Latest developments of CFDEMcoupling

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The History
The Network
The Team

Latest Development of CFDEMcoupling

The History

CFDEM project

As a consequence of the **need for suitable simulation tools** to capture the **industrial processes** of the partners of the CD-Lab. a scientific Open Source software for **numerical simulations of fluid-particle systems** was developed and a **frame for sustainable growth** was established.

JKU JOHANNES KEPLER UNIVERSITY LINZ

CD-Lab. on Part. Flow Mod. – S. Pirker JKU Linz

LIGGGHTS

19.2.2010 LIGGGHTS beta released

CFDEM coupling

25.10.2010 CFDEMcoupling beta released

2009

2010

International Companies start using CFDEMproject software

DCS Computing GmbH

10.01.2012 DCS Computing GmbH founded by Christoph Kloss & Christoph Goniva

2011

2012

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Organization

Professional Base:

Scientific Base:

DCS Computing GmbH

CFDEM project

Open Source Software for num. simulation of granular Systems (DEM)

LIGGGHTS

CFDEM coupling

Open Source Software for num. simulation of fluid-granular Systems (CFD-DEM)

Sandia National Laboratories

LAMMPS

OpenFOAM

esi get it right®

Latest Development of CFDEMcoupling
The Community

Vibrant community has been established: **CFDEMproject users** comprise **world-class companies and dozens of universities and research institutes**.

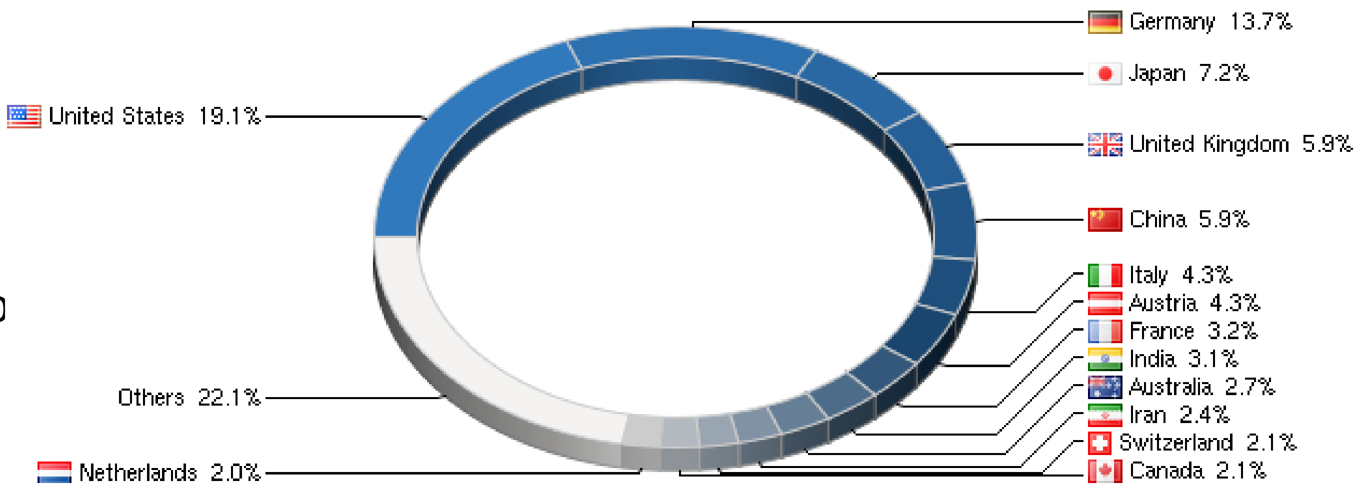
Software used in **2 EU Projects** (Pardem, ULCOS)

Software used in **projects** with 6 out of 9 **industrial partners of the CDL**

LIGGGHTS is now an **official Ubuntu Science Package**

MEC Award for PhD thesis with highest industrial potential to C. Kloss

CFDEM community
on www.cfdem.com
has 1200 users, and
8600 unique site visito
from 92 countries
within 8 months



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The Team

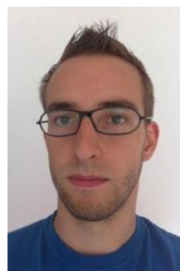
Promoted by a team of **young and motivated researchers** the **CFDEMproject grows** and develops. There is a demand of even more **development power**, thus **expansion will proceed.**

Supervision

Christoph
Goniva

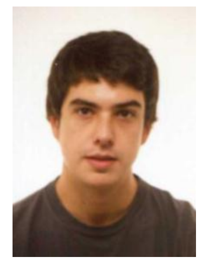
Christoph
Kloss

Alice
Hager



Michael
Friedl

Klemens
Gruber



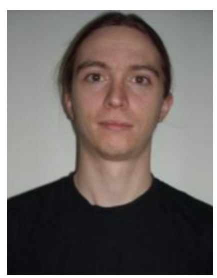
Roberto
Aristegui

Daniel
Nasato

?

Mr./Mrs. X.

Stefan
Amberger



Philippe
Seil

Patrick
Wijerama

Josef
Kerbl

?

Richard
Berger

2009

2012

Discrete Modelling of Fluid-Particle Systems

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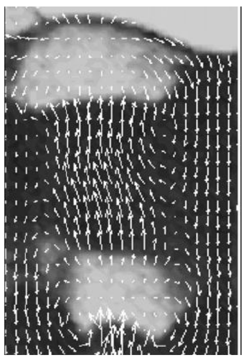
Discrete Modelling of Fluid-Particle Systems

CFDEM project

How to model particulate flow?

… as the romans said: "divide et impera"

Particulate Flow



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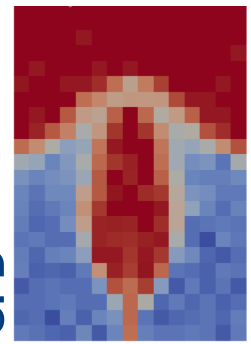
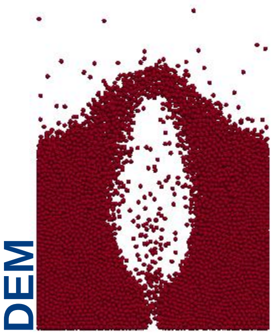
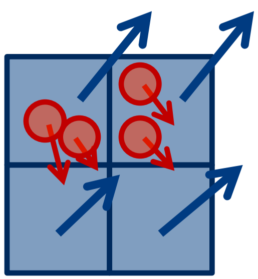
CFD



+

DEM





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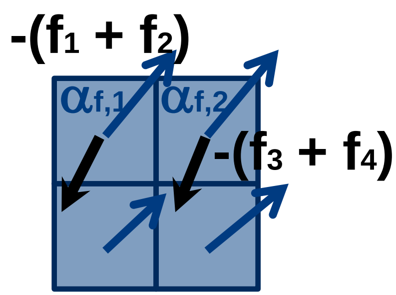
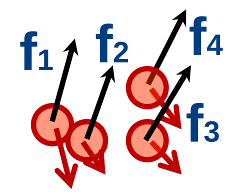


CFD with adapted voidfraction and momentum sources

+



DEM with force on particles coming from CFD

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Discrete Modelling of Fluid-Particle Systems

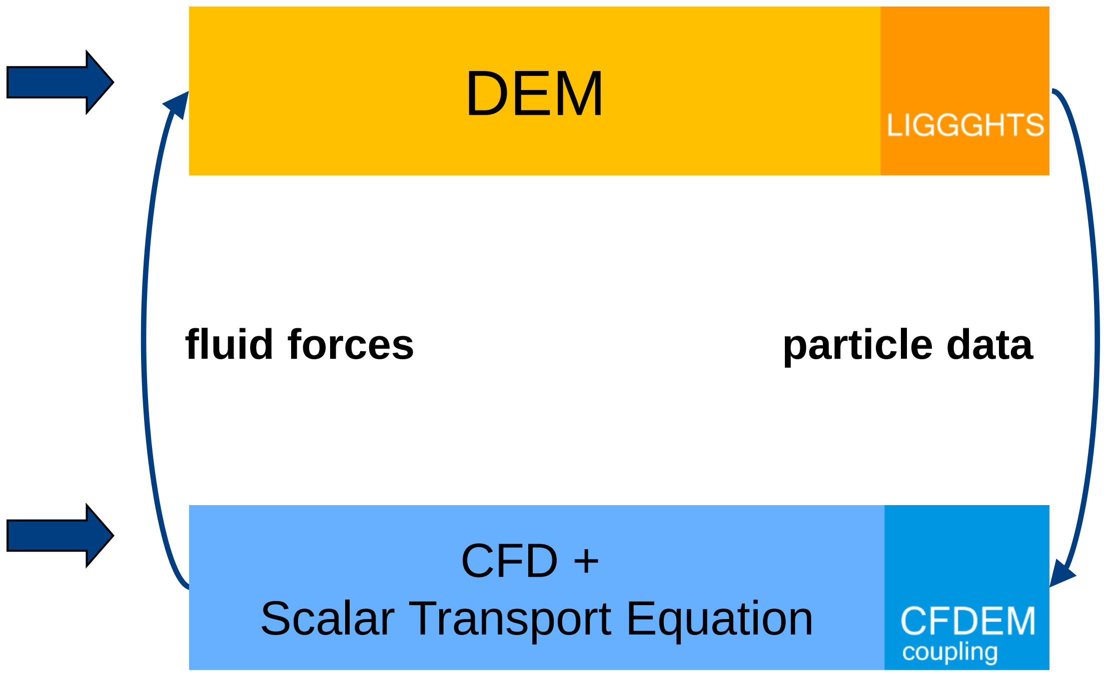
Real Problem — multiple interacting phases

Model — multiple coupled solvers

Granular Flow

Fluid Flow

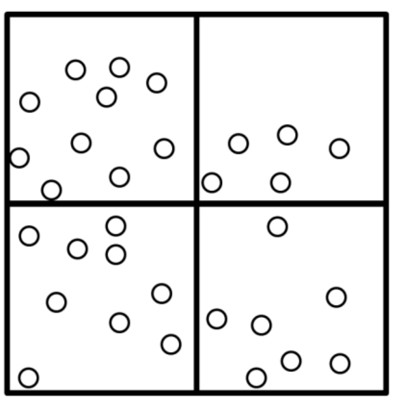
Scalar Transport Eqn.
(e.g. Dust/HeatTransfer)



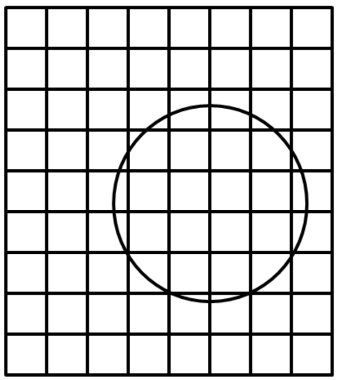
Fluid-particle interaction

Computational Fluid Dynamics (CFD)

Discrete Element Method (DEM)



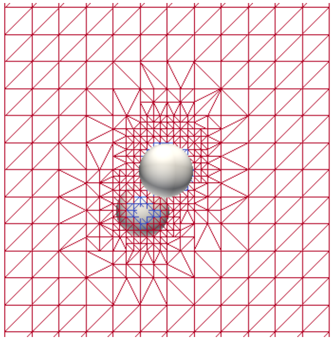
- unresolved CFD-DEM
- **resolved CFD-DEM**

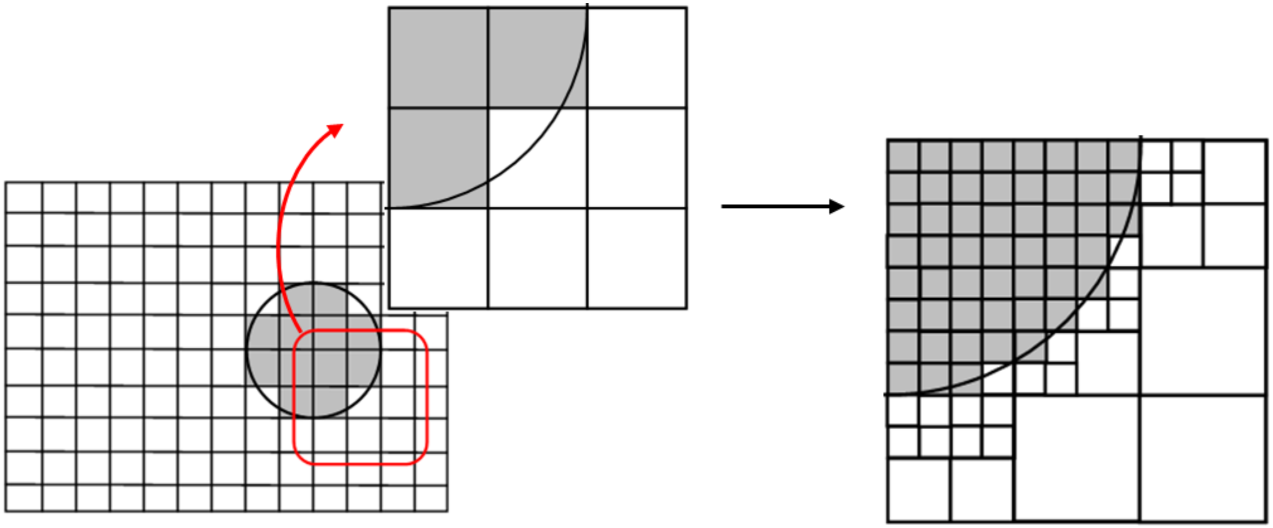


Resolved CFD-DEM

Resolved CFD-DEM

- Dynamic local mesh refinement:
  - The overall mesh is as coarse as the flow problem permits
  - The mesh in the particle-covered area is refined
- Implemented in OpenFOAM®





