when considering **cohesive gas-particle** flows
  - Cohesive influence on the filtered drag force closure
  - Need for **faster (automated) closure development**



Sundaresan et al., AIChE J., 54, 2008. Igci & Sundaresan, Ind. Eng. Chem. Res, 50, 2011; Yu et al., Powder Technology, 184, 2008

Workflows & ML::Need4Speed::Model I

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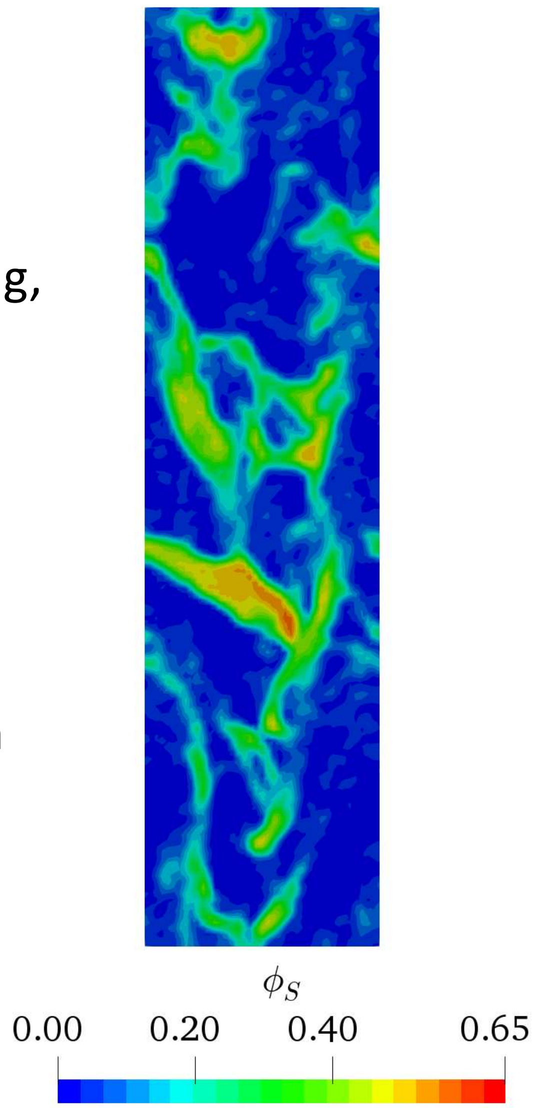
- Performing and then **filtering of "fine grid" simulations**
  - **Euler-Euler Approach**
    - Fluid and solid phase motion via continuum ansatz
    - complex particle-particle interactions (cohesion) challenging, but possible. **However, not the current focus…**
  - **Euler-Lagrange Approach**
    - Classical continuum-based ansatz only for fluid phase
    - Individual particle motion via Newton's equation of motion
    - Large variety of models for **particle-particle** interactions
    - ✓ **Our current focus**



"ML-empowered" closure development

Workflows & ML::Need4Speed::Model II

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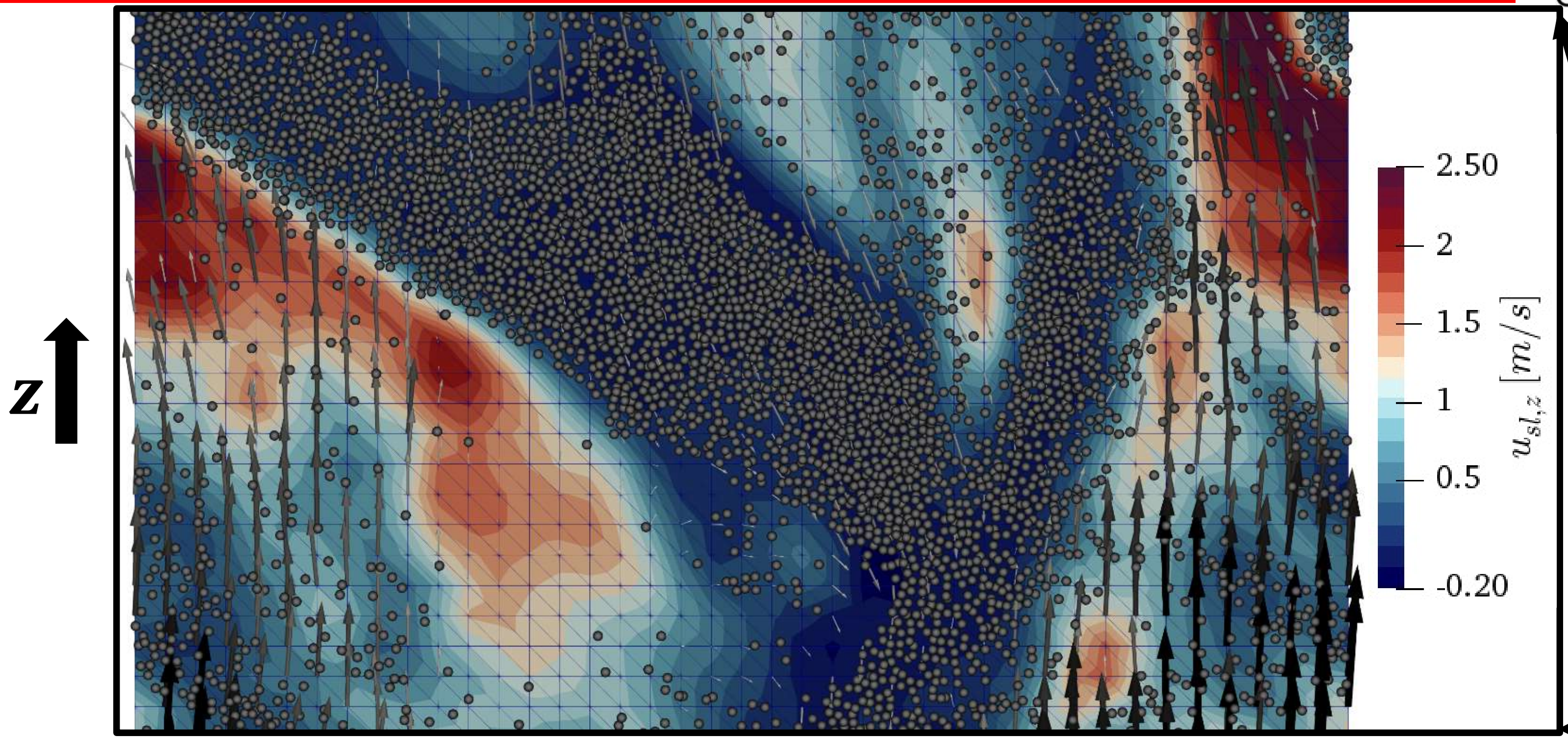
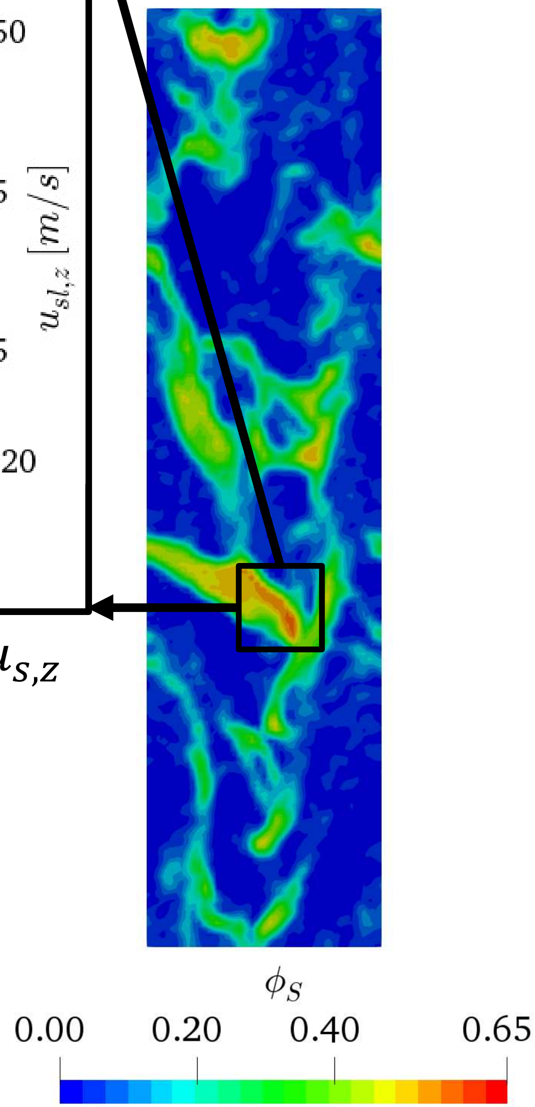


$$u_{sl,z} = u_{g,z} - u_{s,z}$$



- **First "filtering" step**: mapping Lagrangian quantities onto the fine Eulerian grid
- **Second filtering step**: Filter all relevant quantities using a defined filter length → $\bar{\phi}_s, \tilde{\boldsymbol{u}}_g, \tilde{\boldsymbol{u}}_s$

Workflows & ML::Need4Speed::Model III

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- Correction tensor $\boldsymbol{H}_d = \frac{drag\ in\ \boldsymbol{inhomogeneous\ state}}{drag\ in\ \boldsymbol{hypothetical\ homogeneous}\ state}$

- This means it must fulfill the following properties:
  - $\boldsymbol{H}_d \rightarrow \mathbf{1}$ for sufficiently small filter sizes (i.e., ”well-resolved” simulations)
  - $\boldsymbol{H}_d \rightarrow \mathbf{1}$ in the dilute limit (i.e., a single particle sedimenting at its terminal speed)
  - $\boldsymbol{H}_d \rightarrow \mathbf{1}$ in the dense limit (i.e., a particle suspension sedimenting at steady state)

- **Previous approach**: correlation functions based on just few features (“markers”): $\bar{\phi}_s, \Delta_f, \widetilde{\boldsymbol{u}}_{sl}$:
  - Complex to build, limited applicability (poor training, not rigorous)
  - limited accuracy for larger filter lengths

- **Novel approach:** usage of **neural networks**
  - Fast, accurate & rigorous (many markers), and easy to integrate (e.g., Keras2CPP)
  - previously **only applied to dry systems**

Jiang et al., Chem. Eng. Sci. , 230, 2021. Lu et al., Ind. Eng. Chem. Res., 61, 2022

Workflows & ML::Need4Speed::Model Details

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- Keras® framework in Python
- DNNs with three hidden layers are optimal
- Rectifying Linear Unit (ReLU) activation function
- Training: mini-batch gradient descent method (MB size: 1024), Mean Absolute Error (MAE) is the cost function
- Training time: 2D with 25 epochs → 0.5 hours, 3D with 50 epochs → 3.5 hours
- Hyperparameter search: up to 80 hrs in 3D

