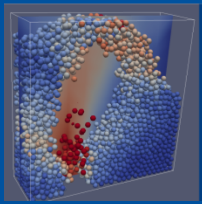

CFDEM project | CFDEM coupling | LIGGGHTS | DCS Computing GmbH

LIGGGHTS and CFDEM coupling - Modelling of macroscopic particle processes based on LAMMPS technology

DEM6 Conference, Golden (CO), 05 August 2013

Christoph Kloss[1,2] *, Christoph Goniva[1,2] , Stefan Pirker[1]

www.cfdem.com | www.jku.at/pfm | www.dcs-computing.com

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2 DCS Computing GmbH, Linz, Austria

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Outline

I. **Introduction**
Industrial perspective of macroscopic particle processes, CFDEMproject

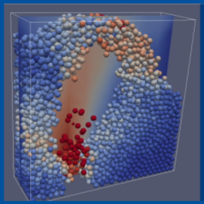
II. **Modelling Approaches**
CFD-DEM (resolved and unresolved), coarse-graining, MP-PIC

III. **Scalability, Efficiency and Maintainability**
Parallelization (distributed and shared mem), benchmarks, code design

IV. **Applications**
Iron/steelmaking, bulk solids handling, environmental eng., fluidized beds, minerals processing, agricultural

V. **Conclusions**

VI. **Acknowledgements**



I.

Introduction

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The Importance of Bulk Solids

Macroscopic particle processes from an industrial perspective:

- Production, handling, storage, transport and processing of particles and granular materials is of **paramount importance in all sectors of industry**.
- **40% of the capacity of industrial plants** is **wasted** due to granular solid problems (**)
- **Between 1 and 10% of all the energy** is **used in comminution**, i.e. the processes of crushing, grinding, milling, micronising (*)

photo from: Whiddon, P.: http://www.flickr.com/photos/pwhiddon/

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* Holdich, R. (2006): Fundamentals of Particle Technology; Midland Information & Publishing

** Ennis, B. J., Green, J., Davies, R.(1994): Particle technology. The legacy of neglect in the US", Chem. Eng. Prog, 90, 32-43.

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The Importance of Bulk Solids

Macroscopic particle processes from an industrial perspective:

- More than **50% of all products** sold are either granular in form or involve granular materials in their production*.
- **40% of the value added** in **chemical industry** is linked to particle technology**.
- Many industrial solid particle systems display **unpredictable behaviour**, leading to losses of resources, energy, money, time
- **State-of-the-art simulation tools show lack of predictive capability**

photo from: Whiddon, P.: http://www.flickr.com/photos/pwhiddon/

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* Bates, L. (2006): The need for industrial education in bulk technology", Bulk Solids Handl., 26, 464-473.

** Ennis, B. J., Green, J., Davies, R.(1994): Particle technology. The legacy of neglect in the US", Chem. Eng. Prog, 90, 32-43.

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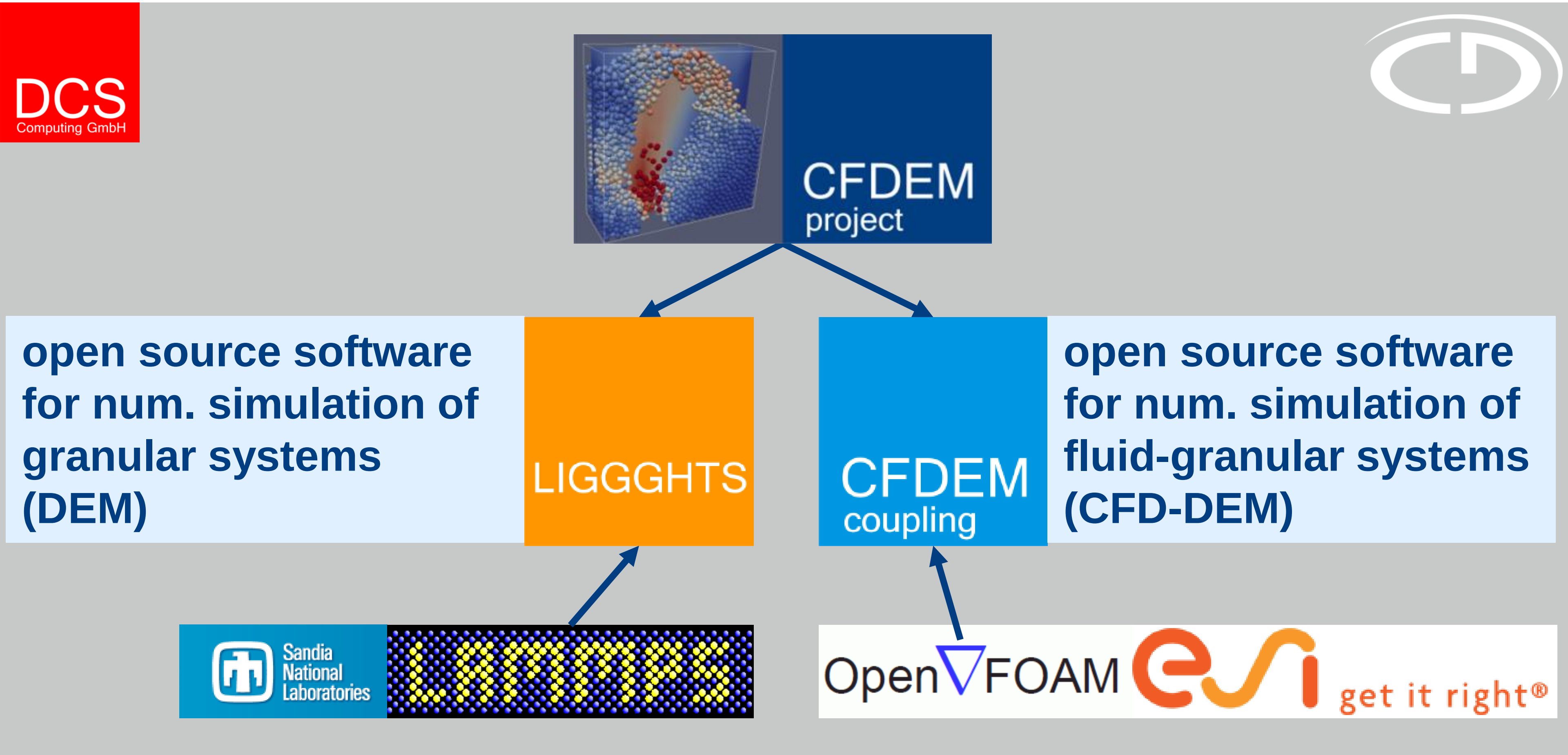
The Framework

Professional Base:

Scientific Base:



open source software for num. simulation of granular systems (DEM)

open source software for num. simulation of fluid-granular systems (CFD-DEM)

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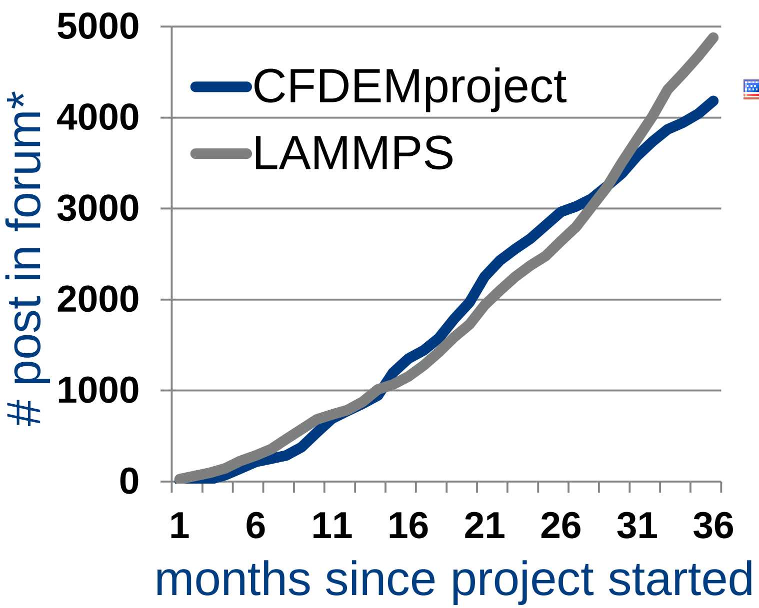
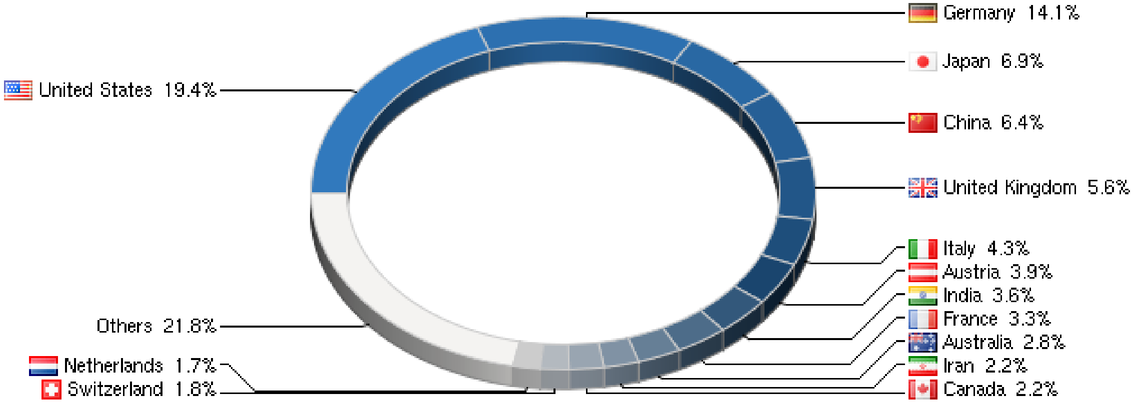
CFDEM Community after 3 yrs

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

Shown below are number of post in forums (left) and regional distribution of visitors.





From 28 Aug 2011 to 03 Jul 2013 (22 months):

23,898 unique site visitors from 112 countries

LAMMPS is one of the standard molecular dynamics (MD) codes

*from www.cfdem.com and http://sourceforge.net/mailarchive/forum.php?forum_name=lammps-users

III.

Modelling Approaches

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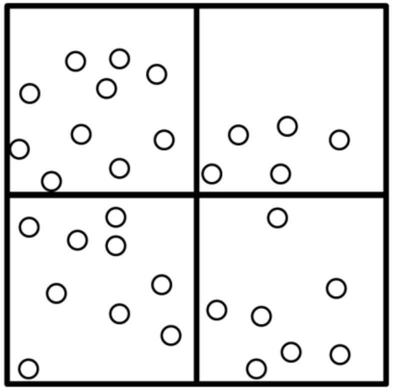
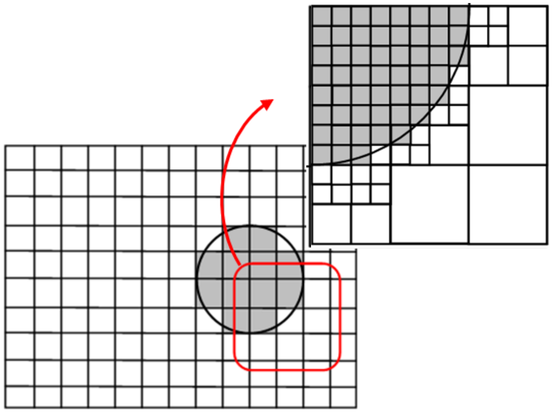
CFD-DEM

Fluid-particle interaction

CFDEM coupling **Computational Fluid Dynamics (CFD)** + **Discrete Element Method (DEM)** LIGGGHTS



- **unresolved CFD-DEM** ←
- **resolved CFD-DEM** →



- CFD-DEM[1]
- coarse grained CFD-DEM [2]
- MP-PIC[3]

- Immersed Boundary Method
- Fictitious Domain Method

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) 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

3) 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

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Unresolved CFD-DEM

Unresolved Discrete Modeling of fluid particle systems comes in different flavors…

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

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Unresolved CFD-DEM

Theoretical background – non-resolved CFD-DEM:

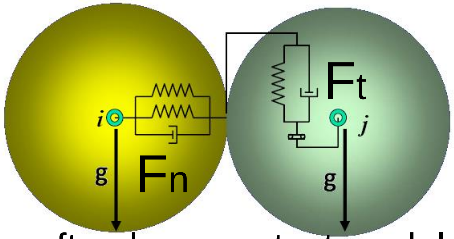
Navier-Stokes equations for the fluid in presence of a granular phase

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

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

Lagrangian Particle Trajectory for Particles

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



soft-sphere contact model:
linear spring-dashpot

α_f	fluid volume fraction
u_f	fluid velocity
τ, p	stress tensor, pressure
$\rho_{f,p}$	fluid/particle density
K_{fs}	fluid solid momentum exchange term
β	drag coefficient

LIGGGHTS+CFDEMcoupling
Unresolved CFD-DEM

Theoretical background – coarse grained CFD-DEM:

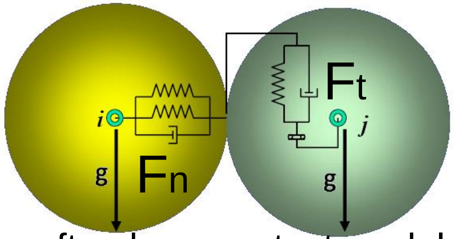
Navier-Stokes equations for the fluid in presence of a granular phase

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

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

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

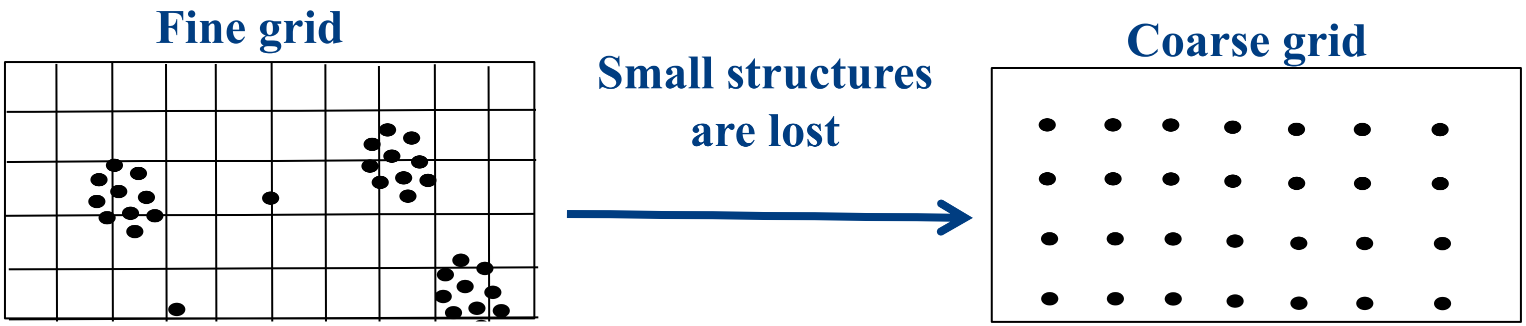
Scaling laws from dimensional analysis

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

- 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**

LIGGGHTS+CFDEMcoupling

Unresolved CFD-DEM



Fine grid

Small structures are lost

Coarse grid

Coarse grained simulations w/ coarser grids require filtered drag laws!

- The effective (filtered) drag is related to the “microscopic” (i.e., standard drag) via:

parcel size correction

fluid grid size correction

particle volume fraction correction

standard drag model

$$\frac{\bar{\beta}_p}{\beta_{p,micro}} = c_{corr}\left(\alpha\right)\left[1 - f\left(F_f, \bar{\phi}_p\right) h\left(\bar{\phi}_p\right)\right]$$

- Functions *f* and *h* are fitted to CFD-DEM data (not shown). The parcel size correction (i.e., the parameter *k* in the expression below) is based on a comparison for the sedimentation velocity:

$$c_{corr} = \exp\left[-k\left(\alpha - 1\right)\right]$$

Collaboration with Stefan Radl (Graz UT)

LIGGGHTS+CFDEMcoupling
Unresolved CFD-DEM

Theoretical background – CFD-DDPM:

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

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

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

Lagrangian Particle Trajectory for Parcels

$$\frac{\partial^2 \mathbf{x}_p}{\partial t^2} = \mathbf{g} + \frac{\beta}{\rho_p \alpha_p} \left(\mathbf{u}_f - \mathbf{u}_p\right) + \mathbf{F}_{\mathrm{int}\; eraction}$$

$$\mathbf{F}_{\mathrm{int}\; eraction} = -\frac{1}{\rho_p} \nabla \cdot \tau_s$$

$$\tau_s = -\frac{\pi}{6} \sqrt{3}\phi \frac{\alpha}{\alpha_{\max}} \rho_p g_0 \sqrt{\Theta}\,\mathbf{u}$$

Characteristics:

- **Fluid equations similar to CFD-DEM**
- **No resolved parcel-parcel interaction**
- **Prevent from overpacking by restoring “granular pressure” from kinetic theory**

Also needs corrections for coarse-graining / coarse-grid simulations!

LIGGGHTS+CFDEMcoupling

Unresolved CFD-DEM

Theoretical background – MP-PIC[1]:

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

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

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

Lagrangian Particle Trajectory for Parcels

$$\frac{\partial^2 \mathbf{x}_p}{\partial t^2} = \mathbf{g} + \frac{\beta}{\rho_p \alpha_p}\left(\mathbf{u}_f - \mathbf{u}_p\right) - \frac{1}{\rho_p} \nabla p + \mathbf{F}_{\mathrm{int}\, eraction}$$

$$\mathbf{F}_{\mathrm{int}\, eraction} = p^* \frac{\alpha_p^\beta}{\alpha_p^{\max} - \alpha_p}$$

Characteristics:

- **Fluid equations similar to CFD-DEM**
- **No resolved parcel-parcel interaction**
- **Prevent from overpacking by restoring “granular pressure”**

1) Basic form of equations following: *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*

Also needs corrections for coarse-graining / coarse-grid simulations!

Collaboration with Stefan Radl (Graz UT)

LIGGGHTS+CFDEMcoupling

Which Model to choose?

Coarse-Grained CFD-DEM

- uses soft-sphere contact models on parcel base
- can handle dense regions and equilibrium state
- Equations **converge to CFD-DEM particles**, which is well established

CFD-DDPM and MP-PIC

- difficulties for dense regions and equilibrium state
- needs additional formulation for particle-wall contact

- Both need corrections (filtered drag laws) for using coarser grids

LIGGGHTS+CFDEMcoupling

Resolved CFD-DEM

Incompressible Navier-Stokes equations (+BC)
conservation of
- mass and
- momentum

$$\rho\frac{\partial \boldsymbol{u}}{\partial t}+\rho(\boldsymbol{u}\cdot\nabla)\mathbf{u}=-\nabla \mathrm{p}+\mu\nabla^2\boldsymbol{u}\text{ in }\Omega \quad (1)$$

$$\nabla\cdot\boldsymbol{u}=0\text{ in }\Omega \quad (2)$$

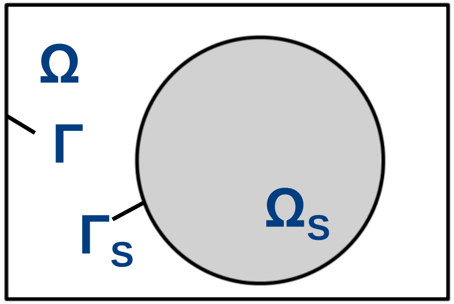
$$\boldsymbol{u}=\boldsymbol{u}_\Gamma\text{ on }\Gamma \quad (3)$$

Interface condition

$$\boldsymbol{u}=\boldsymbol{u}_i\text{ and }\sigma\cdot\hat{\boldsymbol{n}}=t_{\Gamma_S}\text{ on }\Gamma_S \quad (4)$$

Initial condition

$$\boldsymbol{u}(x,t=0)=\boldsymbol{u}_0(x)\text{ in }\Omega \quad (5)$$



u	velocity field
ρ	solid density
$\hat{n}$	outer normal vector
σ	stress tensor

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Resolved CFD-DEM

Integration of the **interface condition**:

$$\int_{\Gamma_s} \sigma \cdot \hat{n} d\Gamma_s = \int_{\Gamma_s} t_{\Gamma_s} d\Gamma_s$$

… applying **Divergence Theorem** and assuming a **Newtonian** fluid:

$$\int_{\Omega_s} -\nabla p + \nabla \cdot (\mu (\nabla u + (\nabla u)^T))\, d\Omega_s = \int_{\Gamma_s} t_{\Gamma_s}\, d\Gamma_s$$

Force:

$$\int_{\Gamma_s} t_{\Gamma_s} d\Gamma_s = \int_{\Omega_s} \overset{\text{pressure component}}{\boxed{-\nabla p}} + \boxed{\nu\rho\nabla^2 u\, d\Omega_s} \leftarrow \text{viscous component}$$

Numerical integration yields

$$f_{drag} = \sum_{c \in \overline{T_h}} \eta(c,t) \cdot V(c).$$

$\boldsymbol{V(c)}$	**… volume of cell c**
$\boldsymbol{\overline{T_h}}$	**… set of all solid-covered cells**
$\boldsymbol{\eta(c,t)}$	**… force at time t, evaluated at the center of cell c**