Local mesh refinement in the area of the particle

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Resolved CFD-DEM

- **Rotating body**

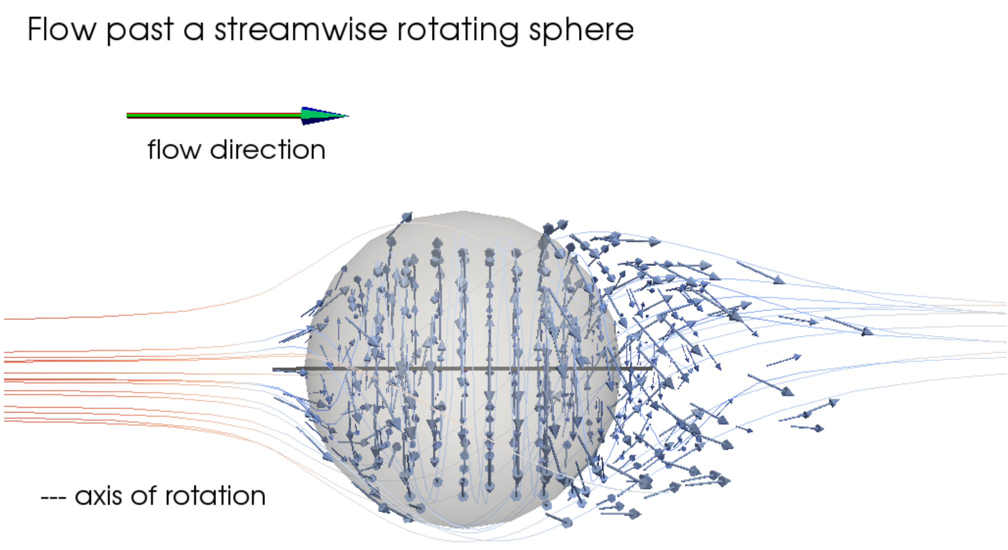
$$u = U + \omega \times r$$

u … particle velocity

U … translational velocity

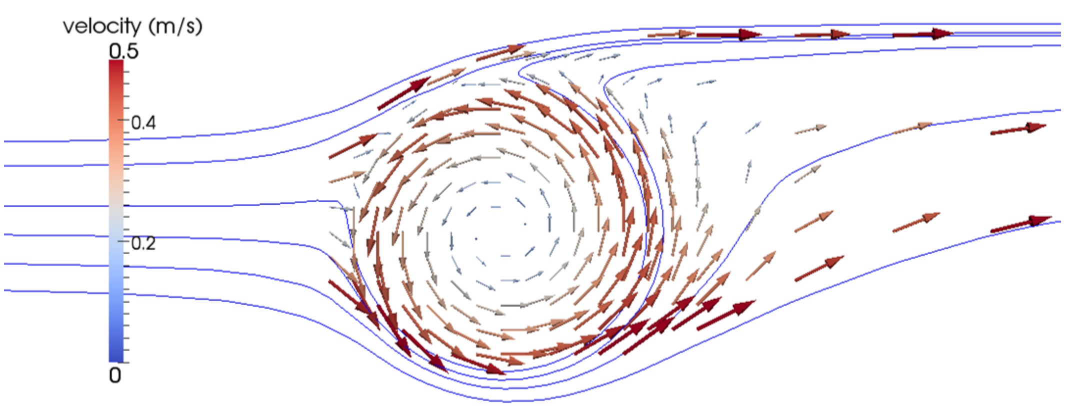
r … positon vector wrt. body center

ω … angular velocity



Rotating sphere

Re = 100
omega = 2 (<=> S_Pa = 1)



→ incorporation of the rotational component

Unresolved CFD-DEM

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Discrete Modelling of Fluid-Particle Systems

Discrete Modeling of fluid particle systems comes in different flavors…

- CFD-DEM[1,2]
- coarse grained CFD-DEM [3]

Topic of this talk

- CFD-DDPM[4]
- MP-PIC[5,6]

1) Goniva, C., Kloss, C., Deen, N.G., Kuipers, J.A.M. and Pirker, S. (2012): "Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations", Particuology, DOI 10.1016/j.partic.2012.05.002

2) Z.Y. Zhou, S.B. Kuang, K.W. Chu and A.B. Yu (2010) : "Discrete particle simulation of particle-fluid flow: Model formulations and their applicability", Journal of Fluid Mechanics 661, 482-510.

3) Radl S., Radeke, Ch., Khinast, J., Sundaresan, S. (2011) : "Parcel-Based Approach for the Simulation of Gas-Particle Flows" , Proc. CFD 2011 Conference, Trondheim, Norway

4) Fluent® Manual

5) Andrews, M.J., O'Rourke, P.J. (1996): "The multi-phase particle-n-cell (MP-PIC) method for dense particle flow", Int. J. Multiphase Flow, 22, 379-402

6) Benyahia, S., Sundaresan, S. (2012): "Do we need sub-grid corrections for both continuum and discrete gas-particle flow models", Powder Technology, 220, 2-6

Latest Development of CFDEMcoupling

Discrete Modelling of Fluid-Particle Systems

Theoretical background – coarse grained CFD-DEM:

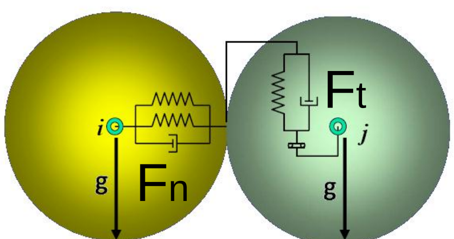
Navier-Stokes equations for the fluid in presence of a granular phase

$$\frac{\partial \alpha_f \rho_f}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \mathbf{u_f} \right) = 0$$

$$\frac{\partial \left(\alpha_f \rho_f \mathbf{u_f} \right)}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \mathbf{u_f} \mathbf{u_f} \right) = -\alpha_f \nabla p + \nabla \cdot \left(\alpha_f \boldsymbol{\tau} \right) + \alpha_f \rho_f \mathbf{g} - \mathrm{K_{fs}} \left(\mathbf{u_f} - \mathbf{u_s} \right)$$

Lagrangian Particle Trajectory for Parcels

$$\frac{\partial^2 \mathbf{x}_p}{\partial t^2} = \frac{\mathbf{F}_n}{m_p} + \frac{\mathbf{F}_t}{m_p} + \mathbf{g} + \frac{\beta}{\rho_p \alpha_p} \left(\mathbf{u}_f - \mathbf{u}_p \right) - \frac{1}{\rho_p} \nabla p$$



soft-sphere contact model:
linear spring-dashpot

Scaling laws from dimensional analysis

$$\Pi_1 = l, \Pi_2 = \frac{k_n}{R_i \cdot \rho_p \cdot v_0^2}, \Pi_3 = \frac{c_n}{R_i^2 \cdot \rho_p \cdot v_0}$$

- l: size ratio of colliding particles, k_n: stiffness, R: radius, ρ: density, v_0: reference velocity
- Density, coefficient of friction, coefficient of rolling friction stay same
- k_n/R must stay constant → scale stiffness with radius
- scaling of particle drag
- Equations converge to particle equation for parcel = particle

Validation of CFD-DEM approach

applied to spout fluidized beds

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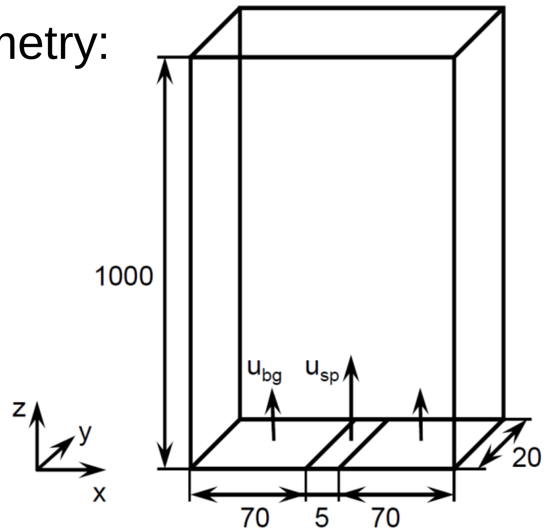
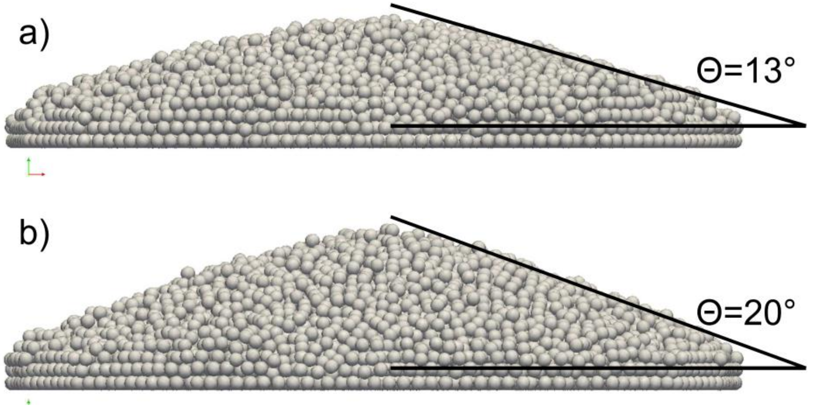
single spout fluidized bed

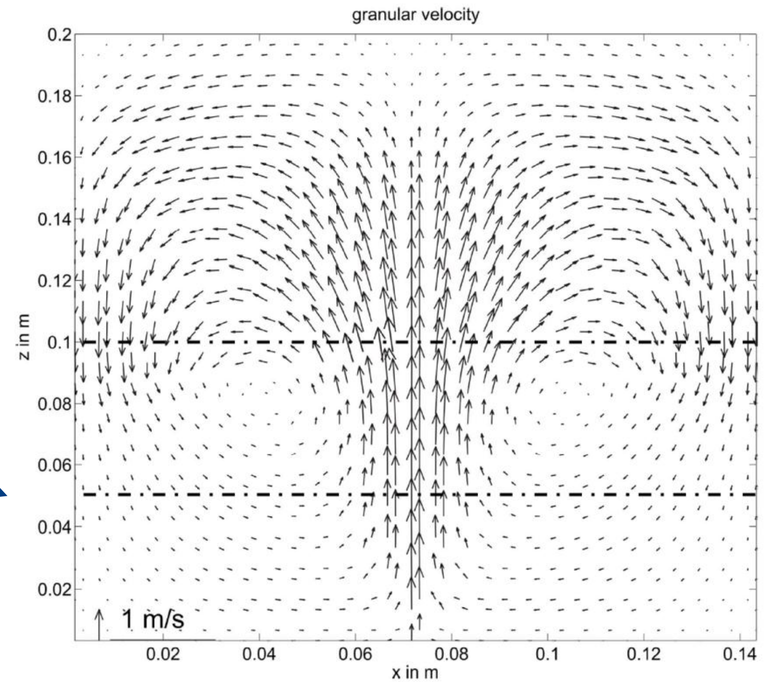
Geometry:



Variation of Rolling friction:



Measurement positions



Goniva, C., Kloss, C., Deen, N.G., Kuipers, J.A.M. and Pirker, S. (**2012**): "**Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations**", Particuology, DOI 10.1016/j.partic.2012.05.002