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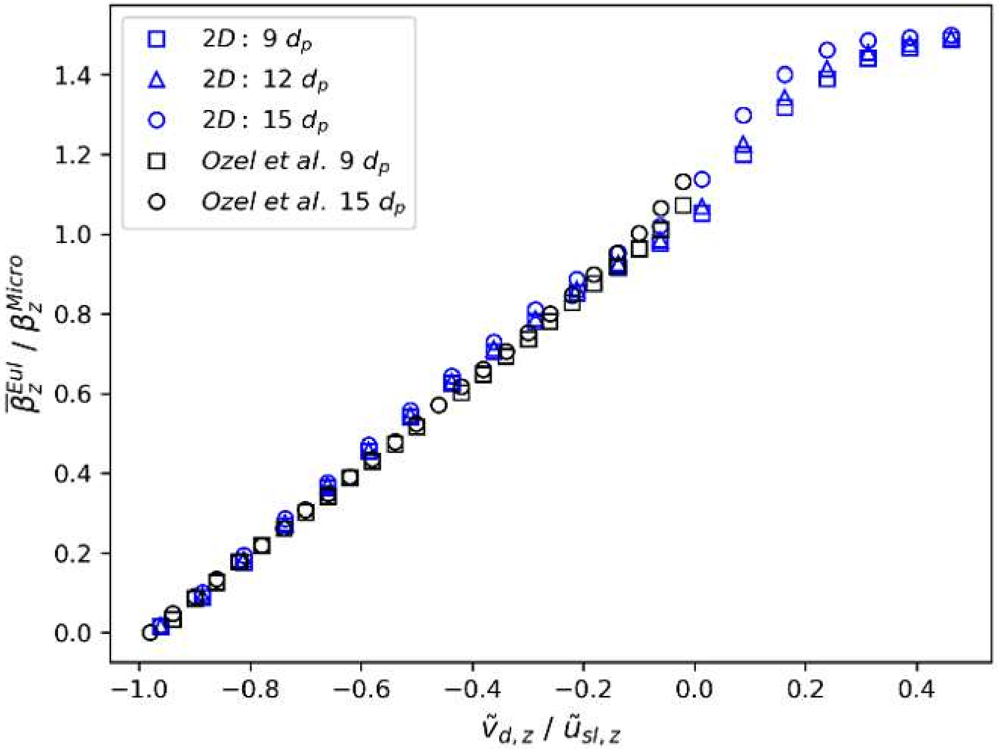
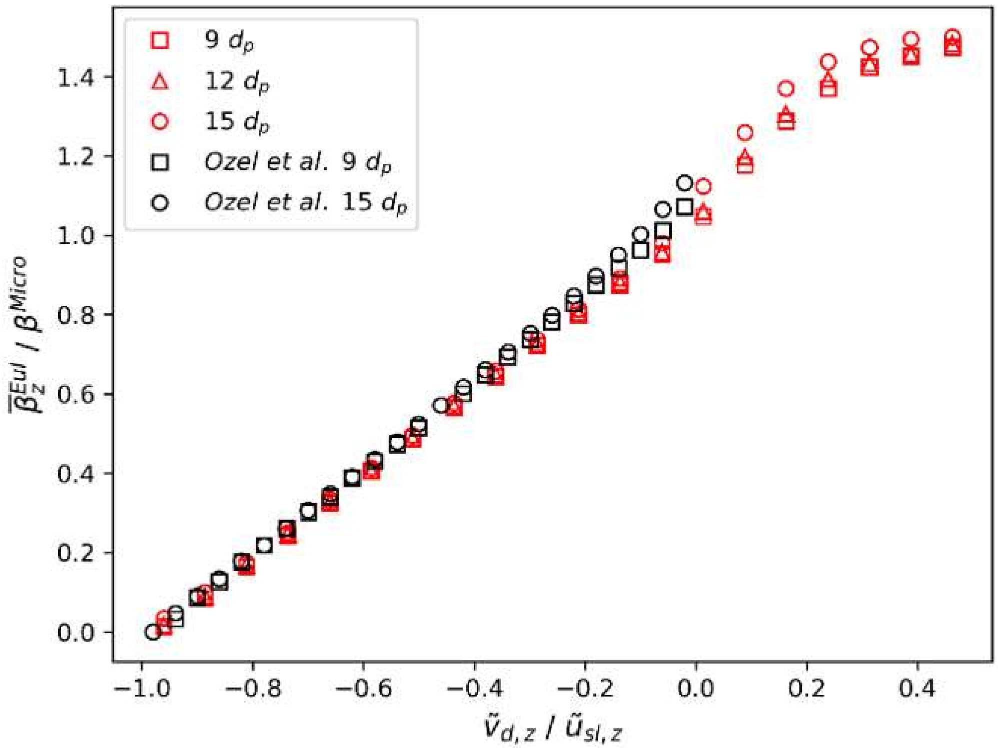
- „Validation“ with previous work





Workflows & ML::Need4Speed::Result I

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- Ansatz for the filtered drag force: $\bar{\boldsymbol{\Phi}}_{d,A} = \boldsymbol{H}_d \, \beta^{Micro} \, \tilde{\boldsymbol{u}}_{sl}$
- …with the closure

$$\boldsymbol{H}_d = \mathbf{1} + \frac{\phi_{s,max} \, u_t}{\bar{\phi}_s \, \tilde{u}_{sl,z}} \boldsymbol{z}$$

- The target and the prediction of the neural network is the **scaled drift velocity**

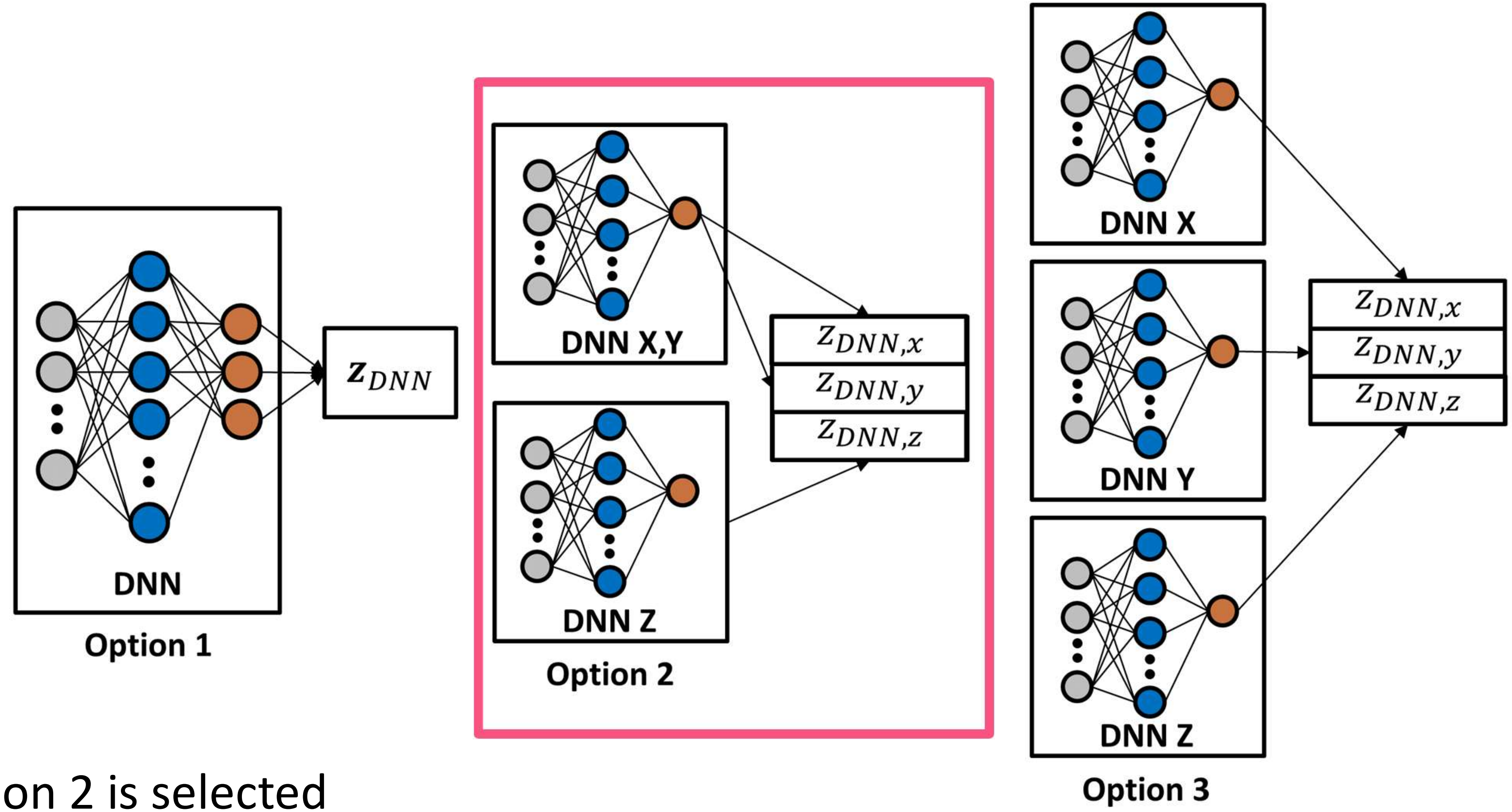
$$\boldsymbol{z} = \frac{\bar{\phi}_s \, \tilde{\mathbf{v}}_d}{\phi_{s,max} \, u_t}$$

- For now, we consider all off-diagonal ("lift like") values of $\boldsymbol{H}_d$ to be zero. However, diagonal elements of $\boldsymbol{H}_d$ are not identical **(anisotropic correction)**

Workflows & ML::Need4Speed::Result II

- Prediction based on vector-valued markers must ensure Galilean invariance

- Three basic options to formulate a drag correction



- Option 2 is selected
  - An internal coordinate system, that respects rotational invariance, can be intuitively spanned

Tausendschön et al., Chem Eng & Technol, 2023 (in press).

