Latest Developments in CFDEM®coupling and LIGGGHTS®

„Dedicated to open source high performance scientific computing in fluid mechanics and particle science”

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Outline

Outline

- Share the **latest news** about **CFDEM®project** and **recent developments**

- Share and exchange modelling **ideas**

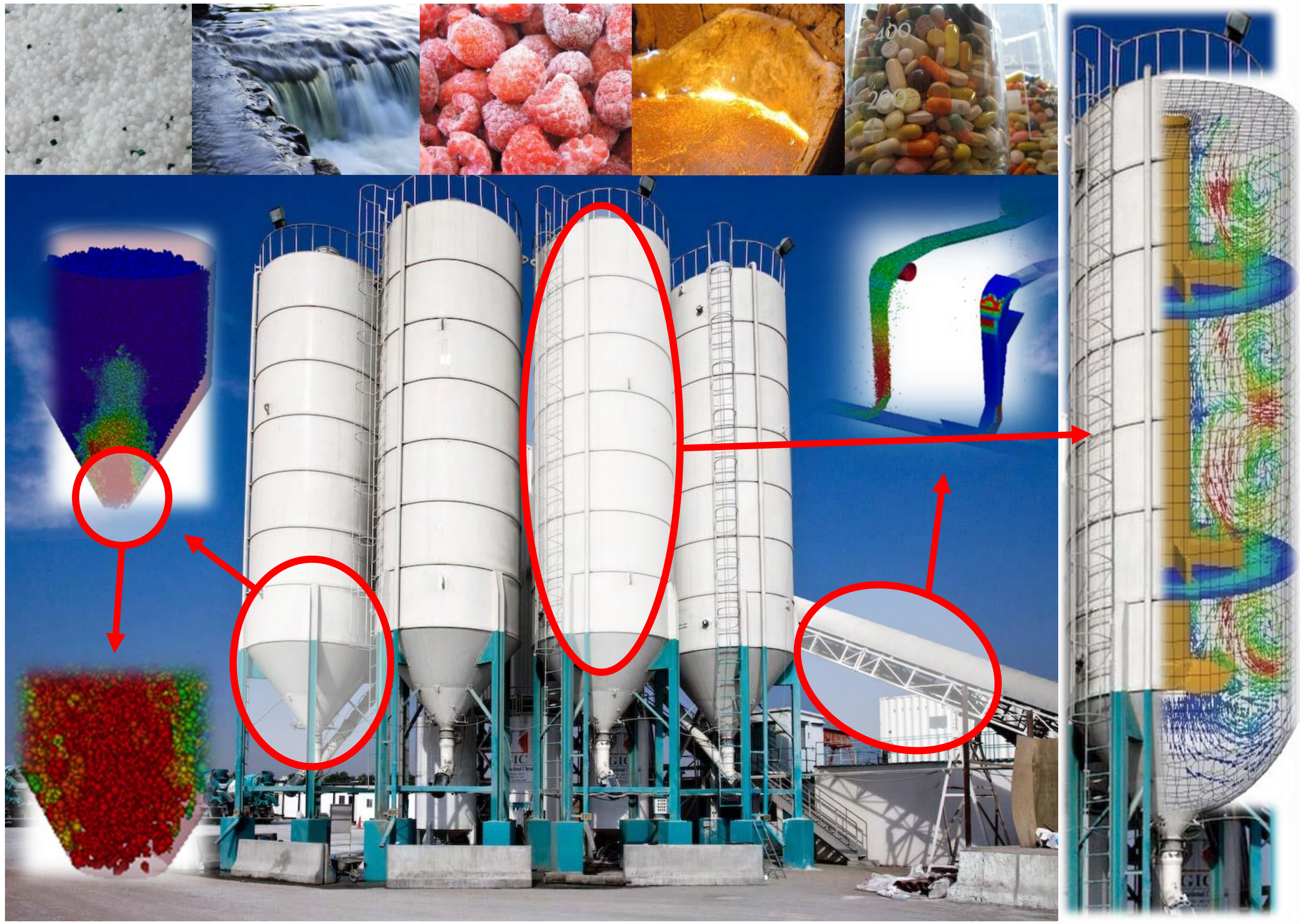
Intro

Modelling Flows of Particles, Gases and Liquids: CFD-DEM technology

Particles & flow processes are everywhere

Sugar, sand, ores, tablets, chemicals, biomass, detergents, plastics, crops, fruits need to be harvested, produced, processed, transported, stored.

DCS Computing is specialized in modelling and engineering solutions for these particle and fluid flow processes.



CFDEM®project latest news

Business Units

DCS COMPUTING GMBH | LIGGGHTS® | CFDEM® COUPLING | CFDEM® PROJECT

I RESEARCH

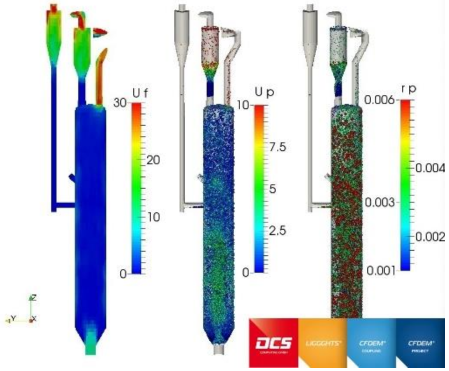
II SIMULATION ENGINES

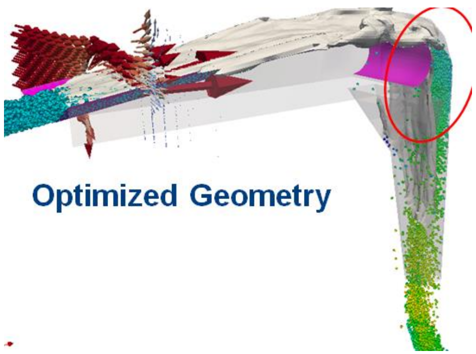
III CAE CONSULTANCY

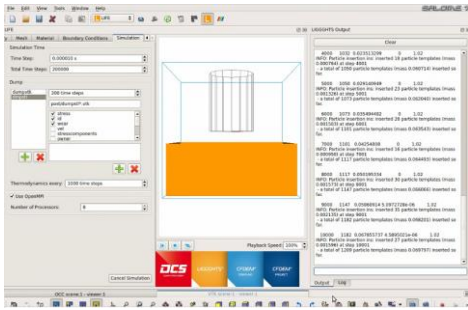
IV CAE Software

$$\Pi_2 = \frac{k_n}{R_i \cdot \rho_p \cdot v_0^2}$$

$$\Pi_3 = \frac{c_n}{R_i^2 \cdot \rho_p \cdot v_0}$$







DCS Computing covers the whole range from physics, code design of simulators, simulation model development, software/workflow development, support and training to actual engineering applications

All levels of creation of value with simulation technology are covered

CFDEM®project latest news

History & Timeline of DCS

- Founded 2012, Headcount 9 (July 2015)
- CAGR 89% (2012 turnover vs 2015 estimated turnover)
- DCS is funded by project cash flow, which is fully driven by the customers' needs and demands.
- DCS activities well balanced over business areas/industries

Impact: CFDEM®coupling workbench (FFG)

Fundament : Technology development with customers, 2 EU FP7 projects

Pre-Development outside DCS

2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020

PhD

DCS founded
Group leaders at JKU

Founders
Full-time

Why use DEM and CFD-DEM?

Over 70% of industrial processes involve particles BUT

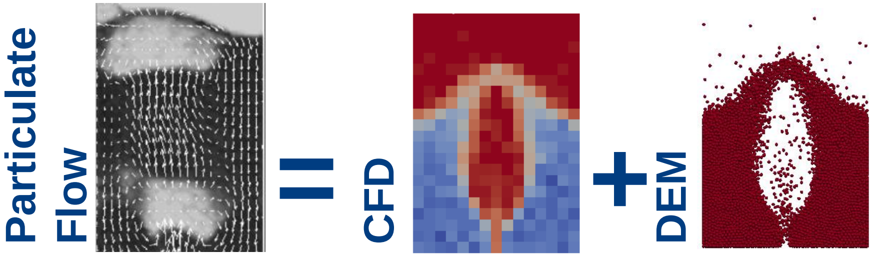
- majority of particle handling/processing operations empirically designed
- Measurement and control is difficult and costly.

(CFD-)DEM is used by **engineers** worldwide to increase profits by:

- **Reducing** need for **physical prototypes**
- **Troubleshooting** operational problems
- Designing more **efficient processes** by providing hard-to-measure information on bulk and particle-scale behavior
- Saving expensive **trial and error**

All processes include fluid-particle interaction

- **neglecting that often leads to errors!**
- Many processes inherently based on fluid-particle interaction
- Measurement is difficult and costly



Theoretical background – coarse grained CFD-DEM:

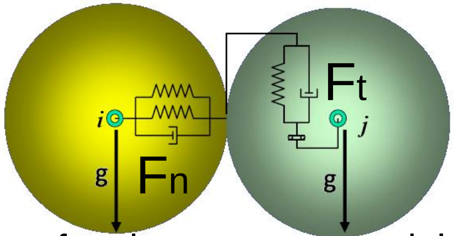
Navier-Stokes equations for the fluid in presence of a granular phase

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

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

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
- **scaling stiffness**
- **scaling of particle drag**
- **Equations converge to particle equation for parcel = particle**