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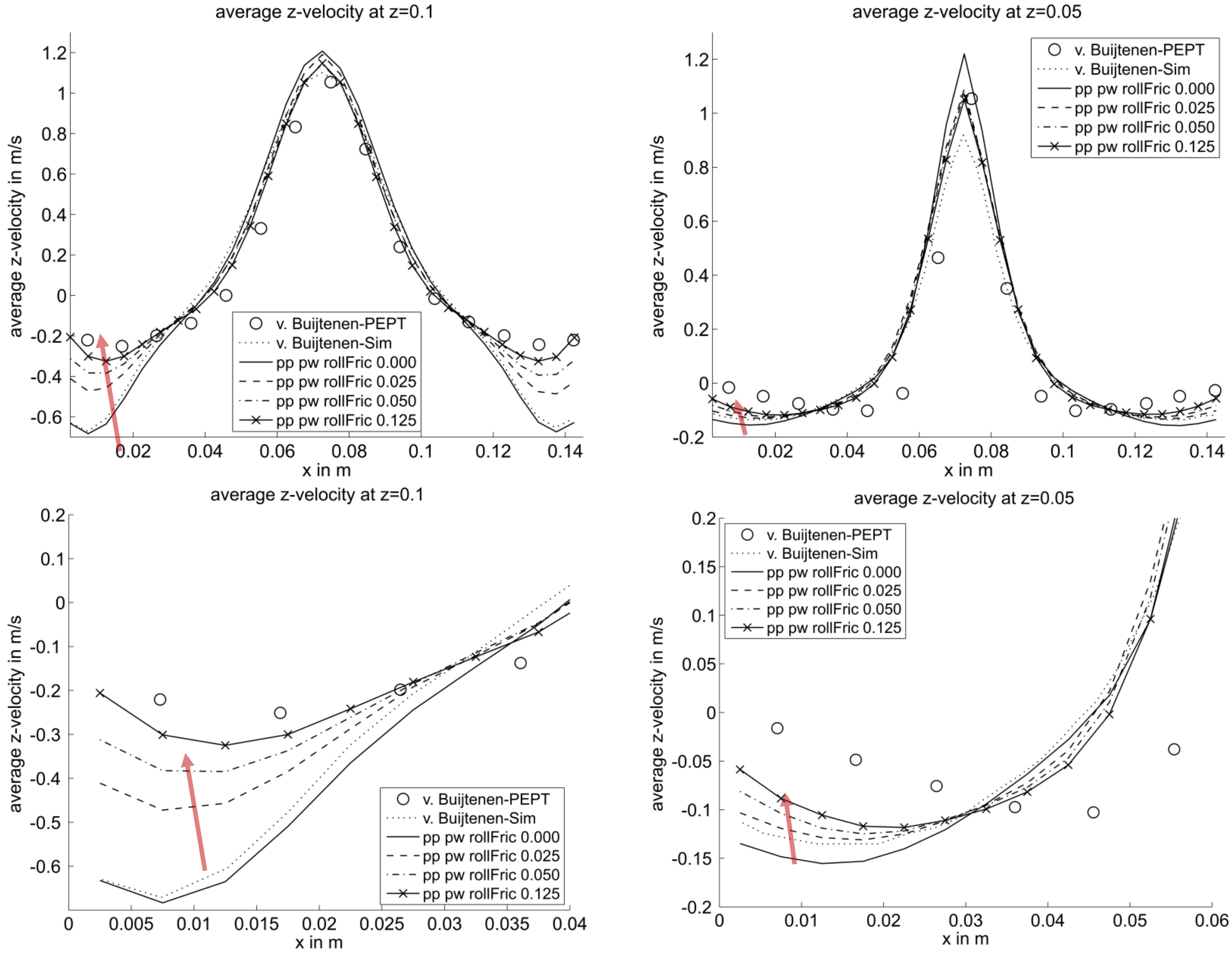
single spout fluidized bed

Variation:
Particle-Particle
+
Particle-Wall
Rolling Friction

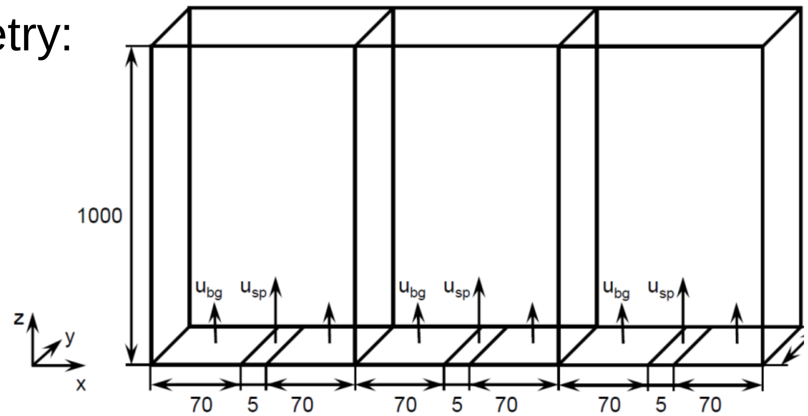
Strong dependency on rolling friction!



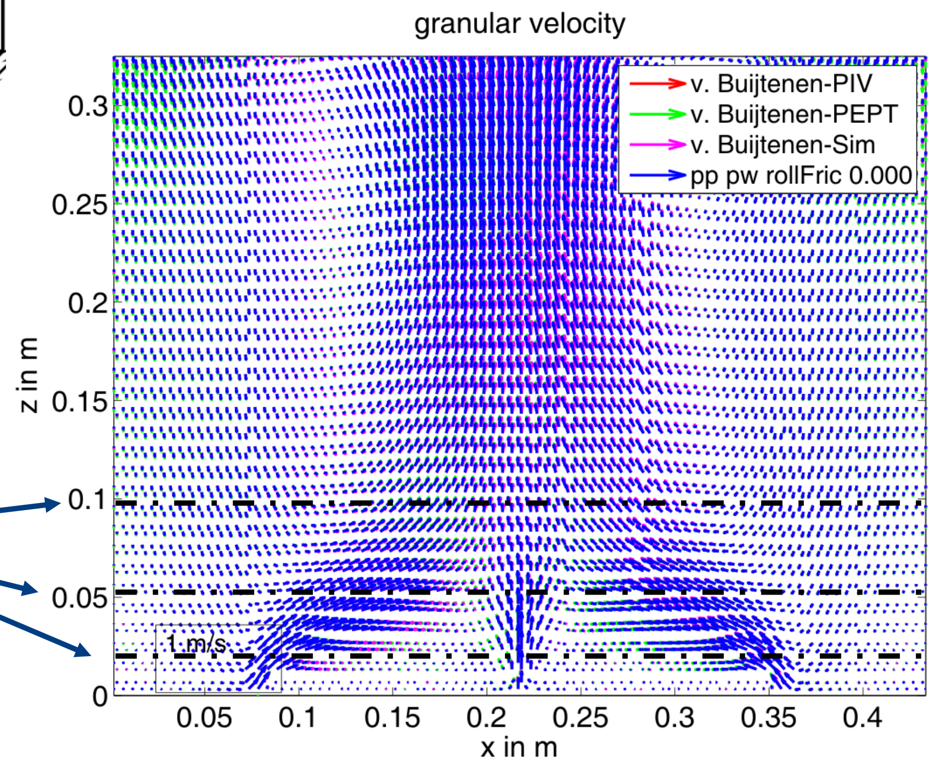
Latest Development of CFDEMcoupling

triple spout fluidized bed

Geometry:

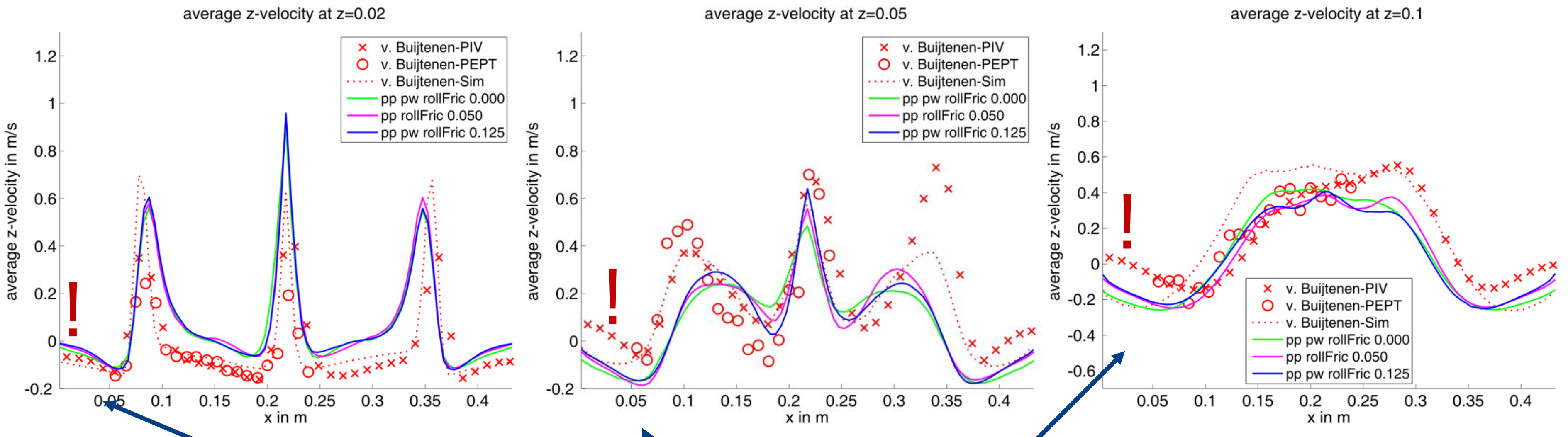


Measurement positions



Latest Development of CFDEMcoupling
triple spout fluidized bed

<u>Variation:</u>
Particle-Particle, Particle-Wall Rolling Friction



Weak dependency on rolling friction!

Validation of parcel approach

applied to spout and bubbling beds

Latest Development of CFDEMcoupling

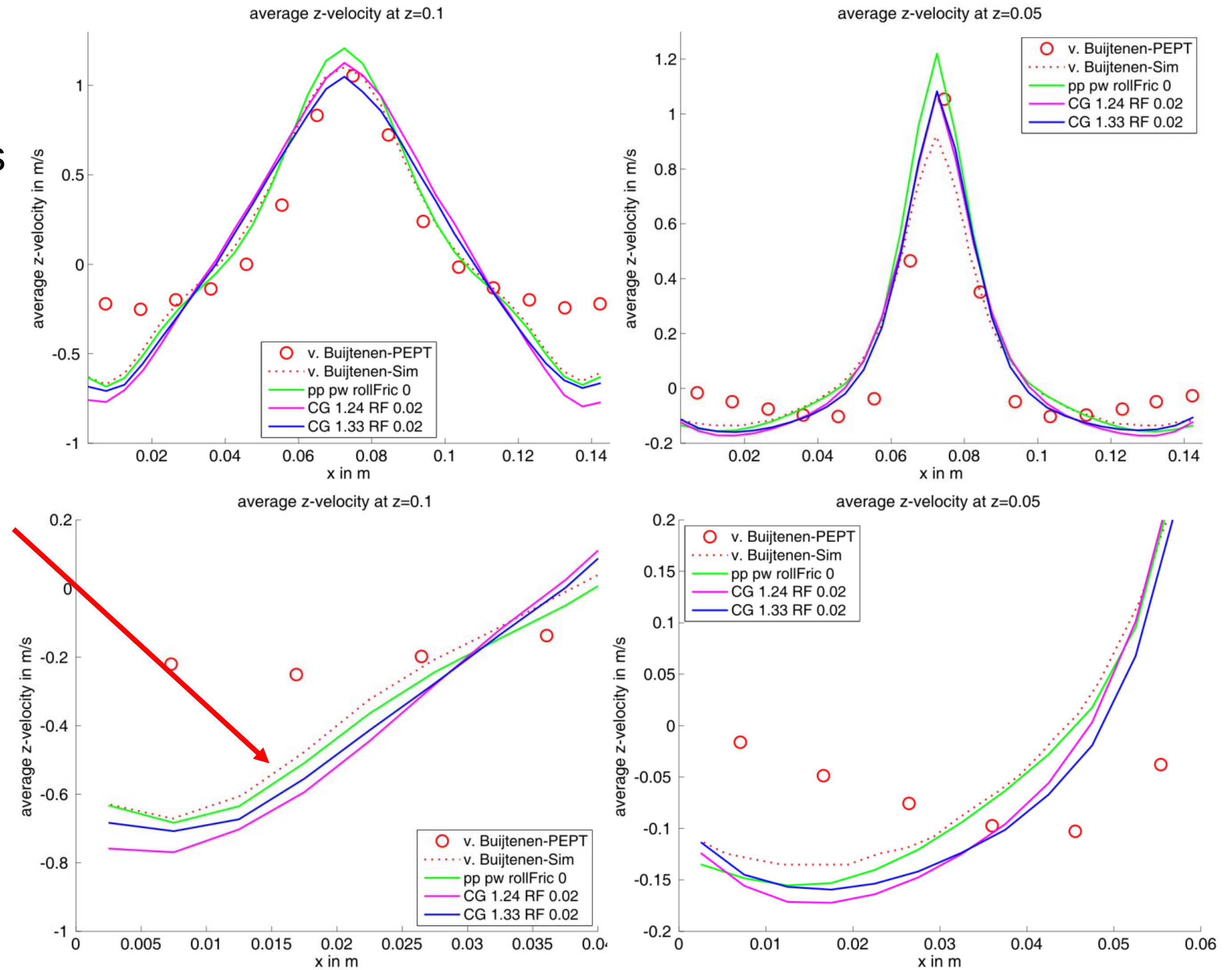
single spout fluidized bed – coarse grained

Variation:

Coarse Graining

1	12000 particles
1.24	6348 **parcels**
1.33	5062 **parcels**

Result is **independent** of coarse graining!!!