Workflows & ML::Need4Speed::Result III

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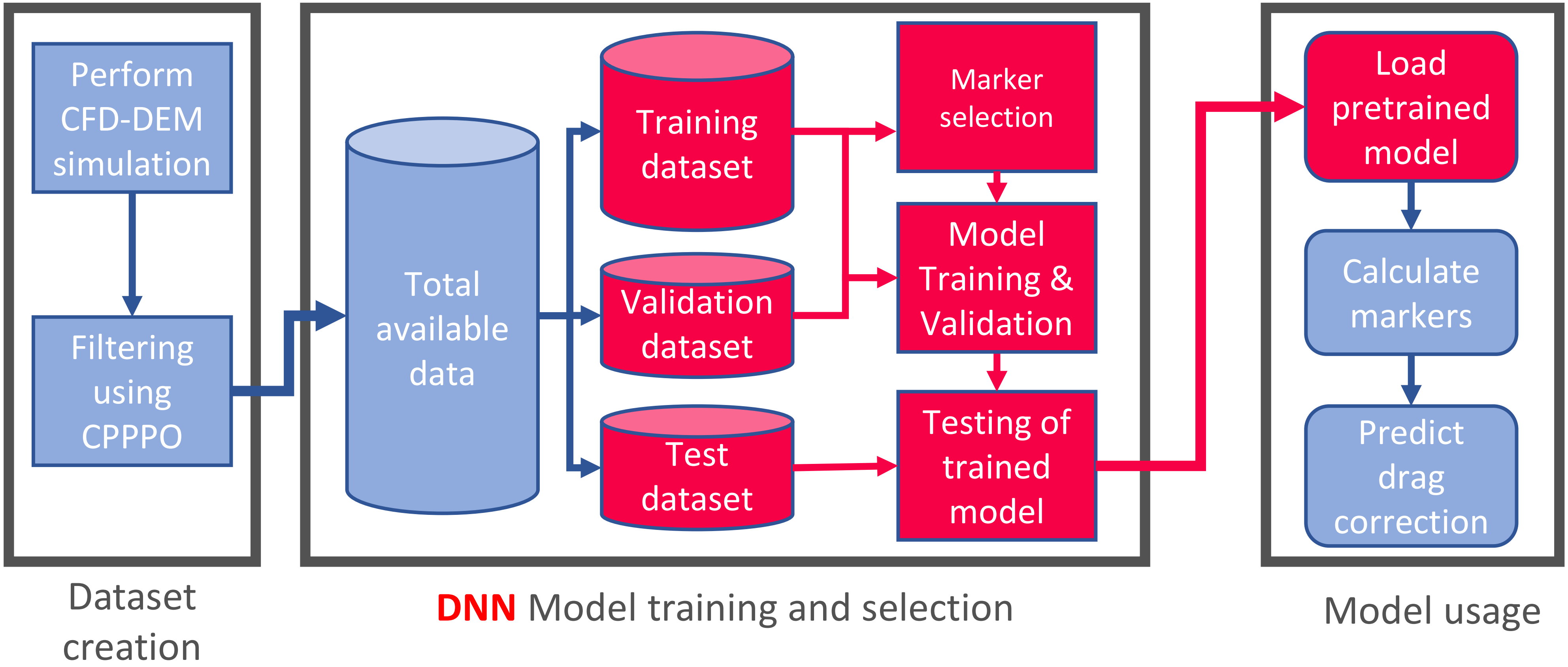


- Markers ("**Features**")

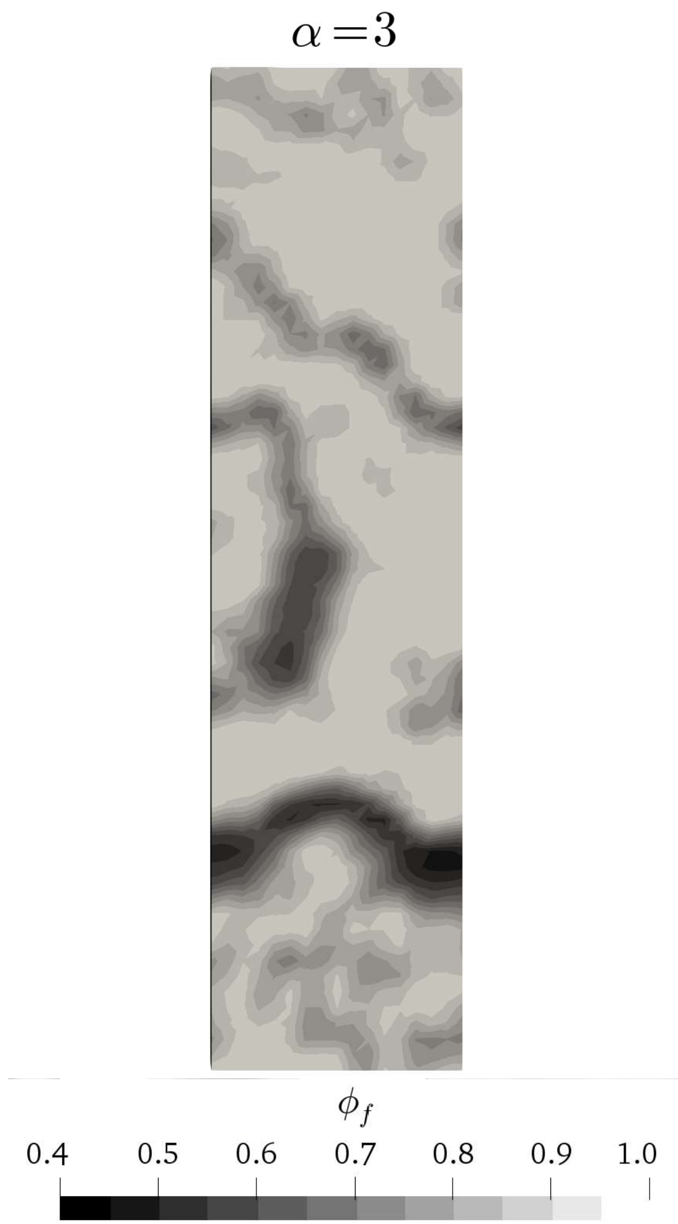
$$\boldsymbol{\psi} = \left(\frac{1}{\Delta_f^*}, \frac{\bar{\phi}_s}{\phi_{s,max}}, \frac{\tilde{\boldsymbol{u}}_{sl}}{u_t}, \overline{\nabla p_z^*}, Bo, \overline{\dot{\gamma}_{sl}}^*, \overline{\dot{\gamma}_s}^*, \frac{\left\| \tilde{\boldsymbol{u}}_{sl,xy} \right\|}{u_t} \right)$$

- All markers min/max normalized prior to usage

Workflows & ML::Need4Speed::Result IV

- Pseudo **2D & 3D CFD-DEM** simulations
  - Domain size is $16\ \Delta_G$ x $2\ (or\ 16)\ \Delta_G$ x $64\ \Delta_G$
  - Total particle volume fraction $\phi_{s,tot}$ = 0.10
  - Filter sizes are: $3\ \Delta_G,\ 4\ \Delta_G, 5\ \Delta_G$
- Scaling of **coarse graining parameters** following Tausendschön et al.
- Dry to **highly cohesive** systems (cohesion from liquid bridges: capillary & viscous)

	$\boldsymbol{\alpha = 3}$
$d_P\ [\mu m]$	450
$\Delta_G\ [\mu m]$	1,350
N_{prime}	285,147
Parcels	10,561
Bo	$0-80$



Tausendschön et al., Powder Technology, 364, 2020

Workflows & ML::Need4Speed::Result V

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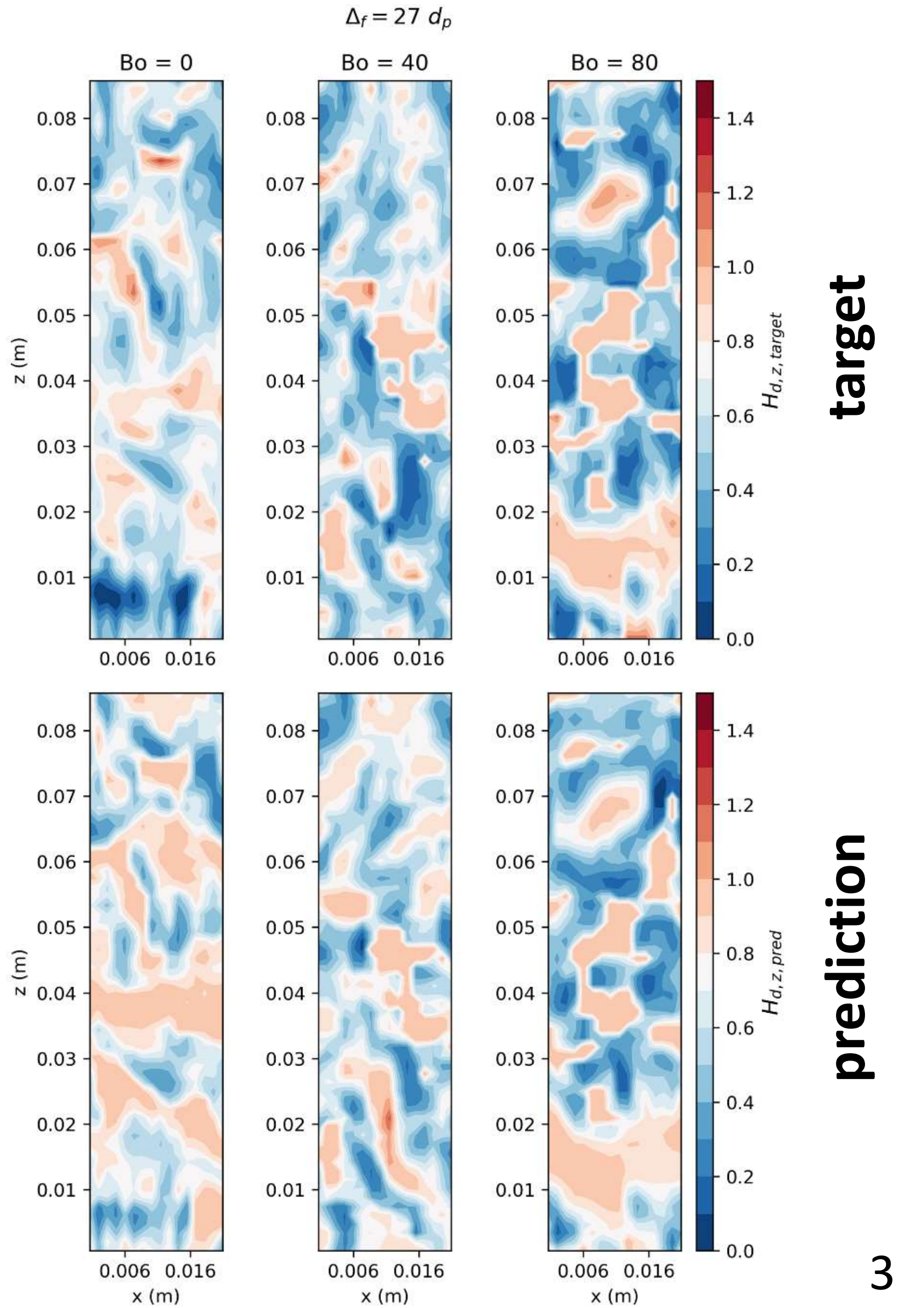
- 2D & 3D, gravitational direction only
- Spatial distribution of the drag correction functions is sensitive to Bond number **("diffuse" versus "focused")** for low and high Bond, respectively)
- Reasonable agreement, except for "extreme" regions (e.g., local maxima in the $\boldsymbol{H}_d$ field)



Tausendschön et al., Chem Eng & Technol, 2023 (in press).