Modelling needs–Fluidized Bed

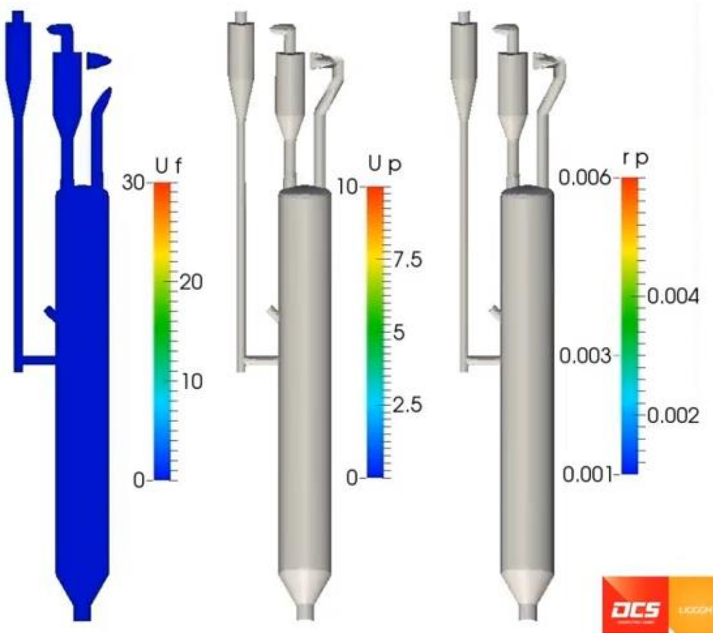
Fluidized Bed Processing

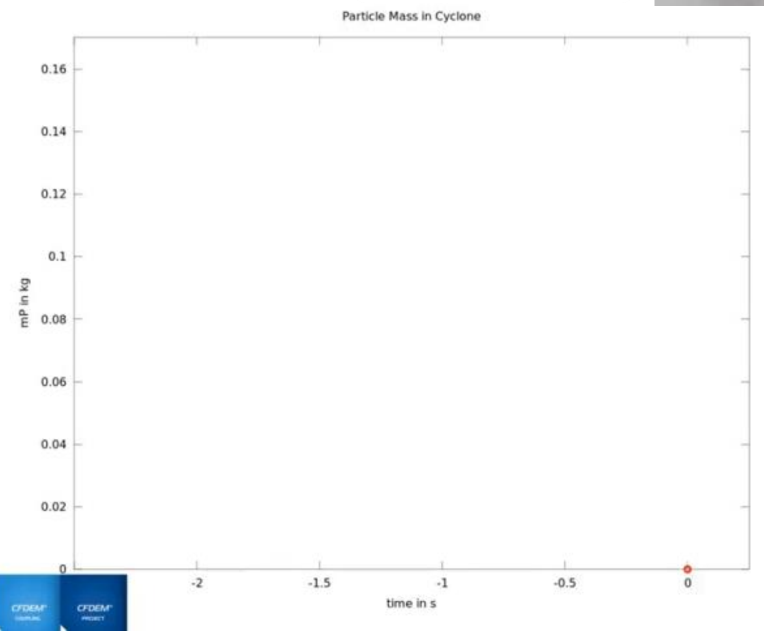
Process with high interphase exchange rates
Applications in most process industries,
including processes w/ high CO2 production

- Optimize heat/mass transfer
- Where do the fines go?, Is there segregation?
- Capture CO2 in the process

NanoSim

SEVENTH FRAMEWORK PROGRAMME





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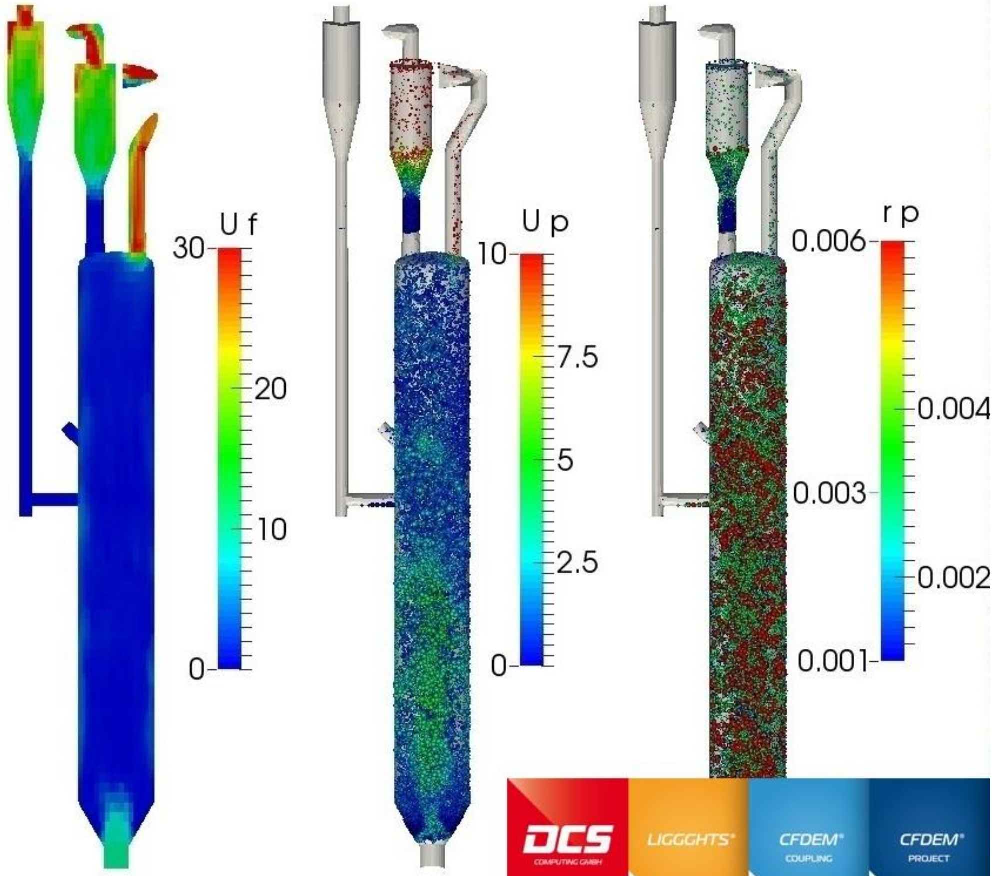
Fluidized Bed Modelling



What needs to be modelled?

- **Particle dynamics** (solid phase)
- **Fluid dynamics** (gas phase)
- **Inter-phase transport processes**
  particle-fluid momentum transfer,
  particle-fluid heat & mass transfer
- **Intra-phase transport processes**
  Intra-Particle heat transfer
  Intra-Particle chemical reactions

CFDEM®project latest news

Eco-system is growing!

What needs to be modelled?

- **Particle dynamics** (solid phase)
- **Fluid dynamics** (gas phase)
- **Inter-phase transport processes**

  particle-fluid momentum transfer,

  particle-fluid heat & mass transfer
- **Intra-phase transport processes**

  Intra-Particle heat transfer

  Intra-Particle chemical reactions

CFDEM®project latest news

Eco-system is growing!

New! First release was a new year gift (31 Dec 2014), next one to follow soon!

For download: www.cfdem.com

parScale ⟷

- **Intra-phase transport processes**

  Intra-Particle heat transfer

  Intra-Particle chemical reactions

CFDEM®project latest news

Eco-system is growing!

Mastermind

(right hand side)

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parScale ⟷

- **Intra-phase transport processes**
  - Intra-Particle heat transfer
  - Intra-Particle chemical reactions

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Chemical Reaction Modelling

PaScal Library for Particle-Based Modelling of Chemical Reactions

- The particle scale simulation tool with interface capabilities to LIGGGHTS, OpenFOAM, FLUENT, NEPTUNE_CFD, as well as to the reaction modelling tool REMARC.

  various particle-scale models to be able to solve complex reaction-diffusion problems, and will have subroutines to model drying or devolatilization processes

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Software Testing

Software Testing

- The test harness is a development tool to **build binaries, run test cases** and **check for consistency** with previous versions.
- It can perform this jobs on the **local machine** or an **external cluster**.
- The **web-based frontend** allows to check the results of all test cases for several builds at once and from your working computer
- The test harness was originally developed for the development of LIGGGHTS® and was extended to cover also CFDEM®coupling and ParScale.
- CI server is used to **check automatically for new commits** to the projects and **start (if required) the test harness**.
- If something is broken, **notification email** to the user is sent.
- In active use for development

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Testing: LIGGGHTS®

liggghts-src-unstable-3.0.x

LIGGGHTS

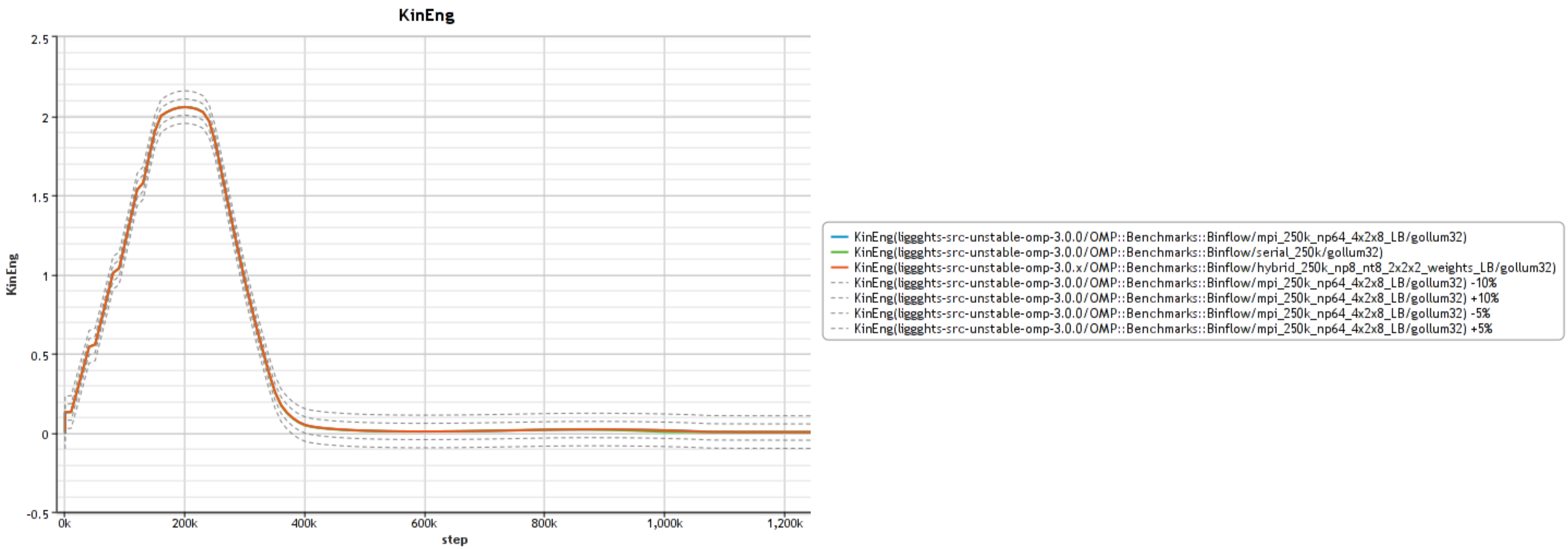
Show version consistency compared to liggghts-src-unstable-3.0.2