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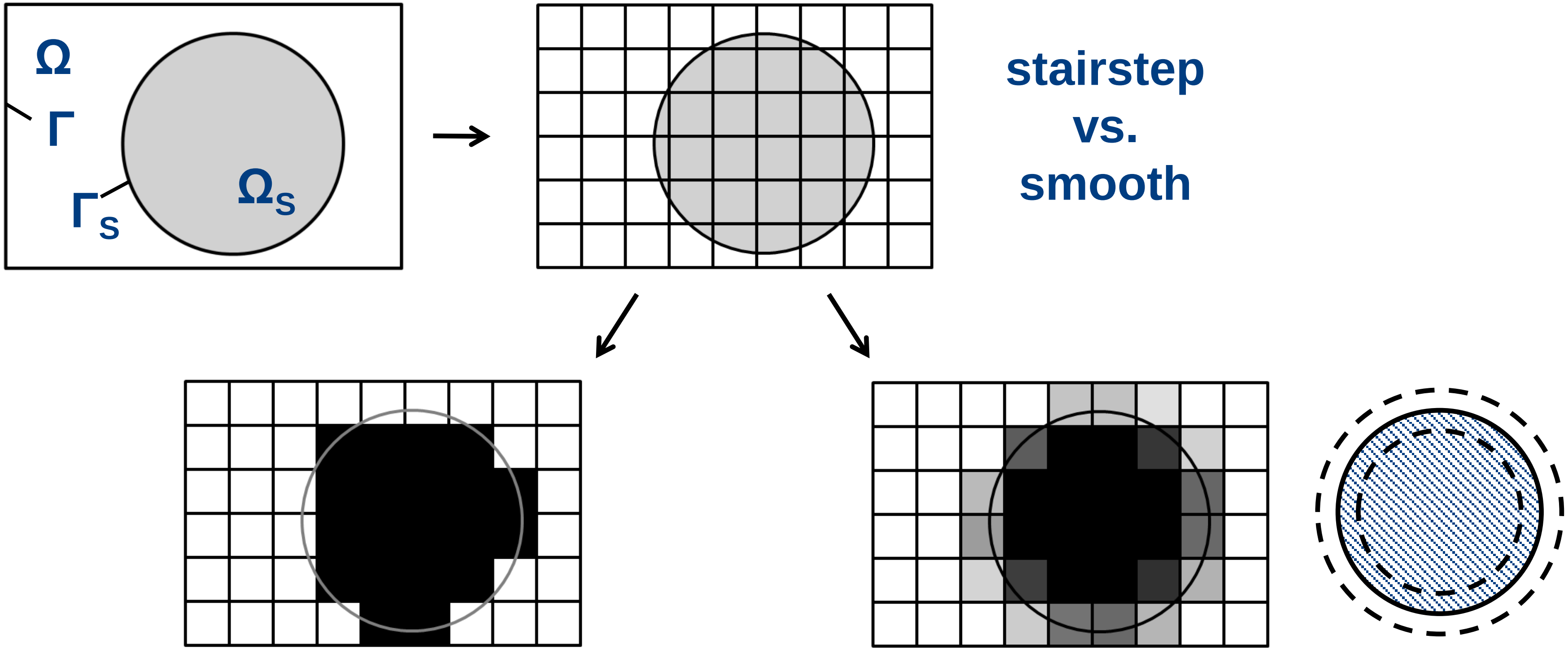
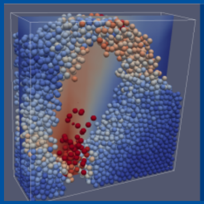
Resolved CFD-DEM



stairstep
vs.
smooth

stairstep representation:
- + fast
- + good results for high resolution
- - numerical troubles for dense packings

smooth representation:
- + higher accuracy in terms of volume representation
- + better numerical stability



III.

Scalability, Efficiency and Maintainability

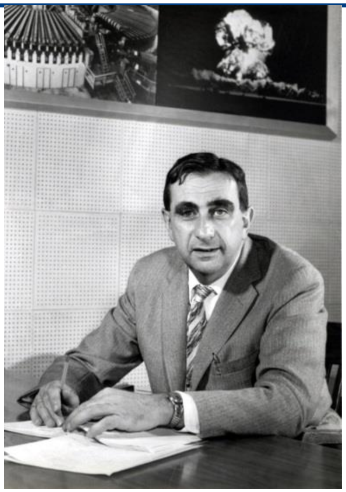
LIGGGHTS+CFDEMcoupling

Some wise words...

A state-of-the-art calculation requires 100 hours of CPU time on the state-of-the-art computer, independent of the decade.

-- *Edward Teller* ("father" of the hydrogen bomb and co-founder of Lawrence Livermore National Laboratory)

(stolen from Steve's quote board)



Problem: Computational time increases with:

- Smaller particles
- Larger application
- Higher flow dynamics

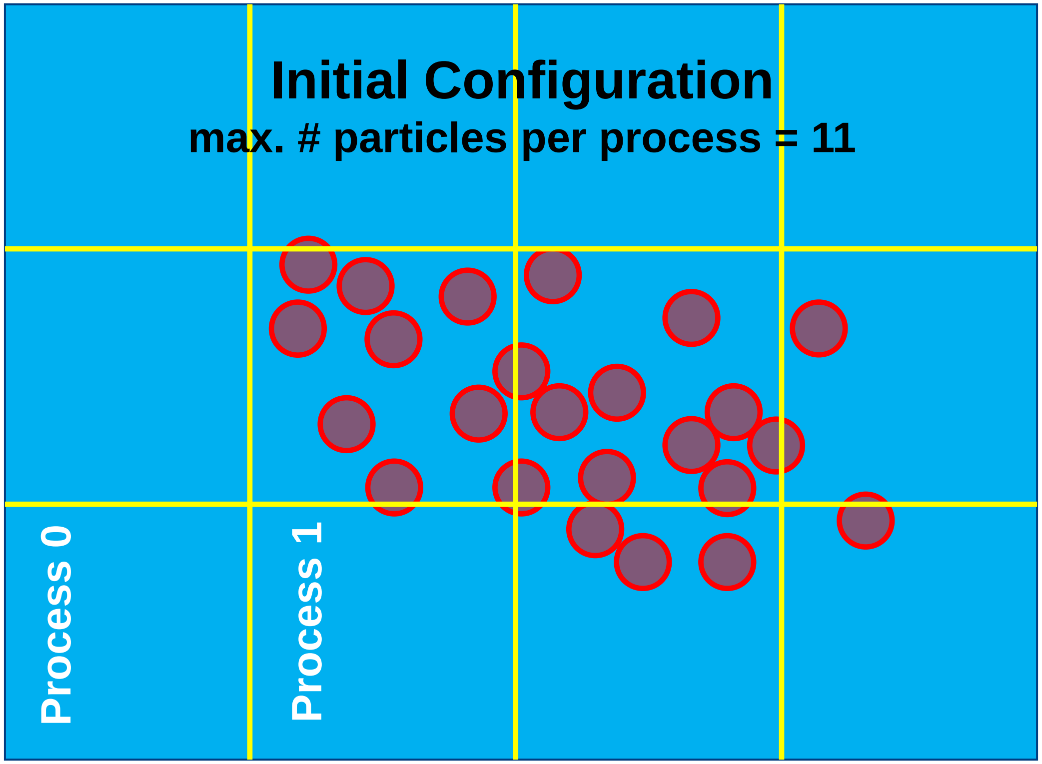
Solution:

- **Efficiency and Parallel Scalability** – harnessing availabe CPU ressources
- **Parcel approach** – particle coarse graining of 10 reduces sim. time by 1000

LIGGGHTS MPI Parallelization

How to distribute load between MPI processes?

If each process handles a different # of particles,
some of them will be idle (low efficiency)



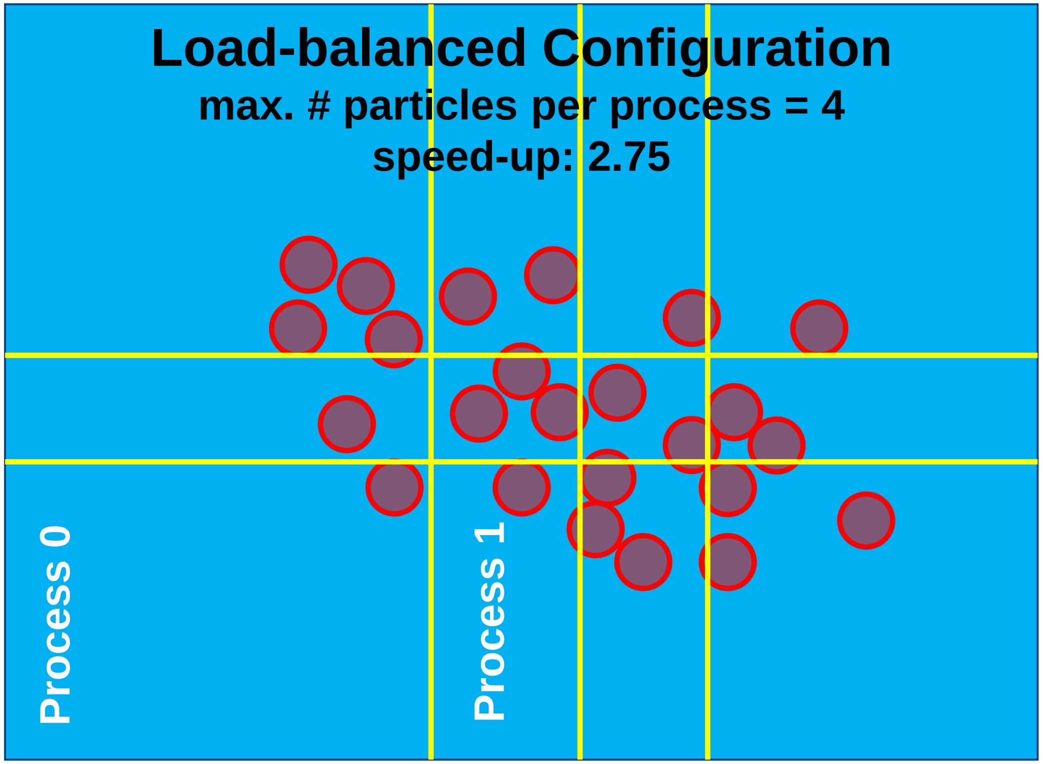
Thanks to:

LIGGGHTS MPI Loadbalancing

How to distribute load between MPI processes?

Load-balancing leads to better density distribution

Strategy: cuts in x and y direction so that each slice holds equal # of particles



Load-balanced Configuration

max. # particles per process = 4

speed-up: 2.75

Thanks to:

Sandia National Laboratories

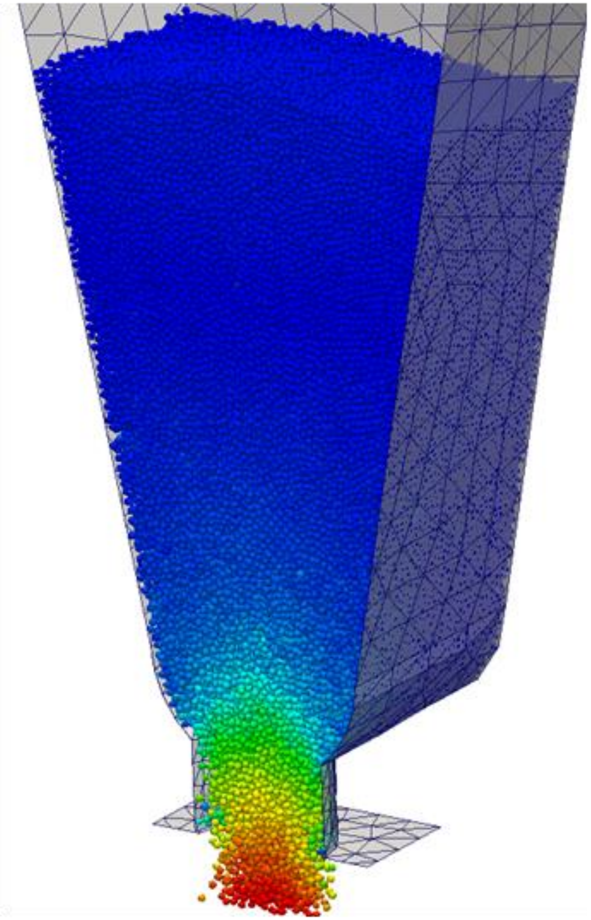
TEMPLE UNIVERSITY®

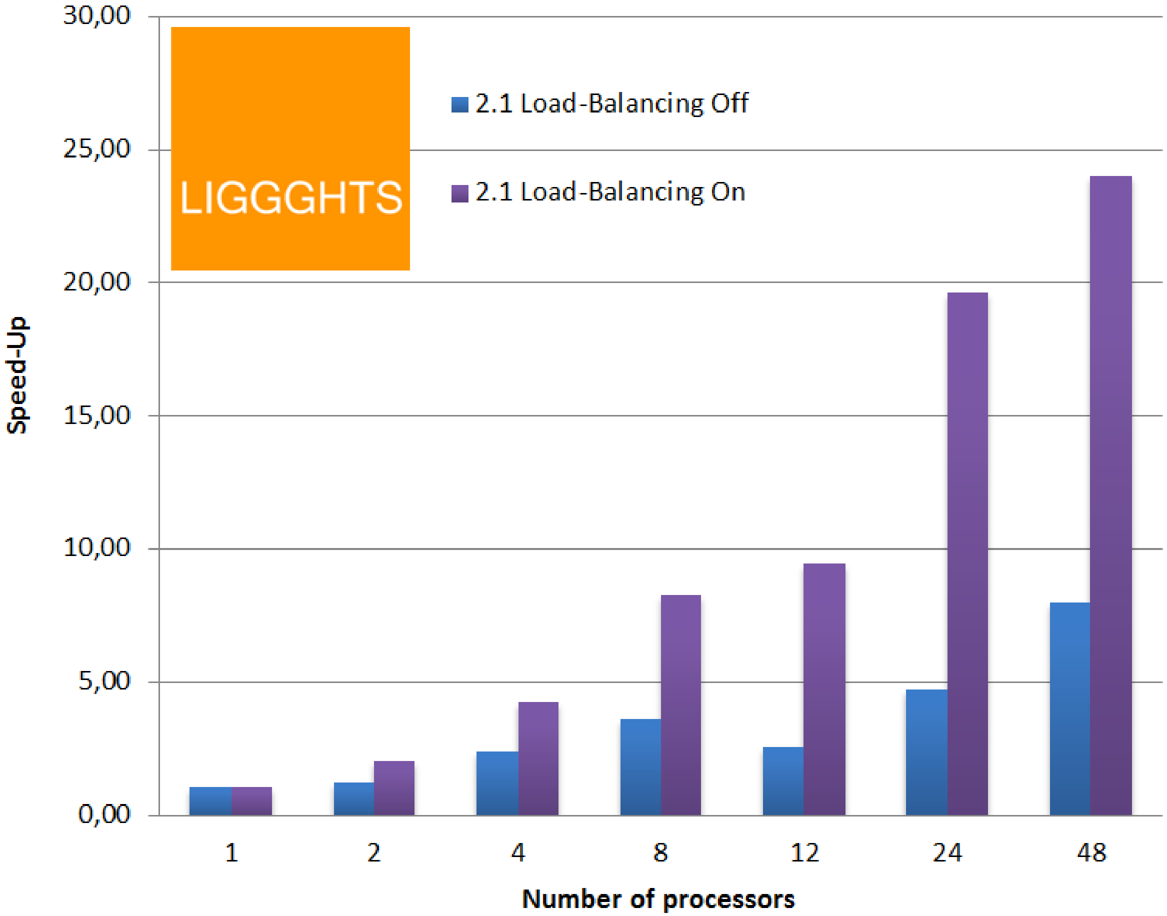
ICMS Institute for Computational Molecular Science

LIGGGHTS MPI Loadbalancing

Strong Scalability for Small-Scale Simulation of Hopper Discharge

300k particles, 400k stime-steps, run on small-scale cluster



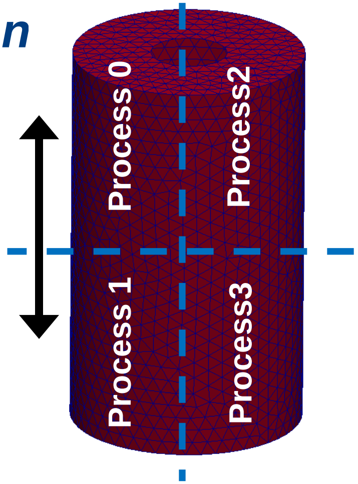


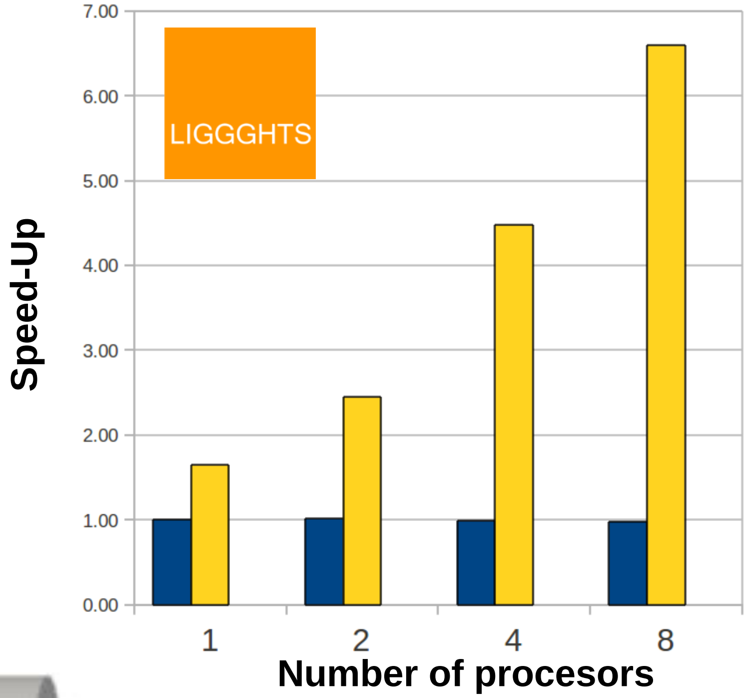
LIGGGHTS+CFDEMcoupling

LIGGGHTS Parallelization

Mesh Movement Parallelization

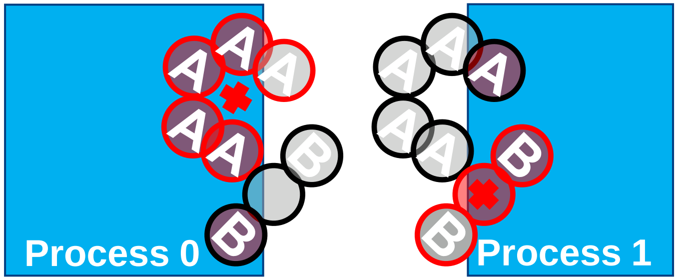
- vibratory oscillation of sample mesh
- blue: LIGGGHTS 1.5.3,
- yellow : LIGGGHTS 2.0)

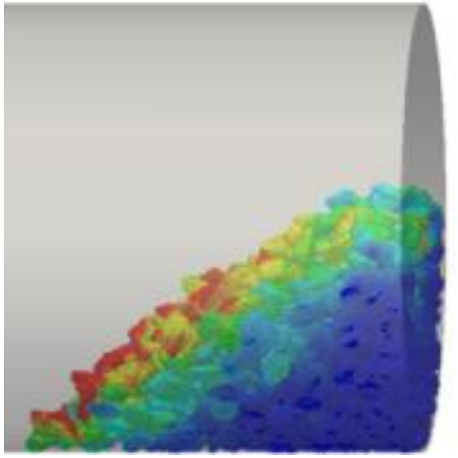


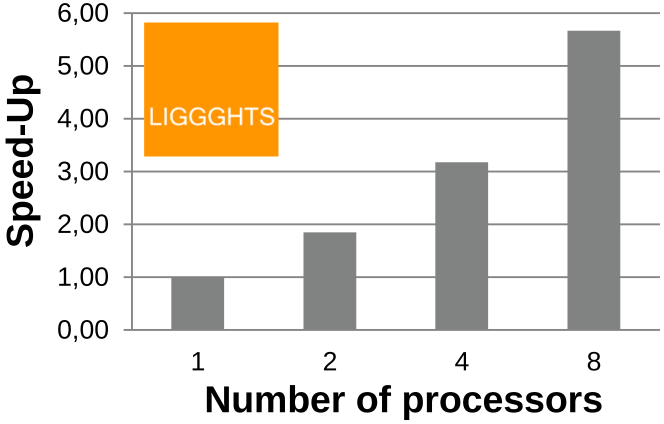


Multisphere Method Parallelization

- test case: angle of repose



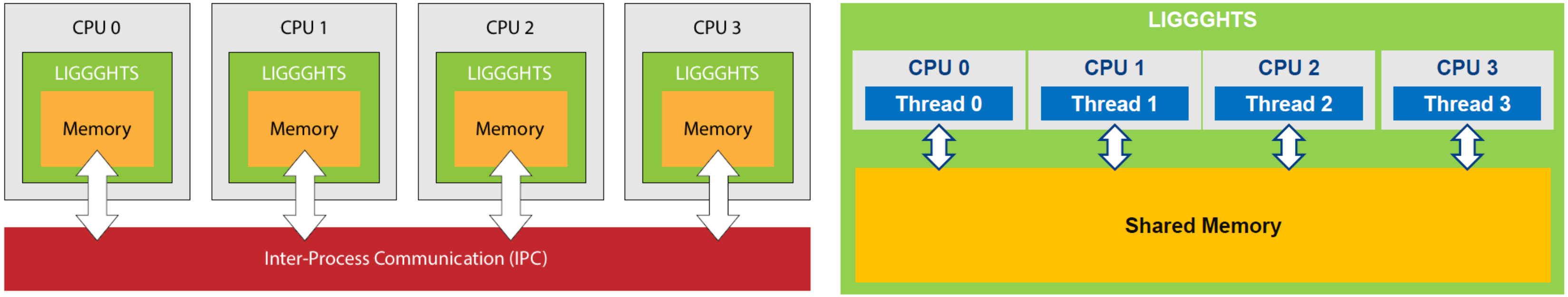




LIGGGHTS+CFDEMcoupling

LIGGGHTS & Shared Memory

- Need to make LIGGGHTS fit for hybrid **shared-distributed cluster architecture** (left: MPI parallelization, right: shared memory parallelization)