Workflows & ML::Need4Speed::Result VI

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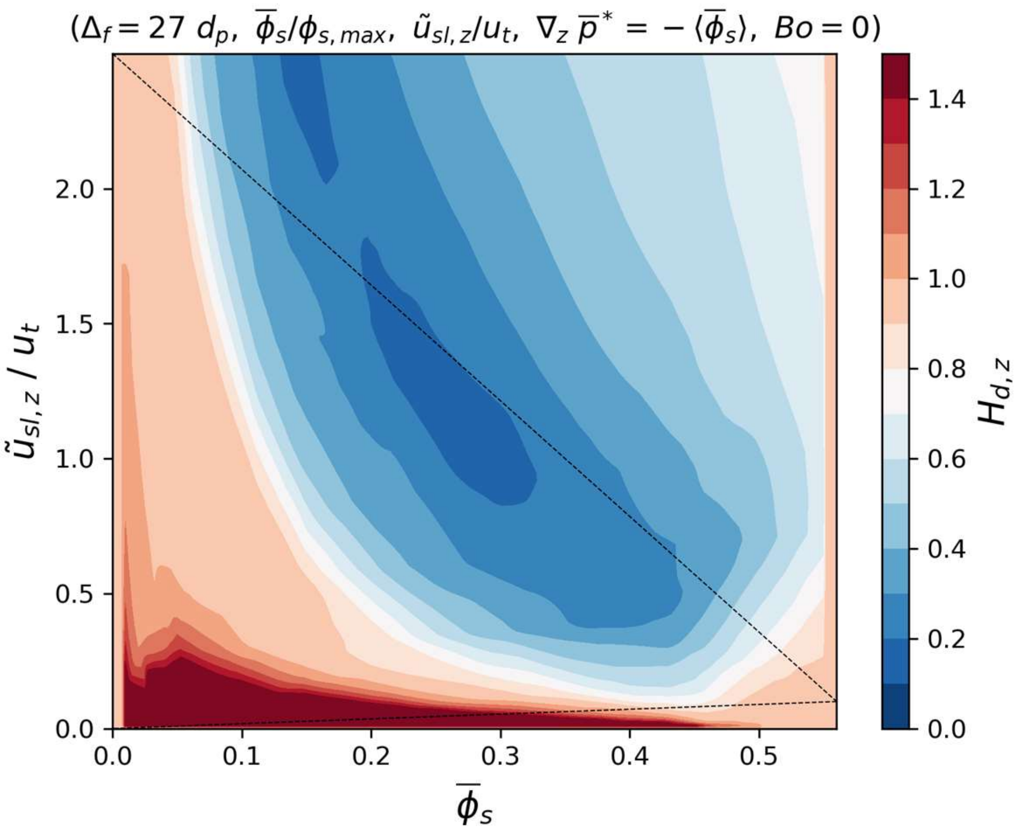
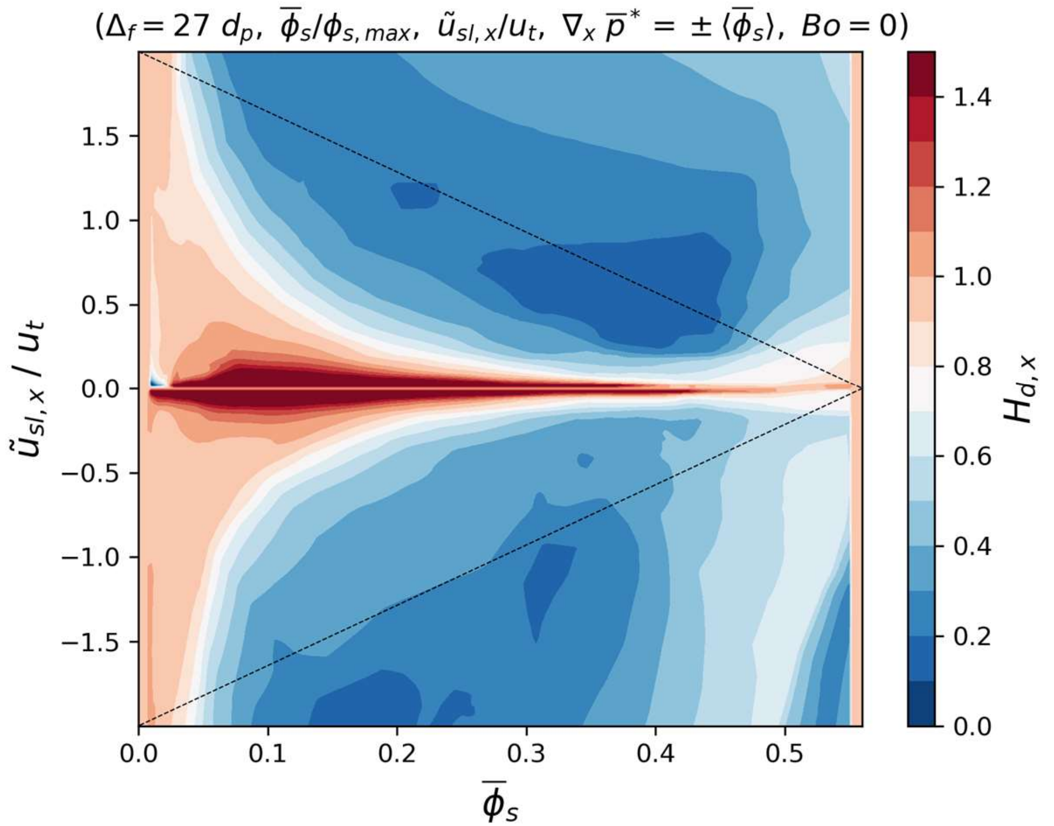
- Distribution of correction values in $\bar{\phi}_s - \tilde{u}_{sl}/u_t$ plane

Gravitational direction



Lateral direction



- Significant and non-trivial change with Bond number

Tausendschön et al., Chem Eng & Technol, 2023 (in press).

Workflows & ML::Need4Speed::Result VII

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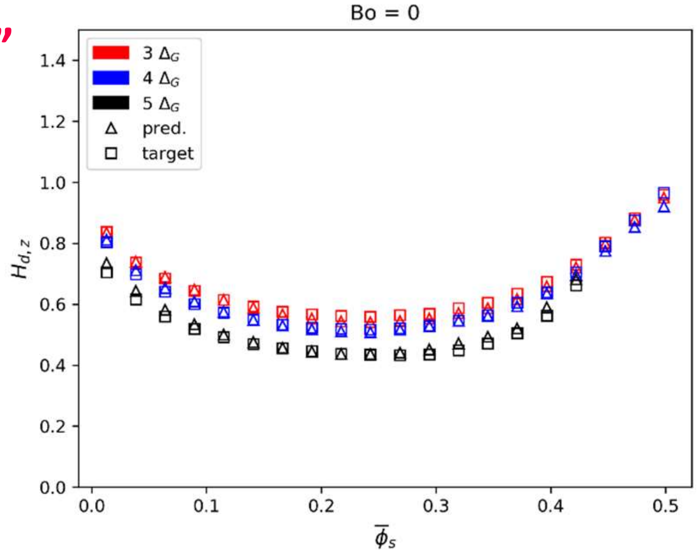
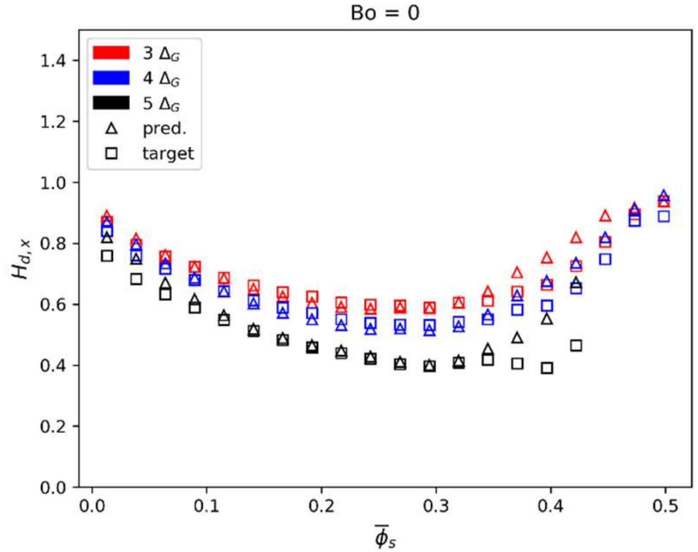
"bin-averaged" data (non-cohesive)