	✔	✖	⚠
examples	175	2	15
local	3	0	145

pascal-master-0.x

PaScal

	✔	✖	⚠
pascal-examples	3	1	0



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Testing: CFDEM®coupling

CFDEMproject Test Harness | Overview | Comparisons | Search | Status | Andreas Aigner

Comparison

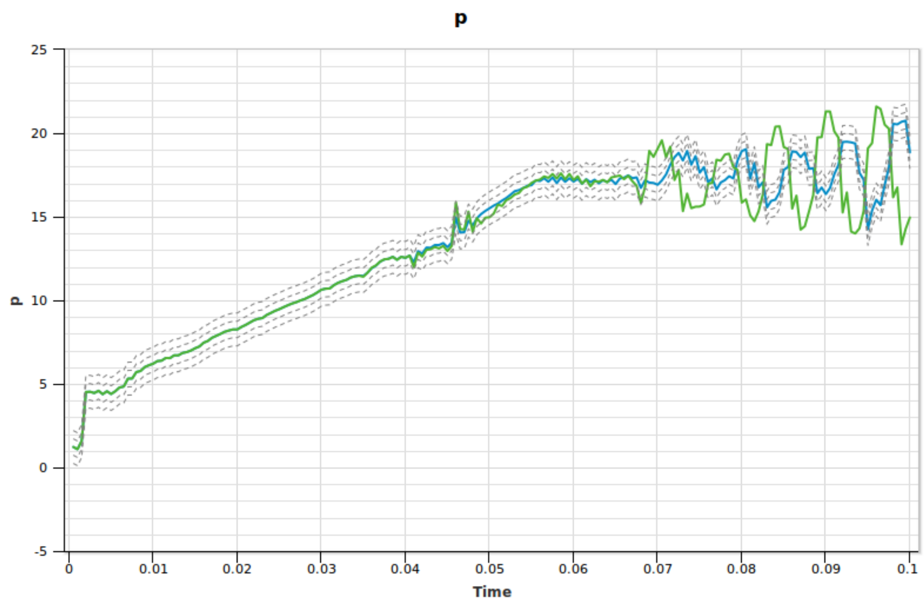
+ Add all

a. CFDEMcoupling-DCS-master-2.8.x-liggghts-src-unstable-3.2.x-OF-2.3.x/CFDEMcoupling-DCS-master-2.8.x-liggghts-src-unstable-3.2.x-OF-2.3.x/DCS-examples::tutorials::cfdemSolverPiso::ErgunTestMPI/cfdemrun/glados
b. CFDEMcoupling-DCS-master-liggghts-src-unstable-OF-2.4.x/CFDEMcoupling-DCS-master-liggghts-src-unstable-OF-2.4.x/DCS-examples::tutorials::cfdemSolverPiso::ErgunTestMPI/cfdemrun/glados

Overview | Logfile | Input Script | Files | Fix Timing | Plots | Probes

probes: **(3e-05, 0, 0.0001)**

p(3e-05, 0, 0.0001)



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Highcharts.com

U(3e-05, 0, 0.0001)

CFDEMcoupling-DCS-master-2.8.x-liggghts-src-unstable-3.2.x-OF-2.3.x

Consistency: None

Detail:

CFDEMcoupling-DCS-master-liggghts-src-unstable-OF-2.4.x

Consistency: 0.0

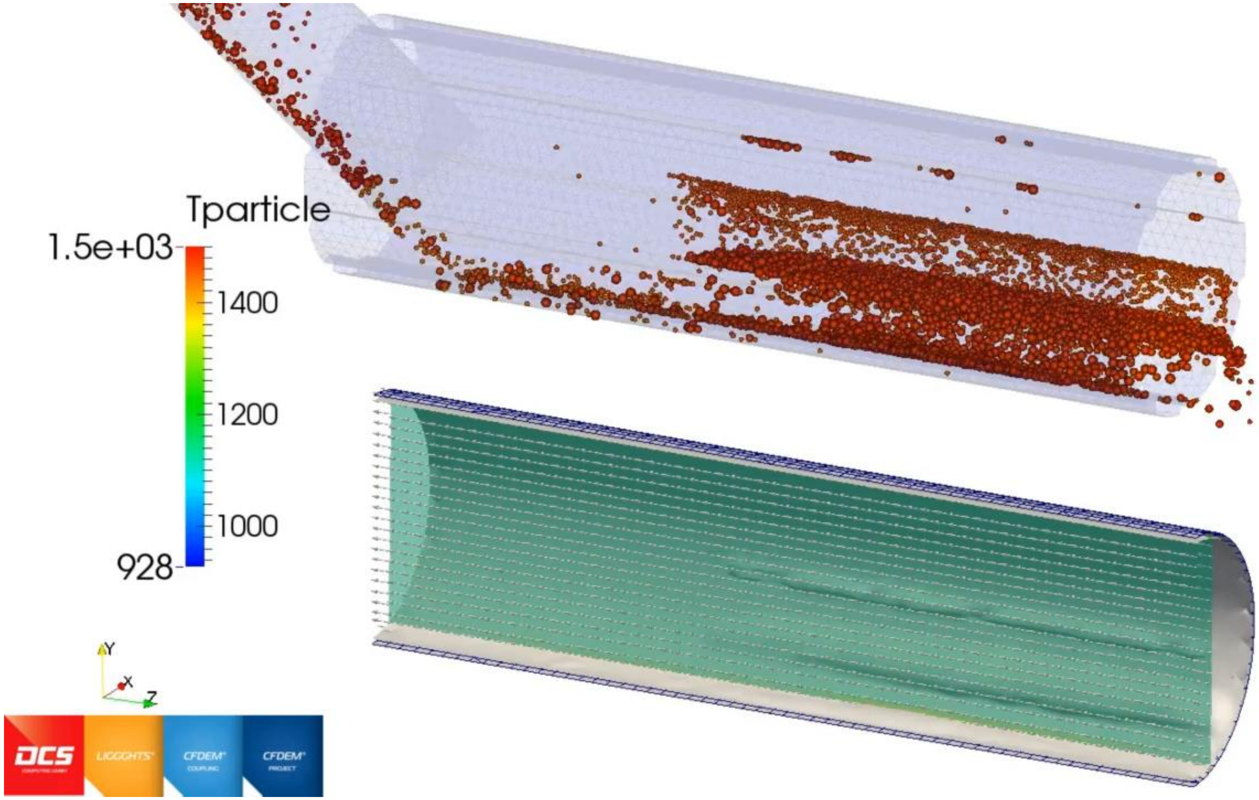
Detail:

- plot thermo_KinEng inconsistent: 0.000000
- plot thermo_rke inconsistent: 0.000000
- plot thermo_dragtota inconsistent: 0.000000

Recent Developments on CFDEM®coupling

Generic Scalar Transport Model coupled CFD-DEM simulations

Generic scalar transport model class that can be hooked onto different solvers, where sub-models for scalar transport can be implemented (temp., species, etc)



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CFD-DEM domain decomposit.

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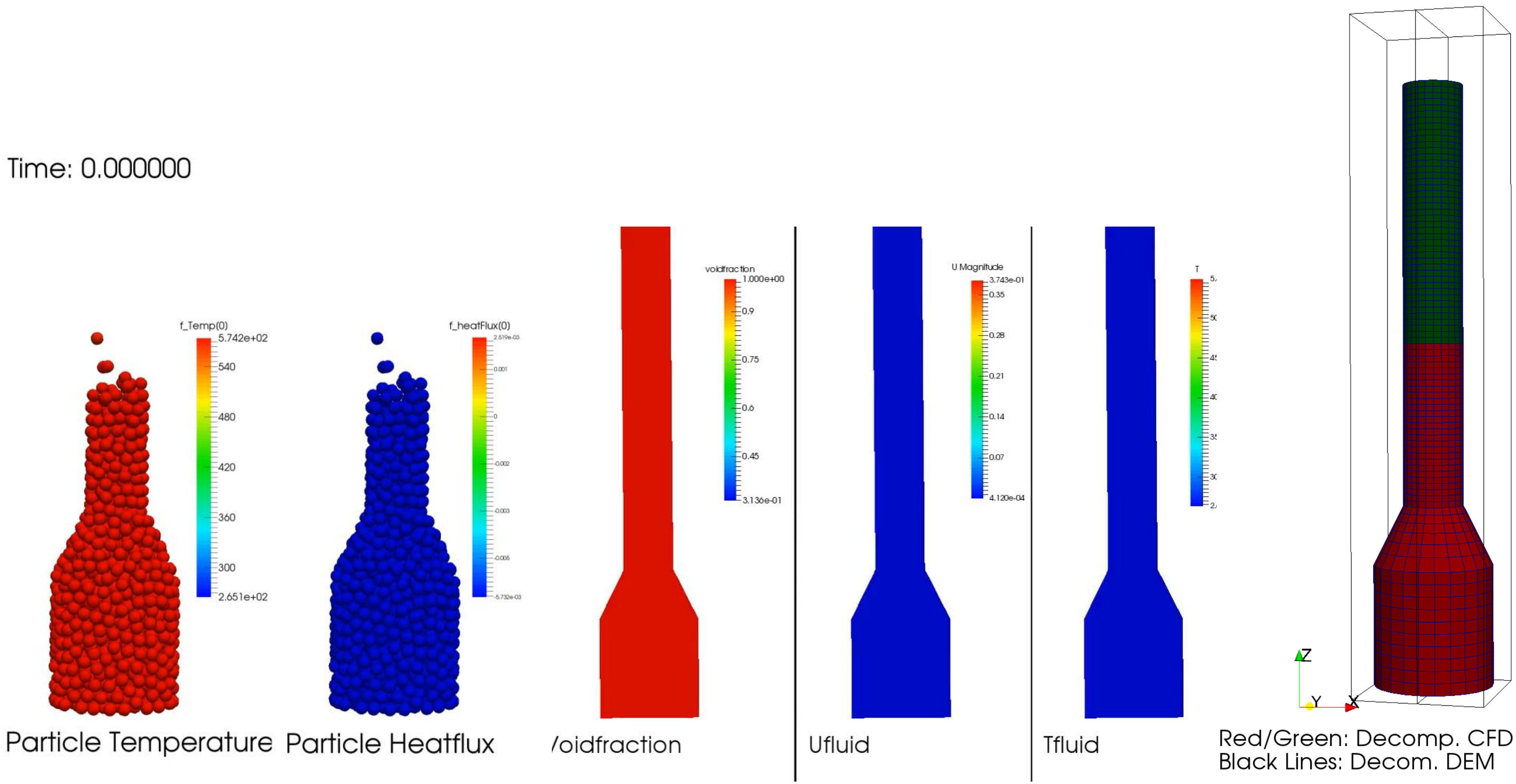
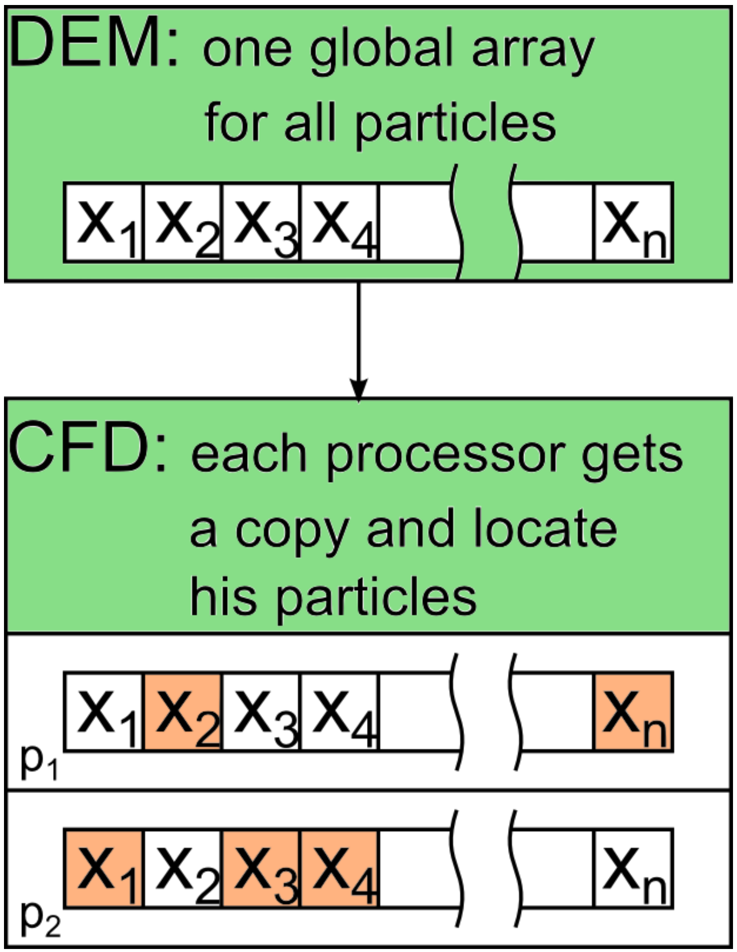
Moving bed reactor with convective heat transfer