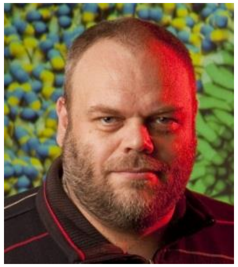


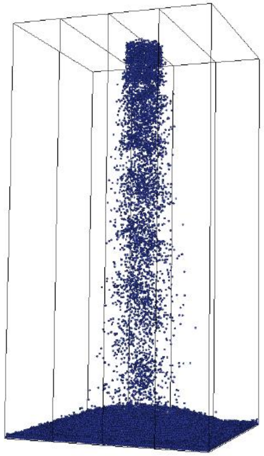
- **Box filling: preliminary result (right)**

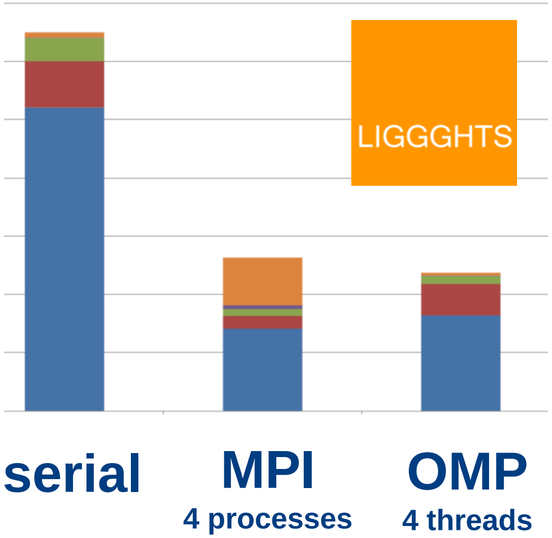
  67 k particles, 4 core CPU

- **Work by Richard Berger (JKU),**

  collaboration with Axel Kohlmeyer (Temple)







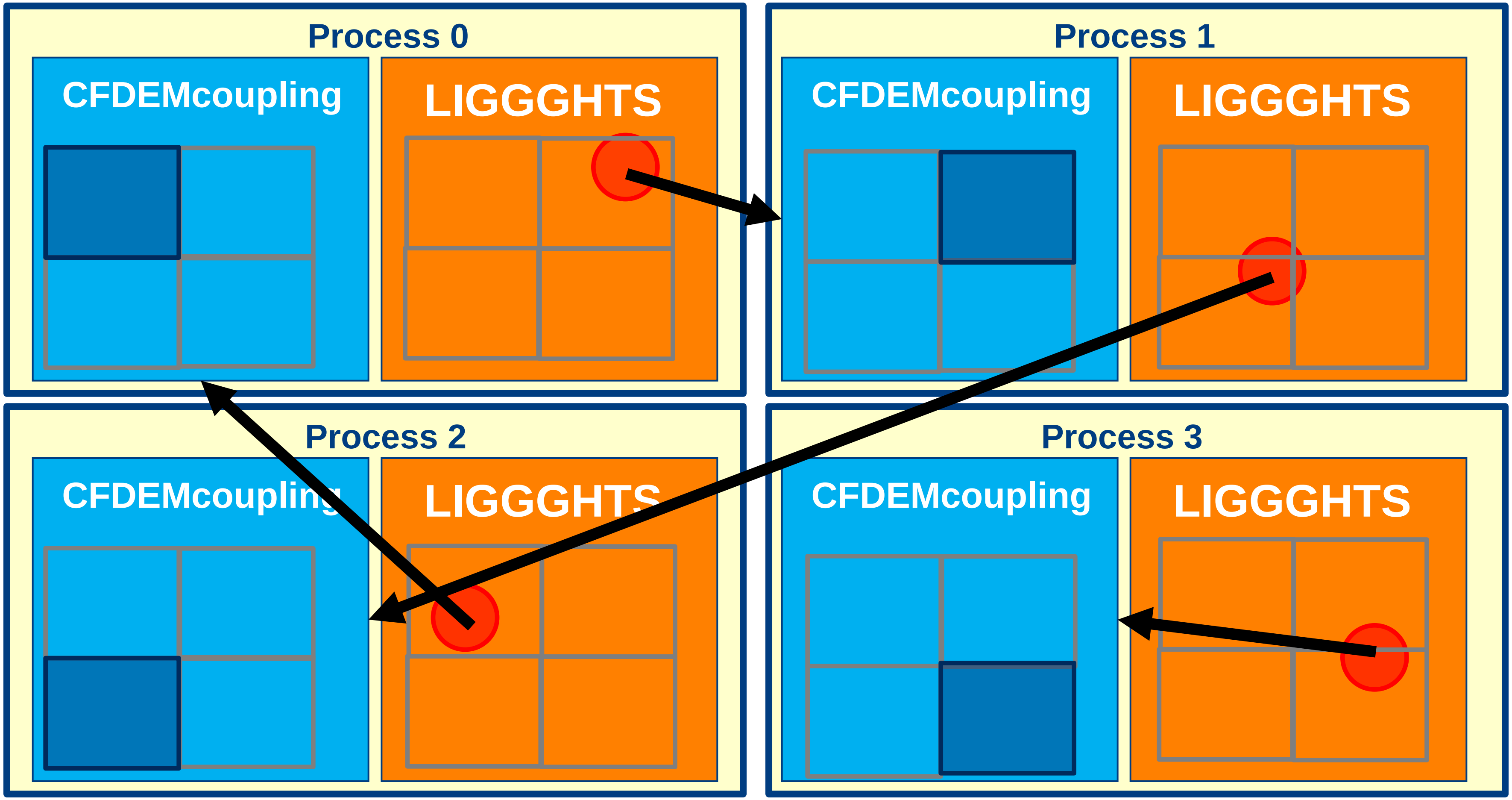
LIGGGHTS+CFDEMcoupling

CFDEMcoupling Scalability

Many2Many CFDEMcoupling communication scheme:

Step 1: Communicate particles using an existing communication pattern

(based on position in previous coupling step)



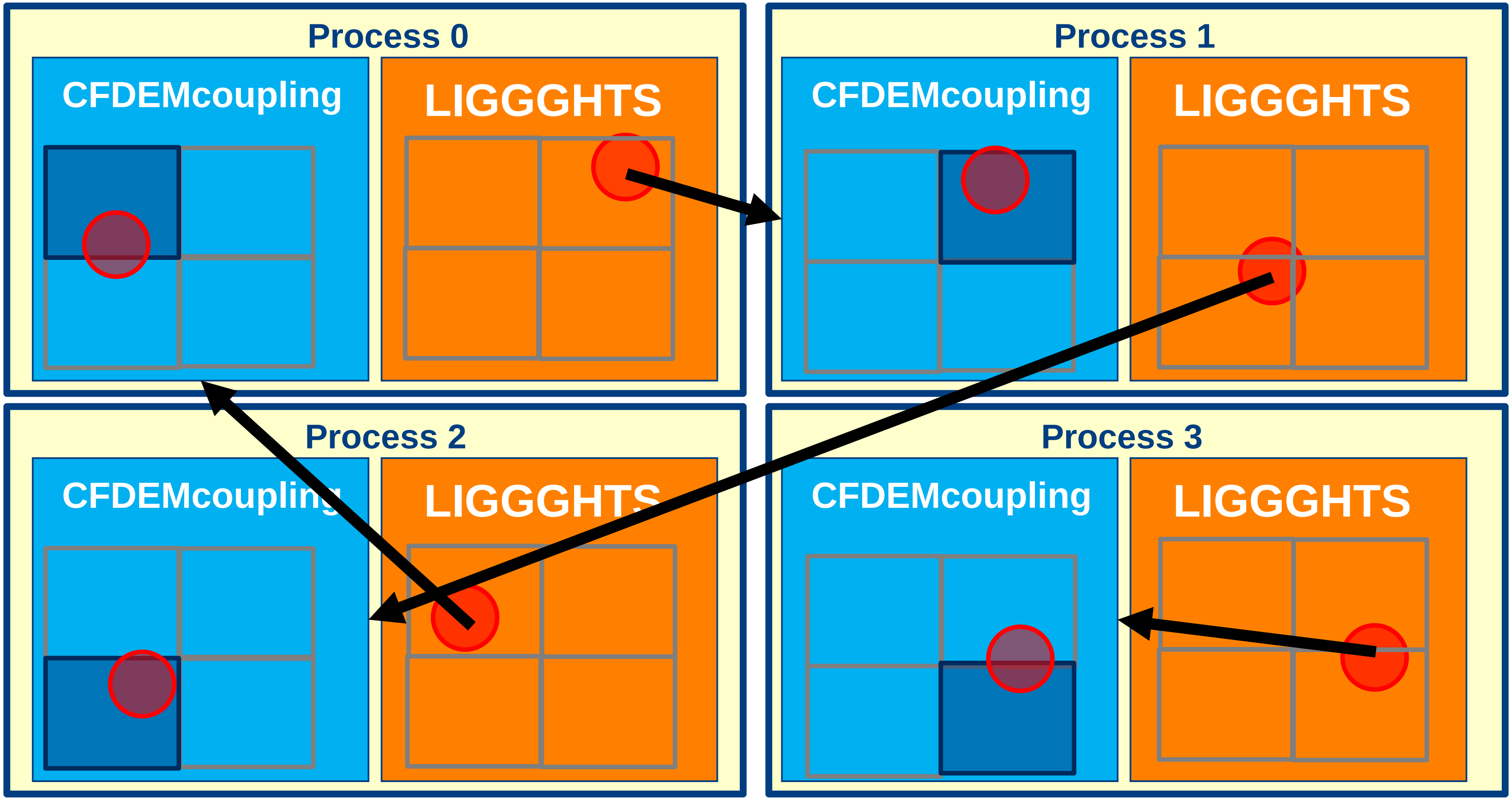
LIGGGHTS+CFDEMcoupling

CFDEMcoupling Scalability

Many2Many CFDEMcoupling communication scheme:

Step 2: Detect CFD domain passover (“defector” particles)

(based on current position)

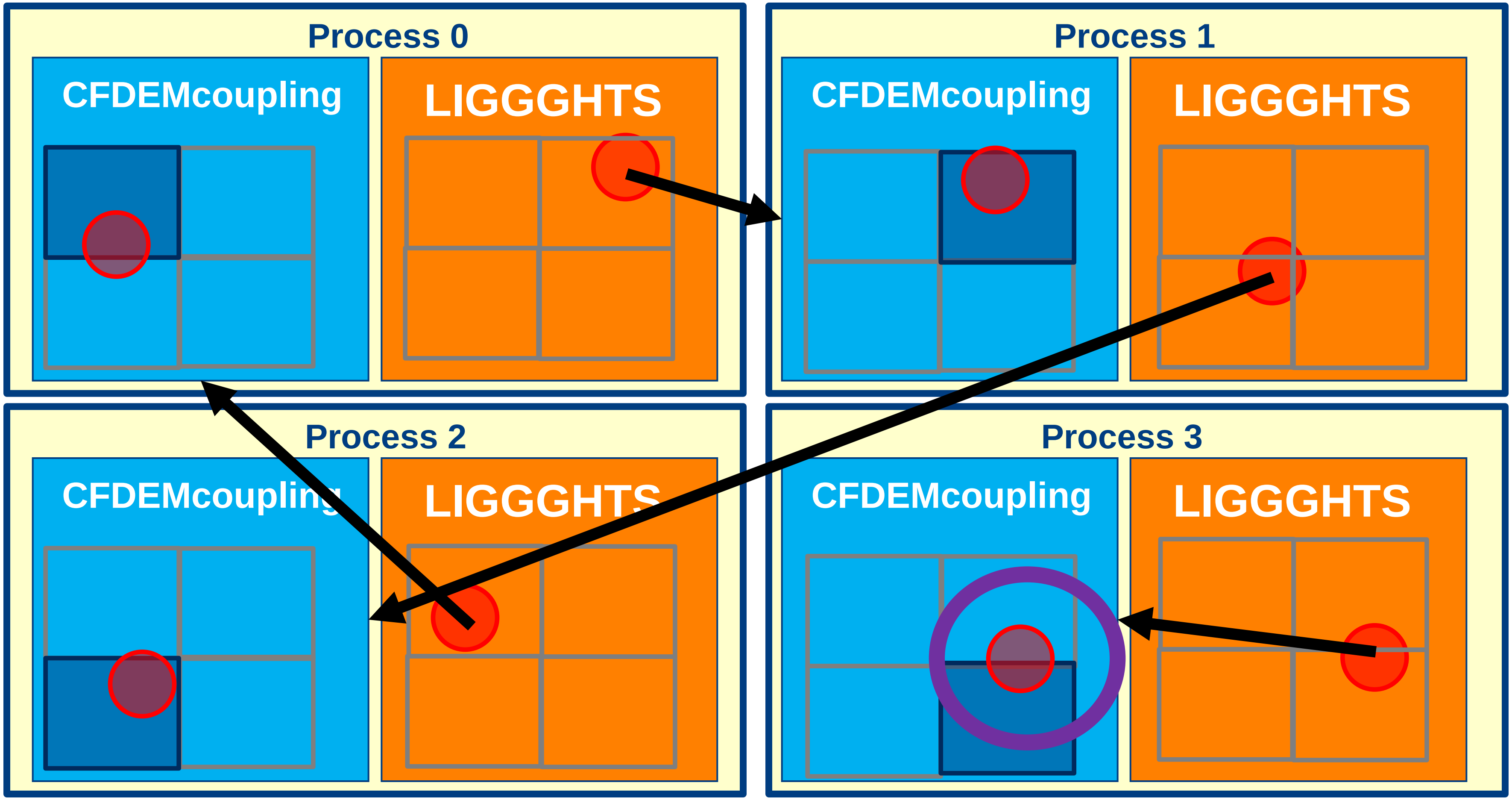


LIGGGHTS+CFDEMcoupling

CFDEMcoupling Scalability

Many2Many CFDEMcoupling communication scheme:

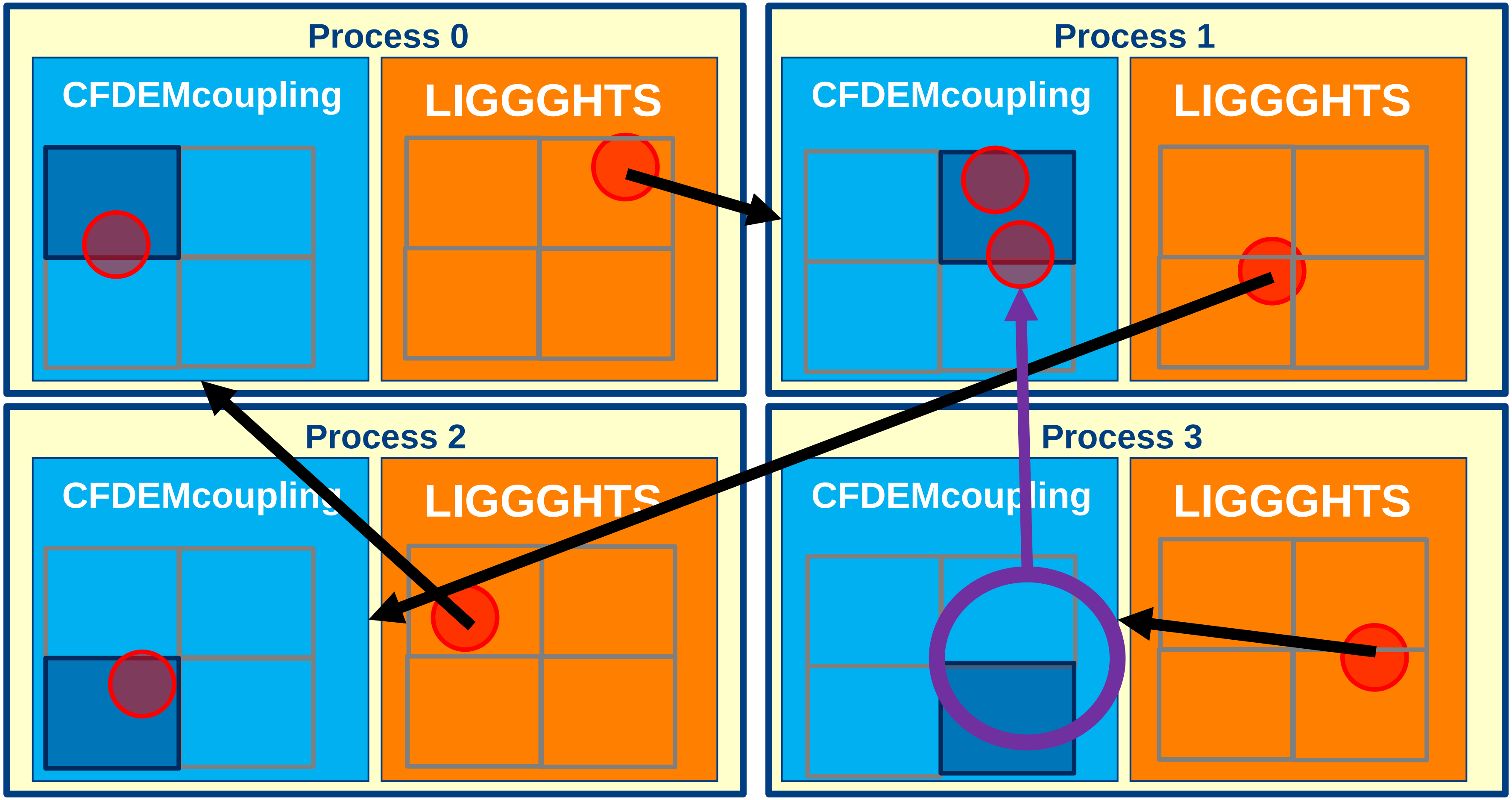
Step 3: Communicate “defector” particles to new host processors
(based on current position)



CFDEMcoupling Scalability

Many2Many CFDEMcoupling communication scheme:

Step 4: Update communication pattern for “defector” particle

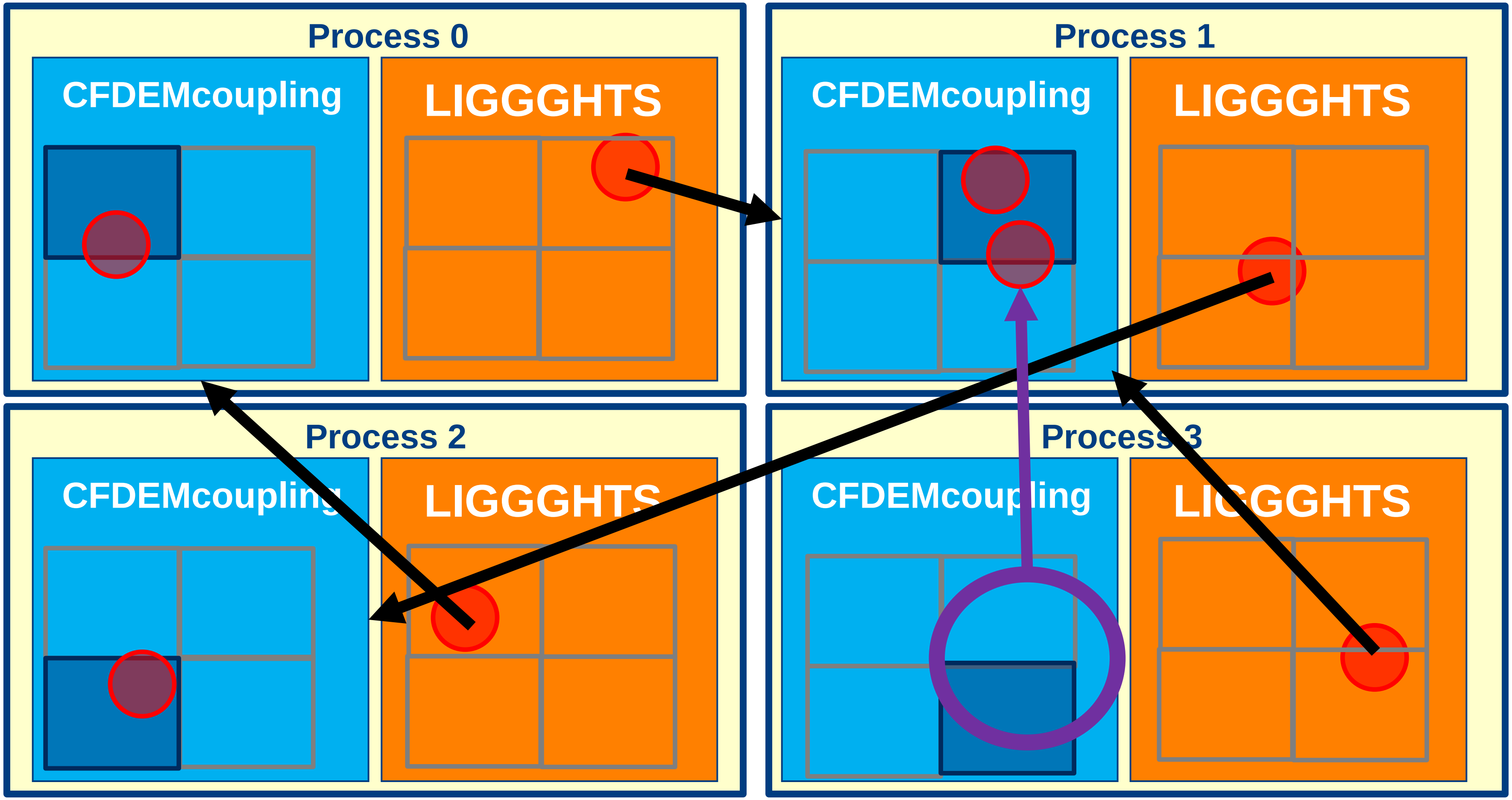


LIGGGHTS+CFDEMcoupling

CFDEMcoupling Scalability

Many2Many CFDEMcoupling communication scheme:

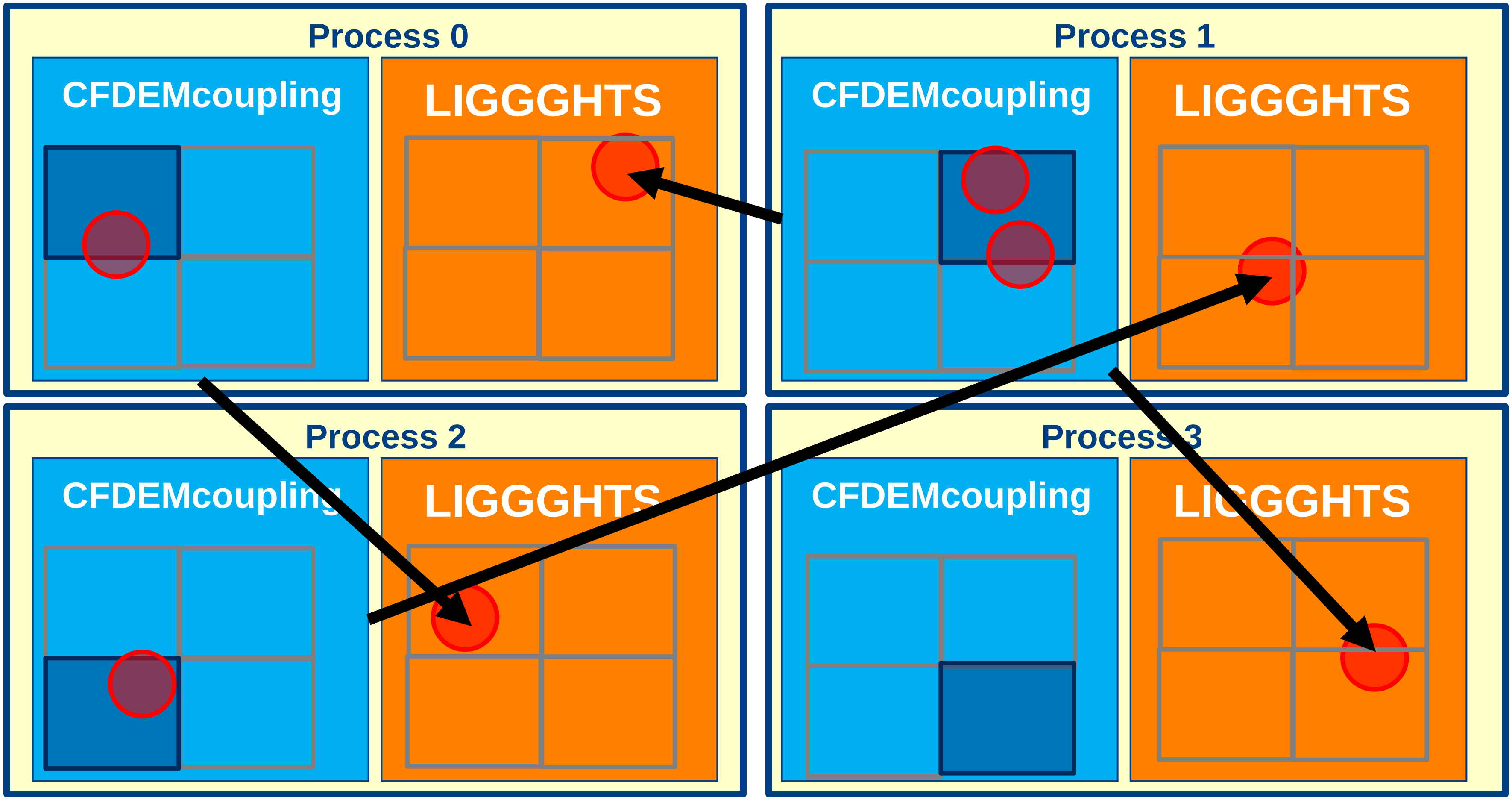
Step 5: Reverse Communication of dragforces etc.



CFDEMcoupling Scalability

Many2Many CFDEMcoupling communication scheme:

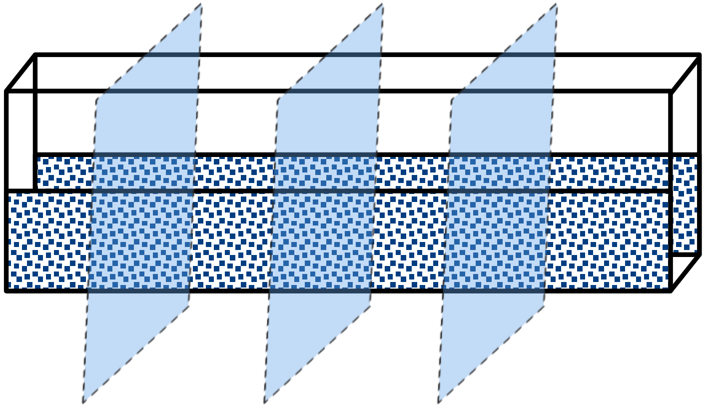
Step 5: Reverse Communication of dragforce



LIGGGHTS+CFDEMcoupling

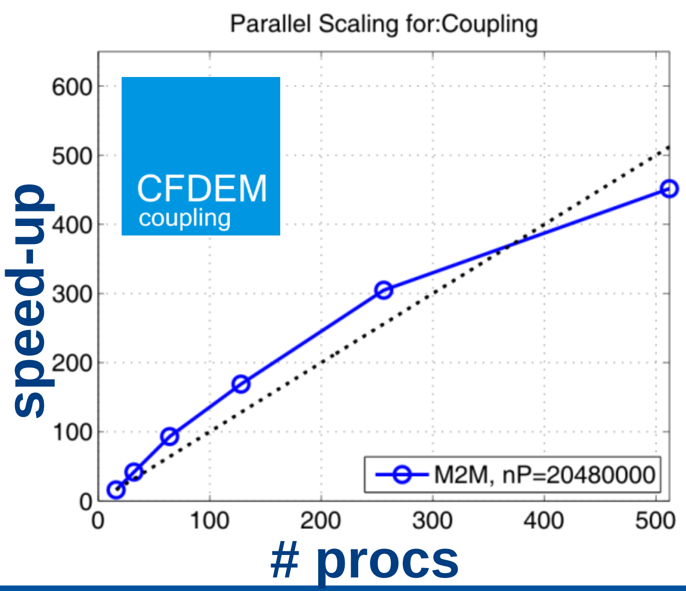
CFDEMcoupling Scalability

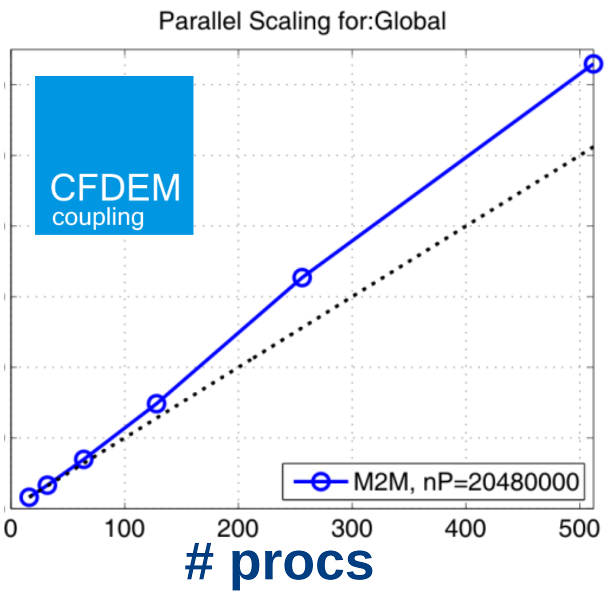
Fluidized Bed Scaled-Size Scalablity up to 512 Processors:

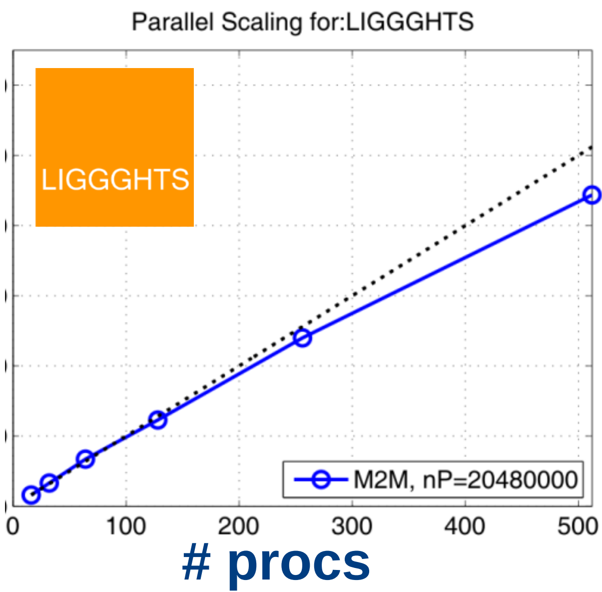


- 10.24 x 0.002 x 0.1 m / 10240 x 2 x 100 cells
- time step: CFD 1e-4s, DEM 1e-5 s

  coupling every 10 DEM steps
- Particles d_P = 0.3 mm
- **n_{proc} = 1 to 512, n_P= 2.048e7**







LIGGGHTS+CFDEMcoupling

Maintainablility

Re-write for mesh walls was incorporated in LIGGGHTS 2.X:

- **Parallelization of mesh handling** (mentioned before)
- Usage of **MPI-enabled templatized container classes**, models can now conveniently register and access properties.

  Are automatically communicated, and manipulated by mesh movements

```
FixMeshSurfaceStressServo::FixMeshSurfaceStressServo(some arguments) :
  FixMeshSurfaceStress(some arguments),
  xcm_(*mesh()->prop().addGlobalProperty< VectorContainer<double,3> >
                  ("xcm","comm_none","frame_invariant","restart_yes",3)),
```

- **Mesh movements** were **generalized** and can be superposed arbitrarily

LIGGGHTS+CFDEMcoupling

Maintainablility

Re-write for force kernels is in the works, to be incorporated in LIGGGHTS 3.X, planned for release within the next 6 months:

LIGGGHTS

- **Clean-up of force kernels**, every model is then located in exactly one file
- Usage of **templatized contactmodel classes**

```
template<typename Style>
class RollingModel<ROLLING_EPSD, Style> : protected Pointers
{
  RollingModel(some args)
  {
    history_offset = hsetup->add_value("r_torquex_old", "1");
    hsetup->add_value("r_torquey_old", "1");
    hsetup->add_value("r_torquez_old", "1");
    STATIC_ASSERT(Style::TANGENTIAL == TANGENTIAL_HISTORY);
  }
```

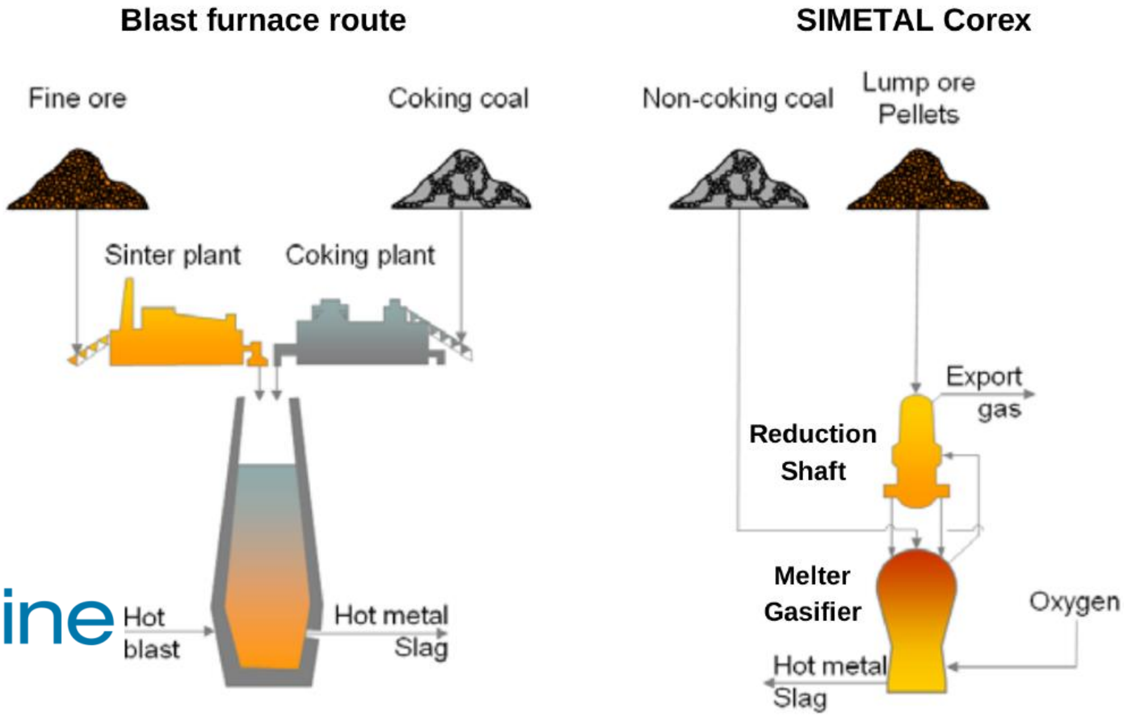
IV.

Applications: Iron/Steelmaking

LIGGGHTS+CFDEMcoupling

BF and Corex Process

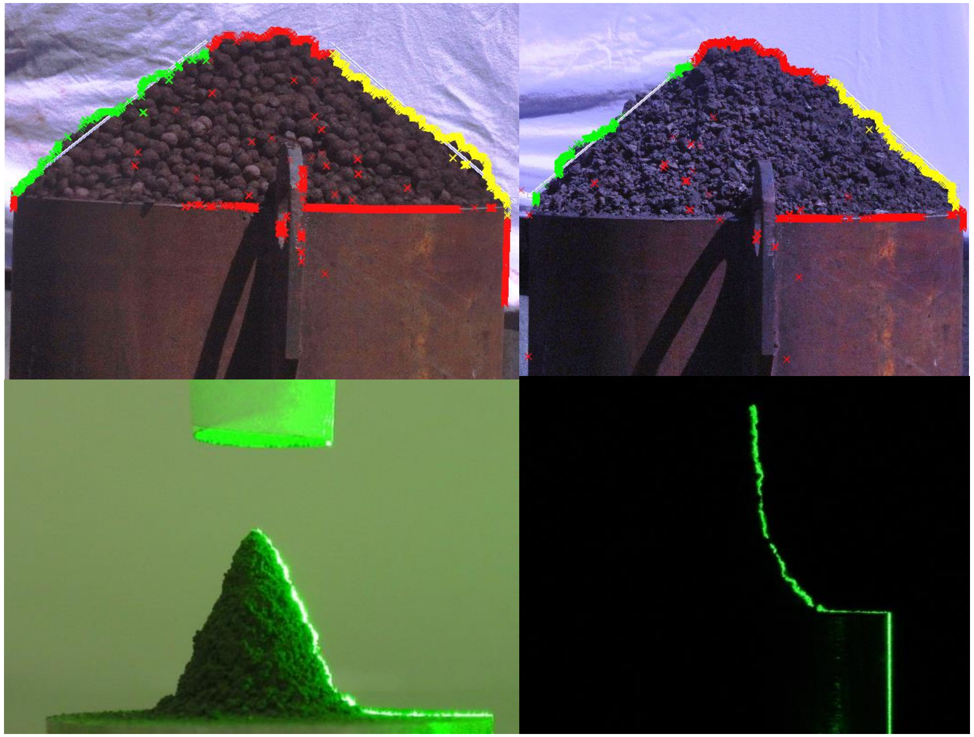
The production of hot metal via a traditional route involves a sinter plant, a coke oven plant and a blast furnace The **SIMETAL Corex® process** represents an alternative process to the blast furnace **where these units are substituted by one single unit**. In this process, a wide variety of coals (non-coking coals) as well as iron oxides, such as lump ores, pellets and sinter are used in a continuous process, consisting of two steps (**reduction shaft** and **melter gasifier**)

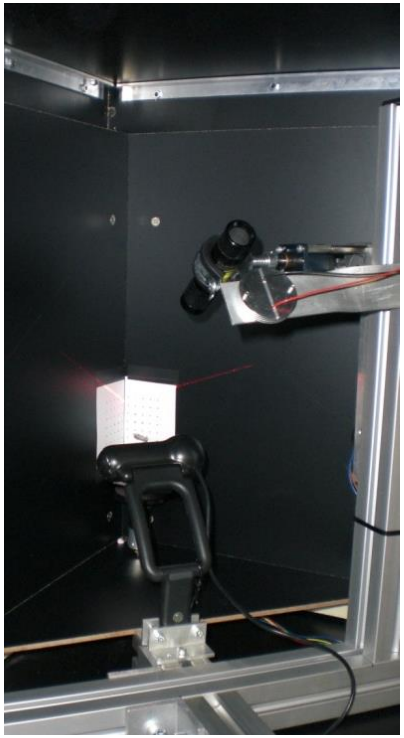


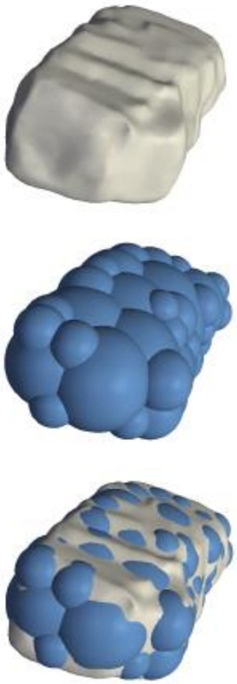
LIGGGHTS+CFDEMcoupling
Calibration and Validation

Calibration

- angle of repose, drop test, shear cell, friction test, shape recognition...



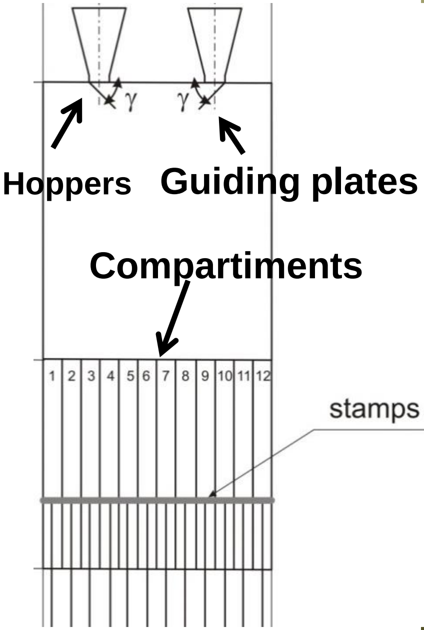


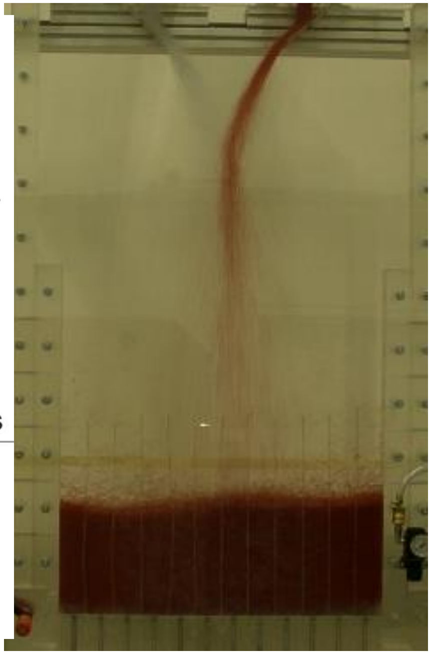


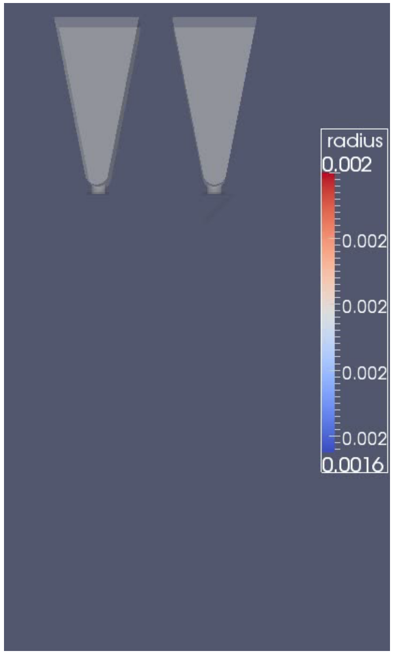
Coal particle and its approximation.