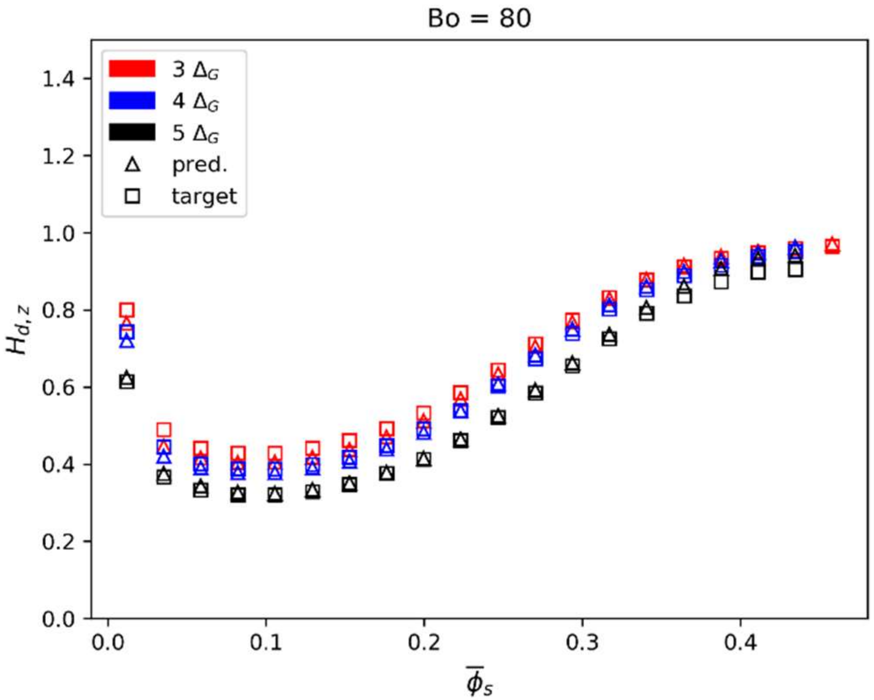
gravitational direction

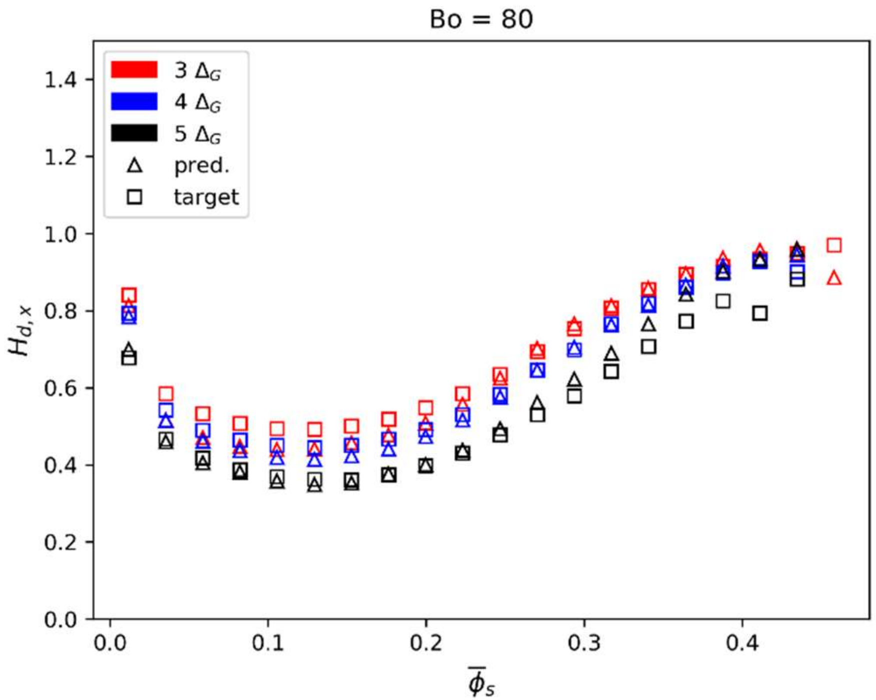


lateral direction



cohesive





Workflows & ML::Need4Speed::Result VIII

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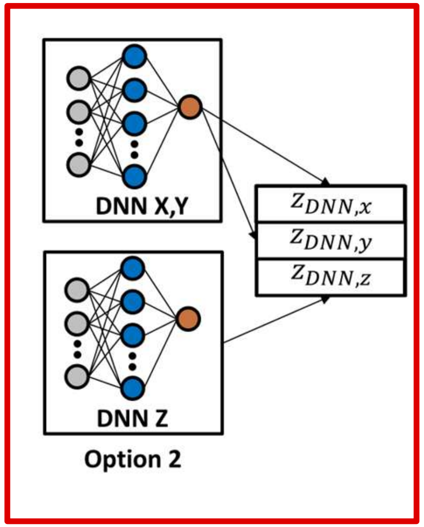
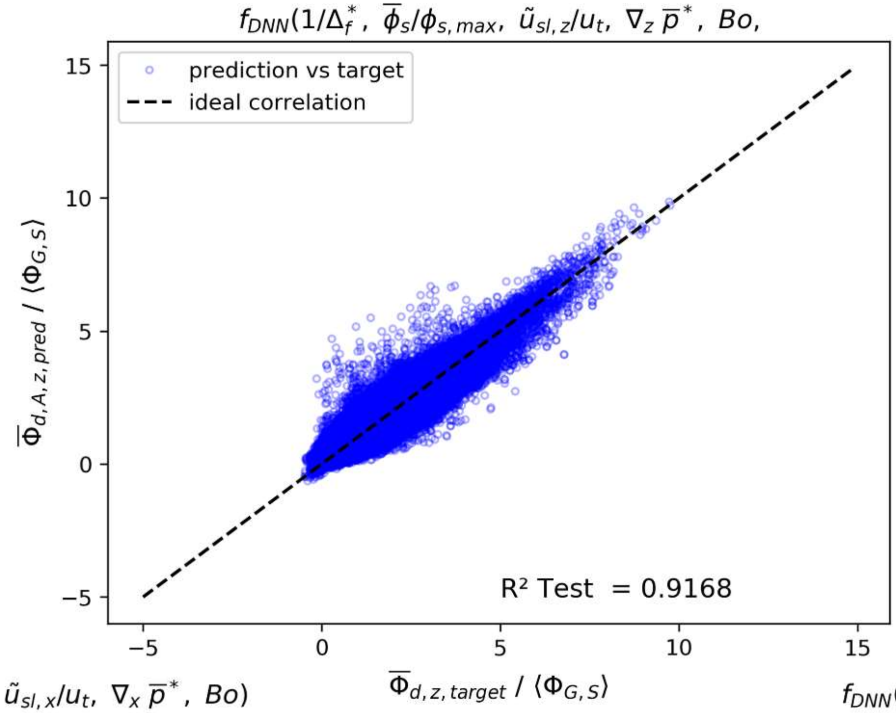
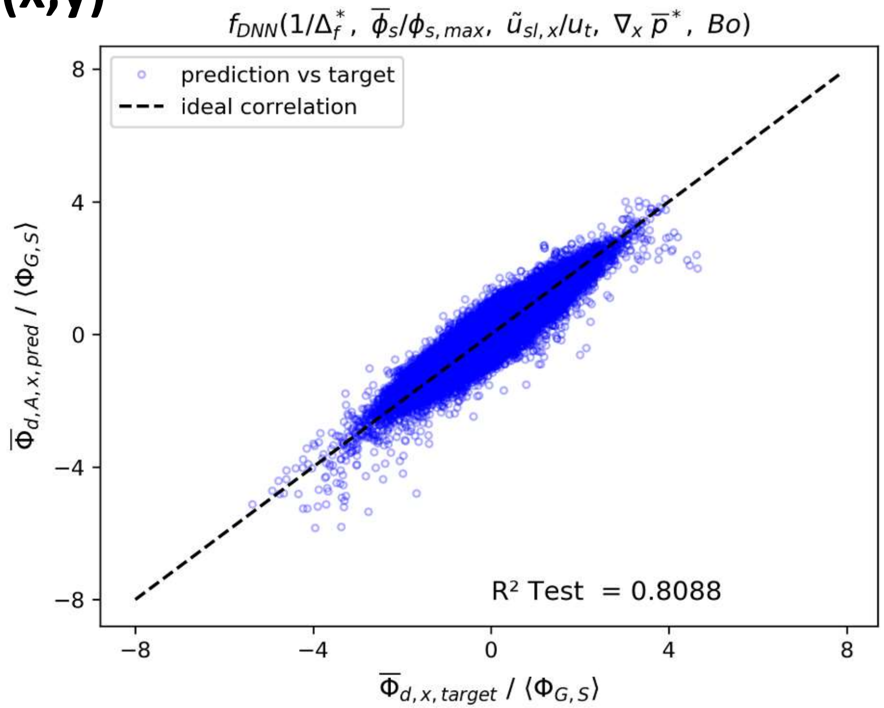


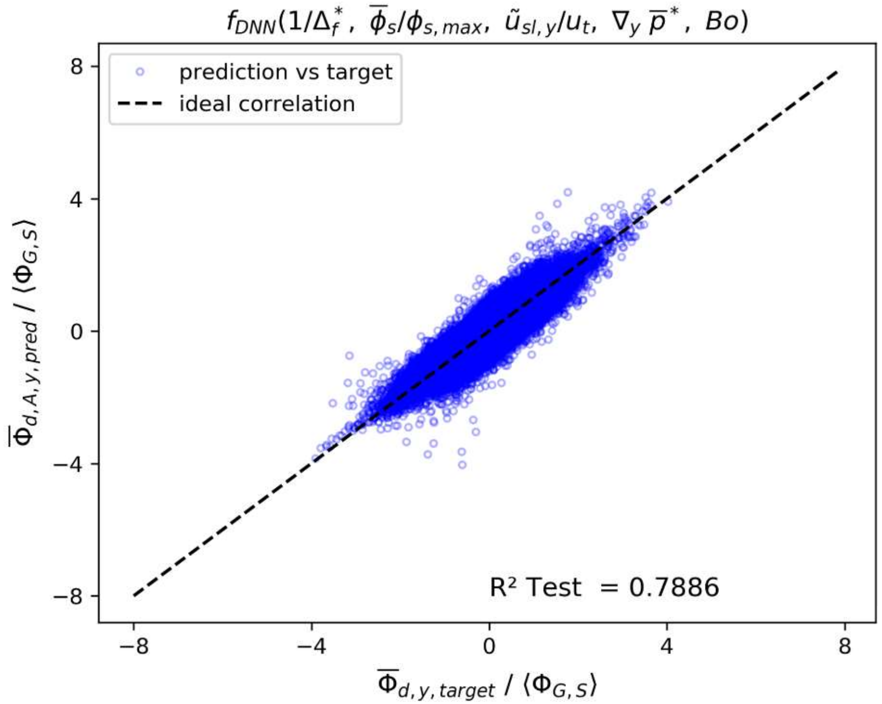


Individual samples ("raw filtered data")

gravitational direction (z)

lateral directions (x,y)





Workflows & ML::Perspectives

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- The "**chicken crossing a street** challenge": calibration has become a standard approach to make simulations "more realistic"
  - Sequential direct calibration approach (Aspherix® calibration)
  - Response surfaces: Superimposing the results of multiple numerically replicated experiments for a range of parameters

- **Common challenges**
  - lack of **graphical calibration workflows, or even the workflow**
  - absence of a **clear & FAIR data handling strategy**

Irrespective of the calibration method, the workflow needs to handle a huge amount of data

Coetzee, Powder Technology, 2017. Roessler et al, Powder Technology, 2019. Do et al, advanced powder technology, 2018. Richter et al, Powder Technology, 2020

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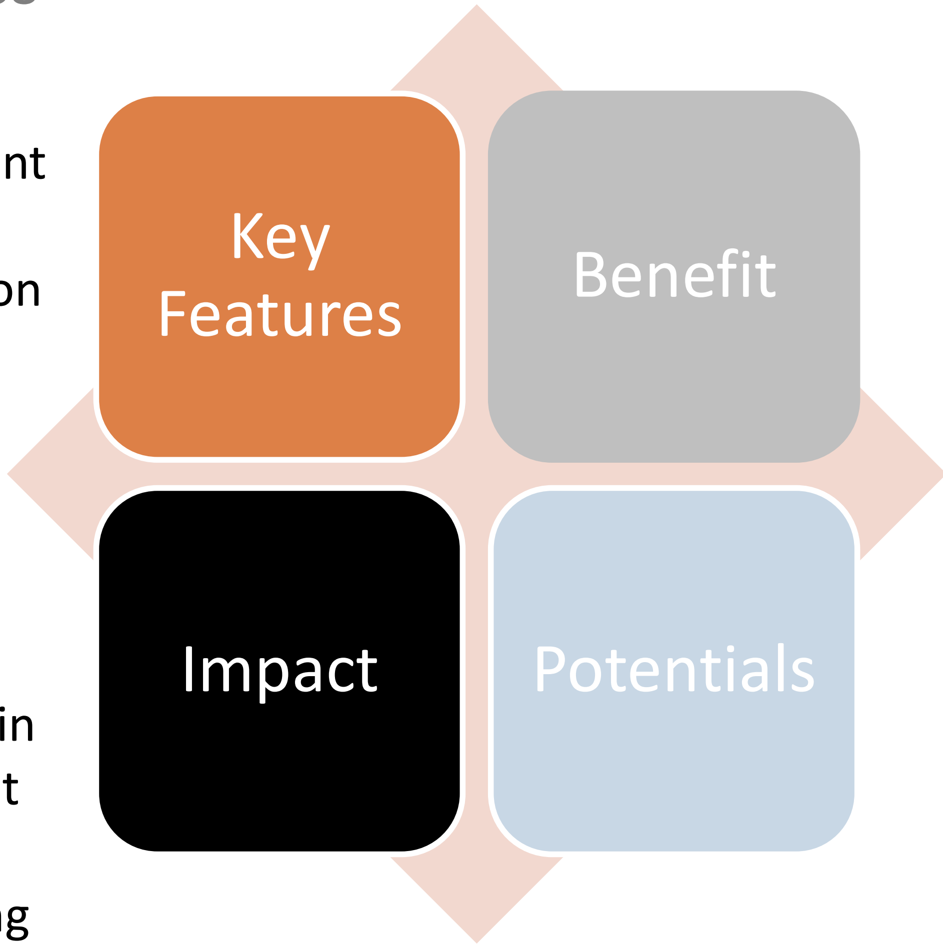
DEMvironment