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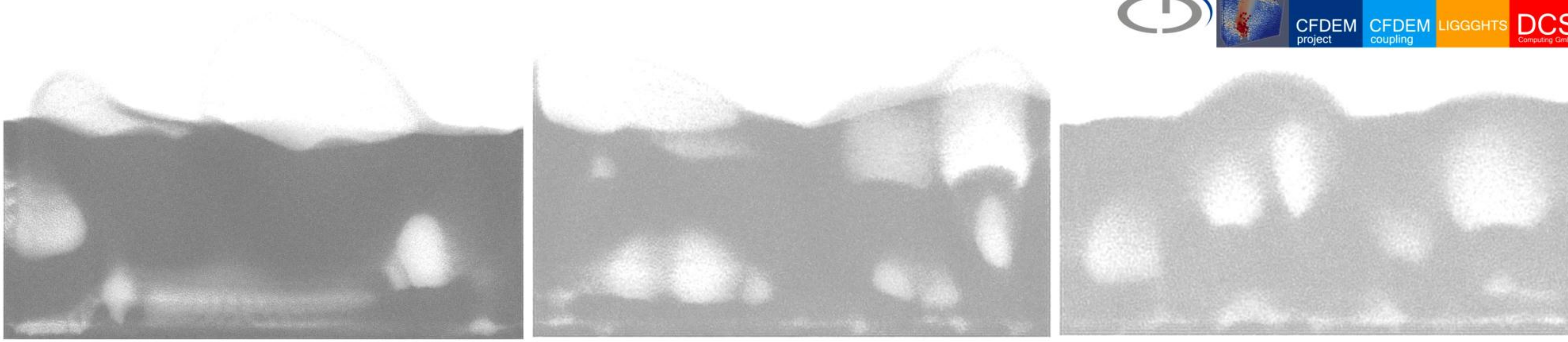
Bubbling Bed – coarse grained

Usf = 0.6077 m/s, dp=0.5mm, nParticles=1.4e6



coarse graining = 1, nParcels=1.4e6 ,

coarse graining = 1.5, nParcels=427.820 ,

coarse graining = 2, nParcels=180.490

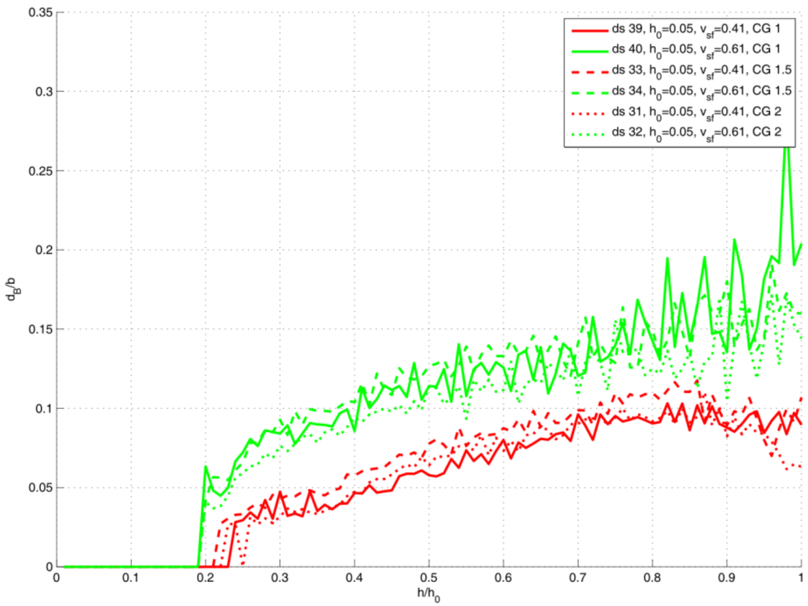
Latest Development of CFDEMcoupling
Bubbling Bed – coarse grained

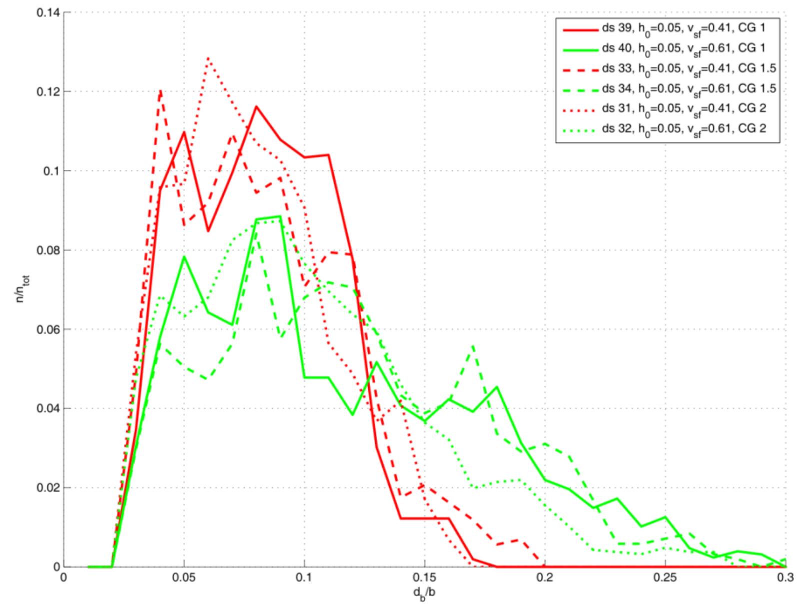
CFDEM project

<u>Comparison of simulations:</u>

Left: bubble diameter for different coarse graining levels and velocities

Right: number of bubbles for different coarse graining levels and velocities





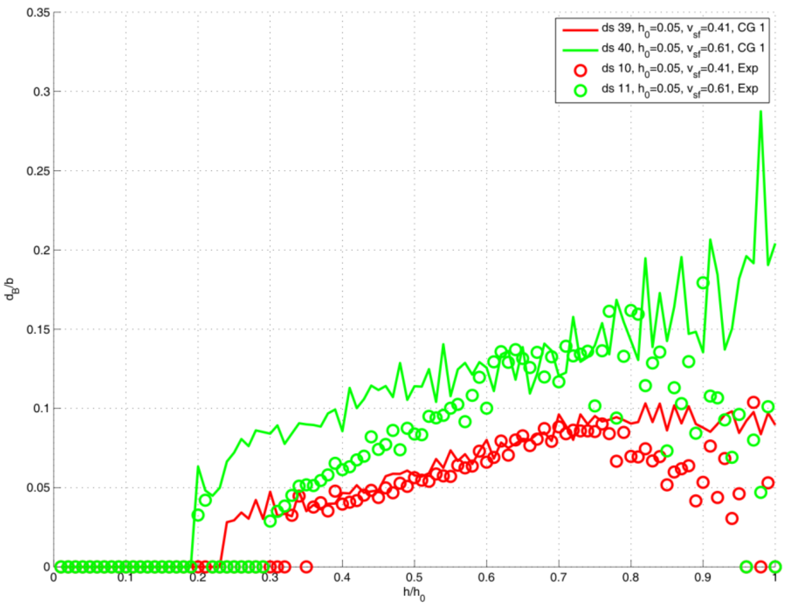
Latest Development of CFDEMcoupling
Bubbling Bed – coarse grained

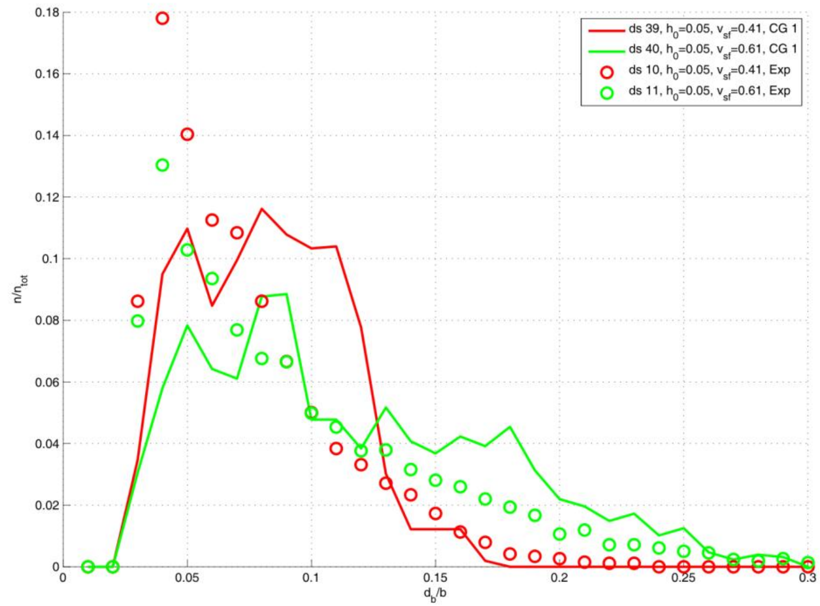
CFDEM project

Simulations vs Experiment:

Left: bubble diameter for different coarse graining levels and velocities

Right: number of bubbles for different coarse graining levels and velocities





Handling Non-Sphericity
multisphere method

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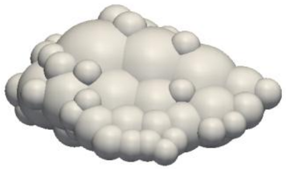
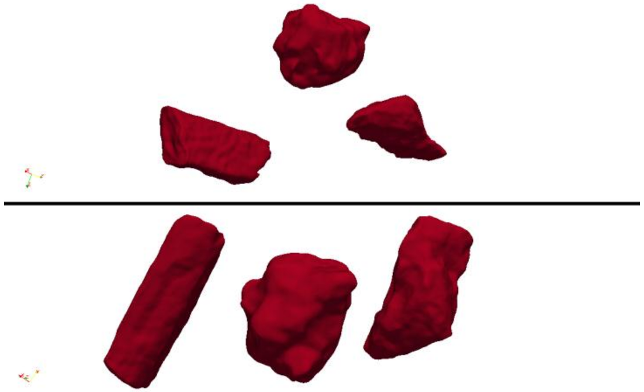
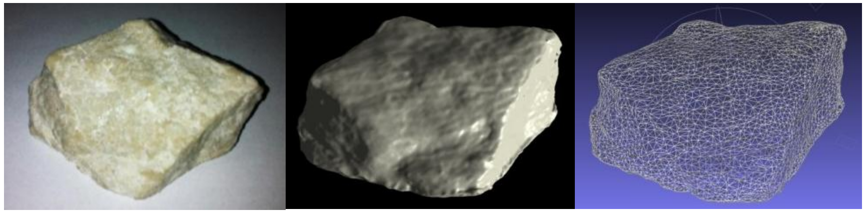
Non-Sphericity and LIGGGHTS

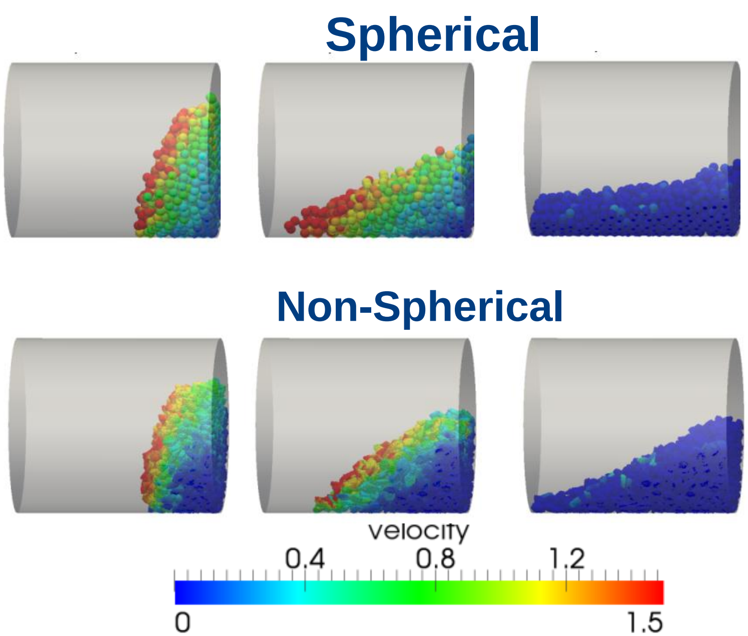
Obviously…

 ≠  ≈ 

Our Approach:
Get closer to real world







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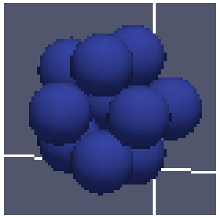
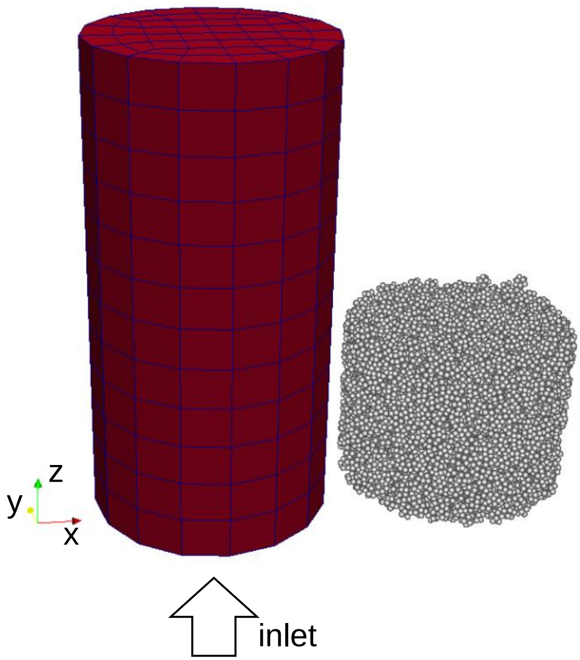
Multisphere validation example