LIGGGHTS+CFDEMcoupling

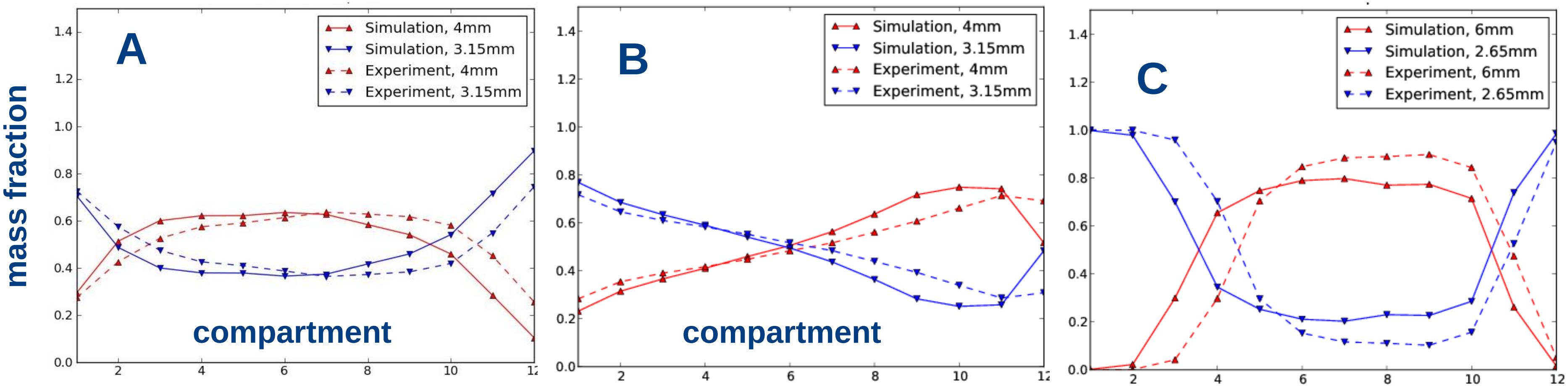
Calibration and Validation





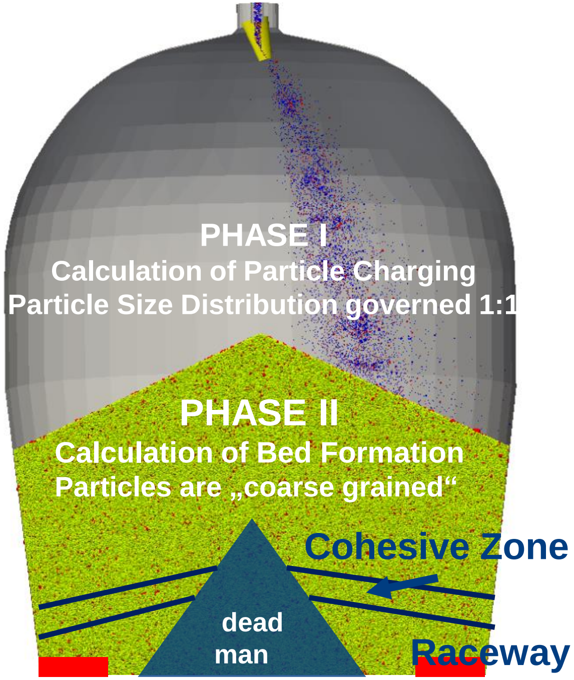


Case	A	B	C
$d_{p,1}$(mm)	4	4	6
$D_{orifice,1}$(mm)	38	38	38
$d_{p,2}$ (mm)	3.15	3.15	2.65
$D_{orifice,2}$ (mm)	34	22	34
$\dot{m}_1$ (kg/s)	0.66	0.66	0.573
$\dot{m}_2$ (kg/s)	0.506	0.113	0.539



LIGGGHTS+CFDEMcoupling

Impact of Charging Patterns



PHASE I

Calculation of Particle Charging

Particle Size Distribution governed 1:1

PHASE II

Calculation of Bed Formation

Particles are „coarse grained“

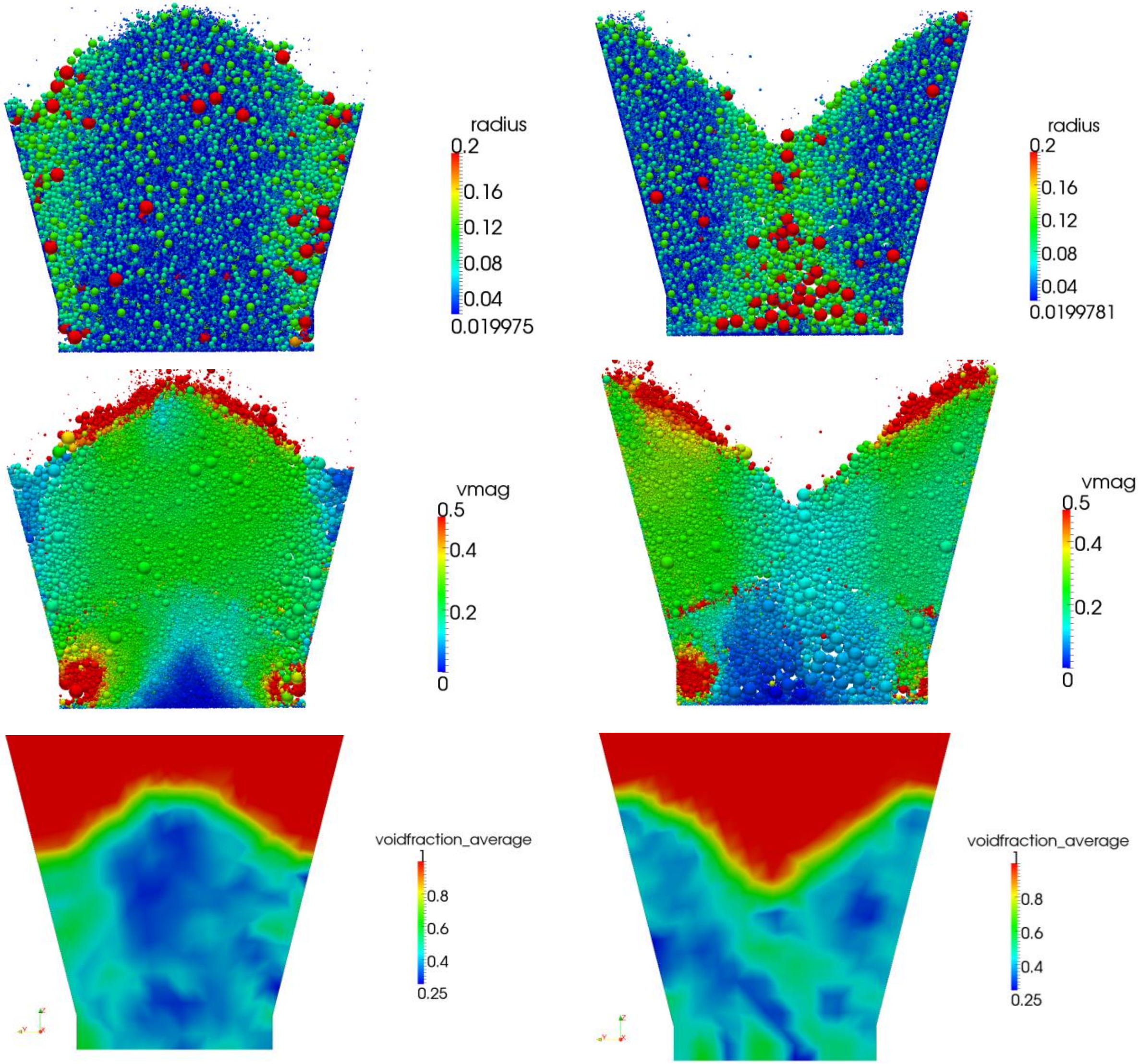
200 sec real-time

~500k parcels

24 procs, 8d sim time

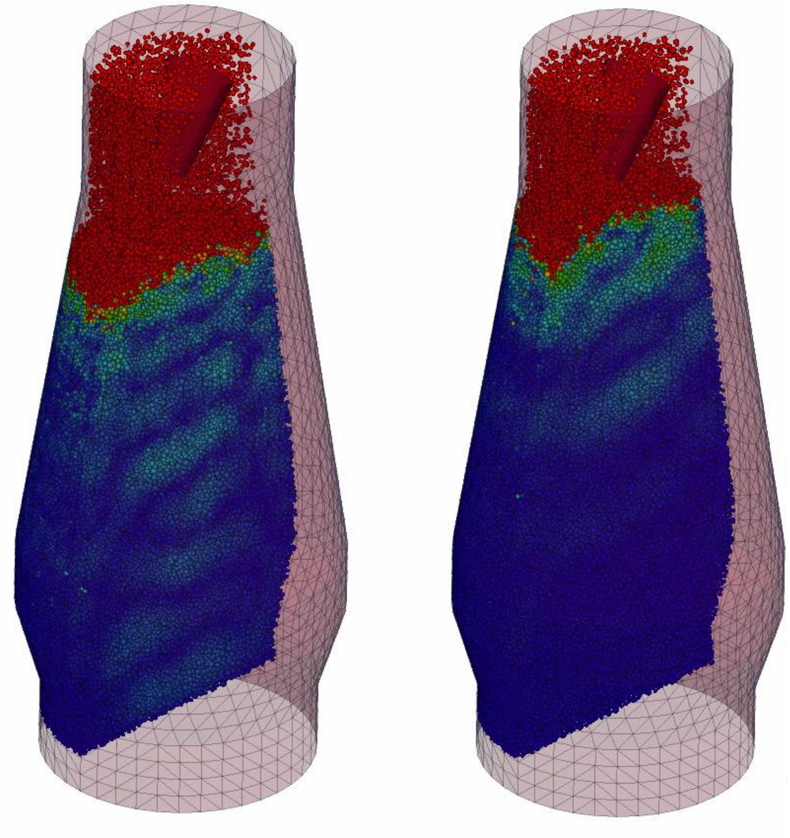
coarse-graining ~6

~100,000,000 particles

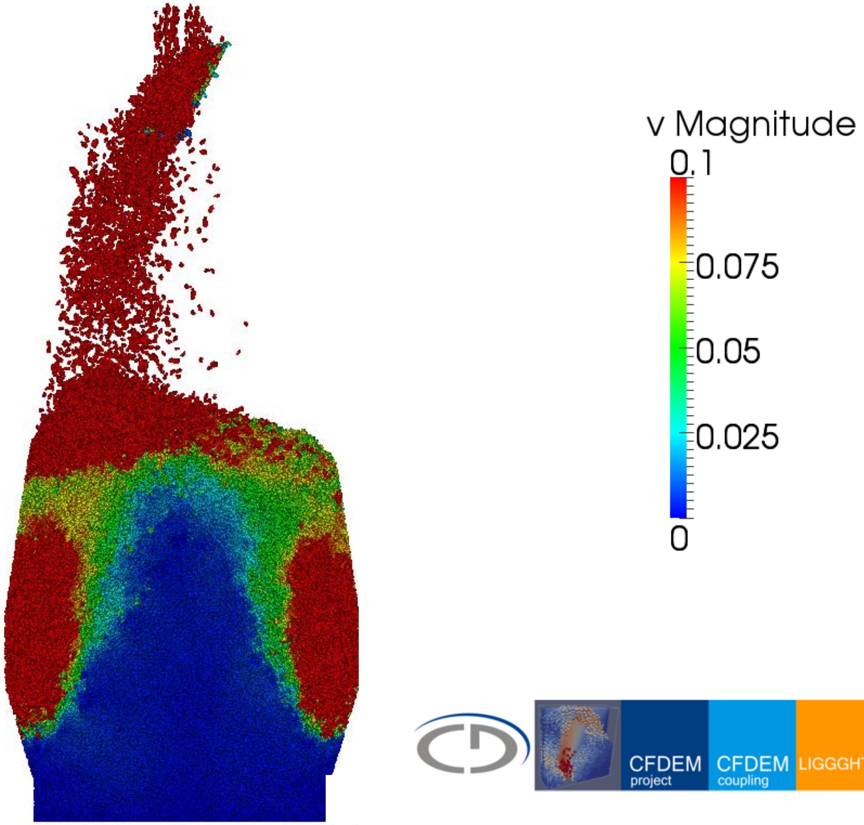


LIGGGHTS+CFDEMcoupling

Blast Furnace



Comparison of flow pattern for different values of non-sphericity modelled by rolling friction



Non-sphericity resolved by multi-sphere method (lower fill-level)

IV.

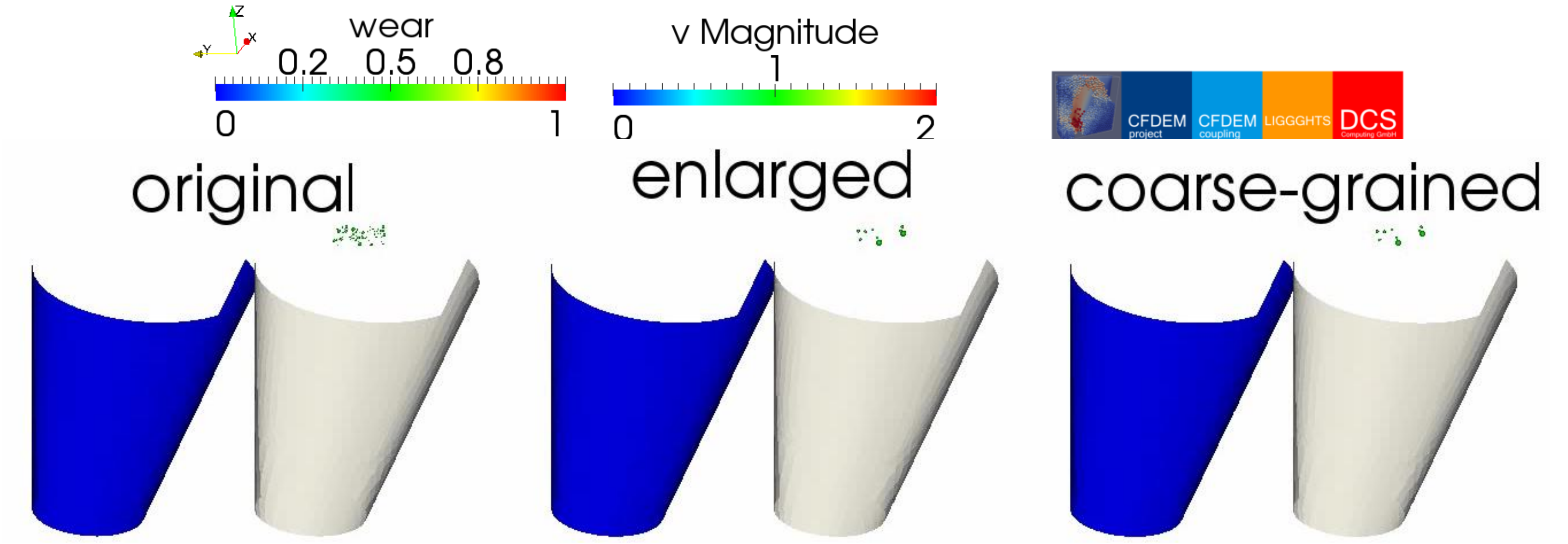
Applications: Bulk Solids Handling

LIGGGHTS+CFDEMcoupling

Case Study: Chute Abrasion

Chute Abrasion Simulation

- **Models: Finnie wear model** and (simplified) **Schiller-Naumann drag**
- Original (un-coarse-grained) system: 3700 particles / sec
- Coarse-grained system: coarse-graining factor 2, 462 particles /sec **(factor 8)**
- **Comparison of simply enlarged and correctly coarse-grained approach**



LIGGGHTS+CFDEMcoupling

Case Study: Chute Abrasion

Chute Abrasion with deformation

- **Finnie wear model** (Finnie 1972) was used to predict deformations

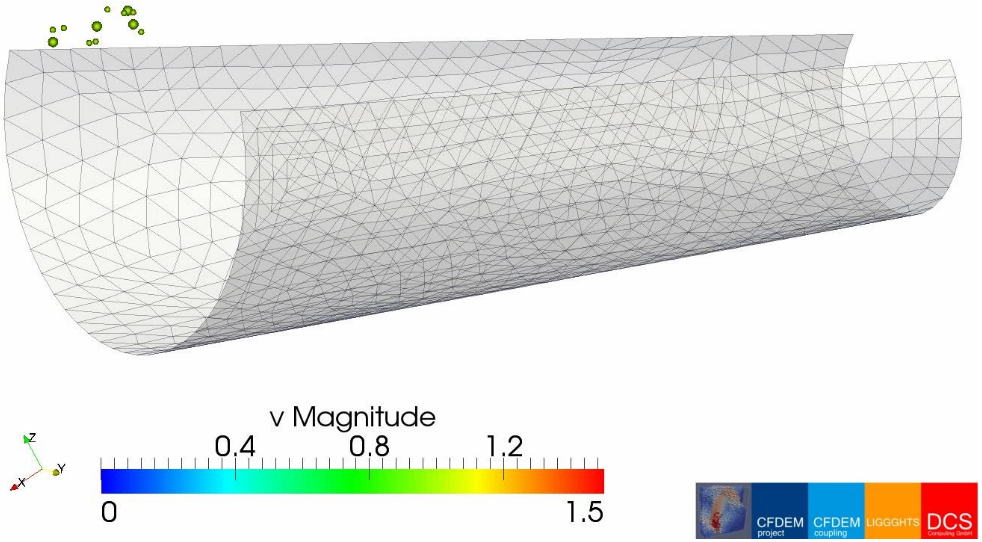
$$E = k_f \left|\mathbf{u}_\mathbf{p}\right|^2 f(\gamma_i),$$

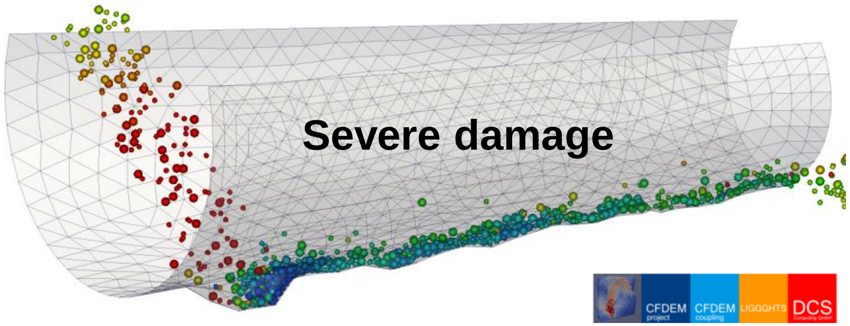
$$f(\gamma_i) = 1/3\cos^2(\gamma_i)\ \ ,\ \tan(\gamma_i) \geq 1/3,$$

$$f(\gamma_i) = \sin(2\gamma_i) - 3\sin^2(\gamma_i)\ \ ,\ \tan(\gamma_i) < 1/3,$$

$$EM = 2k_f \int_{tc,0}^{tc,1} hs(\mathbf{u}_\mathbf{p}\,\mathbf{c}_\mathbf{n})\sin(2\gamma_i)\,\mathbf{u}_\mathbf{p}\,\mathbf{f}_\mathbf{p\text{-}w}\ f(\gamma_i)\ dt.$$

- Deformations were mapped to the mesh nodes based on the point of impact.