A workflow environment for data management of DEM parameter calibration process

- Data management
- Guide for experiment selection
- Steers the calibration workflow



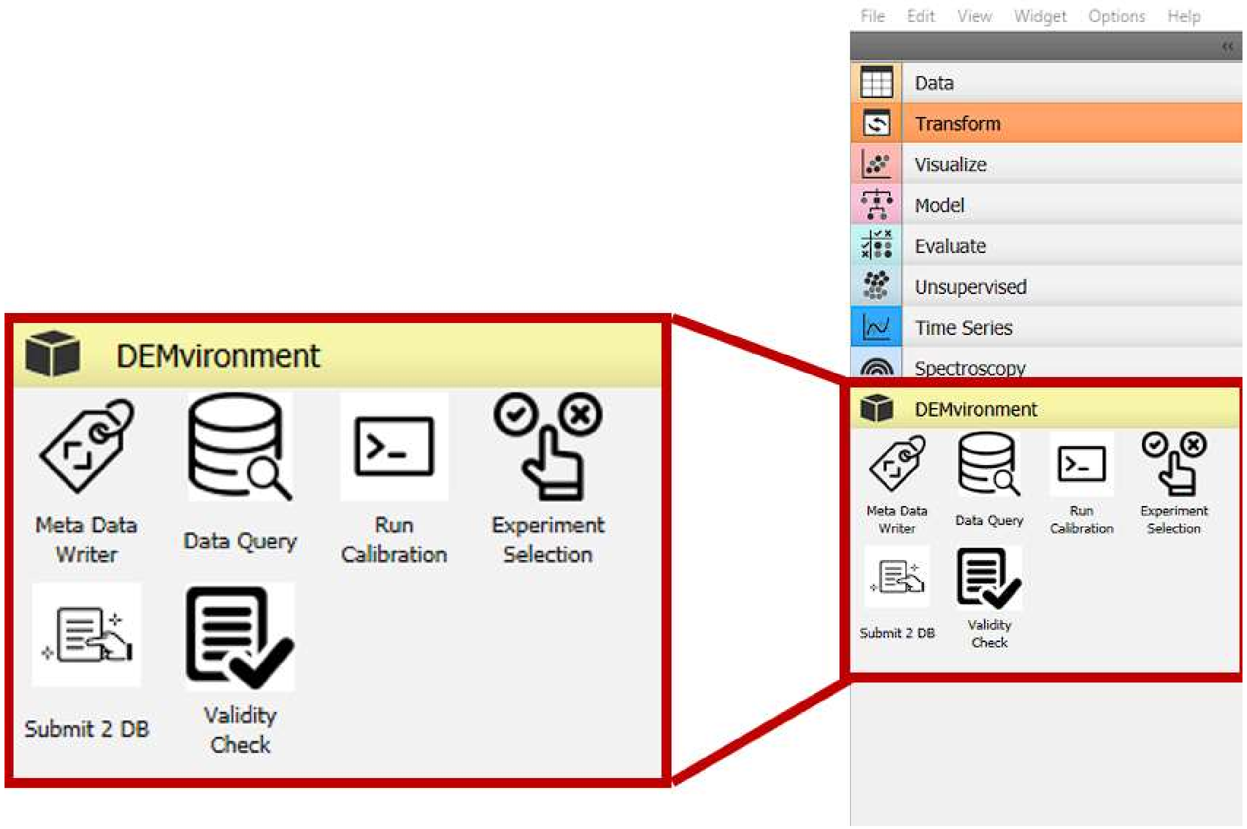
- User-friendly interface
- Automated parameter calibration
- Reproducibility of the process
- Open source

- Speeding up the process
- Increase efficiency in model development
- Increased collaboration among researchers and practitioners

- Allows steering more sophisticated ML algorithms
- Can be applied to other particle simulation techniques

DEMvironment interface

…soon available in Orange3



https://n-ghods.github.io/workflowenv

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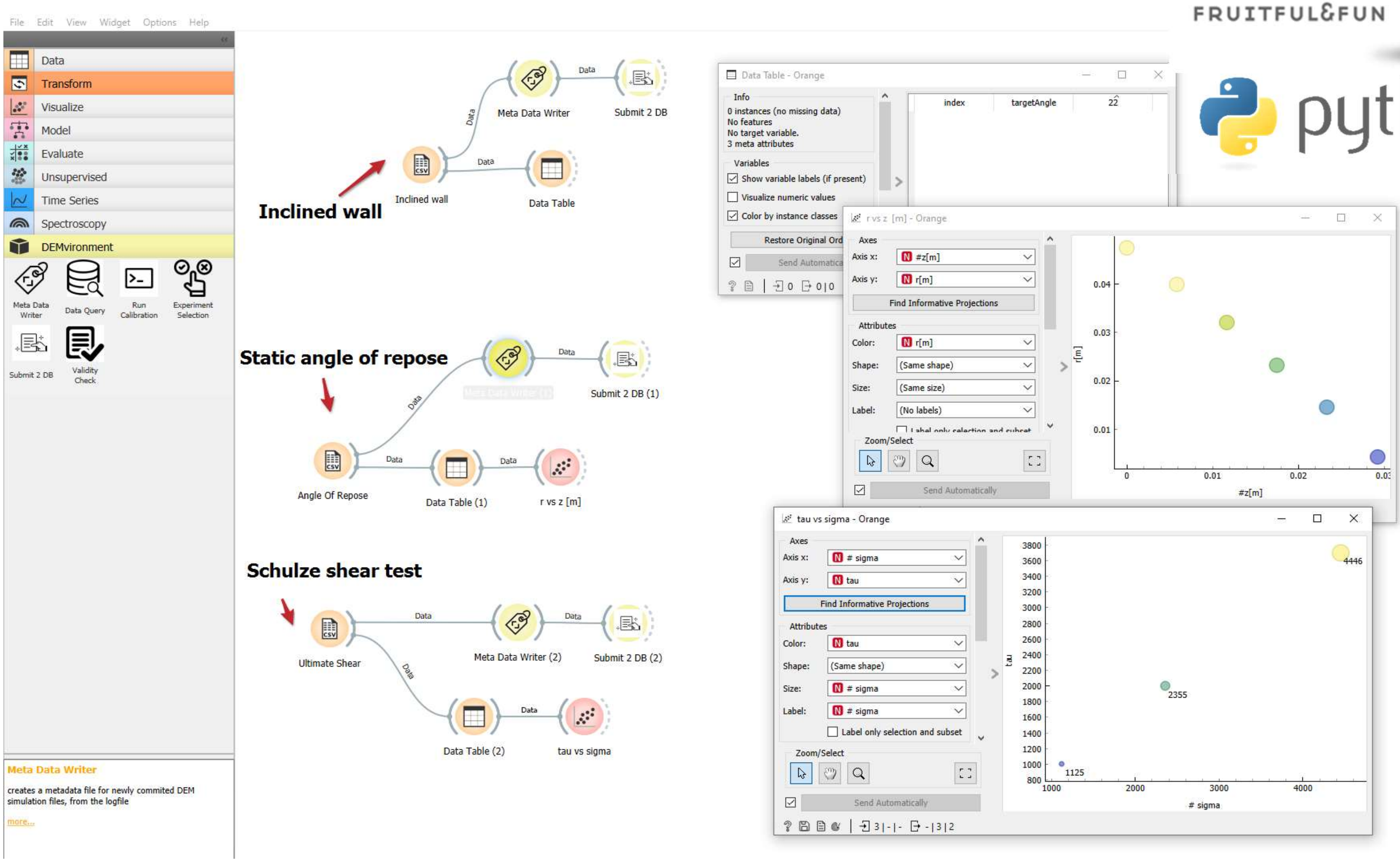
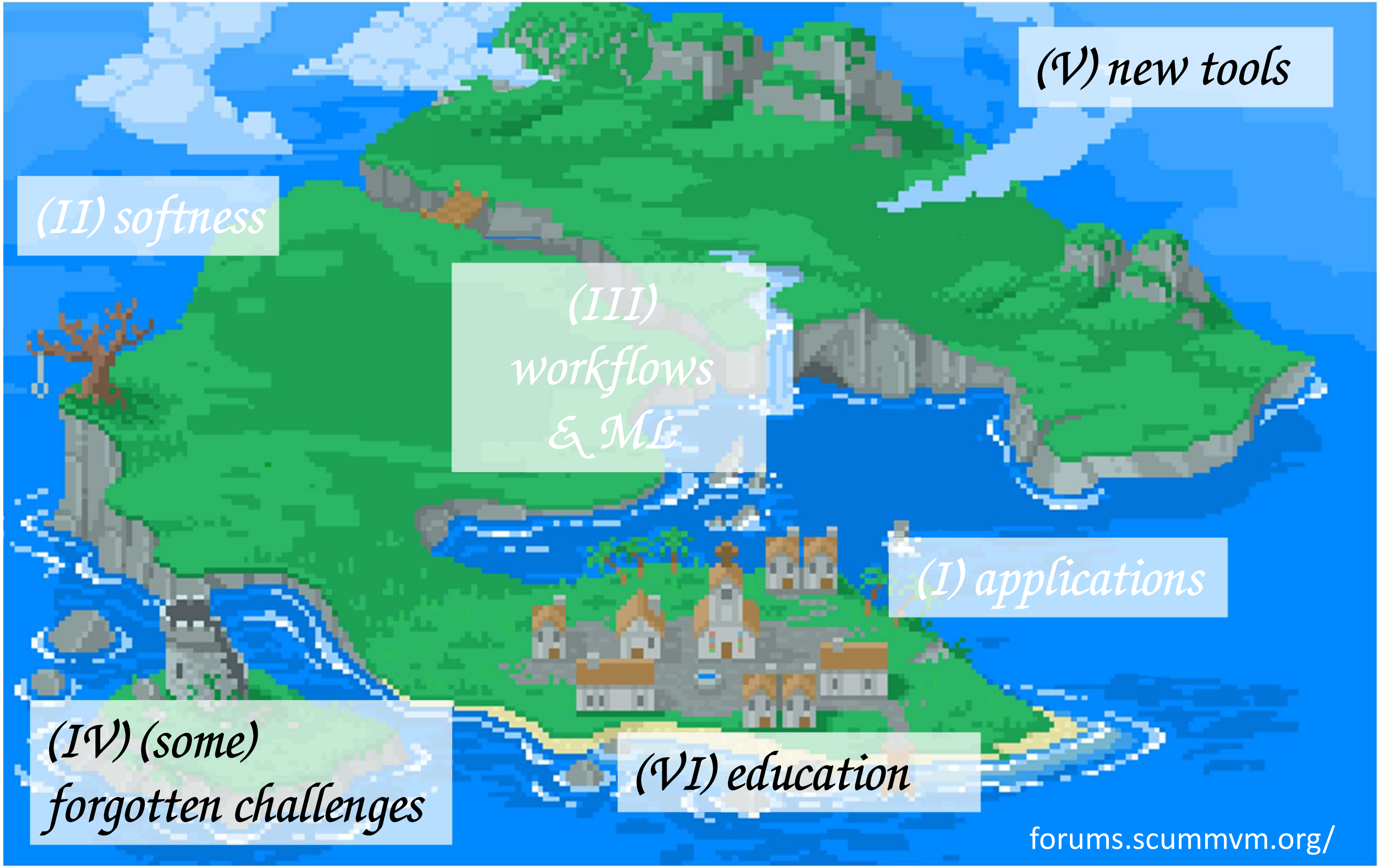
DEMvironment interface