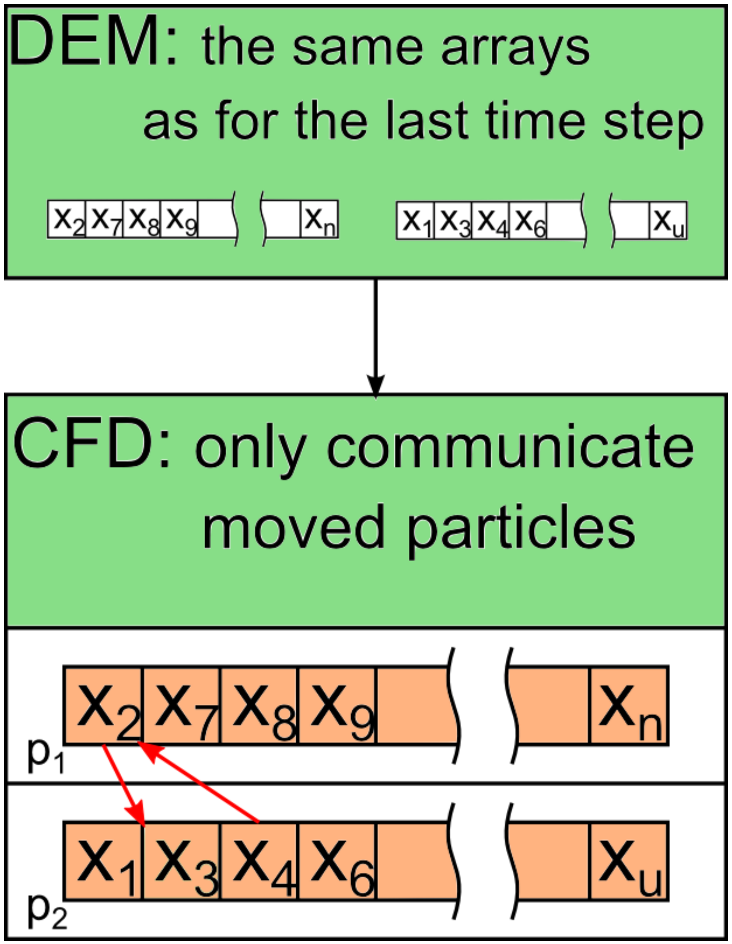


All-to-All vs. Many-to-Many

All-To-All



Many-To-Many



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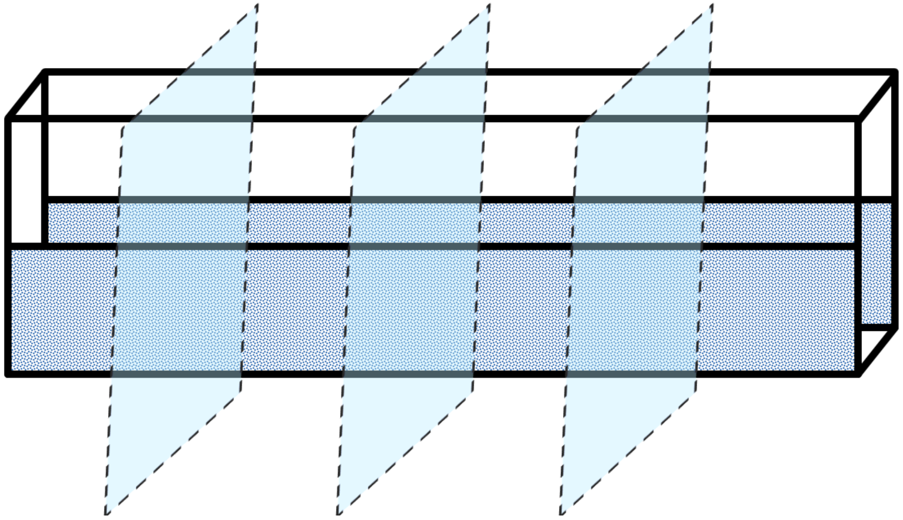
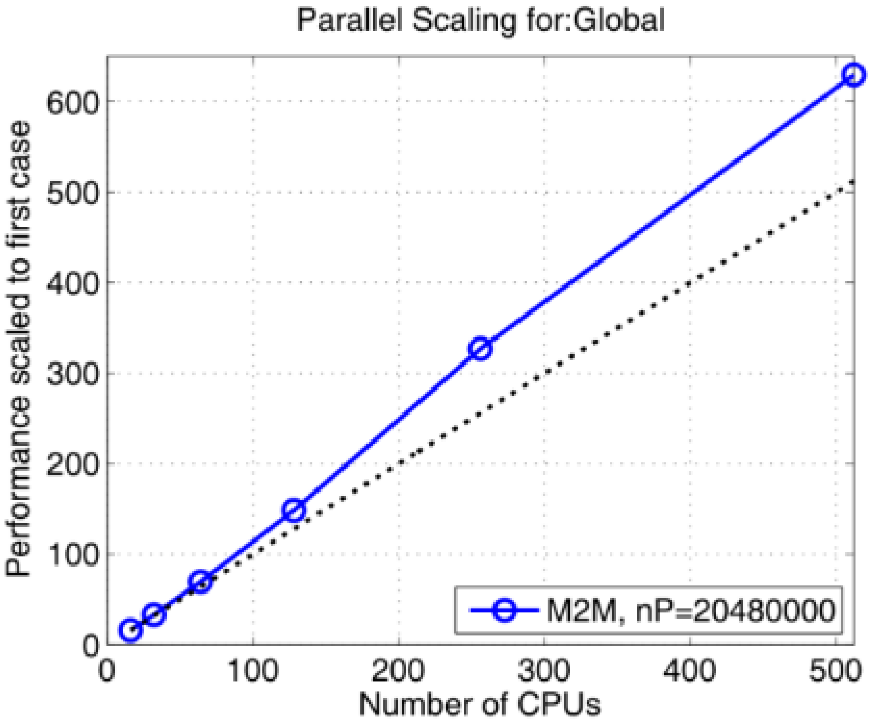
ManyToMany Communication

Test Case	Purpose	Machine used	Version of “many2many” used
Elongated Packed Bed #1	Show feasibility of the approach and its scalability	JKU cluster “MACH” (512 CPUs)	Very early feasibility version
Elongated Packed Bed #2	Show scalability of the final stable version and applicability across clusters	JKU cluster “LISE” (128 CPUs)	Stable version 1.0
Thermal Packed Bed	Compare results to physical lab-scale test-case where experimental data is available	Local workstation and JKU cluster “Gollum” (one blade with 32 cores)	Stable version 1.0

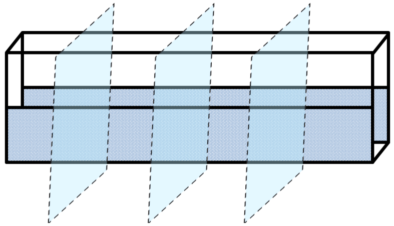
Elongated packed Bed #1

The system consists of a block 10.24 x 0.002 x 0.1 m / 10240 x 2 x 100 cells, filled with particles of d_P = 0.3 mm, and a total particle number of n_P=20.48e6.