Ergun pressure drop of (multi) sphere particle bed

Property	Dimension	Size
x-dimension of domain	[m]	-0.0138 : -0.0138
y-dimension of domain	[m]	-0.0138 : -0.0138
z-dimension of domain	[m]	0 : 0.0553
gravity vector	[m/s2]	(0,0,-9.81)
Particles per clump	[-]	10
# clumps	[-]	2500
Particle diameter	[m]	0.7061 e-3
Clump diameter	[m]	2 e-3
Particle density	[kg/m3]	1000
Clump density	[kg/m3]	440
Fluid density	[kg/m3]	5
Inlet velocity	[m/s]	0:0.2

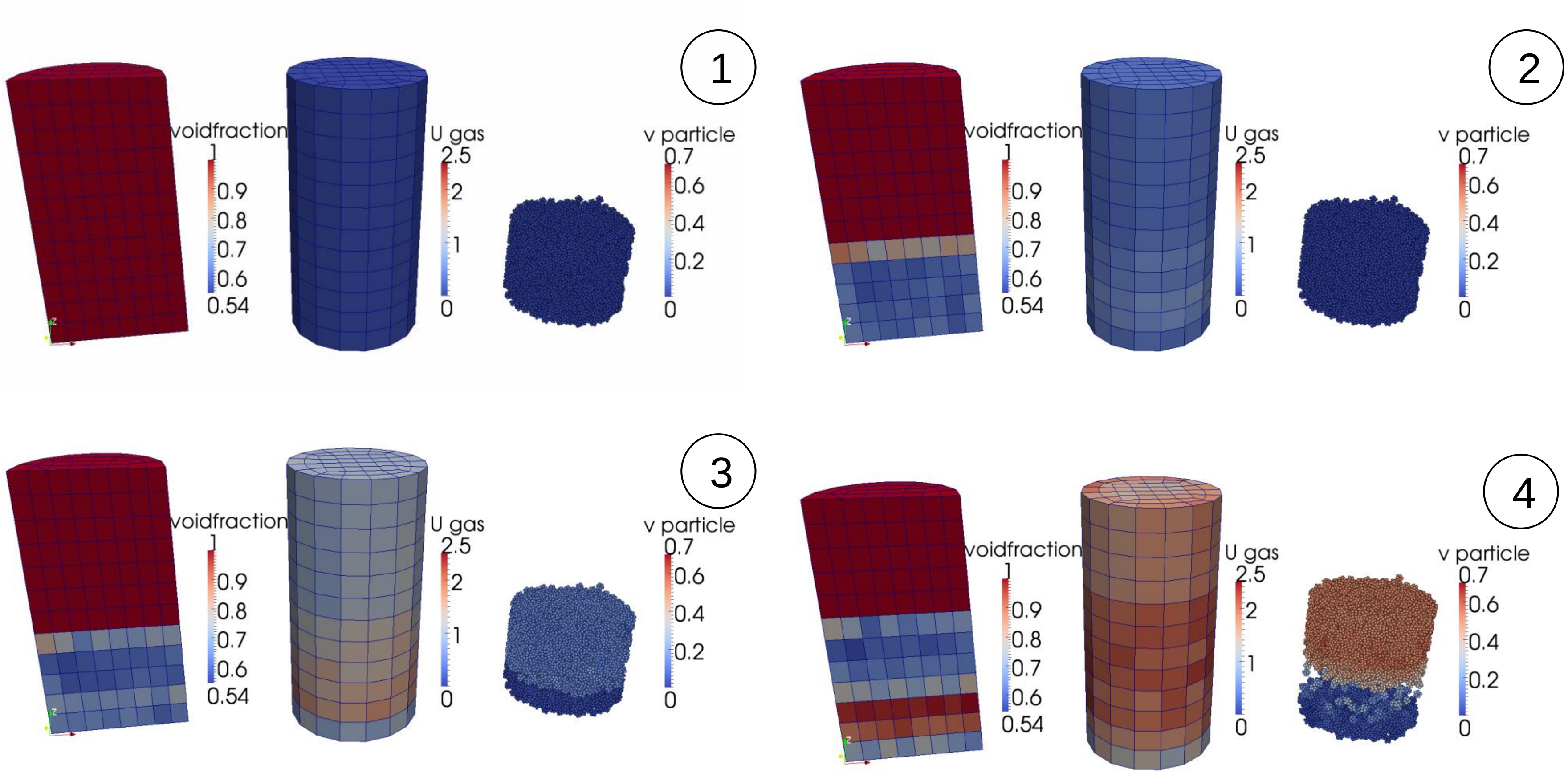




Multisphere validation example

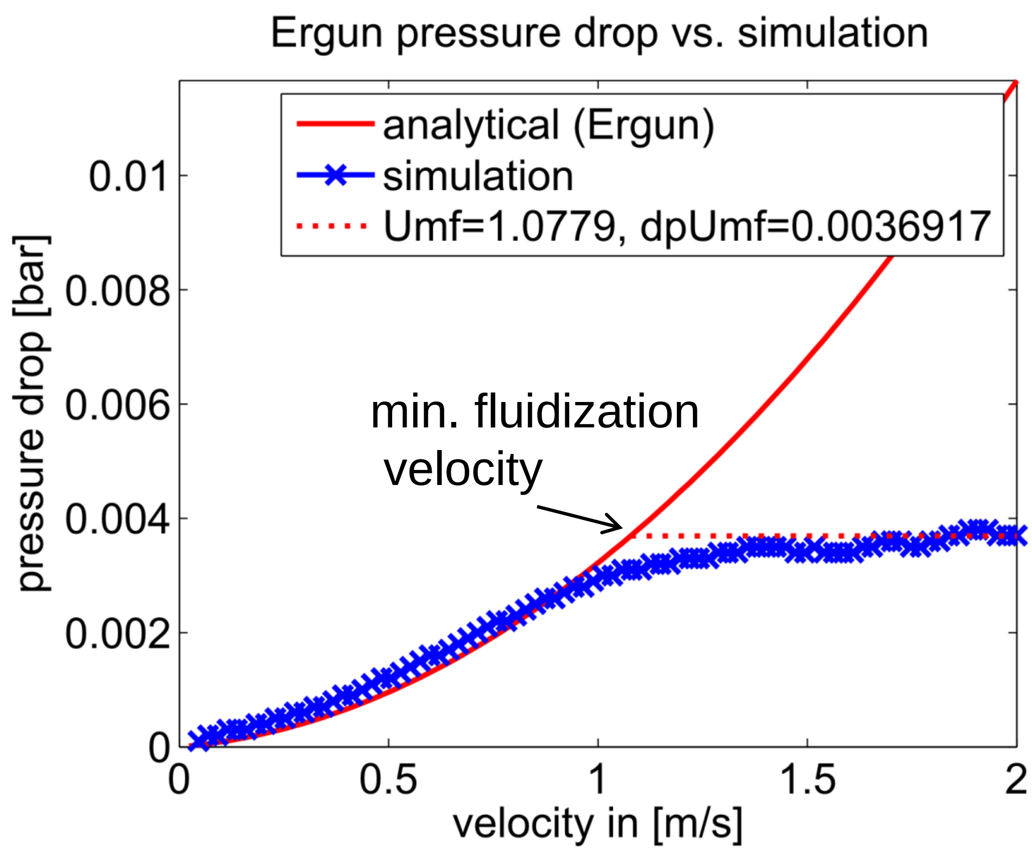
Ergun pressure drop of (multi) sphere particle bed

animation



Multisphere validation example

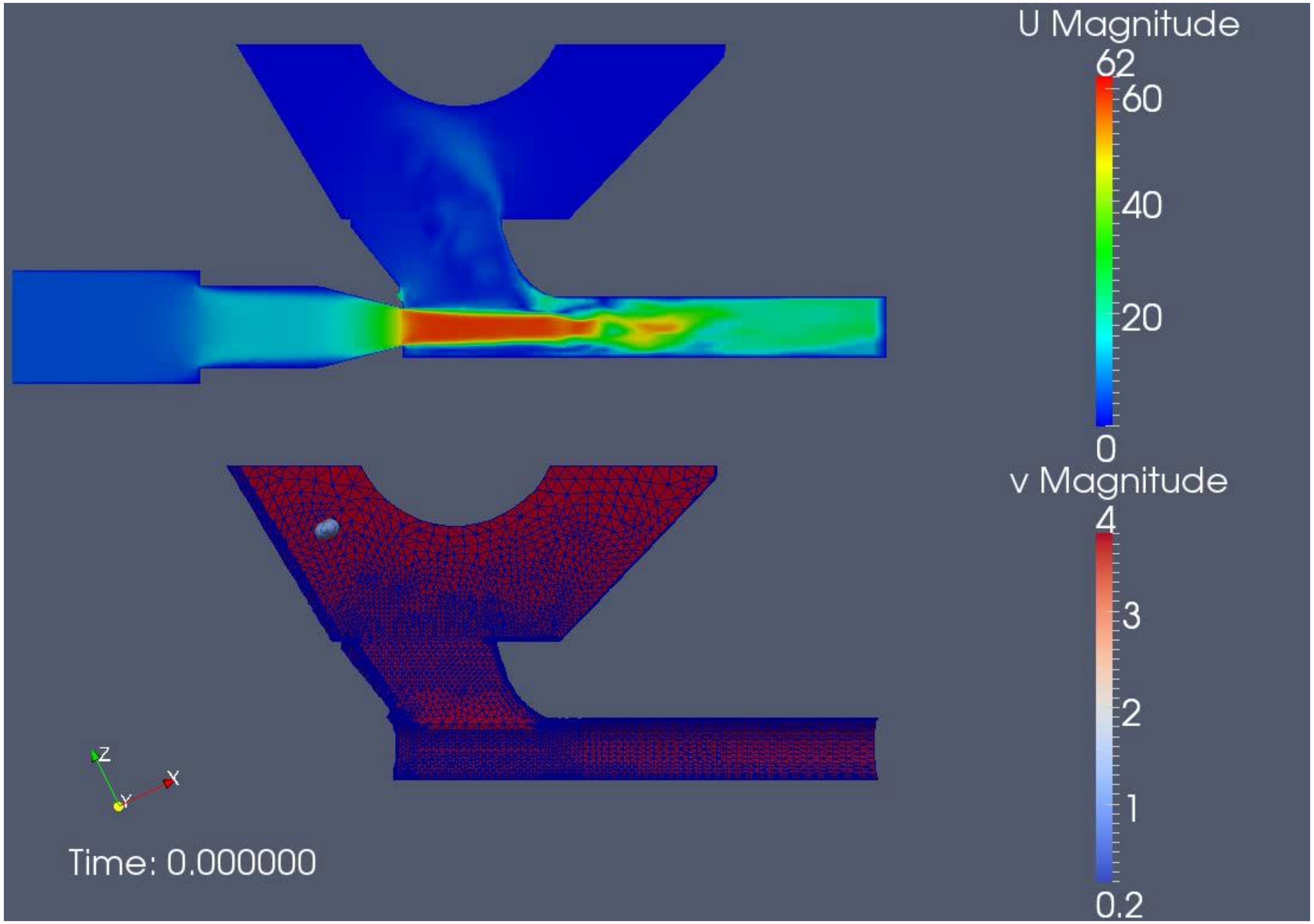
Ergun pressure drop of (multi) sphere particle bed



Latest Development of CFDEMcoupling
Particle Injector

- best case: particles are smoothely given into gas stream
- Note:Upward disturbance due to particles!