…soon available in Orange3



Overview


(V) new tools
(II) softness
(III) workflows & ML
(I) applications
(IV) (some) forgotten challenges
(VI) education
forums.scummvm.org/

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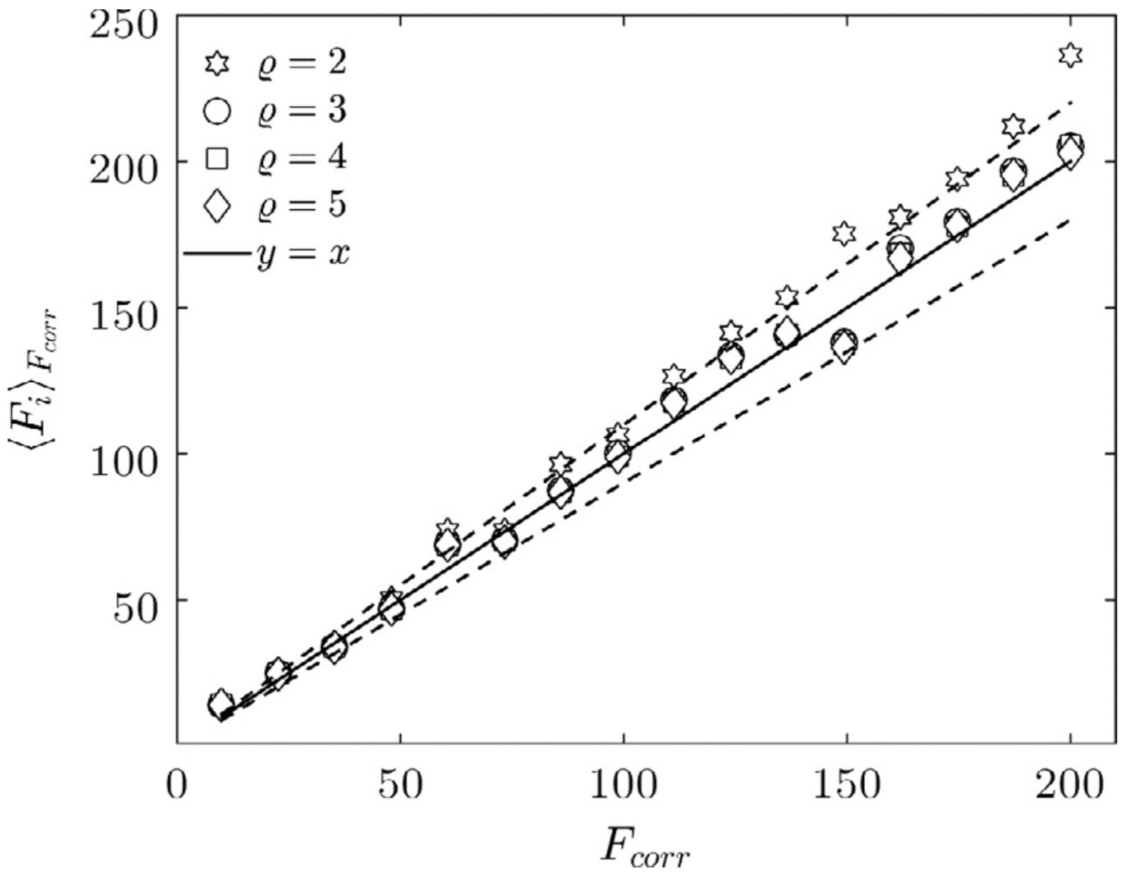
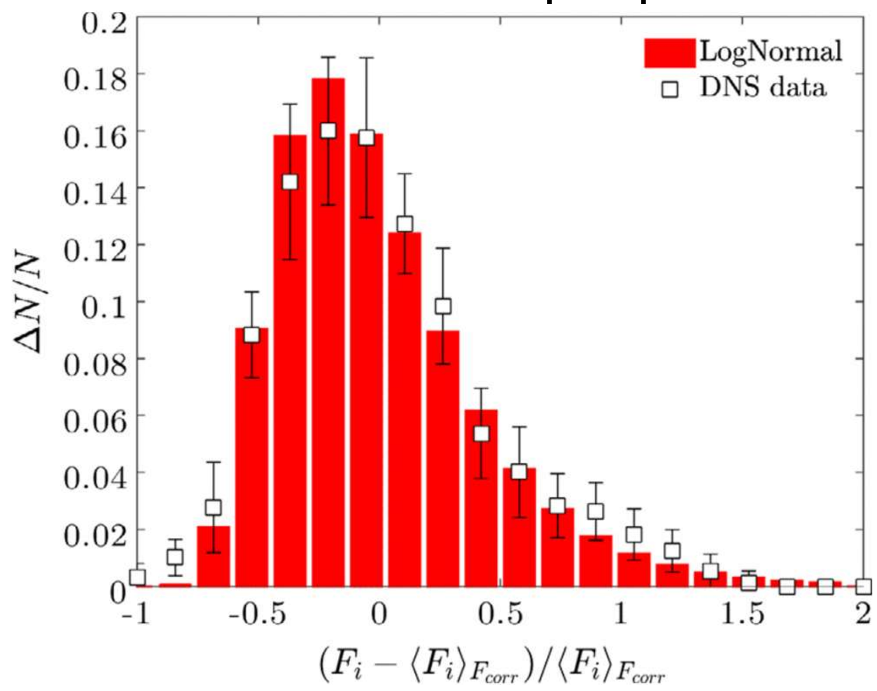
Let us reflect…

What would we need to go "beyond" current CFD-DEM capabilities?

Fluid-particle drag (and Nusselt number) is okay „on average"….



….but there is a wide distribution on a per-particle!



Municchi & Radl, Int J Heat Mass Transfer, 2017

(Some) Forgotten Challenges

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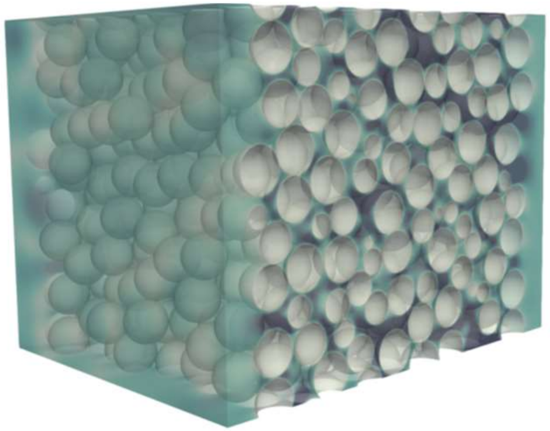
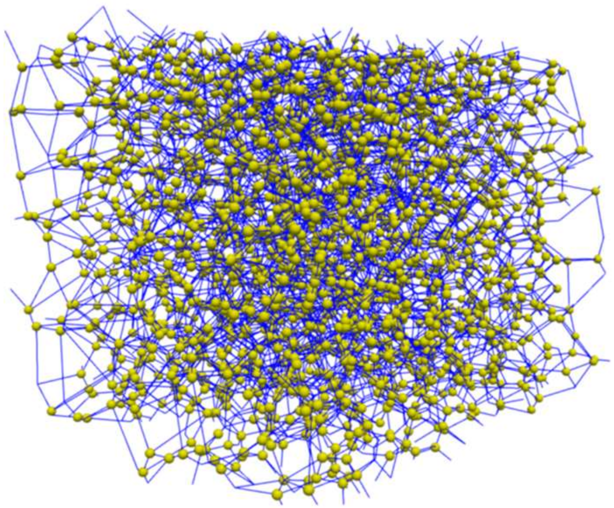
Let us reflect…

What would we need to go "beyond" current CFD-DEM capabilities?

Possible solution: use a pore network model to improve flow prediction…



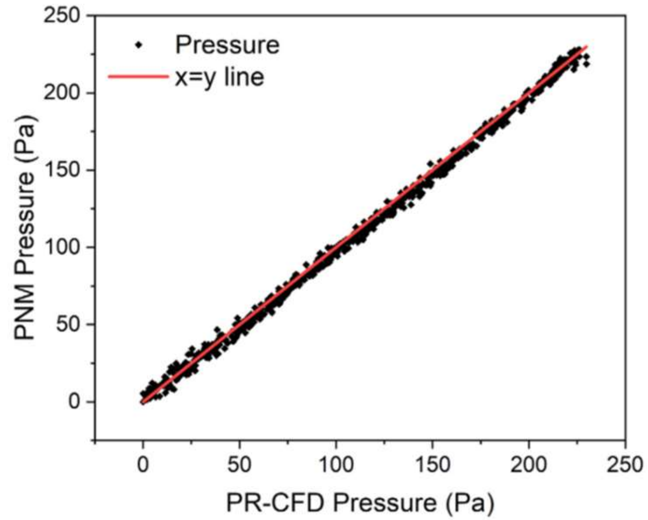
(a)



(b)

Morimoto et al, Computers & Geotechnics, 2022

….with recent success! But what is the computational cost? Is their calibration universal?