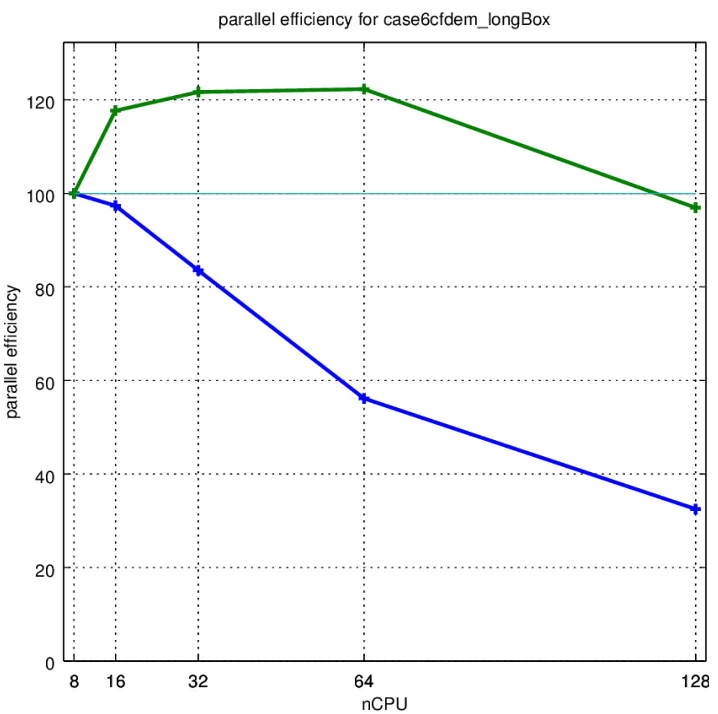


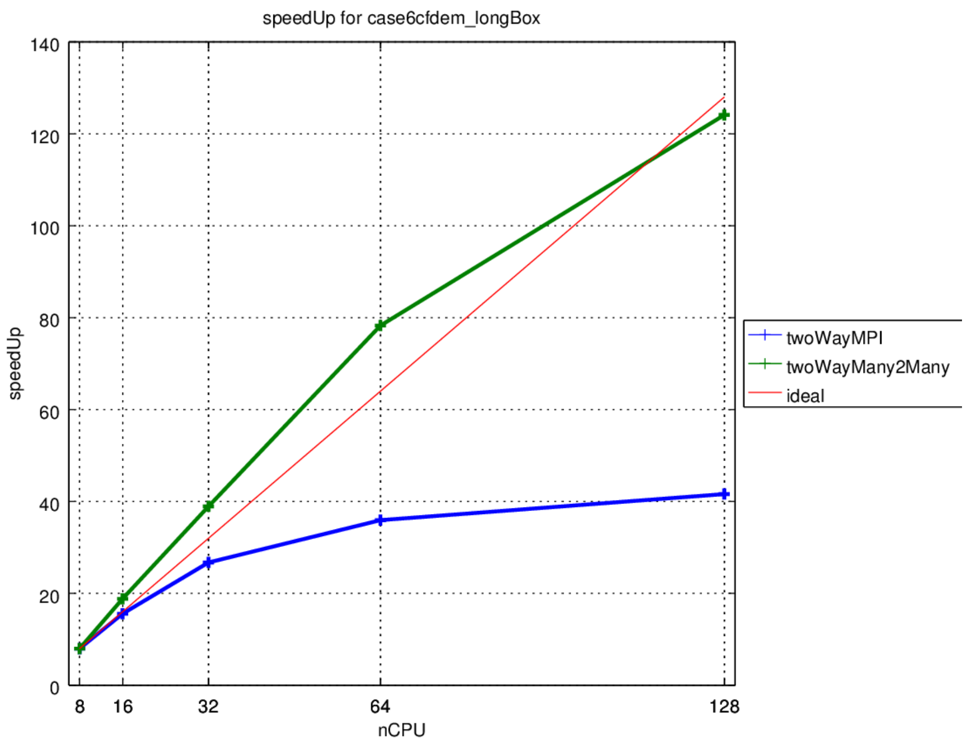
Elongated packed bed #2



Elongated packed Bed #2

The system consists of an elongated block of 64x1x1 m, is filled with 1,1 Mio particles (radius of 0.02m) and represents a packed bed which is seeing gas flow through the bottom walls with a velocity of 0.6077 ms/s, starts to bubble slightly

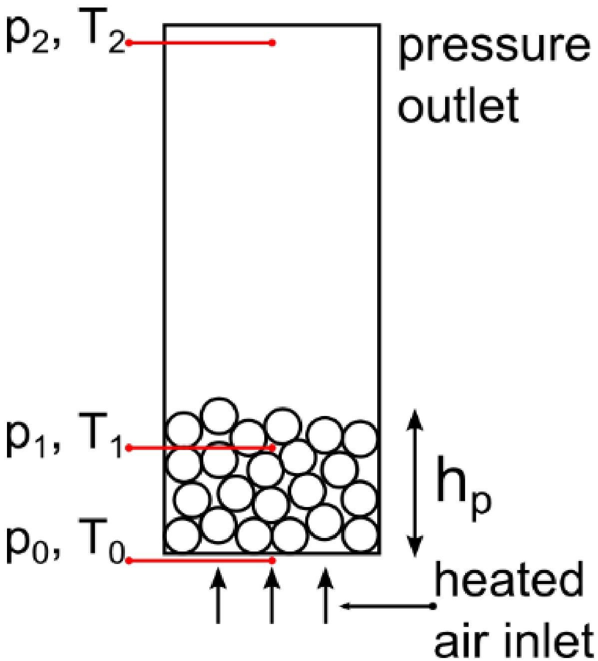


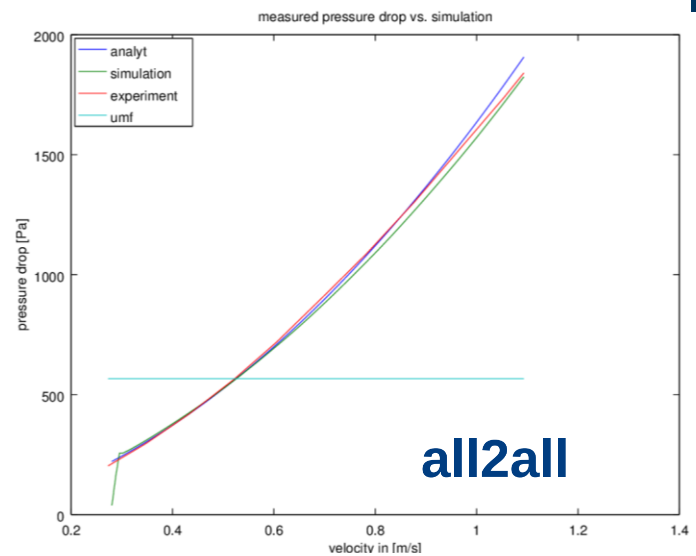


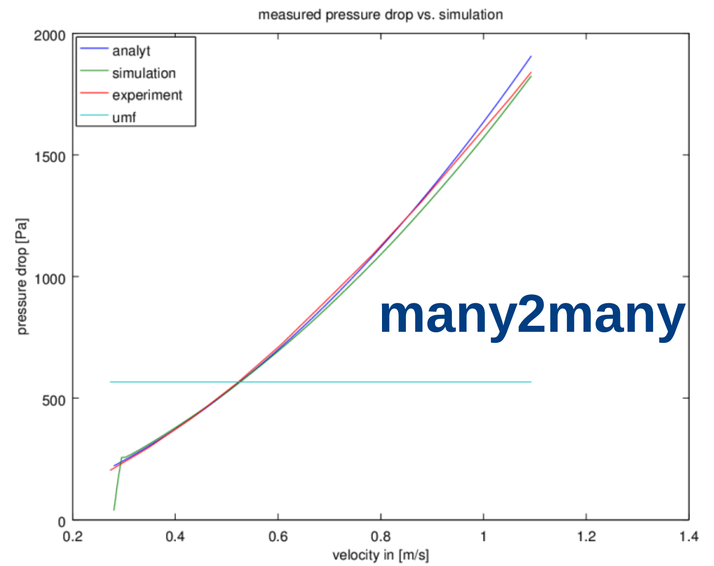
Thermal Packed Bed

Thermal Packed Bed

cylindrical fixed bed (d_{cyl}=0.1m, h_p=0.1m) with heated air inlet where experimental data (courtesy of JKU) was available. Particles are non-spherical poly-propylene-particles with Sauter mean diameter of 3 mm. Pressure and temperature are measured. The packed bed is fixed by a porous plate so it can not fluidize.







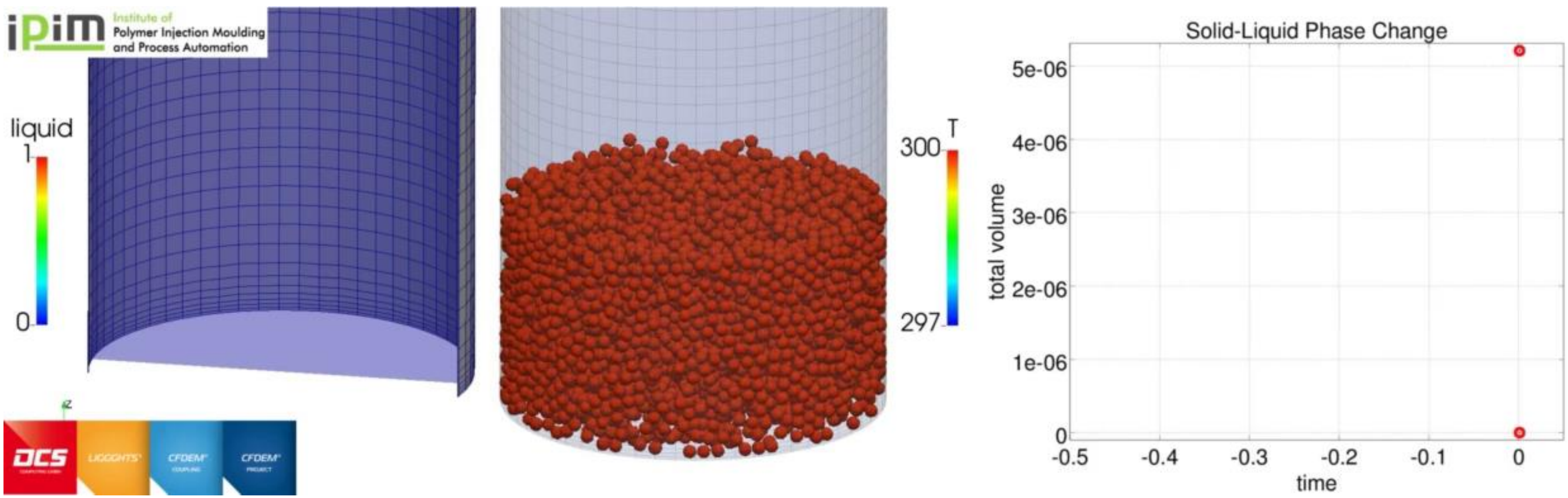
Conclusions:

(i) the numerical method can capture the physics of the process, and
(ii) the Many2Many and the All2All scheme deliver the same mascroscopic result.