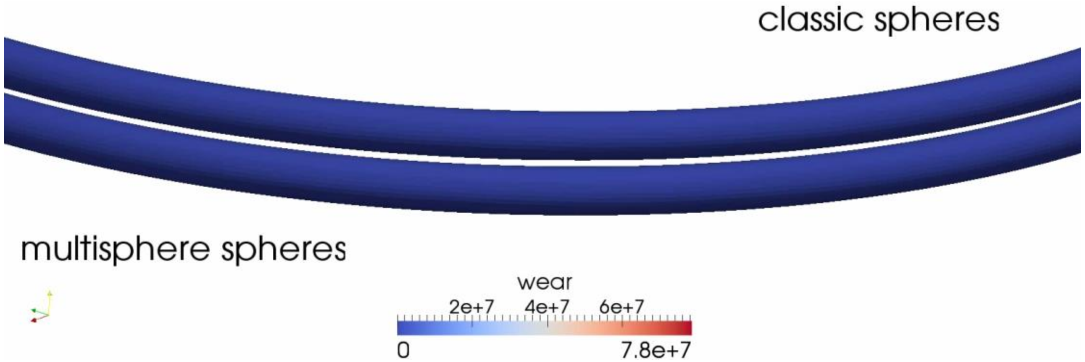
E	**erosion rate**
k_f	**material dependent model parameter**
u_p	**particle velocity**
γ	**impact angle**
f	**dependency on impact angle**

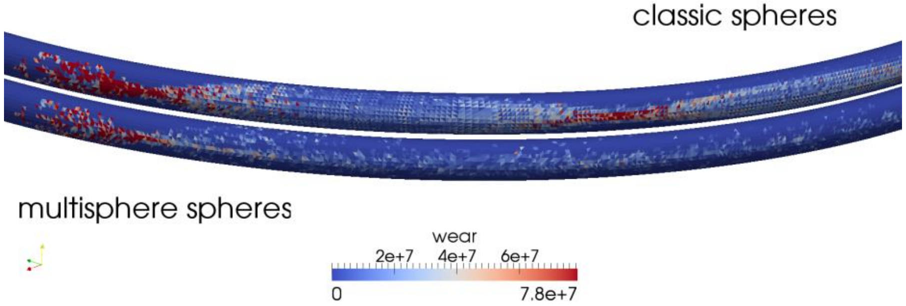
EM	**Eroded Mass**
hs	**Heaviside function**
$f_{p\text{-}w}$	**particle-wall contact force**
c_n	**particle-wall distance vector**

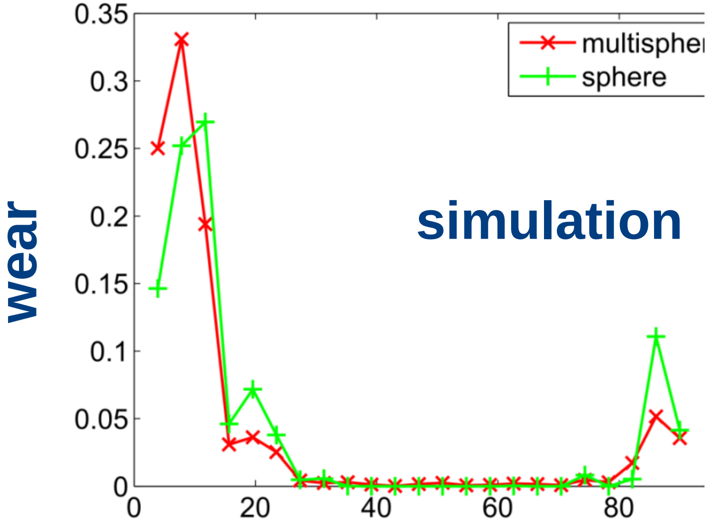
LIGGGHTS+CFDEMcoupling

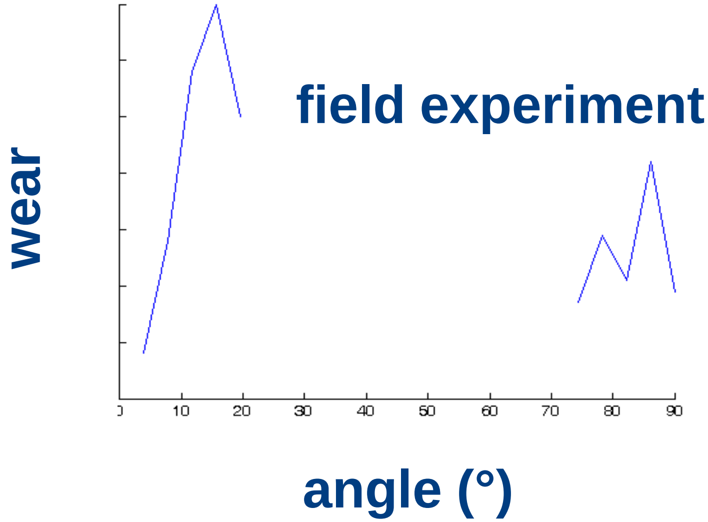
Pneumatic Conveying Erosion

animation









LIGGGHTS+CFDEMcoupling

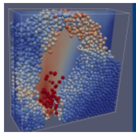
Excavator Simulation

```
simtime  :   0.000
throttle:     0.0%
brake    :    0.0%
gear     :       1
KiZyIn   :       0
HuZyIn   :      -1
LeZyIn   :       0
```

Work by **Christian Richter** and **Andre Katterfeld** (OVGU Madgeburg), in collaboration with TU Dresden, using **OpenModellica** and **Functional Mock-up Interface** (FMI) for coupling

LIGGGHTS+CFDEMcoupling

Transfer Chute Dust Emission



Transport equation for passive dust phase

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \left(\phi \, \mathbf{u}_{pa} \right) = \nabla \cdot \left(D_{diff} \nabla \phi \right) + S_T$$

$$\mathbf{u}_{pa} = \mathbf{u}_f$$

Φ	**dust concentration**
u_f	**fluid velocity**
u_{pa}	**dust phase velocity**
D_{diff}	**diffusion constant**
S_T	**source term**

Assumptions:

- coupling between phases is strong

- loading of the secondary phase << 1

→ treated as passive phase

Manninen, M. (1996): On the mixture model for multiphase flow, VTT Publications 288, Technical Research Centre of Finland

Source term for passive dust phase

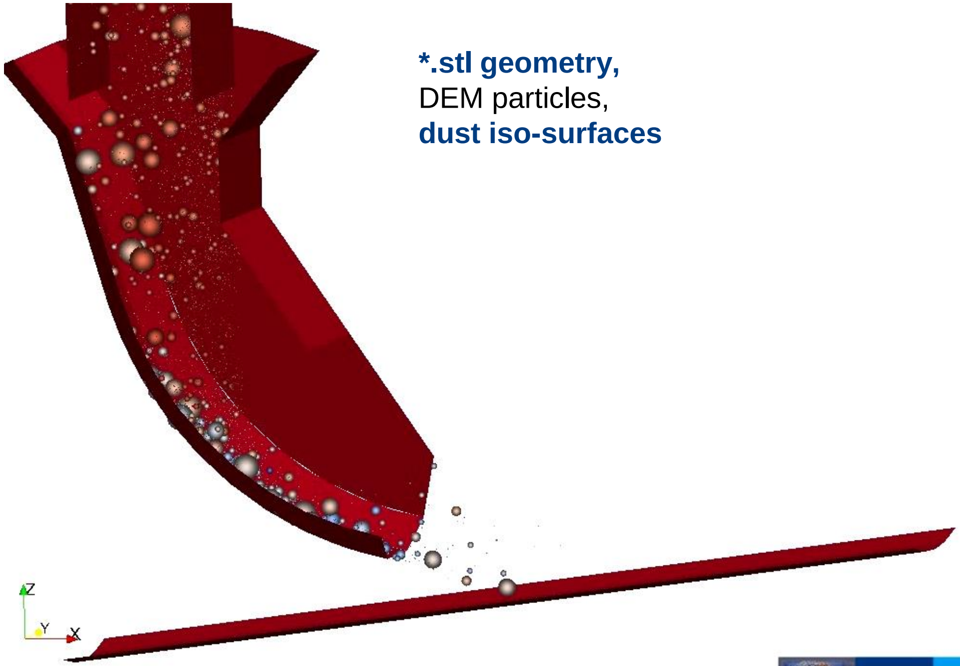
$$S_T = \frac{C \, r_p \left| \mathbf{u}_f \right|^3}{V_{cell}}$$

S_T	**source term**
V_{cell}	**computational cell**
u_f	**fluid velocity**
r_p	**particle diameter**
C	**model constant**

Hilton, J.E. and Cleary, P.W. (2011): "Dust Dispersal Modelling on a Conveyor Chute using a Coupled Discrete Element and CFD Method", 8th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries, SINTEF/NTNU, Trondheim Norway, 21-23 June 2011

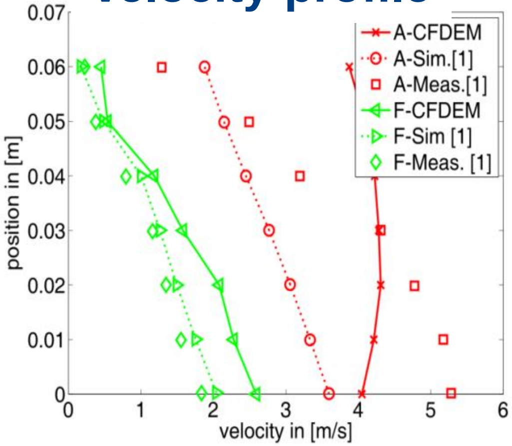
LIGGGHTS+CFDEMcoupling

Transfer Chute Dust Emission

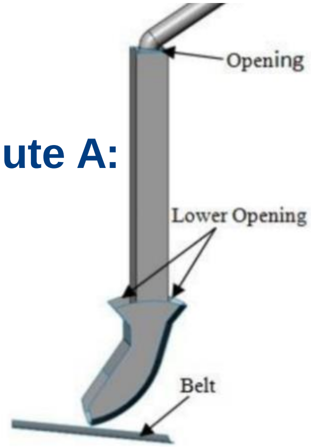


***.stl geometry,**
DEM particles,
dust iso-surfaces

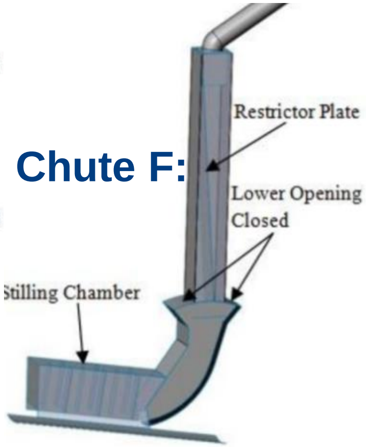
velocity profile



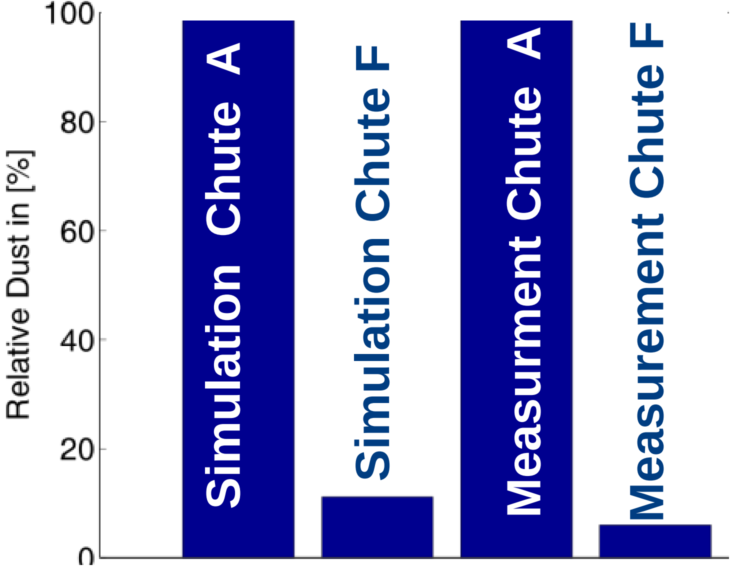
Chute A:



Chute F:



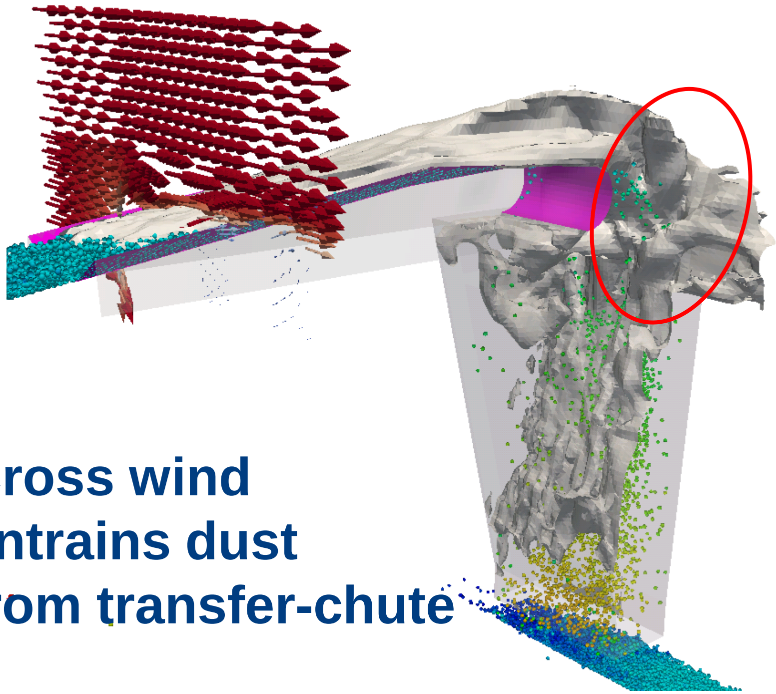
relative dust flux at outlet



LIGGGHTS+CFDEMcoupling

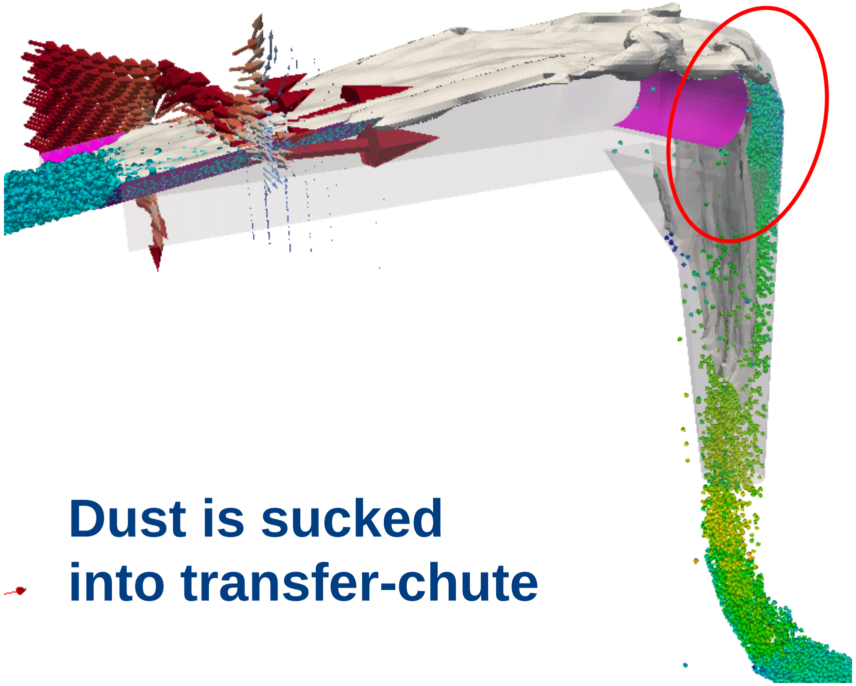
Transfer Chute Dust Emission

Original Geometry



Cross wind entrains dust from transfer-chute

Optimized Geometry



Dust is sucked into transfer-chute

Publications:

Kloss, C., Goniva, C., Katterfeld, A.: Simulation of wear and dust emission at a transfer chute; Cement International, 2012 (10), 2-9

measurem.data from: 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

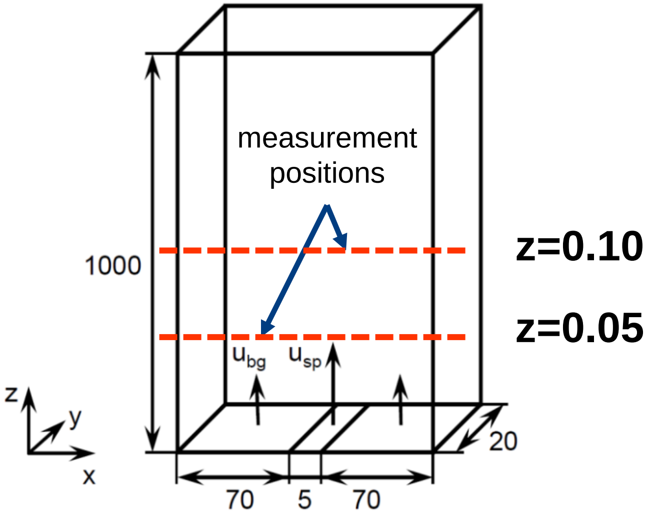
IV.

Applications: Fluidized Beds

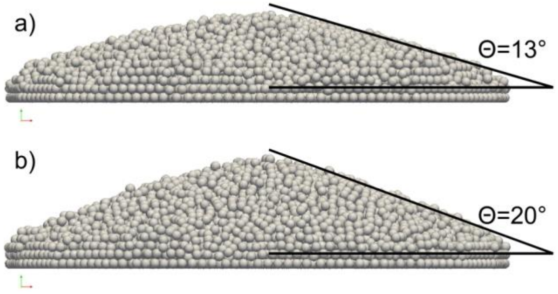
LIGGGHTS+CFDEMcoupling

Single Spout Fluidized Bed

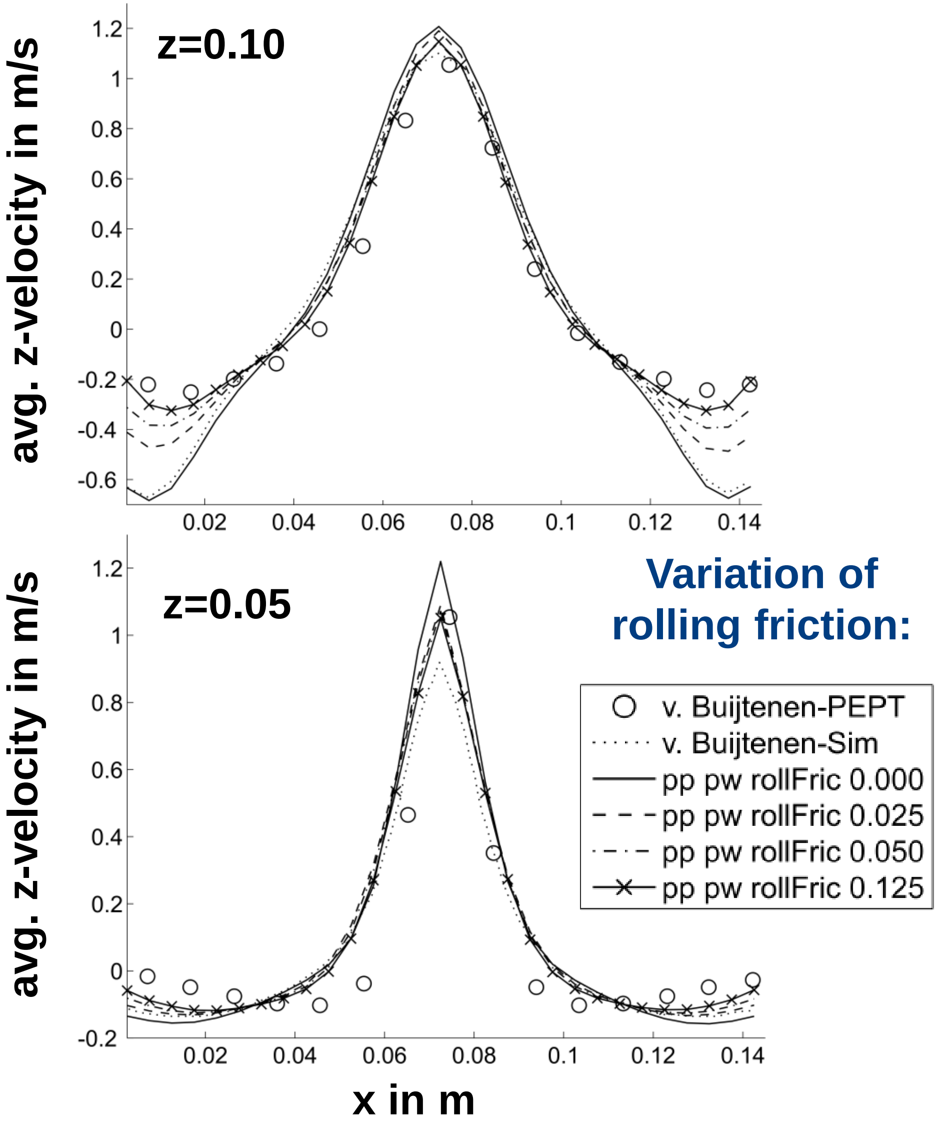
Geometry:



Variation of rolling friction:



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

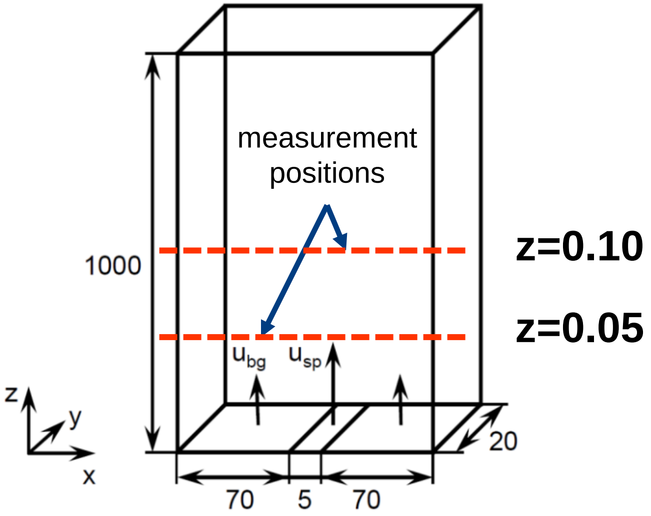


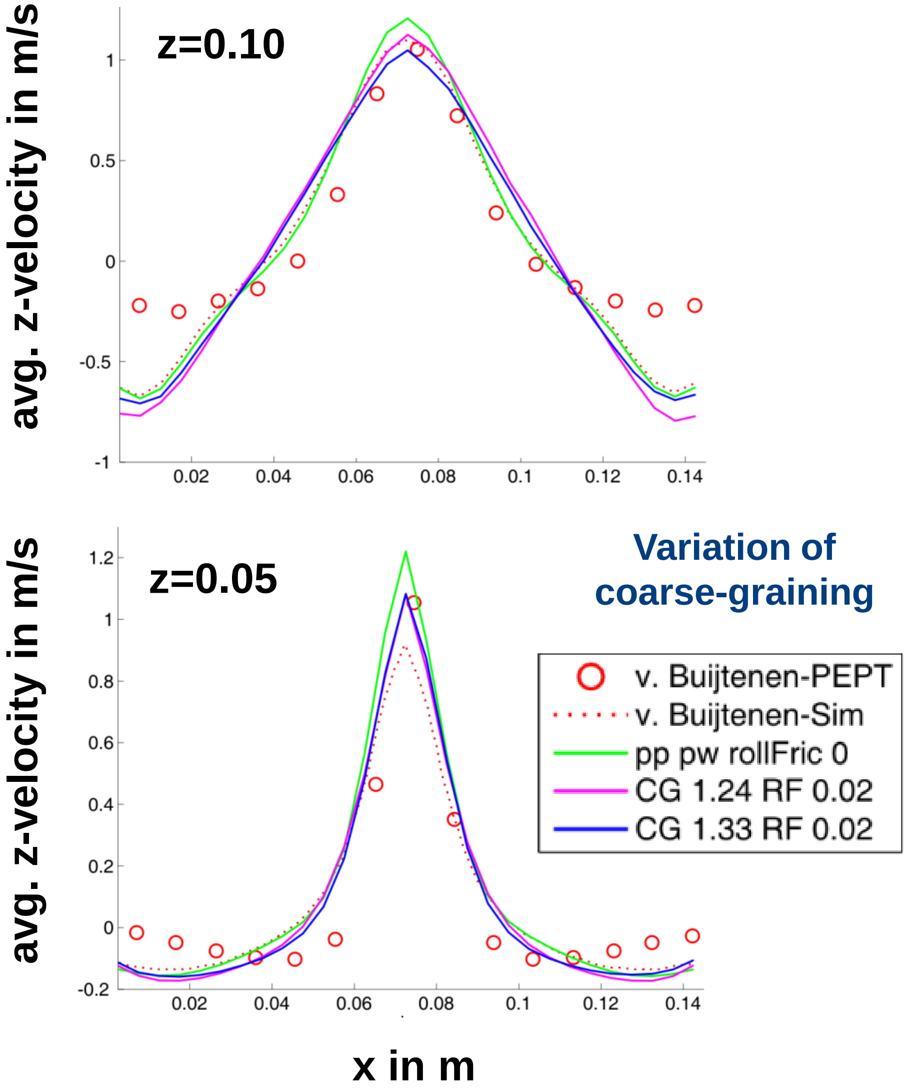
Variation of rolling friction:

LIGGGHTS+CFDEMcoupling

Single Spout Bed Coarse-Grained

Geometry:





Variation of coarse-graining:

CG 1.00	12000 particles
CG 1.24	6348 particles
CG 1.33	5062 particles

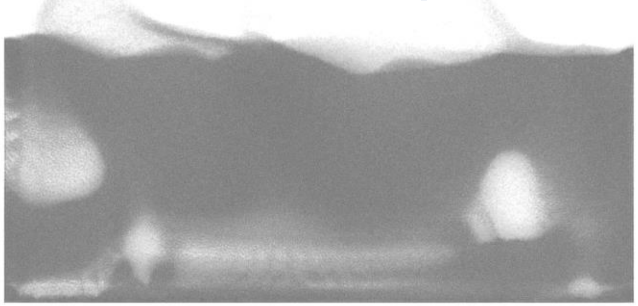
Goniva, C., Kloss, C., Deen, N.G., Kuipers, J.A.M. and Pirker, S. (2012): "Influence of Rolling Friction Modelling on Single Spout Fluidized Bed Simulations", Particuology, DOI 10.1016/j.partic.2012.05.002

LIGGGHTS+CFDEMcoupling

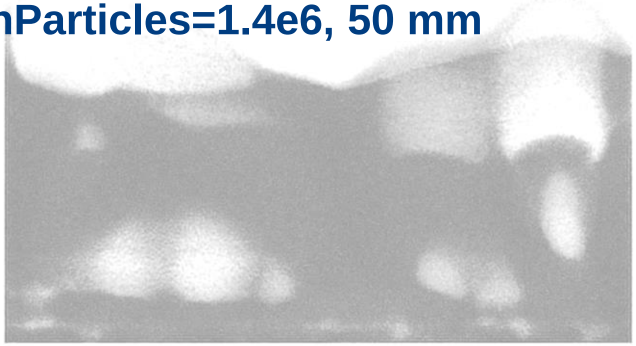
Fluidized Bed Coarse-Graining

Parcel Approach:

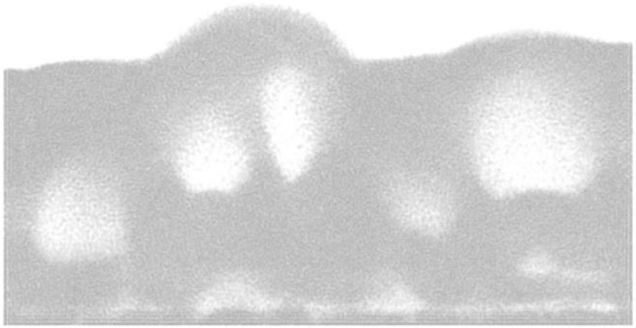
Usf = 0.6077 m/s, dp=0.5mm, nParticles=1.4e6, 50 mm



cg = 1, n_P = 1.4e6

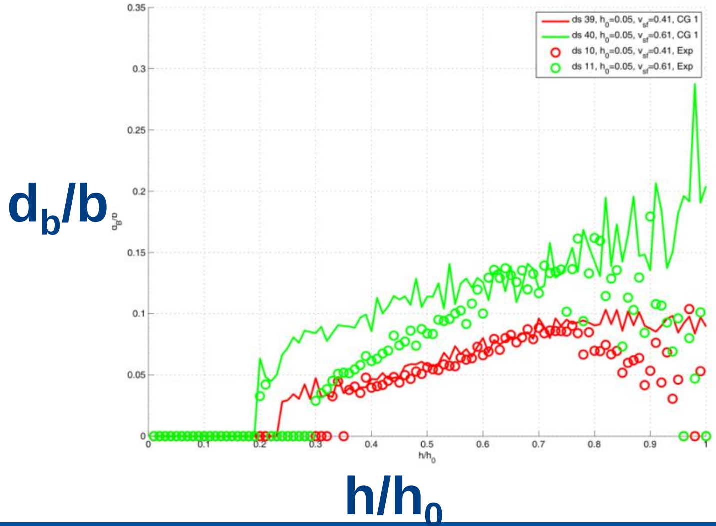


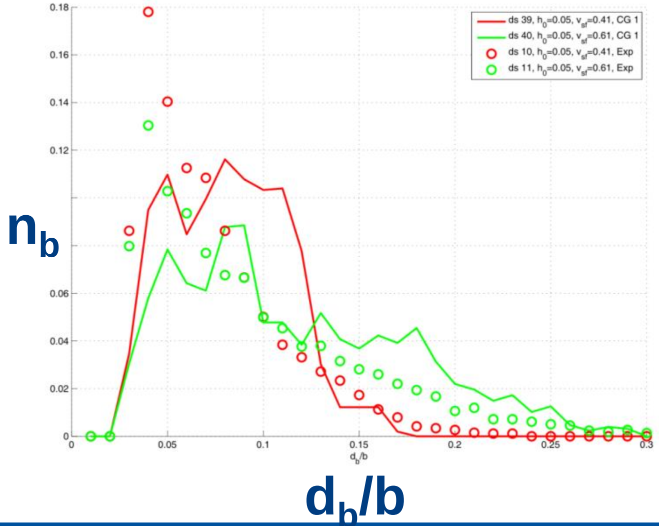
cg=1.5, n_P = 4e5



cg = 2, n_P =1.8e5

Usf = 0.4082 / 0.6077 m/s, dp=0.5mm, nParticles=1.4e6, 50 mm, CG 1





Left: bubble diameter for different coarse graining levels and velocities

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

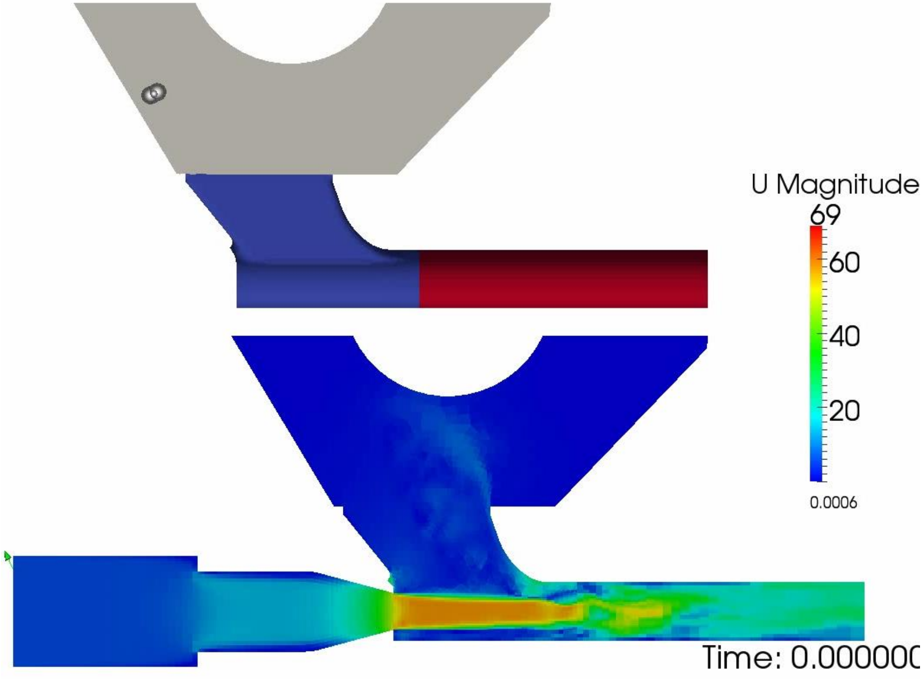
IV.

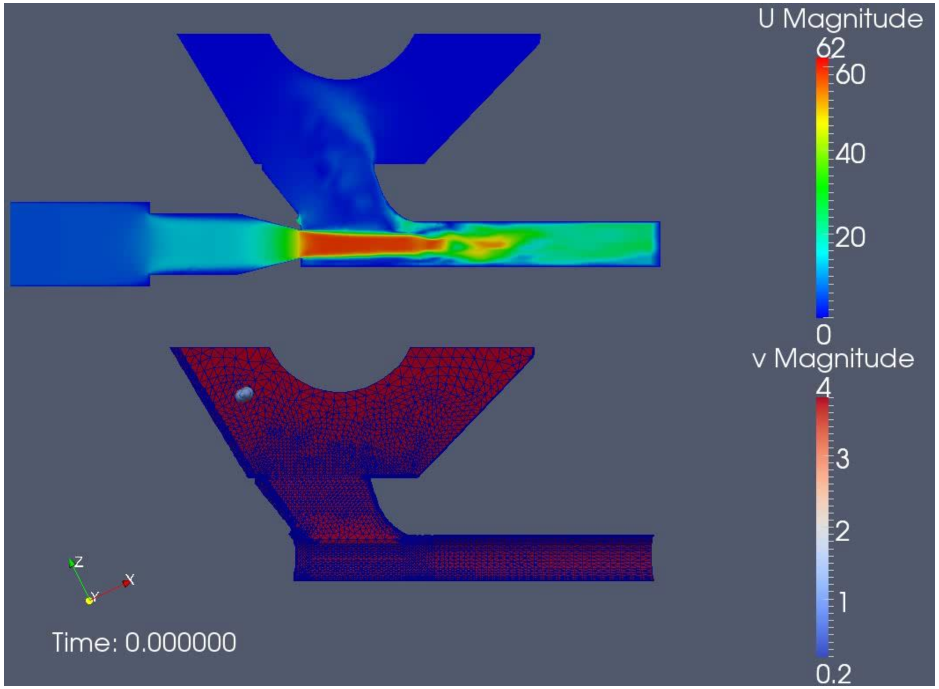
Further Applications & Case Studies

LIGGGHTS+CFDEMcoupling
Agricultural Engineering

CFD-DEM Modelling of Particle Injector for Corn

- **Initial setup (left)**: „bad“ collision – particle blown upward
- **Optimized setup (right)**: particles are smoothely given into gas stream
- Note upward disturbance due to particles



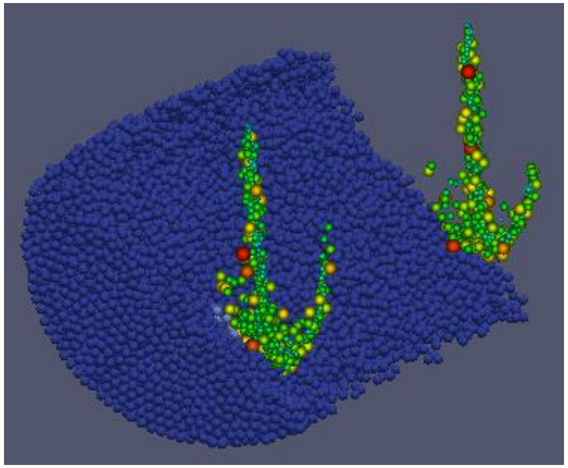


LIGGGHTS+CFDEMcoupling

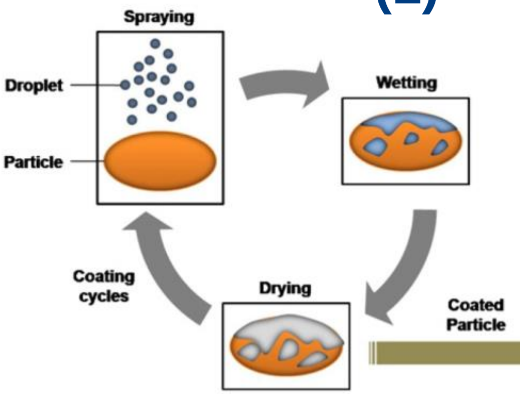
Multi-Phase Flow Applications

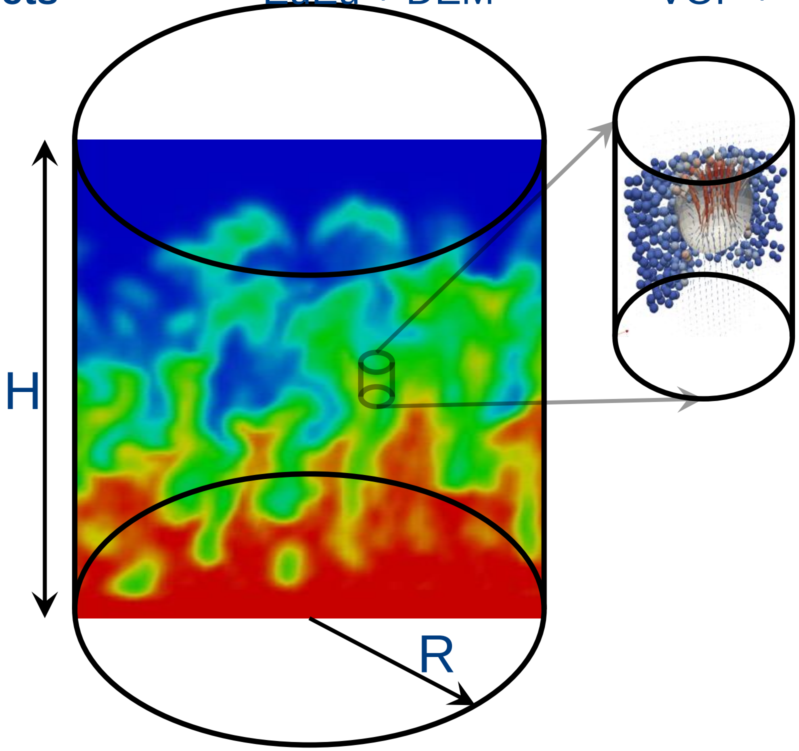
Macro-scale Model **Micro-scale Model** **Macro-scale Model** **Micro-scale Model**

CFD-DEM + Droplets **Wall-film + Droplets** EuEu + DEM VOF + DEM



(1)





(1) Suzzi et al. (2010):“Local analysis of the tablet coating process: Impact of operation conditions on film quality“,CES,65,5699-6715

0 droplet flow Liquid/Gas bubbling flow 1

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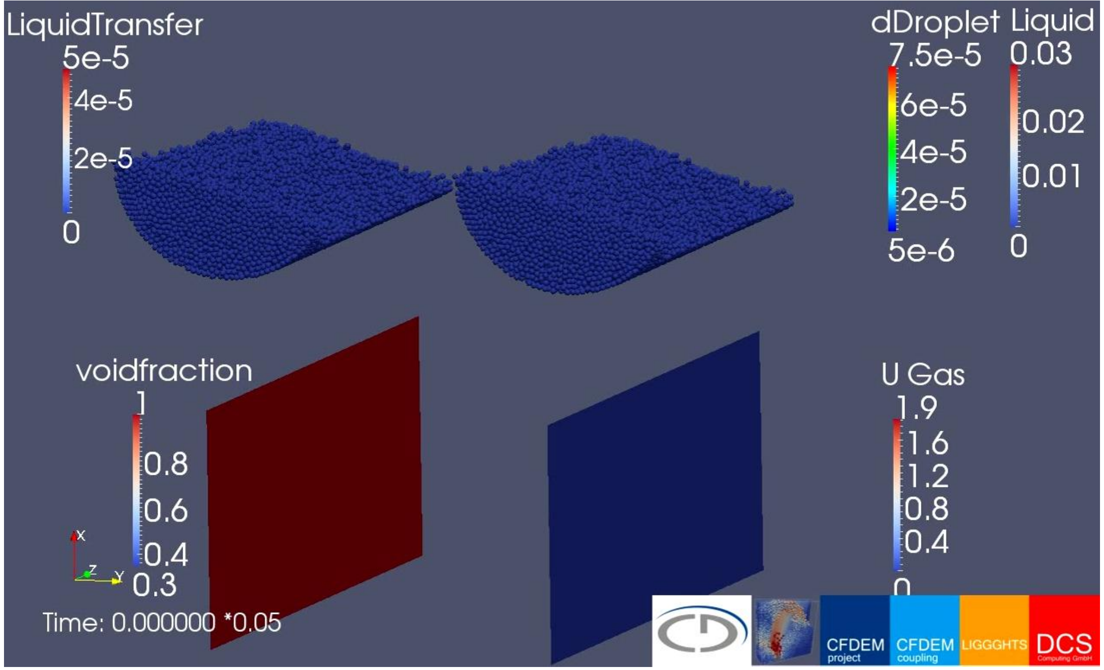
Spray Coating



Physics to be covered

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

Spray modelling

- **Equation of Motion**

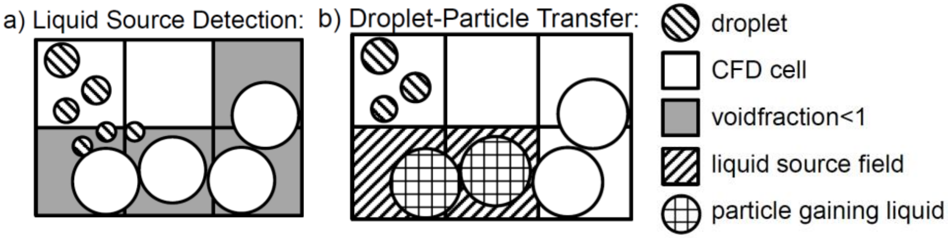
$$m_D \frac{dv_D}{dt} = g(\rho_D - \rho_G)V_D + C_{d,D} A_D \frac{\rho_G (v_G - v_D)|v_G - v_D|}{2}$$

- **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

Floatation cell micro-scale model : VOF Model + DEM

Main Assumption: Bubbles are resolved → particles see only one fluid

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

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

$$\frac{\partial(\rho_f\alpha_f\mathbf{u_f})}{\partial t}+\nabla\cdot(\rho_f\alpha_f\mathbf{u_f}\mathbf{u_f})=\nabla\cdot(\alpha_f\boldsymbol{\tau})-\alpha_f\nabla p+\alpha_f\rho_f\mathbf{g}+\sigma\kappa\frac{\nabla(\alpha_1)}{|\nabla(\alpha_1)|}-\mathbf{K_{sf}}\left(\mathbf{u_f}-\langle\mathbf{u_p}\rangle\right)$$

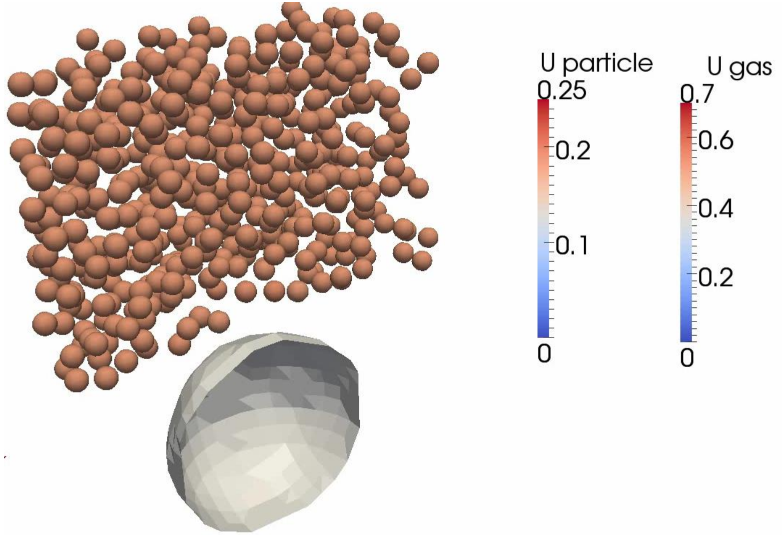
$$\frac{\partial(\alpha_1)}{\partial t}+\nabla\cdot(\alpha_1\alpha_f\mathbf{u_f})-\nabla\cdot(\alpha_1(1-\alpha_1)\mathbf{u_c})=-\alpha_1\frac{\partial(\alpha_f)}{\partial t}$$