Fathiganjehlou et al., Chem Eng Sci, 2023

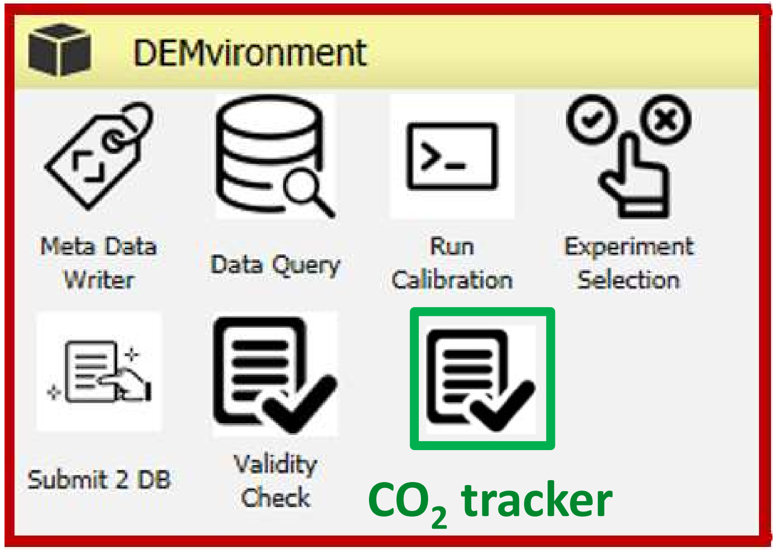
What should happen next…

…tools and their upgrades

https://yopad.eu/p/SoSe23_seminarHannover

- CPPPO's general interface with lagrangian (DEM) data
- Filtering over a fixed number of particles (instead of a fixed region size)
- More filter kernels
- Integration of CO_2 tracker into workflow tool (eco sweet spot of modeling effort)

v2.0



Educational Aspects

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- **Start slow and simple** (analytics first, then simulation; Python first, then C++)
- **Use existing tools** (Orange3, then KERAS/TensorFlow)
- **respect FAIR data management** principles (because only complete data is useful data)
- **Preservation of knowledge** requires a dedicated work package

MATHEGRAM

CALIPER

Grants 813202 & 812638

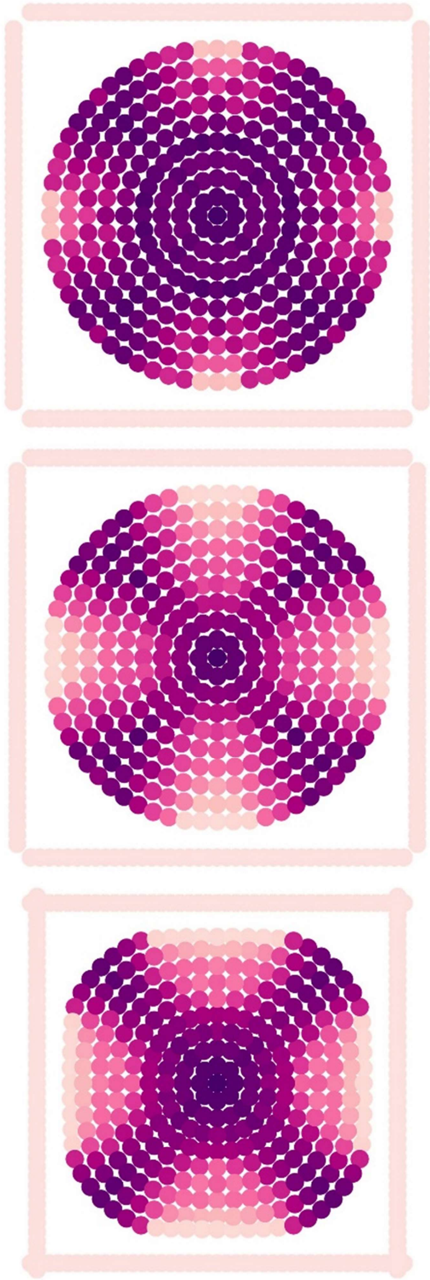
The **Discrete Element Method**

https://imoox.at/course/dem

MOOC starting in fall 2023

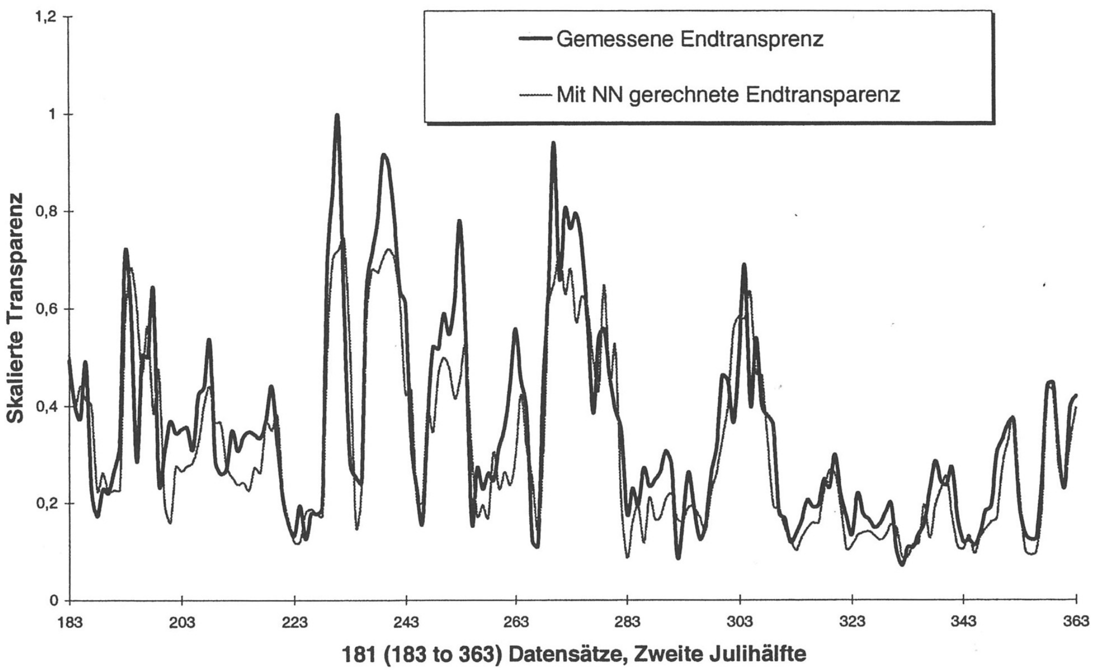
Conclusion I

- **Softness** must be seen in relative terms (pressure/elasticity ratio)
- **Various approaches** exist, simple extension to DEM possible (currently only spheres)
- **Poisson ratio** becomes an additional influence parameter
- Full **flexibility** (SPH, bonded particles, FEM) comes with **significant computational cost**
- advanced **MC DEM together with calibration** a promising strategy



Conclusion II

- **(Cohesive) sedimenting suspensions** are our daily business since many decades. Cohesion may require a **paradigm shift** to a “closure database” approach
- Reading old PhD thesis can give **inspiration** for **new features to be used in ML** (data @ t-Δt, smart NN testing).



Fuchs, Diss. TU Graz, 1999

Conclusion III

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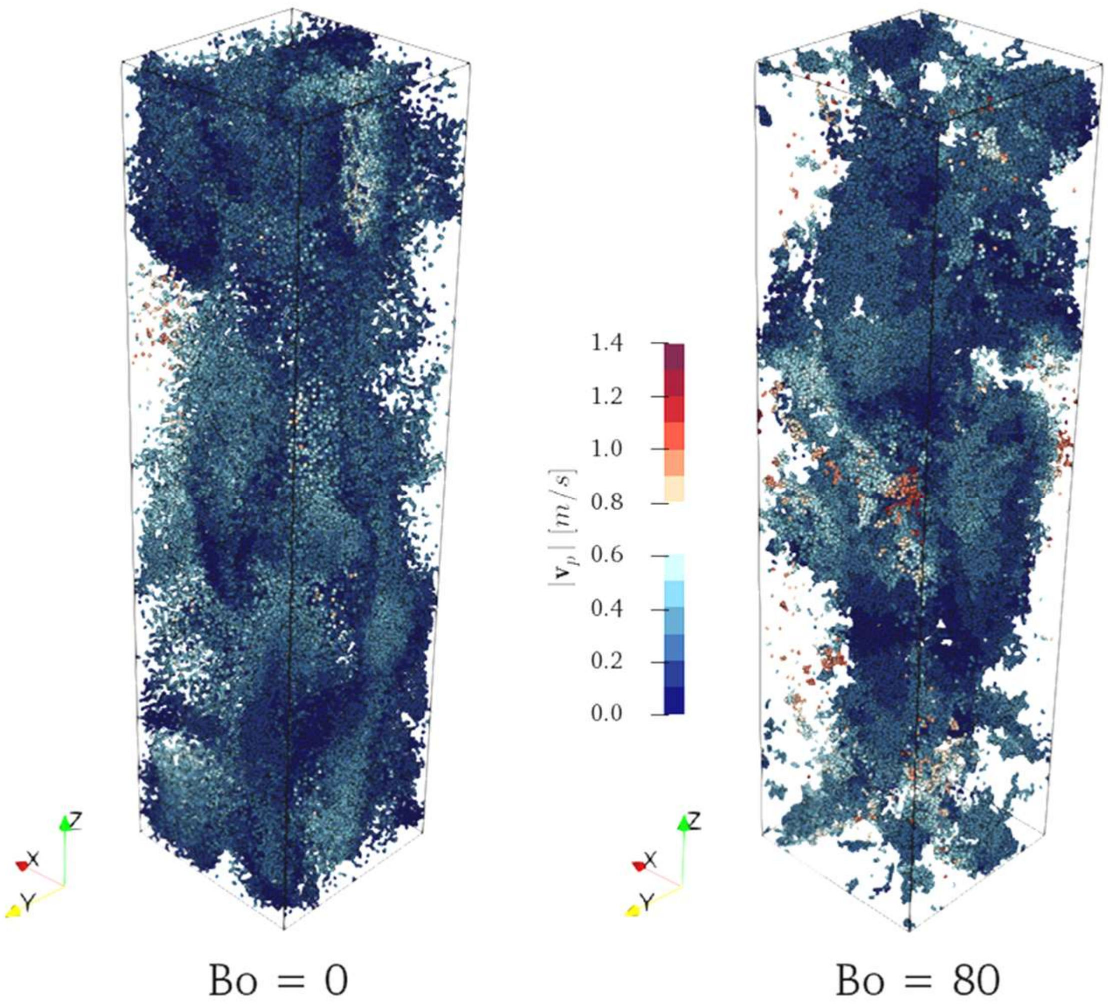
- **Anisotropy** of drag and stress closures must be considered. "Hand fitting" of this **set of 5 marker closures** would be **extremely time consuming** → **central motivation for usage of DNNs.**
- Huge **unexploited potential** when considering individual samples of the filtered drag force. Reasons: fundamental assumption $\bar{\boldsymbol{\Phi}}_{d,A} = \boldsymbol{H}_d \, \beta^{Micro} \, \tilde{\boldsymbol{u}}_{sl}$.
- Drag corrections are **stronger** (i.e., lower drag forces) **for cohesive systems.** Speculated reason: **more compact clusters for high Bo**.
- Options for future work
  - DNN-based closure for **meso-scale stresses.** A posteriori testing of the drag correction models in a **fTFM simulation framework**
  - **"Free" (tabulated, NN-based) force models** for **coarse graining** cohesive powder models

Beyond classical CFD-DEM

Forgotten Challenges and New Tools

Thank you



CALIPER

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska Curie grant agreement No. 812638.