3 Phase Melting CFD-DEM

Result

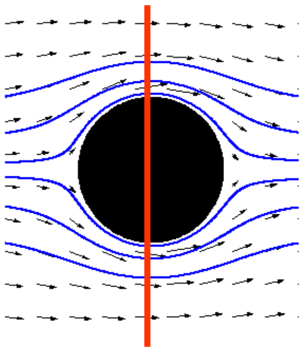
- A model using VOF approach to capture solid-liquid phase change
- Energy equation for particle melting

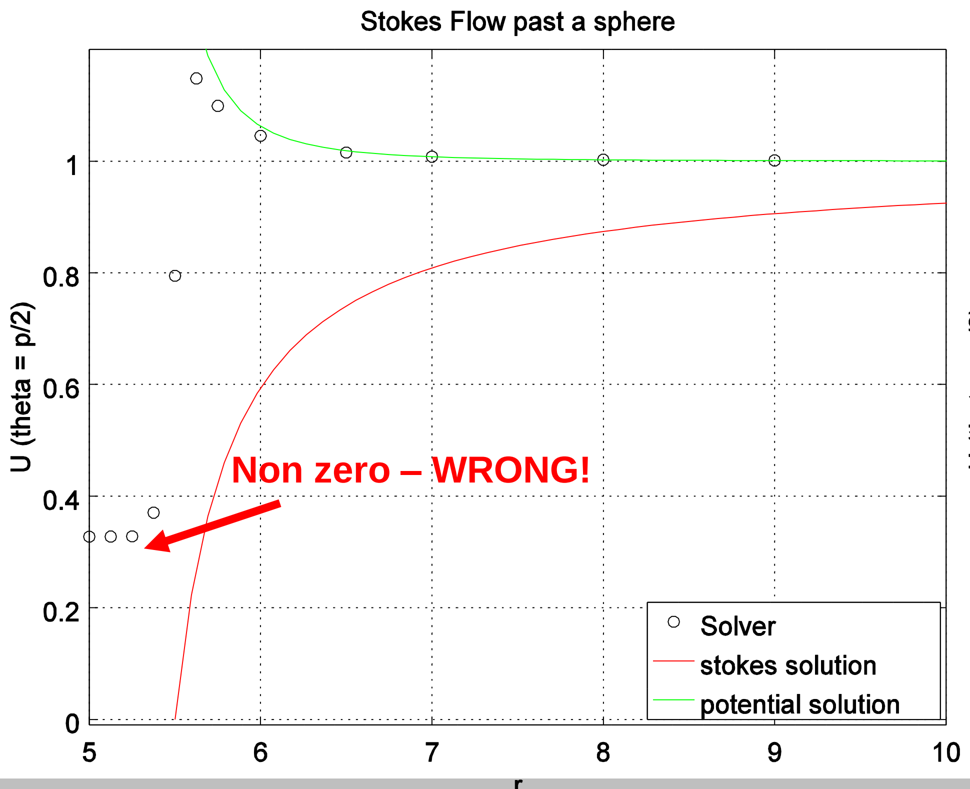


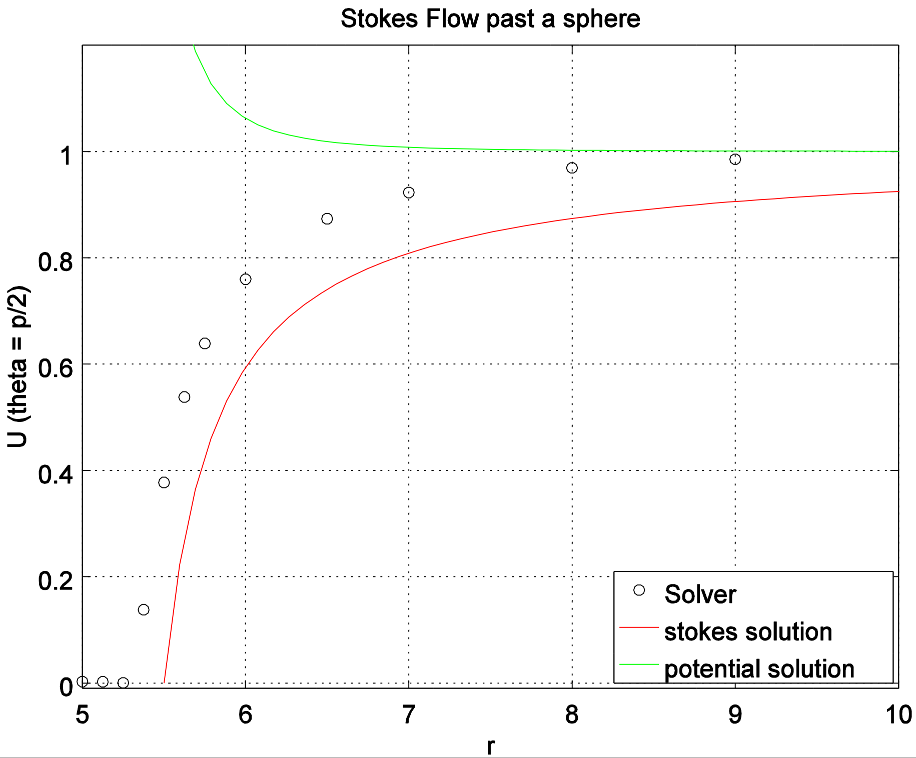
Improved IB Models

Improved Immersed Boundary Model

- Flow past sphere
- Improved solver (right) fulfils no-slip condition on sphere surface