Best Case

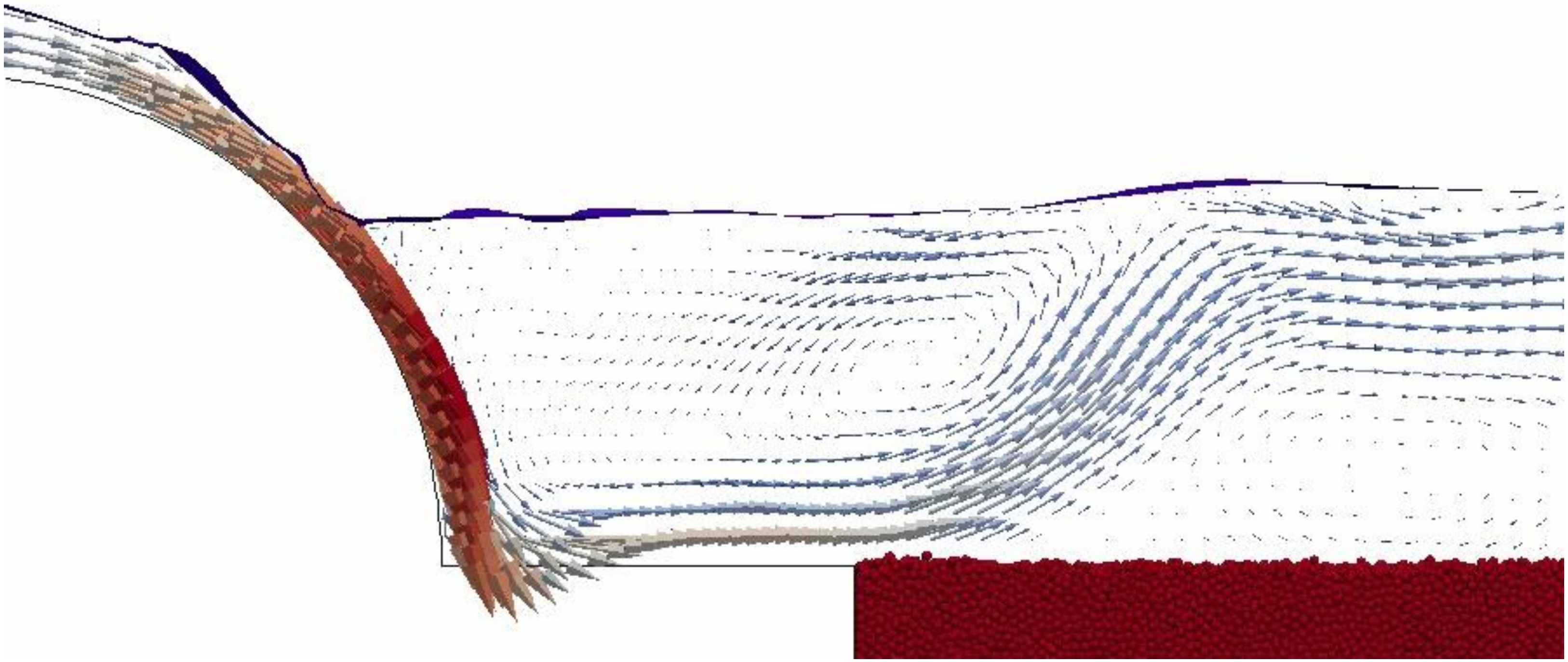


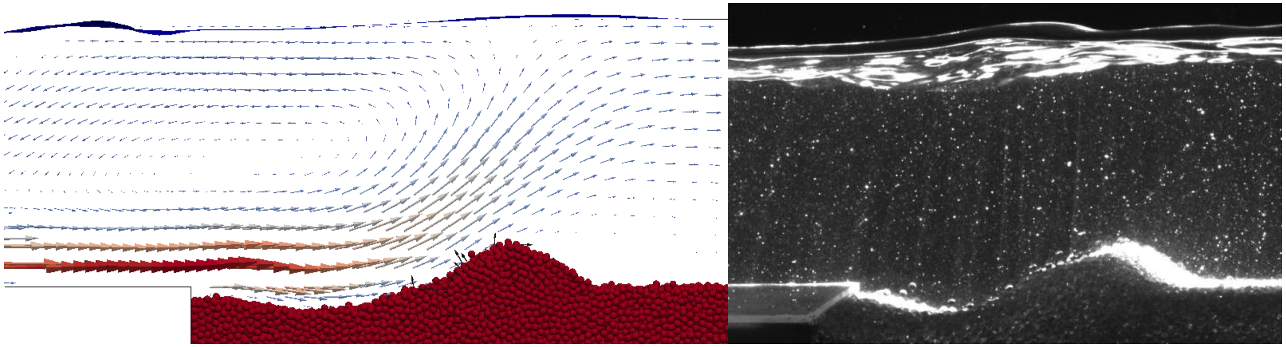
Towards Environmental Flow

river erosion behind a weir

Latest Development of CFDEMcoupling

Scour development

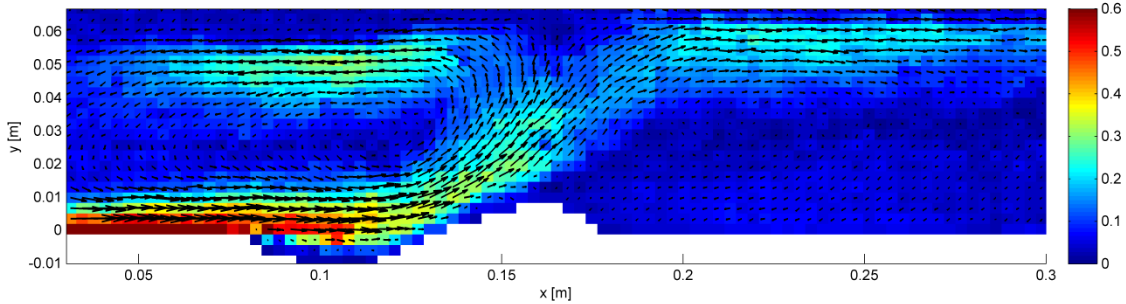




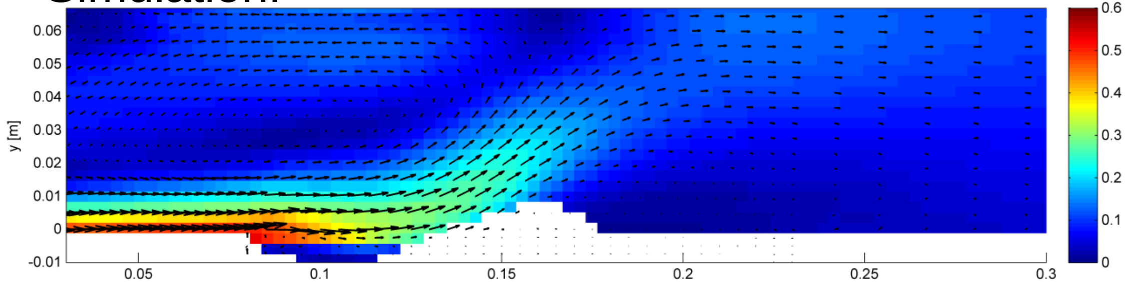
Latest Development of CFDEMcoupling

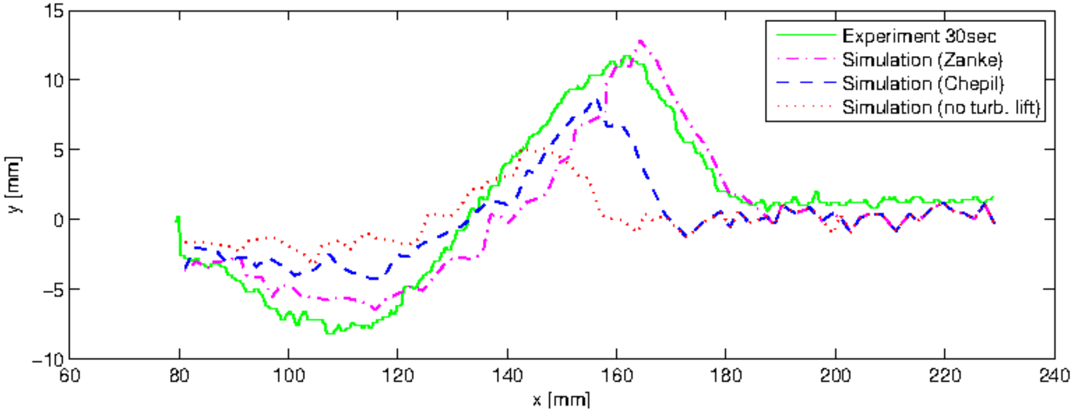
Scour development

Measurement:



Simulation:





Velocity profile

- recirculation mass flow is under predicted
- generally good results

Erosion profile [m/s]

- turbulent lift force
- best performance with a model based on Zanke

Towards Multi-Physics

flotation modelling

joint work with Aalto University

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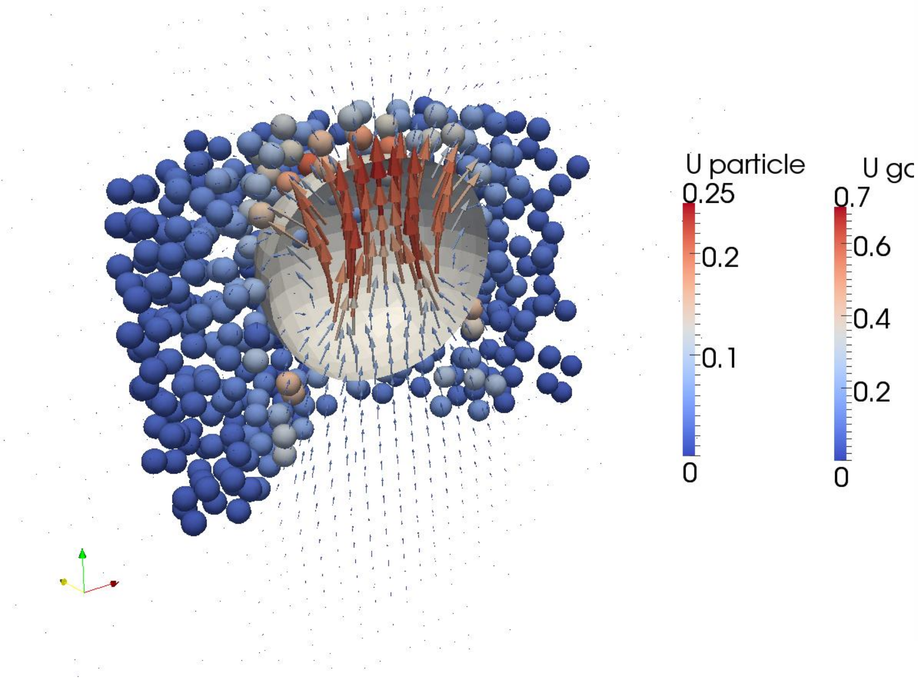
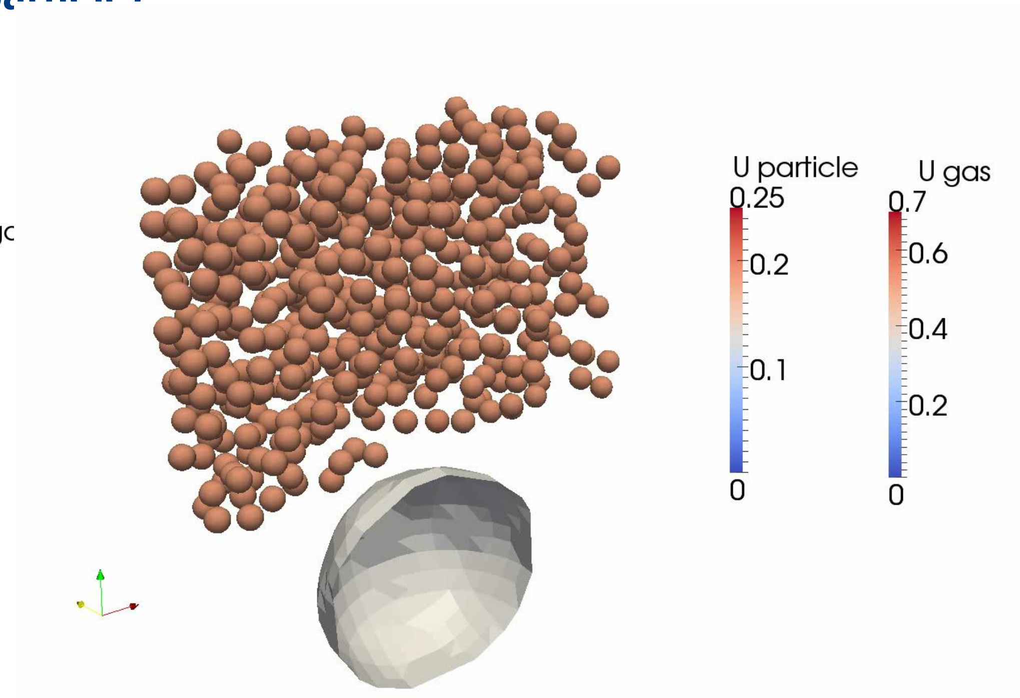
Spray Particle Interaction

Three Phase Interaction Model (fluid+gas+particle):





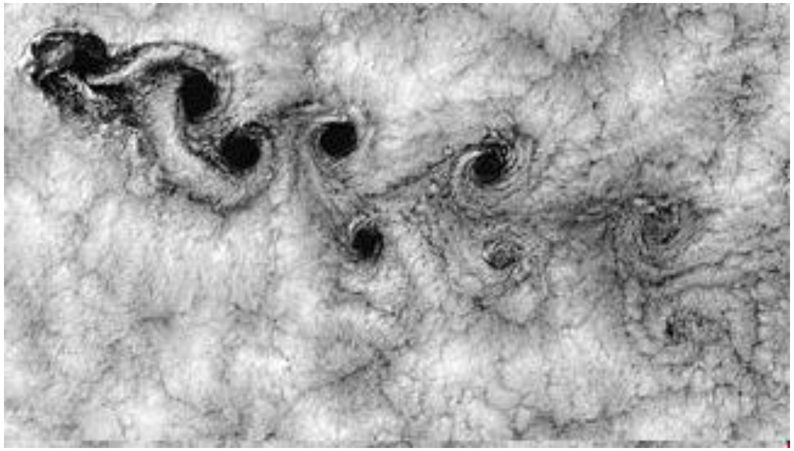
See PhD thesis of Dr. Wierink at www.cfdem.com