Particle, „fluid mixture" based drag

$$\mathbf{K_{sf}}=\frac{\left|\sum_i\mathbf{F_d}\right|}{V_{cell}\cdot\left|\mathbf{u_f}-\langle\mathbf{u_p}\rangle\right|}$$

$$\mathbf{F_d}=\frac{1}{2}\rho\left(\mathbf{u_f}-\mathbf{u_p}\right)\left|\mathbf{u_f}-\mathbf{u_p}\right|C_d\frac{d_p^{2}\pi}{4}\varphi^{1-\chi}$$

$1-\alpha_f$	particle phase volume fraction
u_f	fluid velocity
τ, p	stress tensor, pressure
$\rho_{f,p}$	fluid/particle density
K_{sf}	fluid solid momentum exchange term



G. Wierink: A Computational Framework for Coupled Modelling of Three-Phase Systems with Soluble Surfactants, PhD thesis, Aalto University, 2012

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Minerals Processing

Floatation cell macro-scale model: Two-Phase Euler Model + DEM

Main Assumption: Bubbles are not resolved → particles see mixture

Navier-Stokes equations for each fluid phase “f” in presence of a granular phase “s”

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

$$\frac{\partial \left(\varphi \alpha_f \rho_f \mathbf{u_f} \right)}{\partial t} + \nabla \cdot \left(\varphi \alpha_f \rho_f \mathbf{u_f} \mathbf{u_f} \right) = -\varphi \alpha_f \nabla p + \nabla \cdot \left(\varphi \alpha_f \boldsymbol{\tau} \right) + \varphi \alpha_f \rho_f \mathbf{g} + \varphi \mathbf{M}_f - \alpha_f \mathbf{f}_{\mathrm{fs}}$$

Particle, „fluid mixture“ based drag

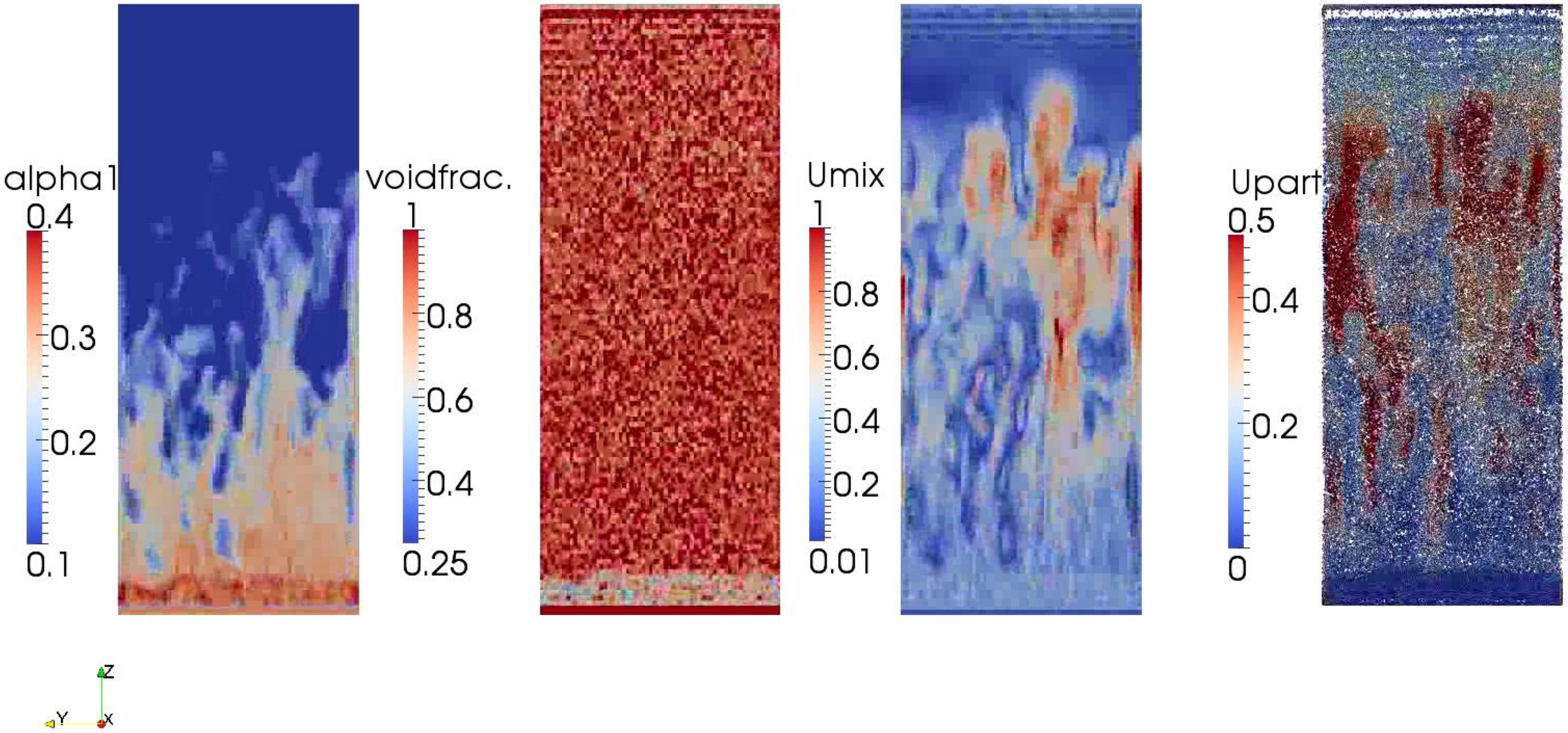
$$\mathbf{f}_{\mathrm{fs}} = \frac{\varphi \cdot \left| \sum_i \mathbf{F_d} \right|}{V_{cell}}$$

$$\mathbf{F_d} = \frac{1}{2} \bar{\rho} \left(\bar{\mathbf{u}} - \mathbf{u_p} \right) \left| \bar{\mathbf{u}} - \mathbf{u_p} \right| C_d \frac{d_p^2 \pi}{4} \varphi^{1-\chi}$$

α_f	fluid phase „f“ volume fraction
$1-\varphi$	particle phase volume fraction
u_f	fluid phase „f“ velocity
τ, p	stress tensor, pressure
$\rho_{f,p}$	fluid/particle density
$\mathbf{f}_{fs}$	fluid solid momentum exchange term

LIGGGHTS+CFDEMcoupling
Minerals Processing

Macro-scale Model: Two-Phase Euler Model + DEM



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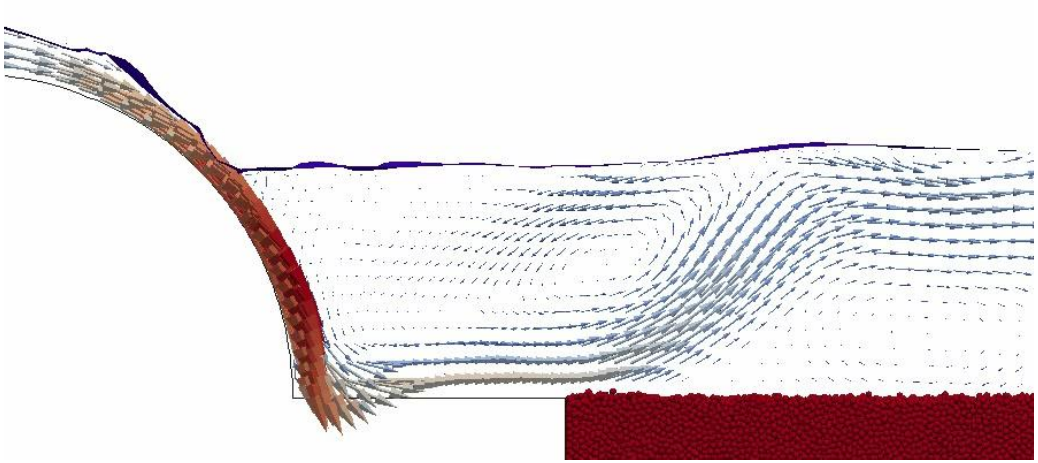
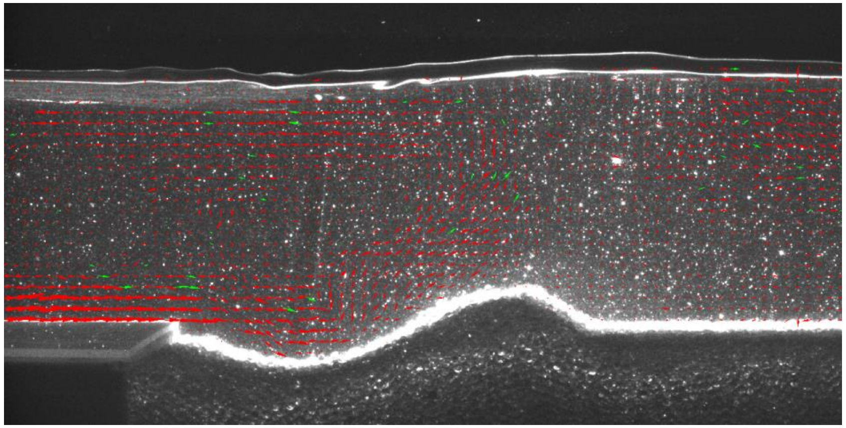
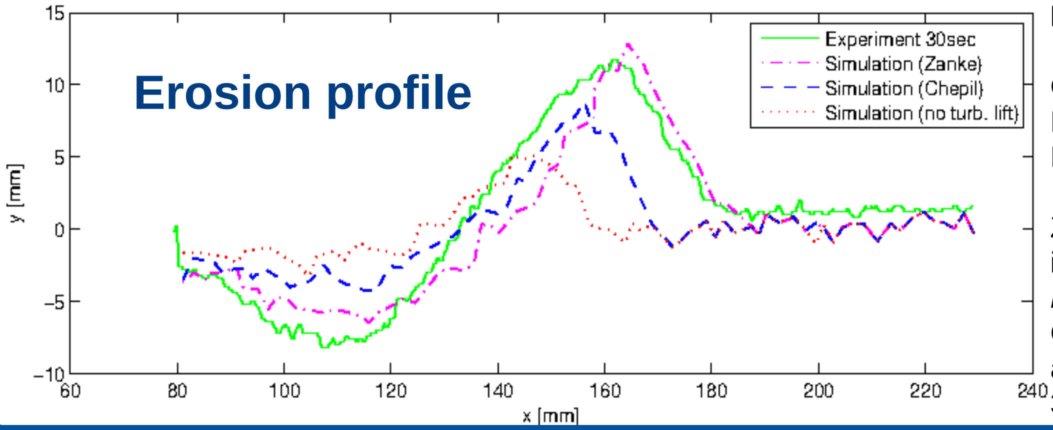
River Bed Erosion

VOF –DEM Modelling of River Bed Erosion

- turbulent lift force is essential; best performance with Zanke (2003) model







Publications:

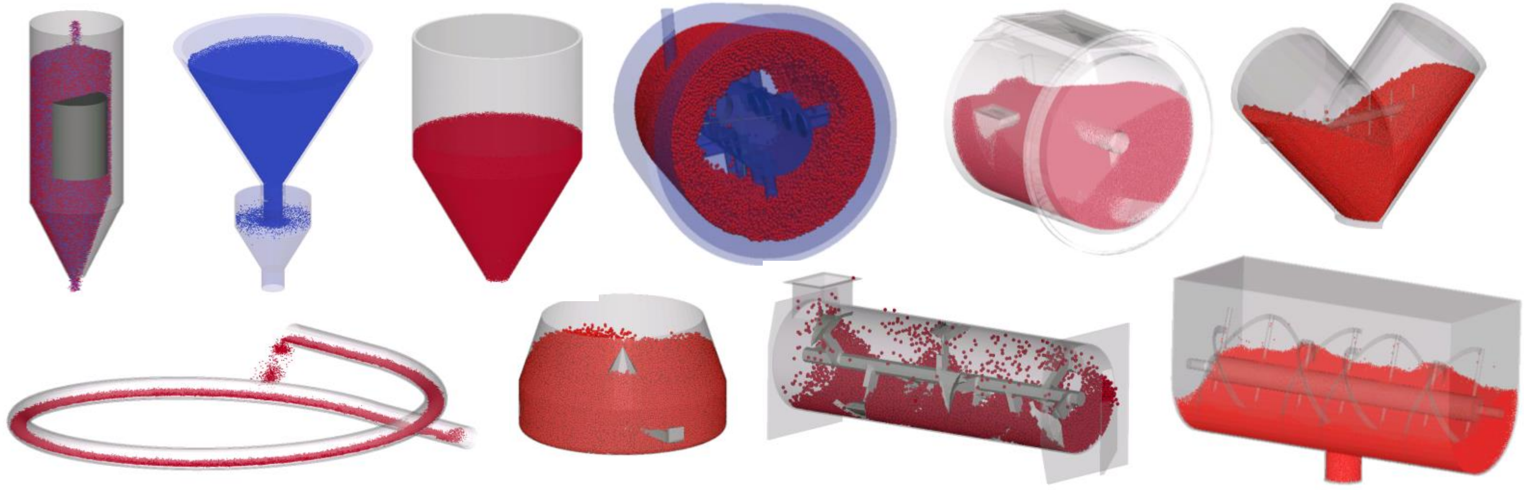
Gruber, K., Kloss, C., Goniva, C: NUMERICAL AND EXPERIMENTAL STUDY OF EROSION IN OPEN CHANNEL FLOW; Proc. IHAR 2012

Zanke, U. (2003). On the influence of turbulence on the initiation of sediment motion. *International Journal of Sediment Research*, pp. 17-31
Chepil, W. (1961). The use of evenly spheres to measure lift and drag on wind-eroded soil grains. Soil Sci. Soc. Am, pp. 343-345

LIGGGHTS Industrial Benchmarks

12 processes were covered by the study:

- Batch processes: Bin flow, Forberg twin paddle mixer, Plow mixer, Fukae vertical shear mixer, V-blender, Ribbon blender, Rotating drum
- Continuous processes: APEC coater, CB mixer, Conditioning cylinder, KM mixer, Revtech process



Download at http://cfdem.dcs-computing.com/media/DEM/benchmarks/LIGGGHTS_Benchmarks.pdf

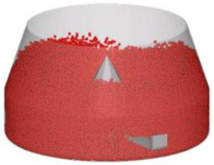
V.

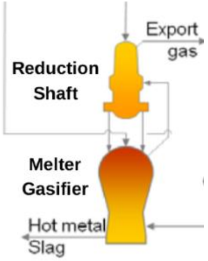
Conclusions

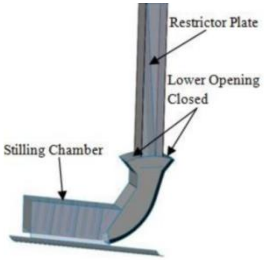
LIGGGHTS+CFDEMcoupling

Conclusions

- Open source simulation software is **driven by the applications,** rules of market apply







LIGGGHTS+CFDEMcoupling
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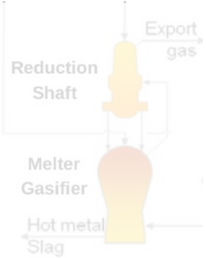
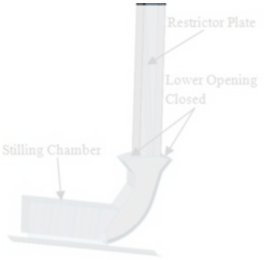
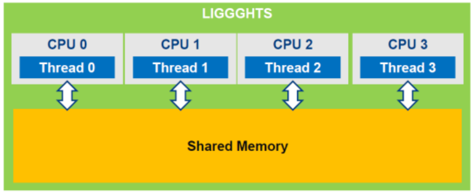
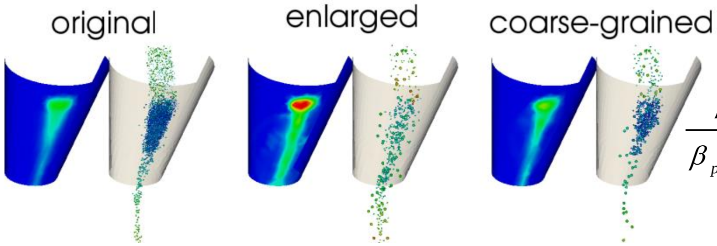




- Providing a **state-of-the-art modelling platform** needs **modelling efforts** and **efforts** to provide a **sophisticated framework** (computer science)





parcel size correction

fluid grid size correction

particle volume fraction correction

$$\frac{\bar{\beta}_p}{\beta_{p,micro}} = c_{corr}(\alpha)\left[1 - f\left(F_f, \bar{\phi}_p\right) h\left(\bar{\phi}_p\right)\right]$$

LIGGGHTS+CFDEMcoupling

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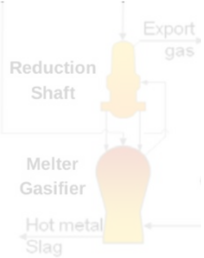

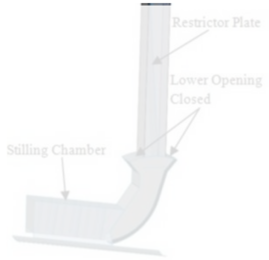

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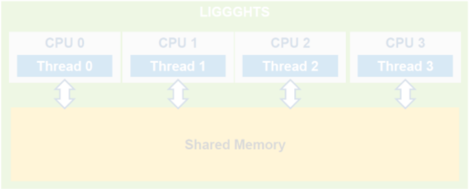

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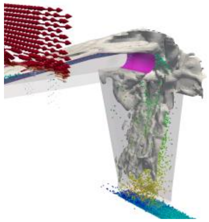
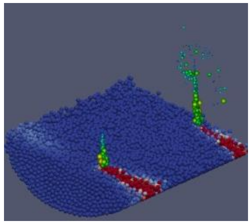
  (2 phase Euler + DEM, VOF + DEM, scalar transport)





- Applications range from iron/steel-making, consumer goods, process, powder metallurgy, refractories production, agricultural, chemical and plastics industries

LIGGGHTS+CFDEMcoupling

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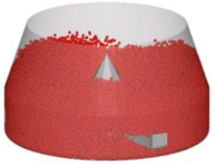

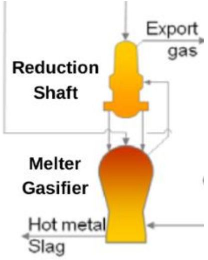

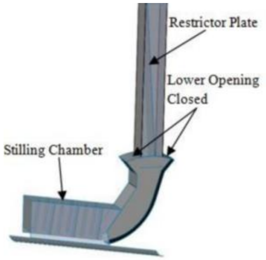

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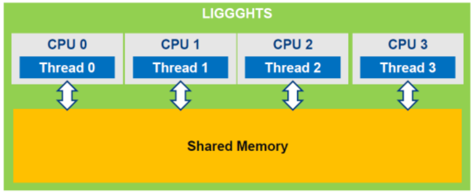

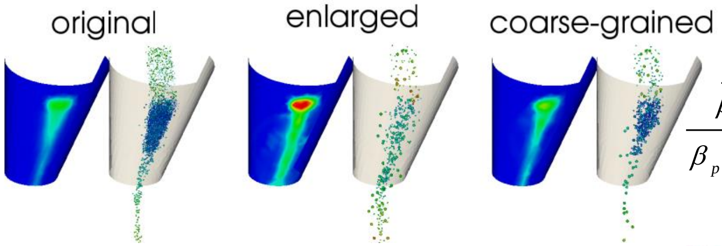

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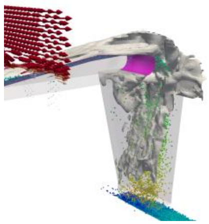

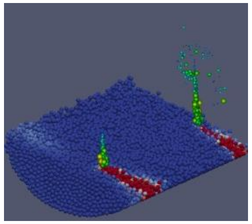

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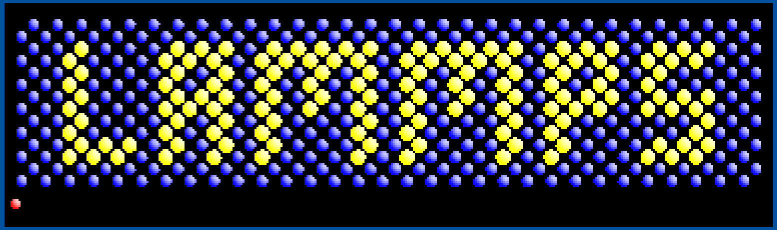
VI.

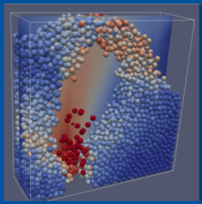
Acknowledgements

Thanks to LAMMPS dev team (Steve, Paul, Axel and others)



and the user community!

We’re willing to contribute back to LAMMPS!



CFDEM project CFDEM coupling LIGGGHTS DCS Computing GmbH

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In alphabetical order:

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