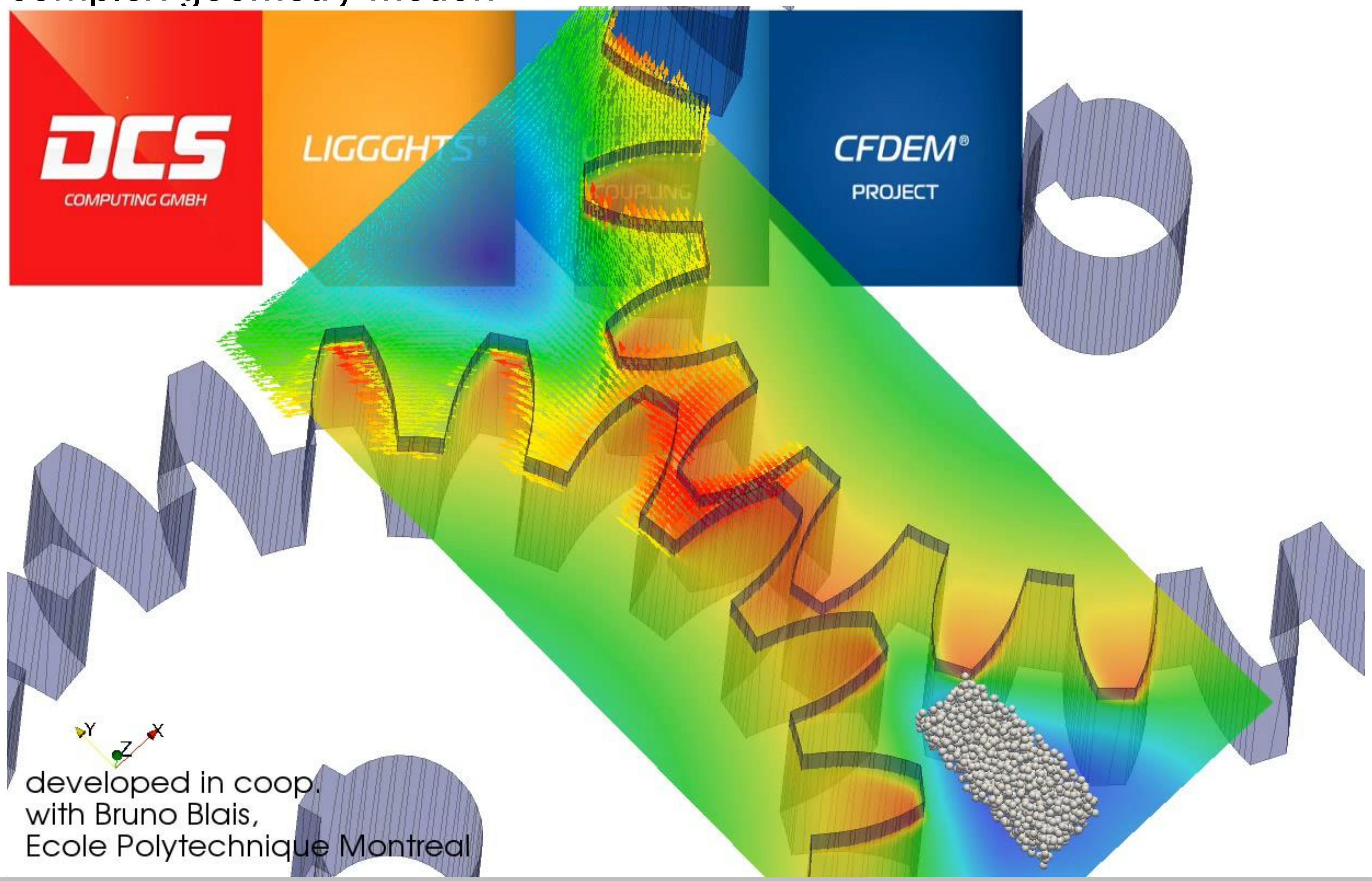






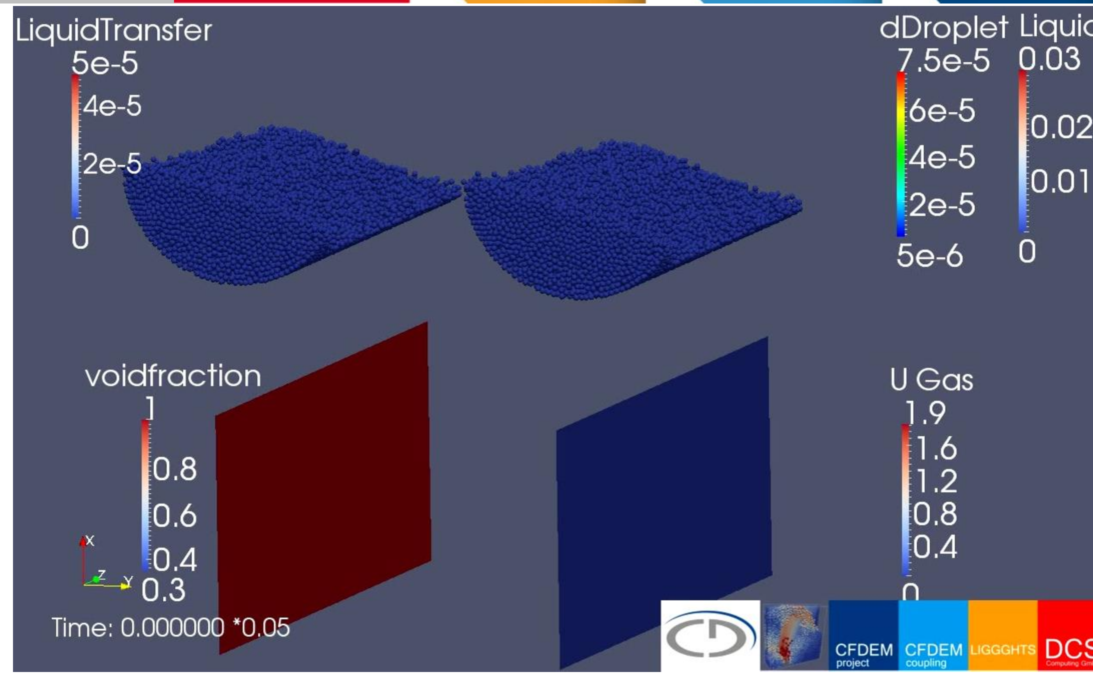
Hybrid IB Model

- First version of a hybrid IB (for solid parts) with CFD-DEM (for particles) model.
- It allows complex geometry motion



Latest Dev. & Outlook

Spray Coating



Physics to be covered

- **Spray modelling**
- **Spray-particle interaction**
- **Liquid bridge forces**
- **Liquid transport** btw. particles

Spray modelling

- **Equation of Motion**

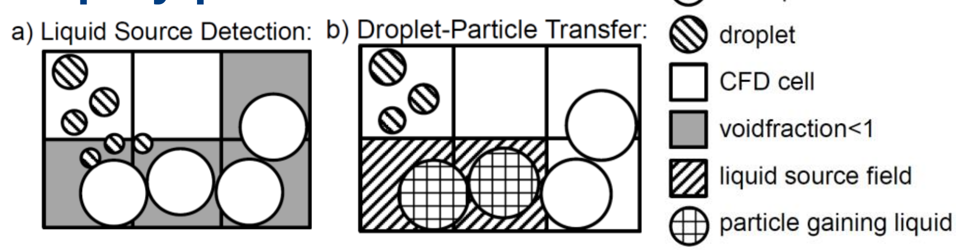
$$m_D \frac{dv_D}{dt} = g\,(\rho_D - \rho_G)V_D + C_{d,D} A_D \frac{\rho_G (v_G - v_D)|v_G - v_D|}{2}$$

- **Drag Law** $C_{d,D} = C_{d,sphere}(1 + 2.632\,y)$

- **Breakup Model (e.g. O'Rourke*)**

$$\ddot{y} + \frac{5\mu_D}{\rho_D r^2}\dot{y} + \frac{8\sigma}{\rho_D r^3} y = \frac{2\rho_G v_{rel}^2}{3\rho_D r^2}$$

Spray-particle interaction

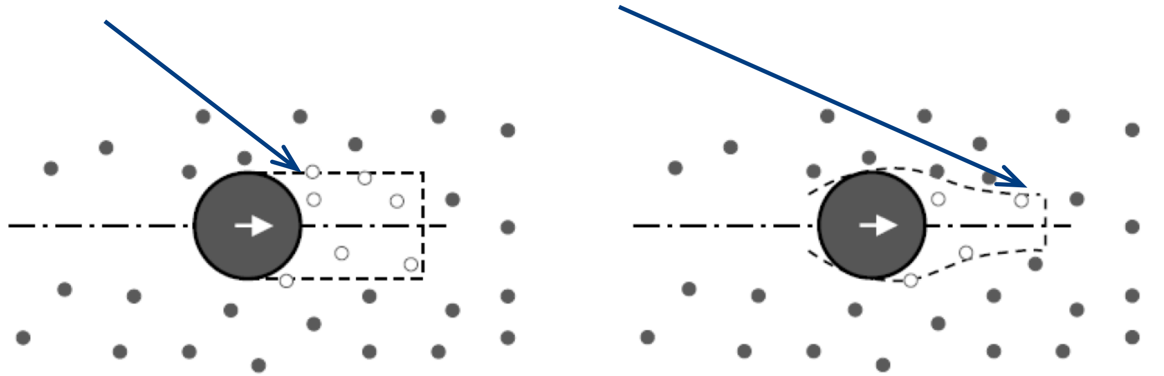


C. Goniva, J. Kerbl, S. Pirker, C. Kloss: Modelling Spray Particle Interaction by a Coupled CFD-DEM Method, Proc. Computational Modelling Conference 2013

Spray Particle Collision Model

Basic Idea:

Particles collect spray on their surface according to their collisional cylinder, which is corrected by Stokes Nr. dependent correlation:



From Goniva, PhD thesis.

Assumptions:

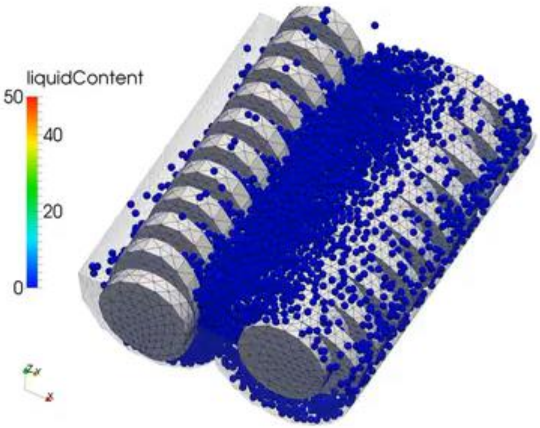
- Collisional regime is dominant.
- Particles are bigger than spray.
- Particle diameter is constant for whole domain.

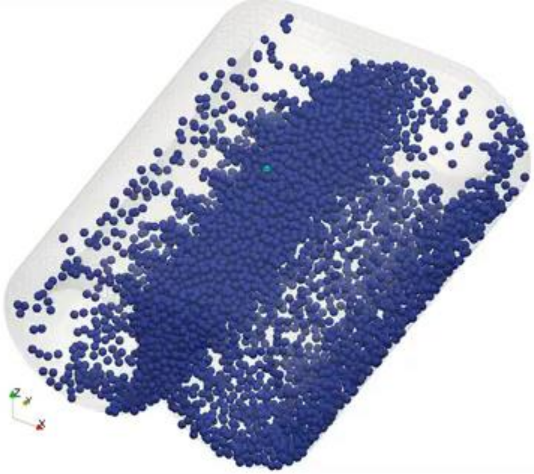
Literature:

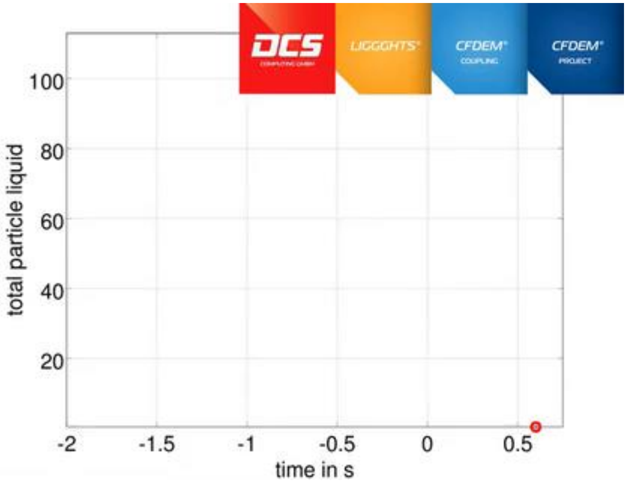
GONIVA C., TUKOVIĆ Ž. and PIRKER S. (2009): “Simulation of offgas Scrubbing by a Combined Eulerian-Lagrangian Model”, International Conference on CFD in the Minerals and Process Industries CSIRO, Melbourne, December 9-11.

HÄHNER F., (1994), “Inertial impaction of aerosol particles on Single and Multiple Spherical Targets”, Chem. Eng. Technol., 17, 88-94.

Spray Coating







Spray modelling

- **Equation of Motion**

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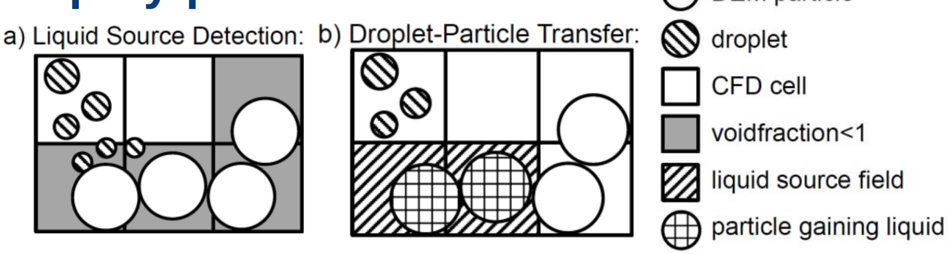
Spray-particle interaction



C. Goniva, J. Kerbl, S. Pirker, C. Kloss: Modelling Spray Particle Interaction by a Coupled CFD-DEM Method, Proc. Computational Modelling Conference 2013

Recent Developments on LIGGGHTS®

CFDEM®project latest news

LIGGGHTS 3.2

DCS COMPUTING GMBH | LIGGGHTS® | CFDEM® COUPLING | CFDEM® PROJECT

Major facelift version

- Revision of src:
  2326 files changed,
  git diff is 3,000,000 lines
- **Revision of documentation:**
  # lines changed:
  1,383 additions 21,065 deletions
- Headers changed (see pic),
  Copyright and License clarified
- Pure LAMMPS functionalities removed completely from src, doc
- New file structure, new packages
- Fixed bugs in the build script
- Other improvements / bug-fixes:
  http://www.cfdem.com/node/42