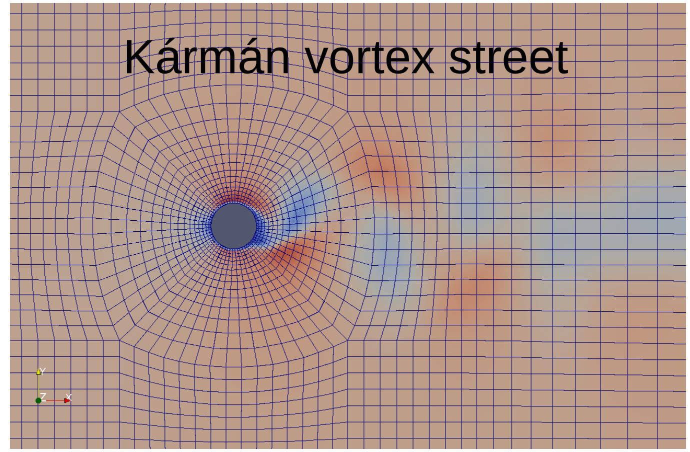
Towards Turbulence Interaction

Particles in von Karman Vortex street

Latest Development of CFDEMcoupling

Particles in von Karman Vortex street





Von Kármán vortex street off the Chilean coast near the Juan Fernandez Islands. (Wikipedia)

d = 0.1 m

nu = 1.5e-4 m^2/s

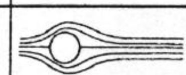
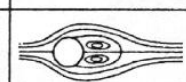
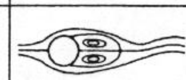
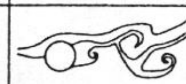
U = 0.5 m/s

Re = U * d / nu = 333

Sr ~ 0.21

Cd ~ 1.2

f = Sr * U / d = 2.1 Hz

Reynolds-Zahl-Bereich	Strömungsbereich	Strömungsform	Strömungs-charakteristik	Strouhal-Zahl Sr	Widerstands-beiwert c_W
$Re \to 0$	schleichende Strömung		stationär. kein Nachlauf	–	siehe Bild 1.12
$3-4 < Re < 30-40$	Wirbelpaar im Nachlauf		stationär. Ablösung symmetrisch	–	$1,59 < c_W < 4,52$ $(Re = 30)$ $(Re = 4)$
$\frac{30}{40} < Re < \frac{80}{90}$	Einsetzen der Kármánschen Wirbelstraße		laminar. Nachlauf instabil	–	$1,17 < c_W < 1,59$ $(Re = 100)$ $(Re = 30)$
$\frac{80}{90} < Re < \frac{150}{300}$	reine Kármánsche Wirbelstraße		Karmansche Wirbelstraße	$0,14 < Sr < 0,21$	
$\frac{150}{300} < Re < \frac{10^5}{1.3 \cdot 10^5}$	unterkritischer Bereich		laminarer Nah-Nachlauf mit Wirbelstraßen-Instabilität	$Sr = 0,21$	$c_W \approx 1,2$

from Schlichting

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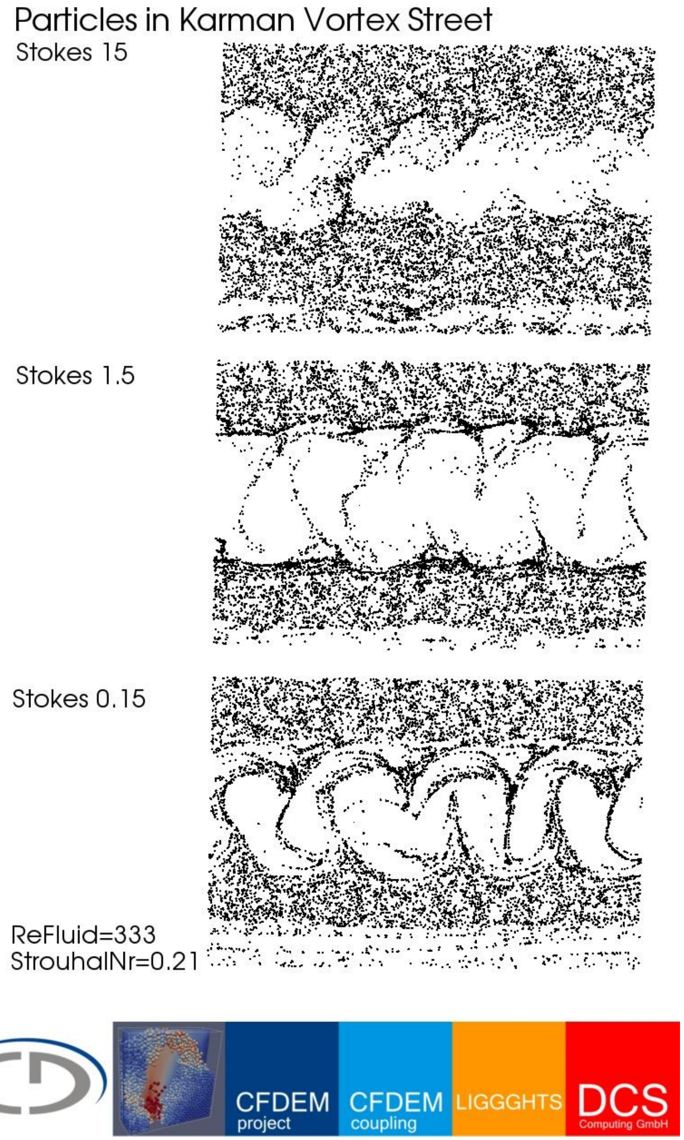
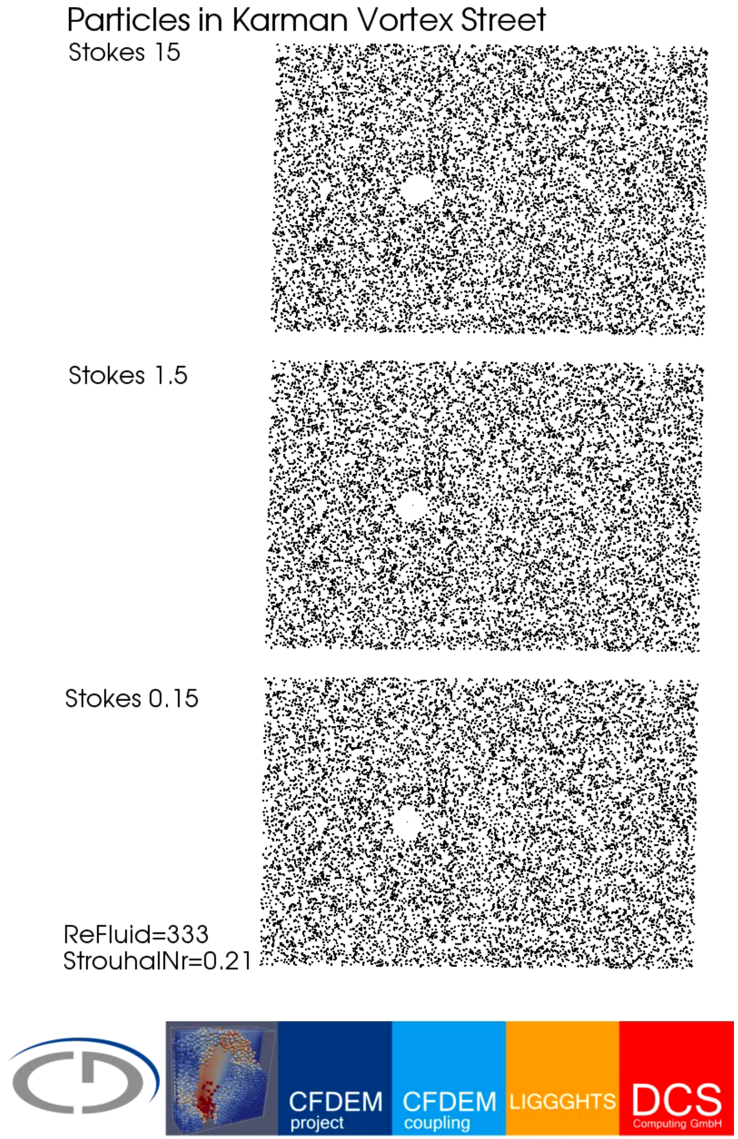
Particles in von Karman Vortex street





Towards Multi-Physics
spray particle interaction

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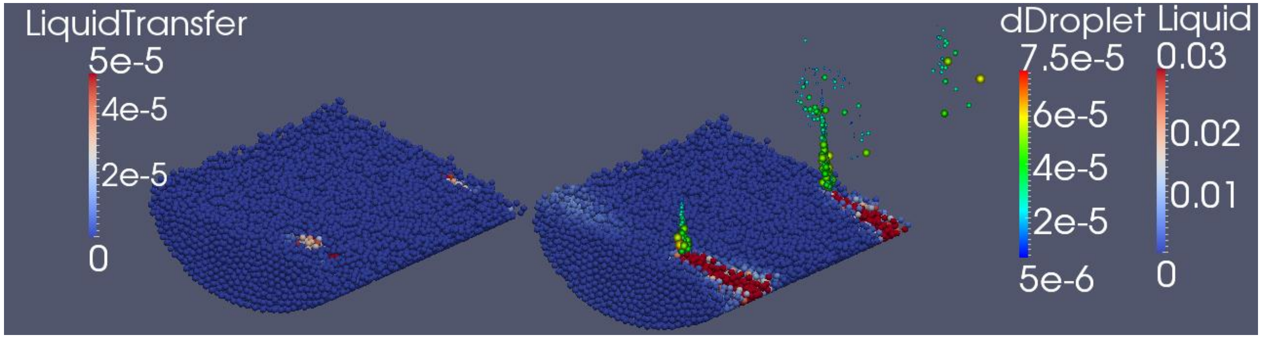
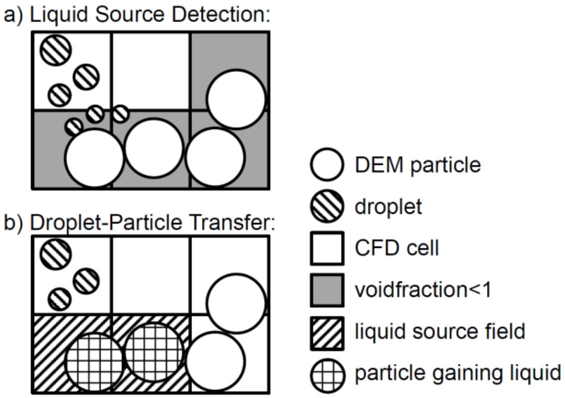
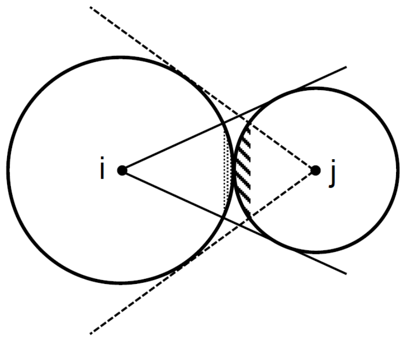
Spray Particle Interaction

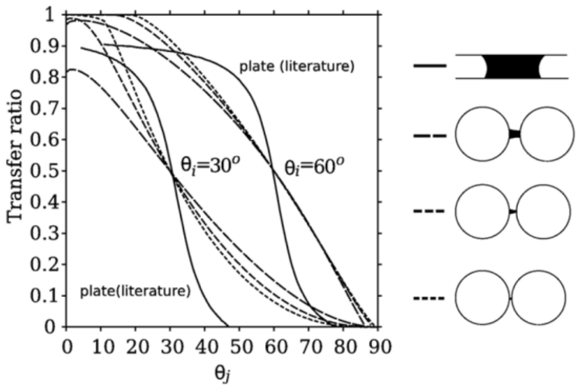
Spray-Particle Liquid transfer Model:

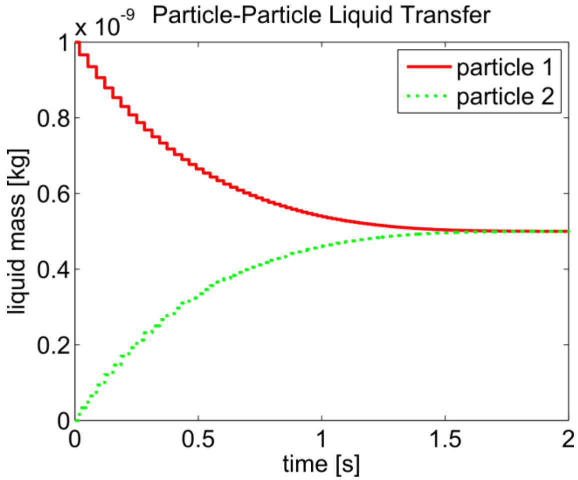




Particle-Particle Liquid transfer Model:







Ch. GONIVA, G. WIERINK, K. HEISKANEN, S. PIRKER & Ch. KLOSS (2012): "MODELLING THREE-PHASE FLOW IN METALLURGICAL PROCESSES", Proc. Int. Conf. on. Computational Fluid Dynamics in the Minerals and Process Industries, Melbourne