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This is the

LIGGGHTS®

DEM simulation engine, released by
DCS Computing Gmbh, Linz, Austria
http://www.dcs-computing.com, office@dcs-computing.com

LIGGGHTS® is part of CFDEM®project:
http://www.liggghts.com | http://www.cfdem.com

Core developer and main author:
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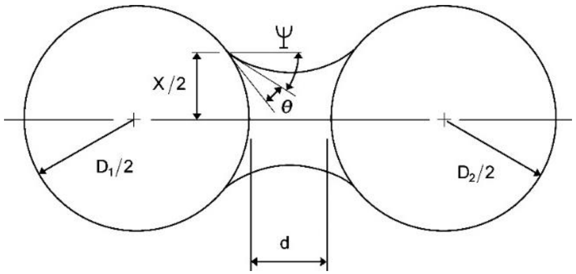
Liquid Bridge Models

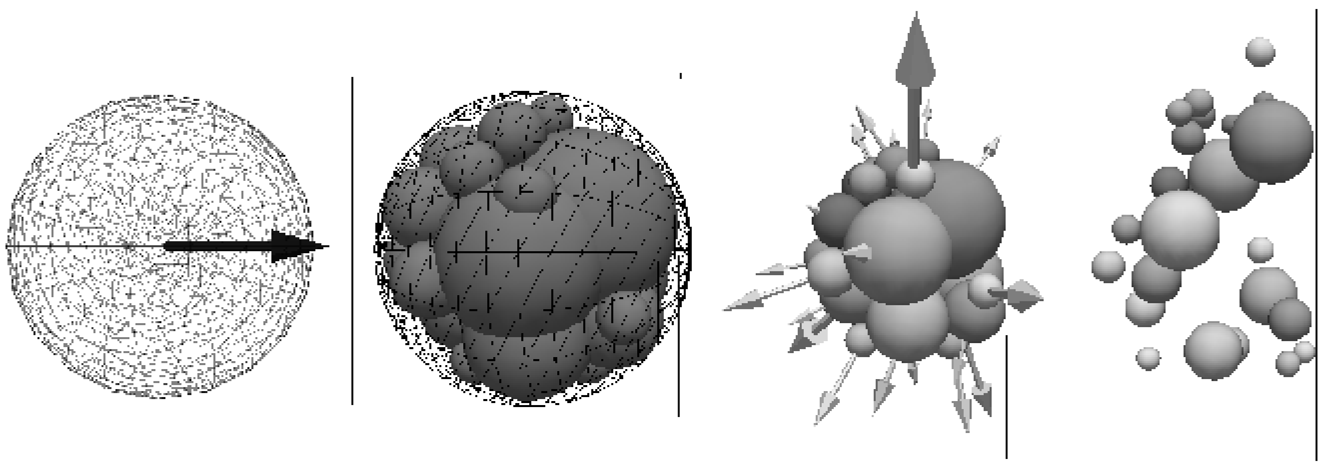
- Particle liquid on leads to
  (a) liquid bridge force [capilary+viscous],
  (b) liquid transfer
- Particles could be assumed to be solid or porous



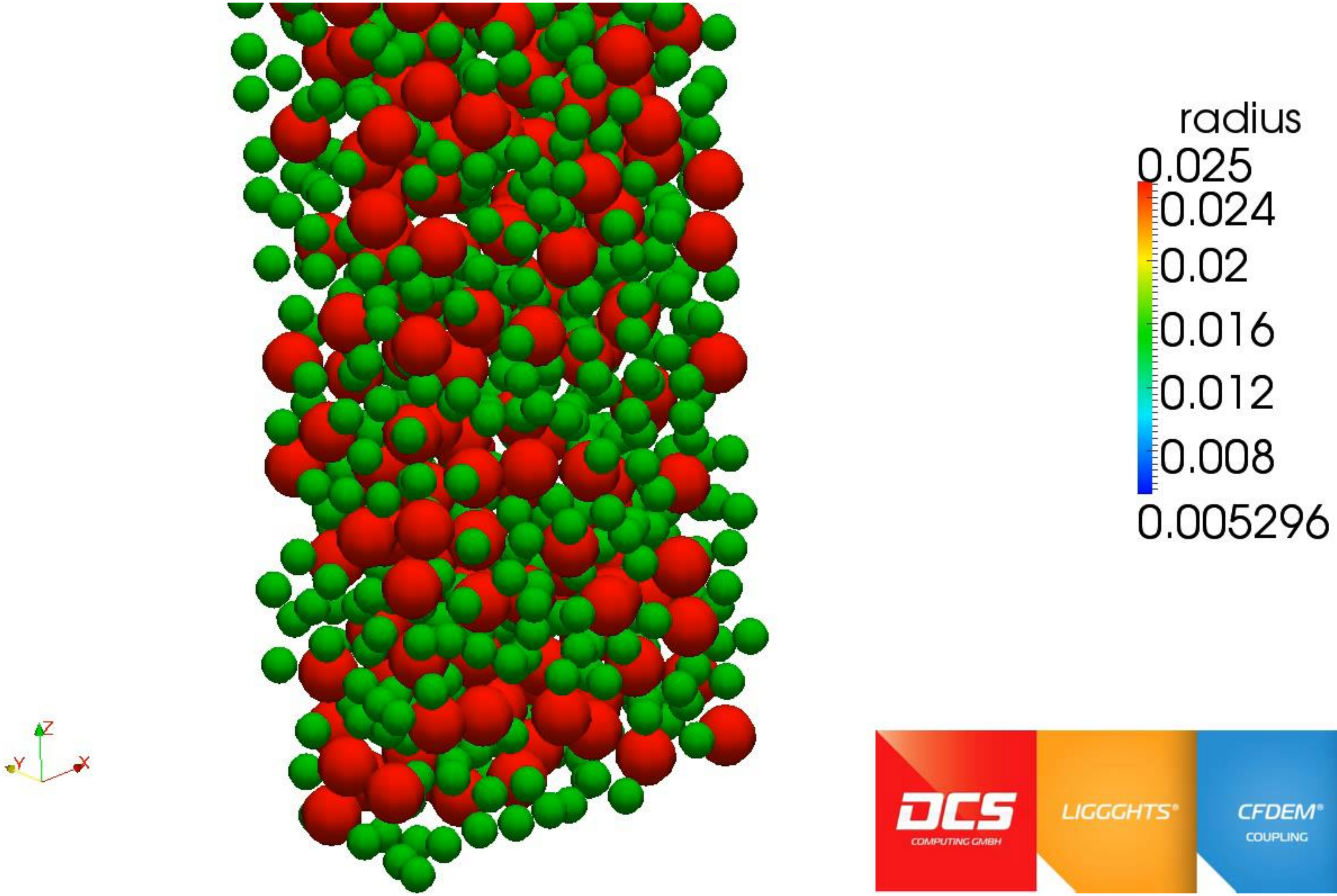
	Washino Kimiaki	Easo
Liquid properties required	• Surface tension • Contact angle • Viscosity • Minimum separation distance ratio for viscosity calculations (~1.0% of smallest particle size); prevents viscous force from becoming exceedingly large • Maximum separation distance ratio, needed because neighbor lists need a cut-off	• Surface tension • Contact angle • Viscosity • Min separation distance • Maximum separation distance ratio, needed because neighbor lists need a cut-off
Volume of liquid involved	Total volume of liquid available between the two spheres multiplied by some user-specified factor (0.05) Currently this 0.05 is hard-coded, but could be easily implemented in a way that the user can specify via script	Shi & McCarthy (2009); contributed fraction depends on relative particle sizes; for equal sized spheres, each contributes approximately 0.067 of its individual liquid volume to the bridge volume
Capillary force	Approximate theoretical solution using minimum energy approach (Rabinovitch, 2005)	Semi-empirical solution to the Young-Laplace equation (Soulie et al, 2006)
Viscous force	Nase et al as quoted in Shi&McCarthy	Nase et al as quoted in Shi&McCarthy
Formation distance	Rupture distance (see below)	Contact distance
Rupture distance	Lian et al, 1993 $$D = \left(1 + \frac{\theta}{2}\right) V^{1/3}$$ Not quite sure how theta_i / theta_j would transfer into a theta_effective in case two particles have different thetas, at first glance it seems that this is not covered in the paper. For now, I am assuming 0.5*(theta_i+theta_j)	Lian et al, 1993 $$D = \left(1 + \frac{\theta}{2}\right) V^{1/3}$$ Not quite sure how theta_i / theta_j would transfer into a theta_effective in case two particles have different thetas, at first glance it seems that this is not covered in the paper. For now, I am assuming 0.5*(theta_i+theta_j)
Liquid transfer between particles	Equal distribution method (Mani et al, 2013)	Equal distribution method (Mani et al, 2013)
Initialization	Specify default amount of liquid per particle in % of weight; can be overridden by set command based on region/and/or other criteria	Specify default amount of liquid per particle in % of weight; can be overridden by set command based on region/and/or other criteria

Particle Breakage

- Particles can break when being processed – usually problem for process
- Breakage processes consume ~2-10% of worlds energy
- Spheres can be replaced by a conglomerate of daughter spheres



Simple Breakage Case



Heat Conduction Coarse Grain

Coarse Graining of Particle-Particle Heat Conduction

- Coarse graining = reproduce behaviour with larger particles
- Coarse graining was verified
- Temp profile over z after 20k time-steps, dt =1e-5s Fine (right) vs coarse (left) (2nd col = position, last col = averaged Temperature)

1	0.005	50	591.642
2	0.015	66	581.198
3	0.025	65	570.333
4	0.035	62	558.195
5	0.045	65	545.371
6	0.055	57	530.978
7	0.065	61	516.799
8	0.075	65	500.365
9	0.085	58	484.331
10	0.095	67	467.624
11	0.105	60	452.264
12	0.115	64	438.969
13	0.125	60	427.378
14	0.135	66	417.807
15	0.145	48	412.965

1	0.005	4073	594.263
2	0.015	4175	584.802
3	0.025	4159	574.599
4	0.035	4163	563.321
5	0.045	4141	550.846
6	0.055	4183	536.907
7	0.065	4153	521.661
8	0.075	4159	505.346
9	0.085	4154	488.244
10	0.095	4151	470.829
11	0.105	4127	453.845
12	0.115	4152	438.122
13	0.125	4147	424.841
14	0.135	4187	415.72
15	0.145	612	412.93