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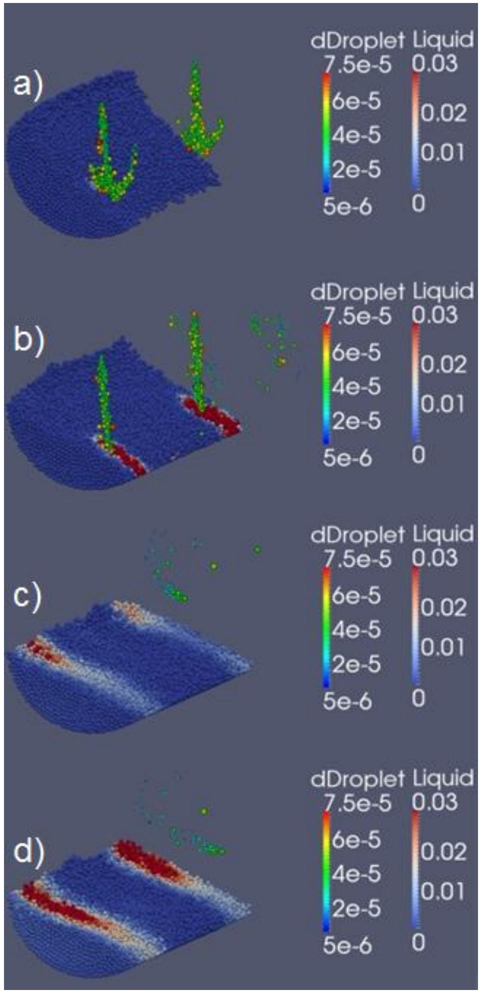
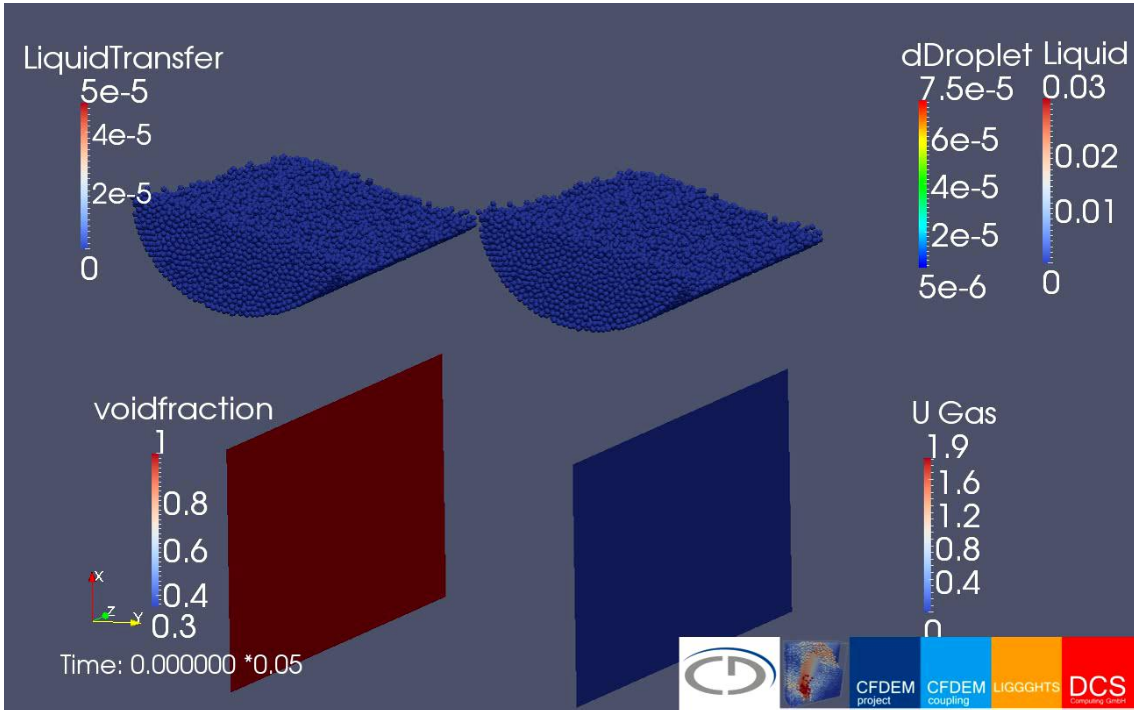
Spray Particle Interaction



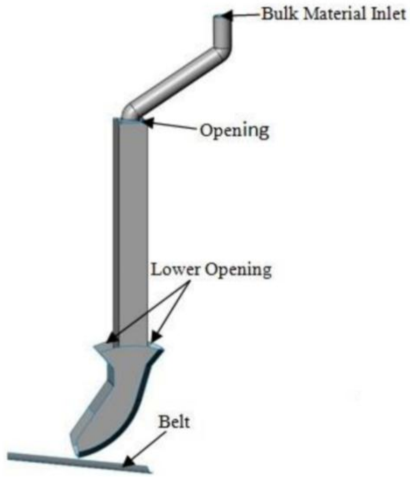


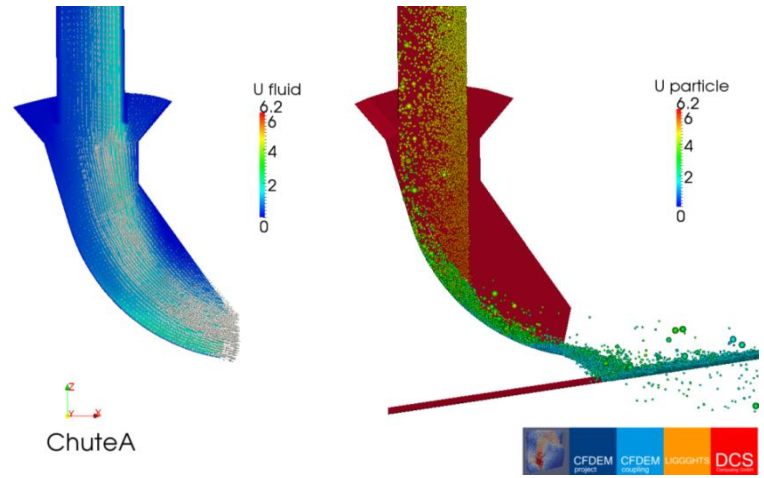
Planned topic for the diploma thesis of Josef Kerbl.

Dust Emission & Propagation

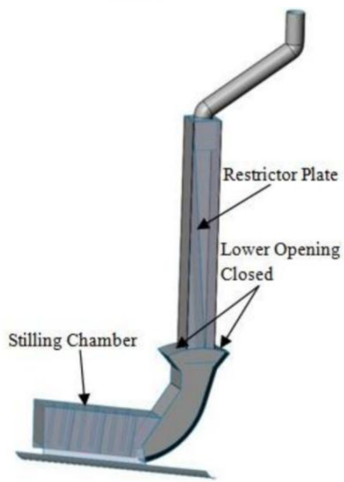
Latest Development of CFDEMcoupling
Dust Emission & Propagation

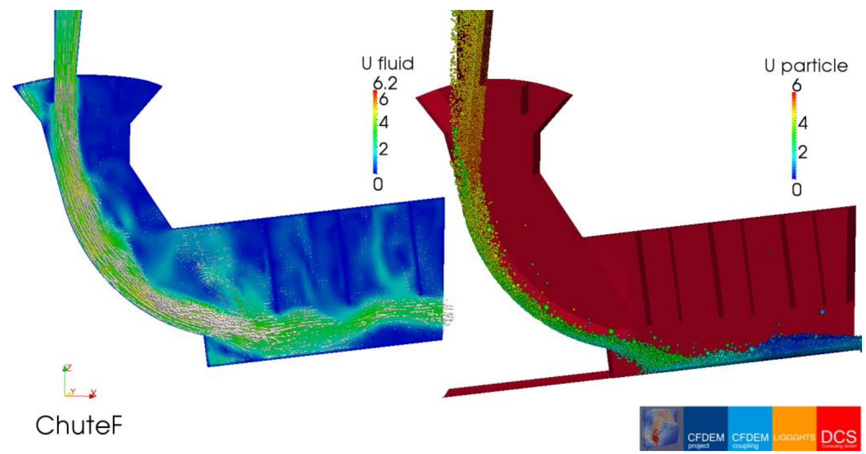
Chute A:





Chute F:





Ch. Goniva, Ch. Kloss, X. Chen, T.J. Donohue, A. Katterfeld (2012): “Prediction of Dust Emissions in Transfer Chutes by Multiphase CFD and Coupled DEM-CFD Simulations”, Proc. Bulk Solids Handling Conference, Berlin

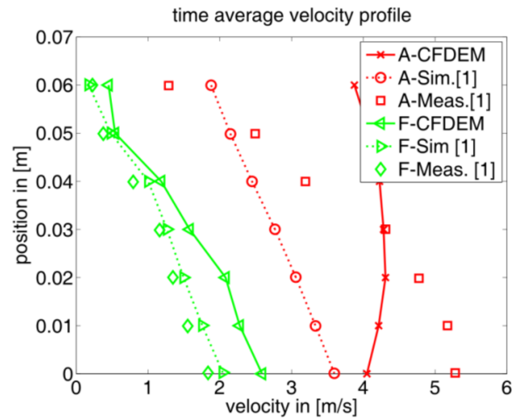
Latest Development of CFDEMcoupling

Dust Emission & Propagation

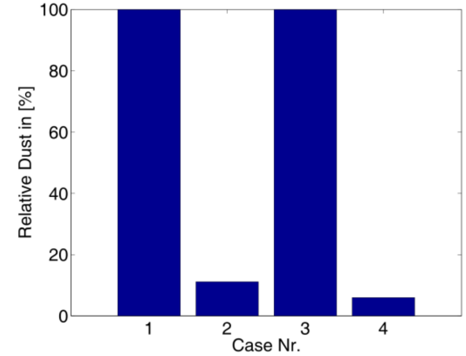
CFDEM project

Validation against measurements:

1: ChuteA CFDEMcoupling,
2: ChuteF CFDEMcoupling,
3: ChuteA measured *,
4: ChuteF measured *

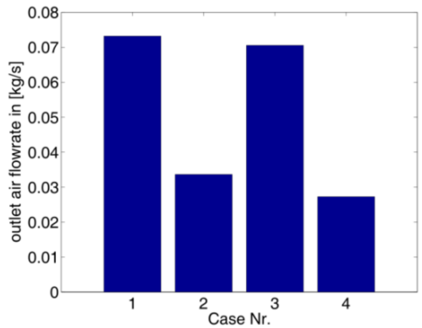


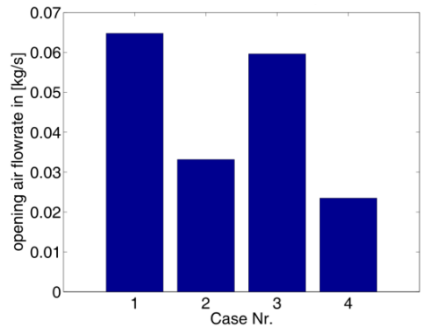
relative dust flux at outlet

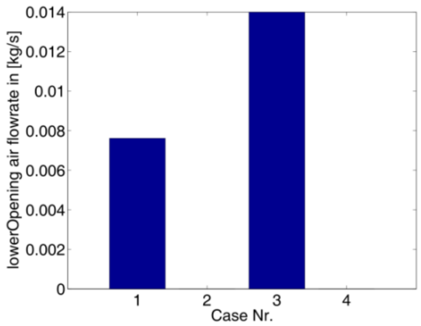


Validation against EuEu Simulations (Newcastle AUS *):

air flowrate at: outlet opening lower opening





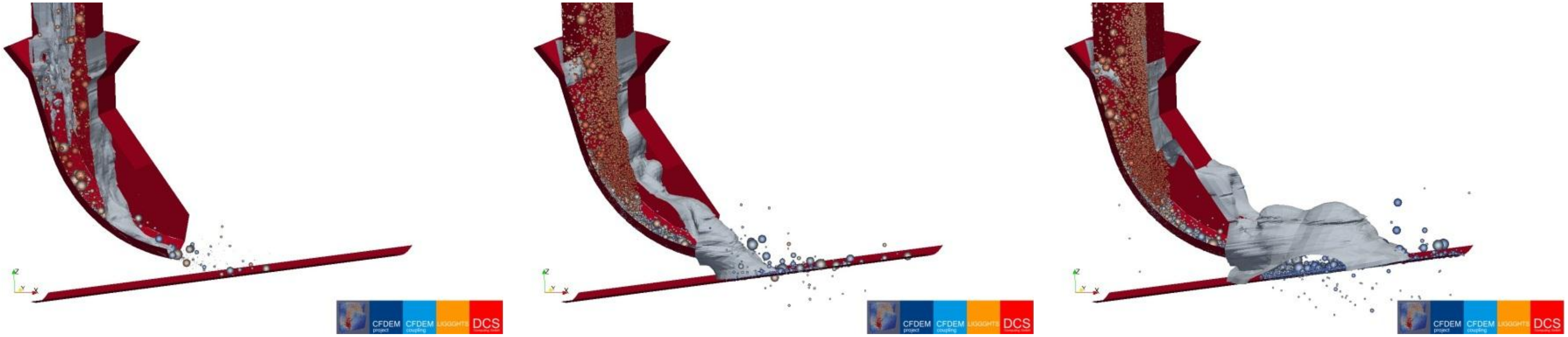


*) Chen, X.L., Wheeler, C.A., Donohue, T.J., McLean, R., Roberts, A.W.: Evaluation of dust emissions from conveyor transfer chutes using experimental and CFD simulation. International Journal of Mineral Processing 110– 111 (2012) pp. 101– 108

Latest Development of CFDEMcoupling

Dust Emission & Propagation

*.stl geometry,
DEM particles,
dust iso-surfaces



Thank you for your attention!
Questions?

www.cfdem.com